# Supporting Information

# In-situ Sequestration of Perfluoroalkyl Substances Using Polymer-Stabilized Powdered Activated Carbon

Chen Liu[1], James Hatton[2], William A. Arnold[3], Matt F. Simcik[4], Kurt D. Pennell*,[1]

[1] School of Engineering, Brown University, Providence, Rhode Island 02912, United States

[2] Jacobs Engineering Group, Inc., Englewood, Colorado 80112, United States

[3] Department of Civil, Environmental and Geo-Engineering, 500 Pillsbury Dr. SE, University of Minnesota, Minneapolis, Minnesota, 55455, United States

[4] School of Public Health, University of Minnesota, Minneapolis, Minnesota, 55455, United States

* E-mail: kurt_pennell@brown.edu; Phone: 401-863-9034

## List of Figures:

**List of Tables:**

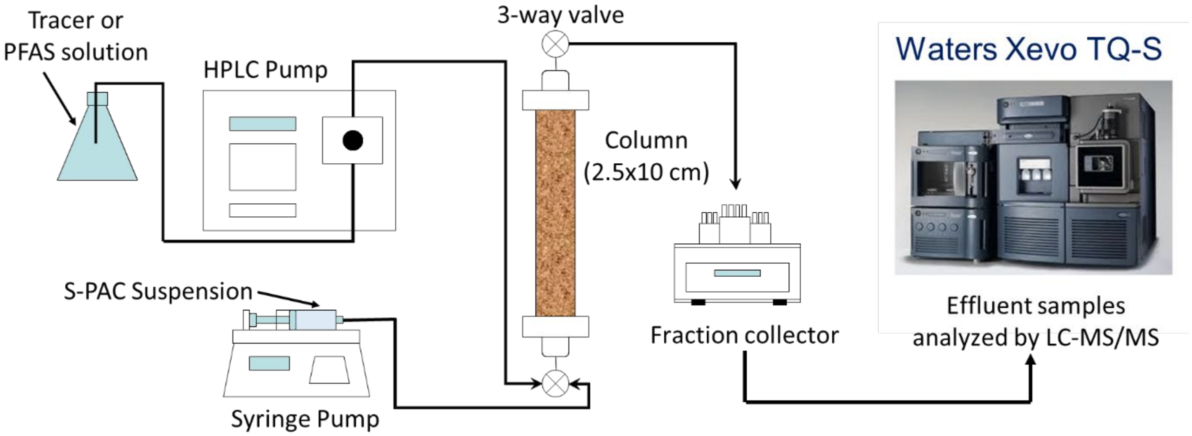


**Figure S1.** Schematic diagram of the experimental system used for the column studies.

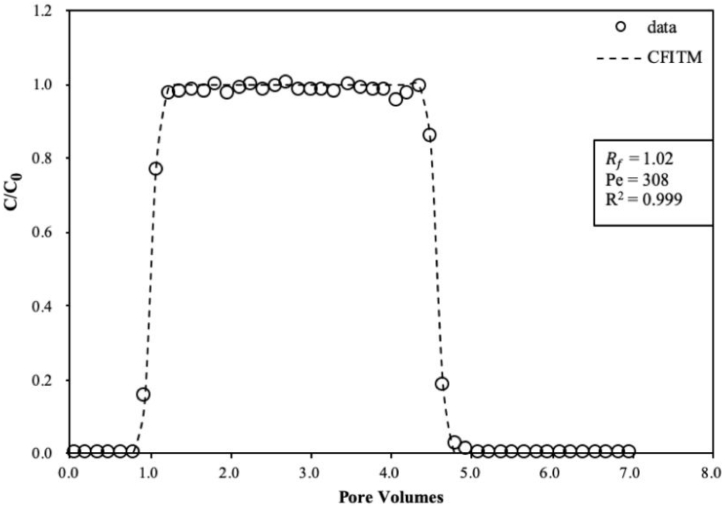


**Figure S2**. Representative bromide tracer breakthrough curve (BTC) obtained for a water-saturated column containing untreated 40-50 mesh Ottawa sand. The pore volume was approximately 20 mL, and the 10 mM NaBr solution was introduced at a flow rate of 0.12 mL/min, yielding a residence time of approximately 2.75 h. Data were fit to a one-dimensional form of the advective-dispersive transport equation using the CXTFIT. [1]

