Supplemental Information

Nonideal Transport and Extended Elution Tailing of PFOS in Soil

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Use of Pentafluorobenzoic acid (PFBA) as the nonreactive tracer (NRT)

PFBA is not a PFAS and is not a surfactant. It is useful as an NRT for characterizing PFOS transport in part because of its similar aqueous diffusion coefficient to that of PFOS and other PFAS of similar size. The aqueous diffusion coefficient for PFBA is $7 \cdot 10^{-6}$ cm^2/s (Bowman and Gibbens, 1992). Aqueous diffusion coefficients of $5\text{-}6 \cdot 10^{-6}$ cm^2/s have been reported for 8-carbon chain PFAS (Sekine et al., 2004; Kuo et al., 2013). The diffusion coefficient for PFBA is much closer to those of the PFAS than are the diffusion coefficients of widely used NRTs such as bromide and chloride, which have diffusion coefficients of $2.1 \cdot 10^{-5}$ cm^2/s and $2.0 \cdot 10^{-5}$ cm^2/s, respectively (Lide and Henry, 1994). The use of paired diffusion coefficients will enhance the representativeness of hydrodynamic characterization provided by the NRT (e.g. Brusseau, 1993).

References:

Bowman, R.S. and J.F. Gibbens. 1992. Difluorobenzoates as nonreactive tracers in soil and groundwater. Ground Water, 30, 8-14.

Brusseau, M.L., 1993. The influence of solute size, pore-water velocity, and intraparticle porosity on solute dispersion and transport in soil. Water Resour. Res. 29, 1071–1080.

Lide, D.R. and V.K. Henry. 1994. CRC handbook of Thermophysical and Thermochemical data. CRC Press, Inc., Boca Raton, FL.

Kuo, C.C., B.A. Noskov, Y.C. Liao, and S.Y. Lin. 2013. The adsorption kinetics of a fluorinated surfactant – heptadecafluoro-1-nonanol, J. Colloids Interface Sci. 402, 131–138.

Sekine, M., R.A. Campbell, D.S. Valkovska, J.P.R. Day, T.D. Curwen, L.J. Martin, S.A. Holt, J. Eastoe, and C.D. Bain. 2004. Adsorption kinetics of ammonium perfluorononanoate at the air–water interface. Phys . Chem. Chem., 6, 5061-5065.

Figures:

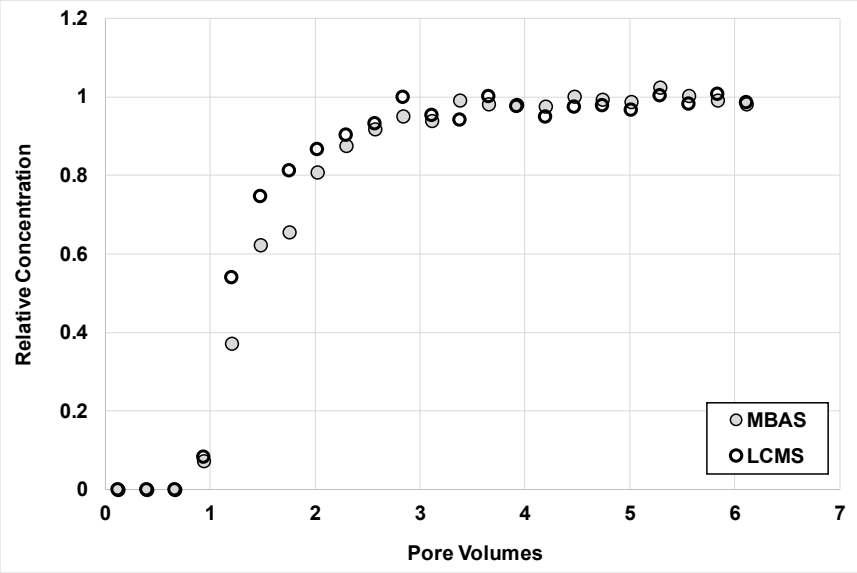

Figure SI-1. Comparison of breakthrough-curve data produced using the two analytical methods for split samples collected during the same experiment. Refer to the main text for descriptions of the two methods.