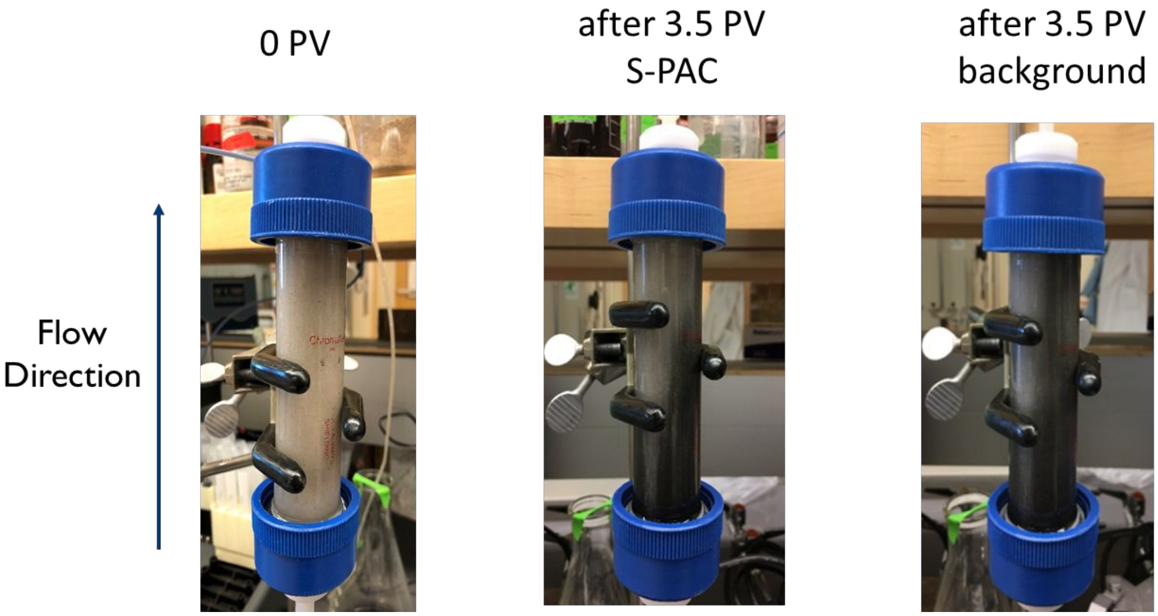


**Figure S3.** Photographs showing the injection of S-PAC and retention PAC (dark color) in a water-saturated column packed with 40-50 mesh Ottawa sand. Approximately 3.5 PV of S-PAC were injected followed by 3.5 PV of background solution (10 mM NaCl) at a flow rate was 0.12 mL/min.

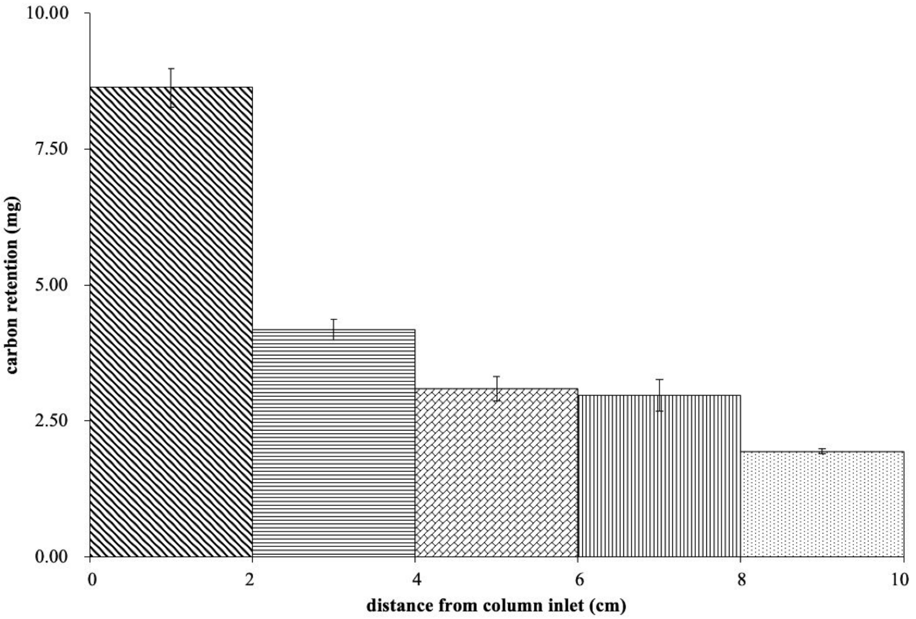
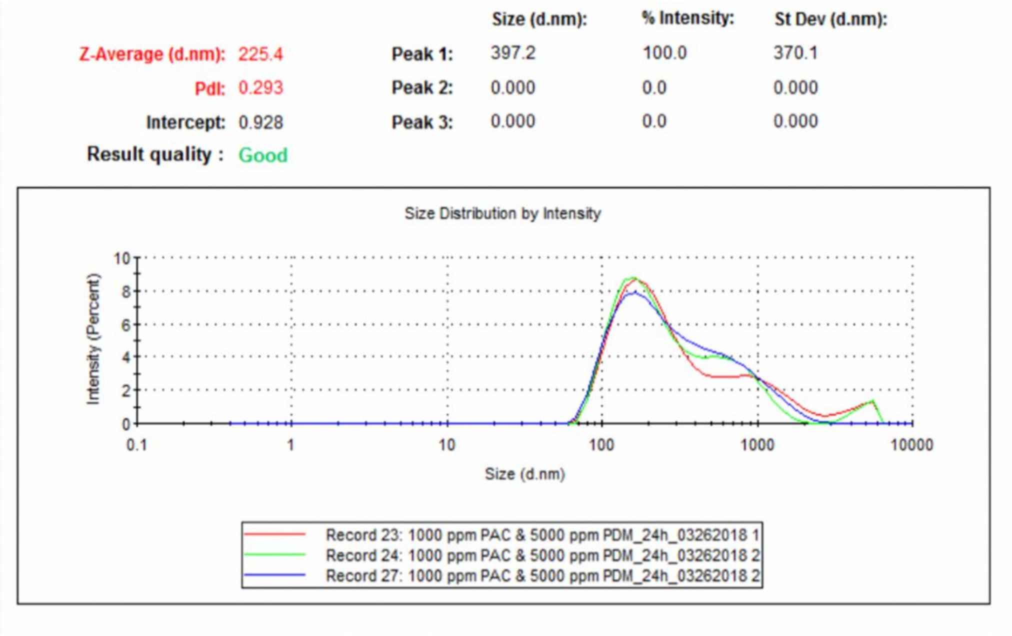
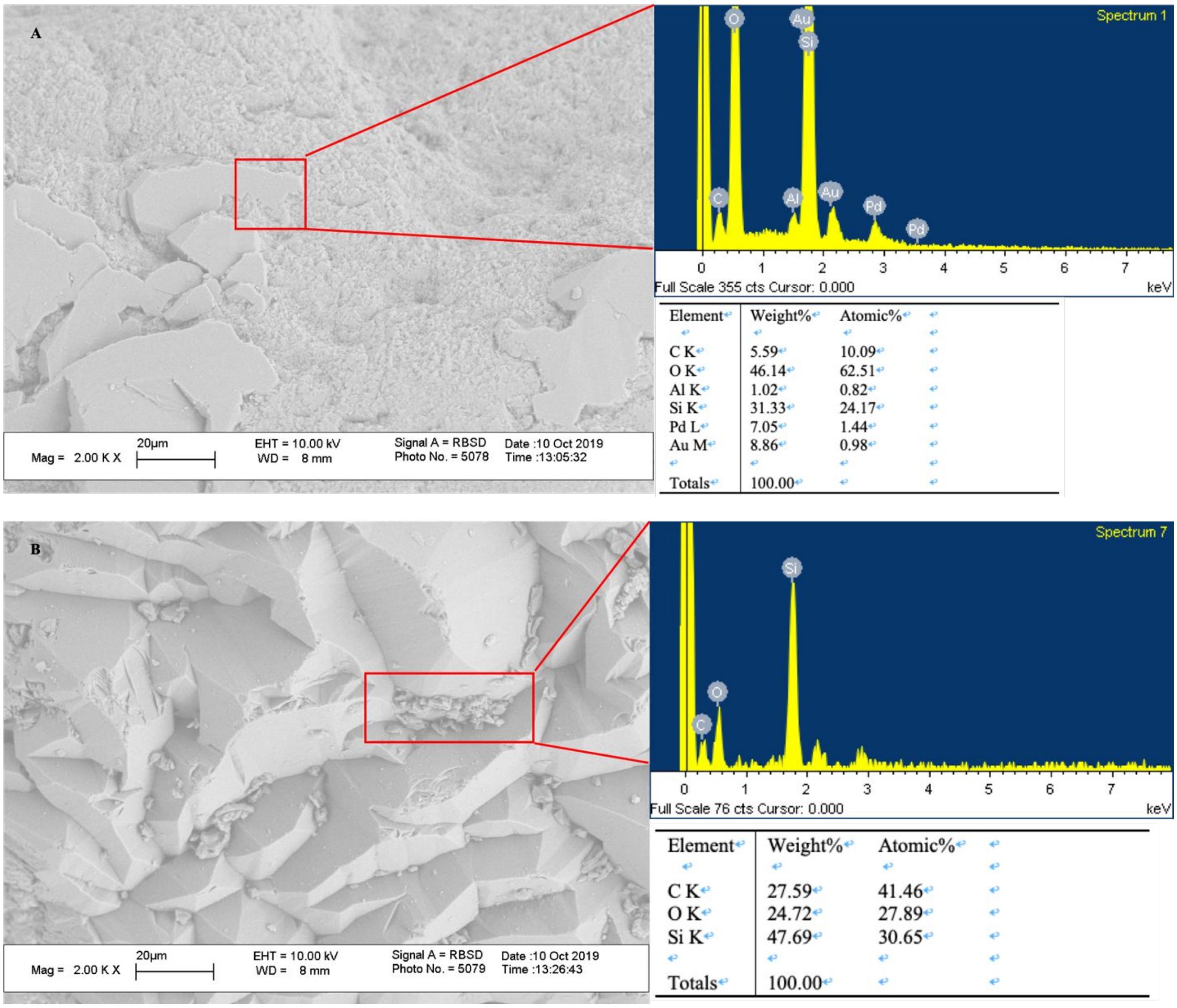