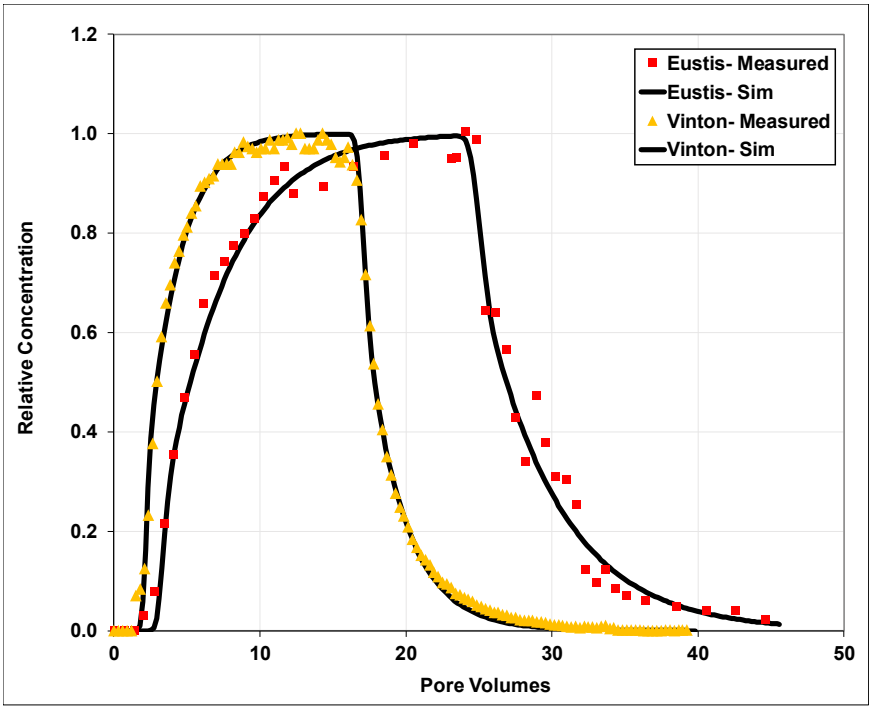

Figure SI-2. Measured and simulated breakthrough curves for transport of the hydrocarbon surfactant SDBS in Eustis and Vinton soil. The simulations are produced using a two-domain model that accounts for nonlinear, rate-limited sorption/desorption (Eustis: $\beta = 0.49$, $\omega = 1.3$; Vinton: $\beta = 0.58$, $\omega = 1.1$).

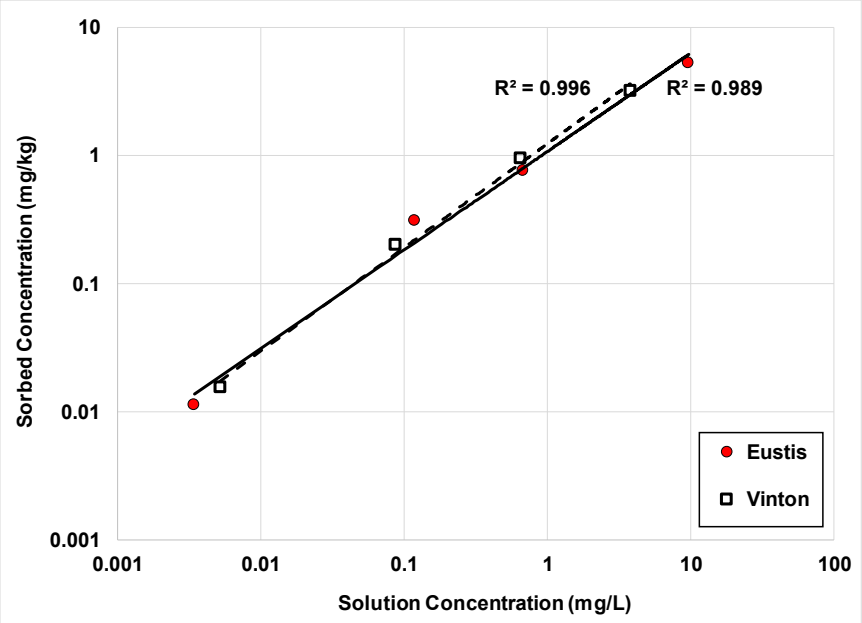

Figure SI-3. Batch sorption data for PFOS with Freundlich isotherms. Eustis: K_f = 1.08 (0.5-2.3) and N = 0.77 (0.5-1); Vinton: K_f = 1.24 (0.8-2) and N = 0.81 (0.7-1). Equivalent K_d values calculated for C_0 = 10 mg/L are 0.63 (0.2-2.4) for Eustis and 0.8 (0.4-1.8) for Vinton. Values in parentheses are the 95% confidence intervals.