**Figure S4.** Distribution of retained carbon after the injection of 3.5 pore volumes of S-PAC into a column packed with water-saturated 40-50 mesh Ottawa sand followed by 3.5 pore volumes of background electrolyte solution (10 mM NaCl) at a flow rate of 0.12 mL/min.



| | | | Size (d.nm): | % Intensity: | St Dev (d.nm): |
|---|---|---|---|---|---|
| Z-Average (d.nm): | 225.4 | Peak 1: | 397.2 | 100.0 | 370.1 |
| PdI: | 0.293 | Peak 2: | 0.000 | 0.0 | 0.000 |
| Intercept: | 0.928 | Peak 3: | 0.000 | 0.0 | 0.000 |
| Result quality : | Good | | | | |

**Figure S5.** Particle size distribution of stabilized PAC obtained by dynamic light scattering using a Zetasizer Nano ZS Analyzer operated in back-scattering mode at an angle of $173^{o}$.



| Element | Weight% | Atomic% |
|---|---|---|
| C K | 5.59 | 10.09 |
| O K | 46.14 | 62.51 |
| Al K | 1.02 | 0.82 |
| Si K | 31.33 | 24.17 |
| Pd L | 7.05 | 1.44 |
| Au M | 8.86 | 0.98 |
| Totals | 100.00 | |

| Element | Weight% | Atomic% |
|---|---|---|
| C K | 27.59 | 41.46 |
| O K | 24.72 | 27.89 |
| Si K | 47.69 | 30.65 |
| Totals | 100.00 | |

**Figure S6.** Images of 40-50 mesh Ottawa sand (A) before and (B) after treatment with S-PAC obtained using a Zeiss Leo 1530 VP Scanning Electron Microscope (SEM) coupled with an Oxford Instruments 7426 Energy Dispersive Spectrometer (EDS).

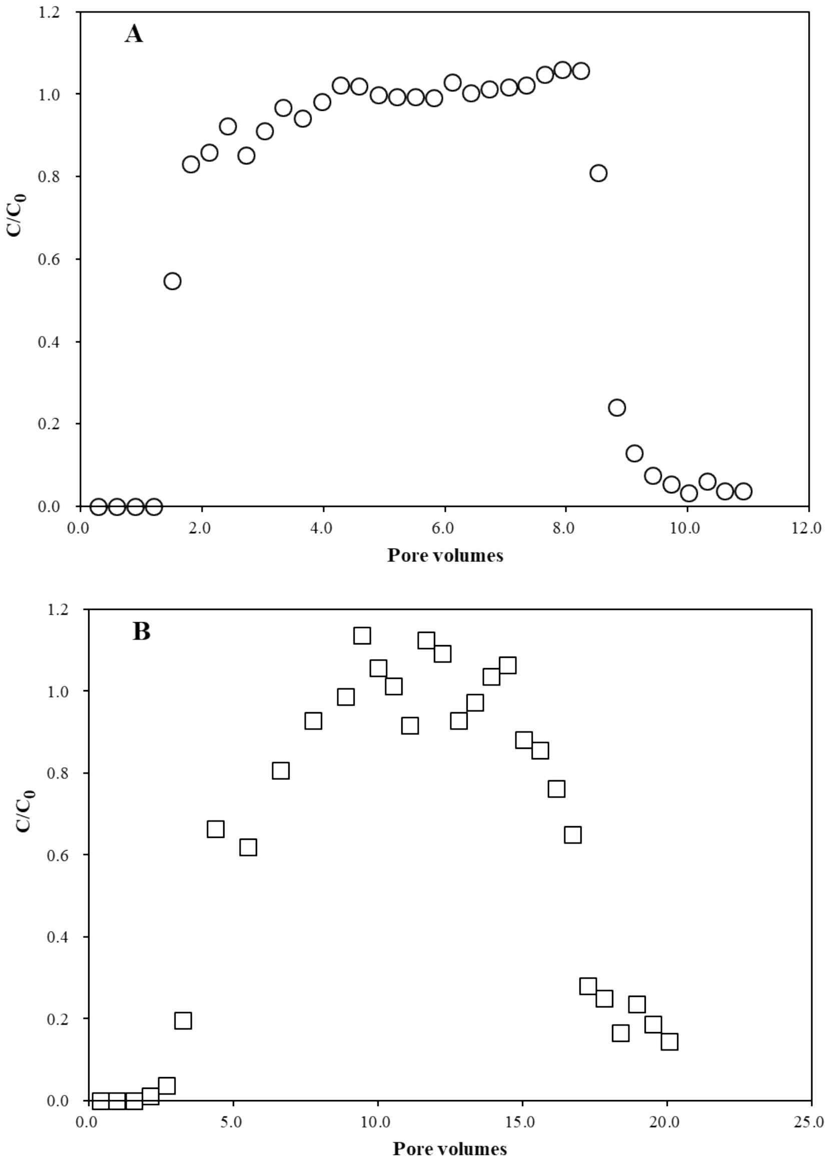


**Figure S7.** Effluent breakthrough curves obtained for pulse injections of aqueous solutions containing either (A) PFOA (100 µg/L) or (B) PFOS (100 µg/L) in water-saturated columns containing untreated 40-50 mesh Ottawa sand at a flow rate of 0.12 mL/min (pore-water velocity of 1 m/day). The pore volume of each column was approximately 20 mL.