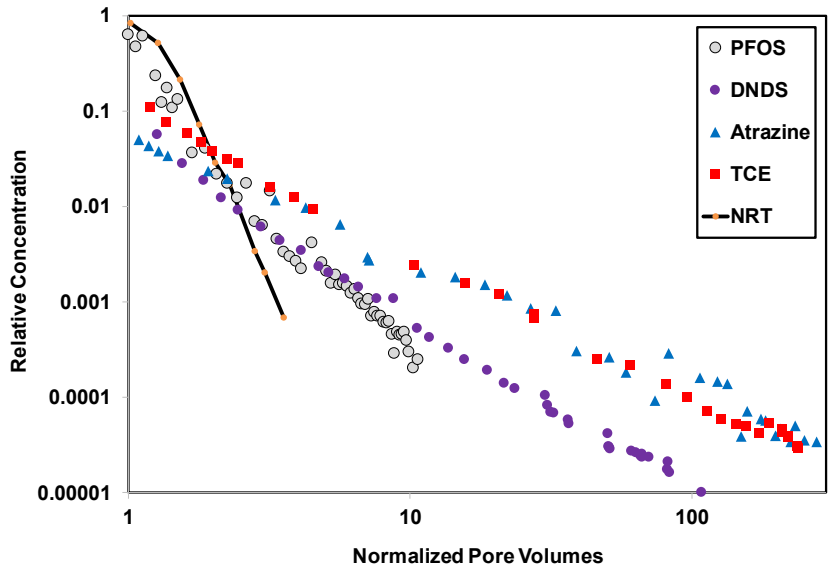

Figure SI-4. Measured elution waves for transport of PFOS, DNDS, two HOCs, and a non-reactive tracer (NRT) in Eustis soil. Plotted with both axes in log scale. The pore volumes are normalized by dividing by the respective retardation factors (NRT = 1, PFOS = 4.2, DNDS = 1.2, atrazine = 3.5, and TCE = 3). The normalized elution curve for a solute undergoing linear, instantaneous sorption/desorption would be identical to that of the NRT curve. See the caption for Figure 9 for the source of the atrazine and TCE data.

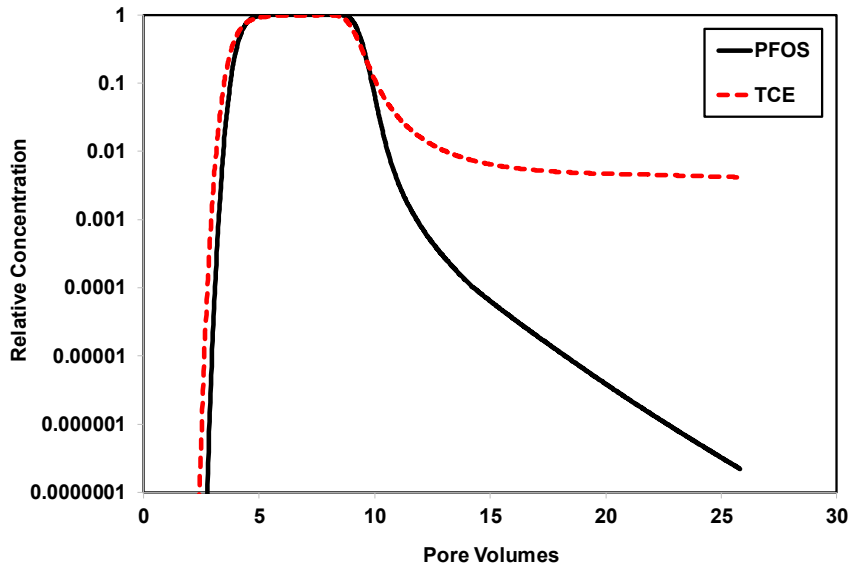

Figure SI-5. Simulated breakthrough curves for PFOS and TCE transport in the Eustis soil for system conditions representing a factor of 100 increase in residence time compared to the conditions used for the miscible-displacement experiments. See the main text for more information.