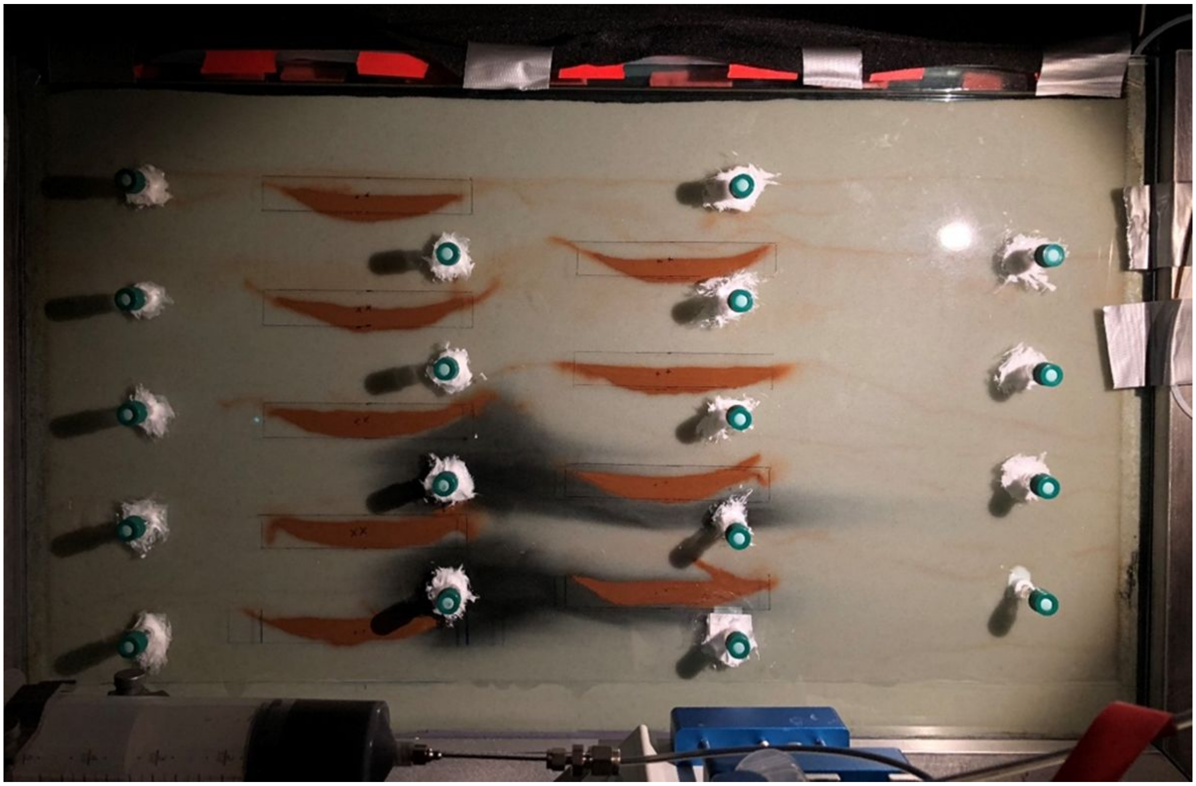


**Figure S8.** Photograph showing retained PAC (dark color) following the injection of 80 mL of S-PAC into side-ports 8 and 9 of the aquifer cell at a flow rate of 0.08 mL/min.

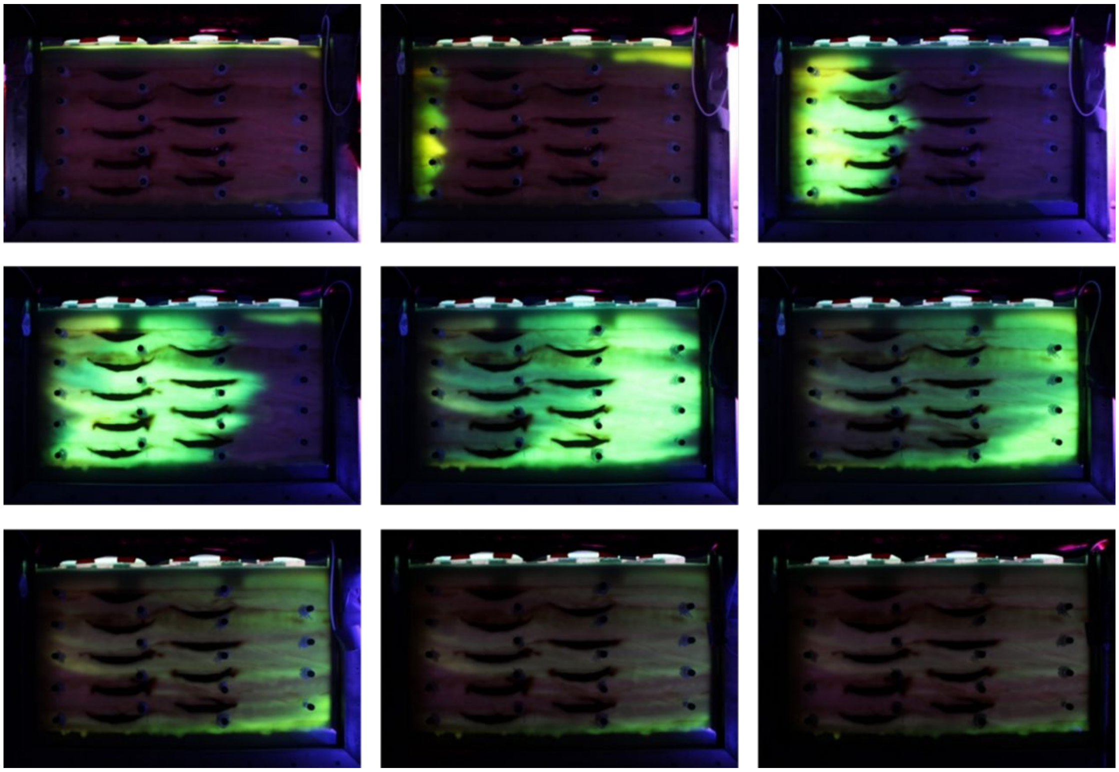


**Figure S9.** Fluorescein tracer test (0.5 PV pulse injection) conducted in the aquifer cell prior to injection of S-PAC at a flow rate of 2.4 mL/min. Images were collected at intervals of 0.26 PV from 0 to 2.12 PV.

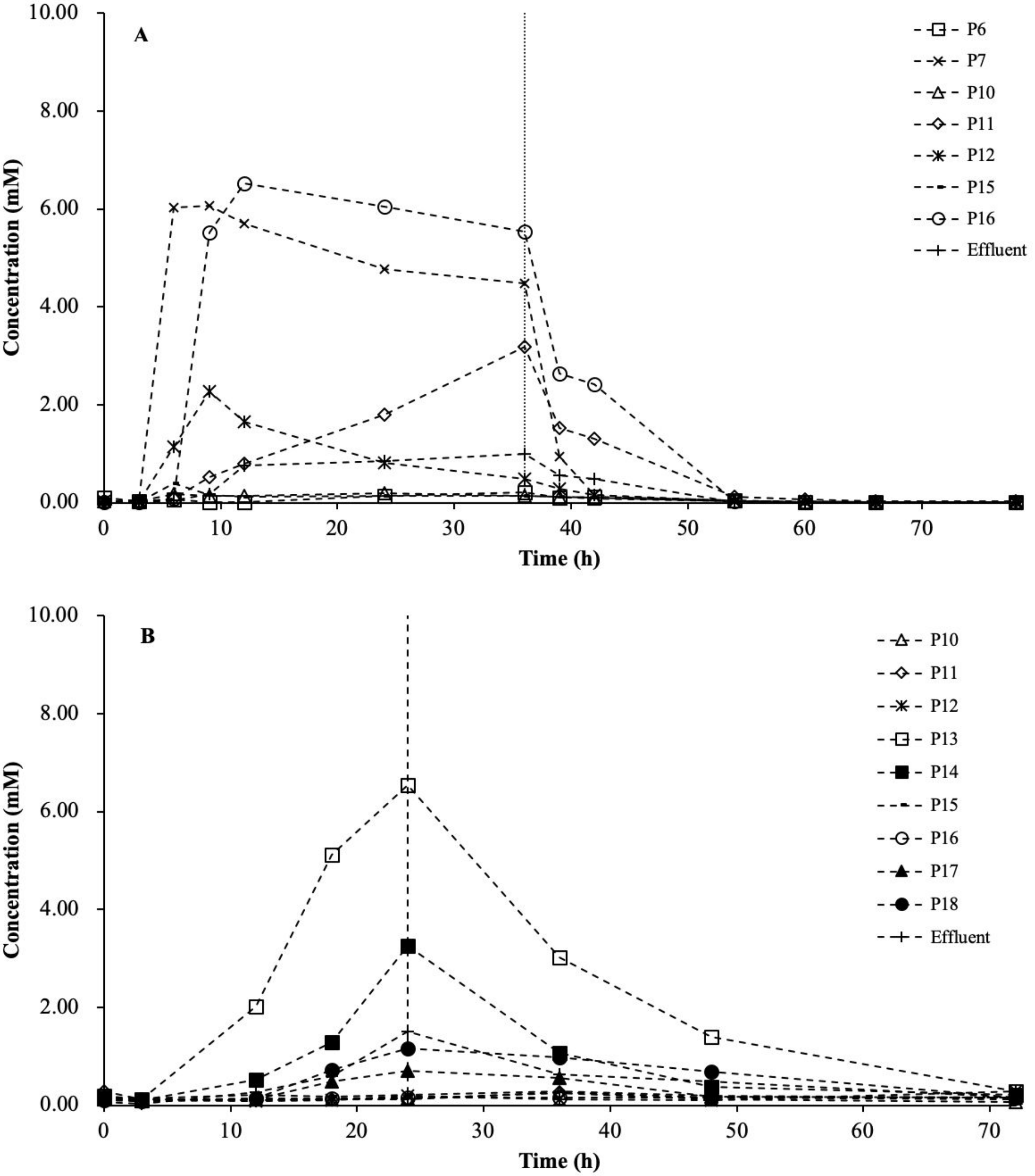


**Figure S10.** Side port and effluent concentration data for pulse injections of non-reactive tracer (10 mM NaBr) in the (A) upper control region and (B) S-PAC treated region of the aquifer cell. The tracer was introduced with 50 µg/L PFOA and 50 µg/L PFOS, and the vertical line indicates when the pulse injection ceased.

**Analytical Parameters for the Mass Spectrometer:**

The Waters TQ-S micro mass spectrometer was be operated in the negative ion electrospray mode with desolvation gas (nitrogen) flow at 450 L/hr and temperature of 55°C. Cone gas flow of 30 mL/min and collision gas (argon) flow at 0.2 mL/min. The source temperature was maintained at 150°C and the electrospray capillary voltage at 0.6 kV. The multiple reaction monitoring (MRM) conditions for PFOA and PFOS are given in Table S1. The method detection limit (MDL) for each compound was calculated based on seven repeated injections of the lowest standard [2]:

$$MDL = s * t_{(n-1,\, 1-\alpha = 0.99)}$$

where $s$ is the standard deviation, $t$ is the student's t-value, $n$ is the number of replicates, and $\alpha$ is the level of significance (for $n = 7$ and $\alpha = 0.01$, $t = 3.14$).

**Table S1.** Multiple reaction monitoring (MRM) parameters used for the detection and quantification of PFOA and PFOS by LC-MS/MS.

| Compound | Internal Standard | Molecular Ion (m/z) | Cone Voltage (V) | Collision Energy (V) | Quant. Ion (m/z) | Cone Voltage (V) | Collision Energy (V) | Confirmation Ion (m/z) |
|---|---|---|---|---|---|---|---|---|
| PFOA | [$^{13}C_8$] PFOA | 413 | 15 | 8 | 369 | 15 | 8 | 169 |
| PFOS | [$^{13}C_8$] PFOS | 499 | 4 | 50 | 80 | 4 | 40 | 99 |

## References

1. Toride, N., F. J. Leij, M. T. van Genuchten. 1995 The CXTFIT code for estimating transport parameters from laboratory or field tracer experiments, U.S. Salinity Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Riverside, CA.

2. Harris, D.C. 2010. Quantitative Chemical Analysis. 8th Ed., W.H. Freeman and Company, New York, NY.