Supplemental Information

Adsorption of PFOA at the Air-Water Interface during Transport in Unsaturated Porous Media

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Additional supporting information:

3 Figures



Figure S1. Surface tensions measured for a homologous series of sodium perfluoroalkyl carboxylates in DI water. All data reproduced from Lunkenheimer et al., (2015), except for C8-2017 (Lunkenheimer et al., 2017) and C8-UAZ (measured in this work). C6 = Perfluorohexanoate, C7 = Perfluoroheptanoate, C8 = perfluorooctanoate, C9 = Perfluorononanoate, C10 = Perfluorodecanoate, and C11 = Perfluoroundecanoate.



Figure S2. Breakthrough curves for transport of a nonreactive tracer (pentafluorobenzoic acid) through columns packed with a 0.35-mm sand. Numbers 0.79 and 0.66 represent water saturations for the unsaturated-flow experiments. The arrival wave extends longer for the 0.79 experiment because a larger input pulse was used. The model simulation is obtained using the ideal, one-dimensional advective-dispersive transport equation, with R (Retardation Factor) = 1 and Peclet Number = 65. Peclet Number is defined as vL/D, with v = mean pore-water velocity, L = system length, and D = hydrodynamic dispersion coefficient. An analytical solution derived by Brenner (1962) was used to solve the transport equation.



Figure S3. Air-water adsorption coefficient (Kai) as a function of PFOA concentration. Label "BTC" represents data obtained from the miscible-displacement experiments; label "ST" represents data obtained from surface-tension measurements.

References

Brenner, H. 1962. The diffusion model of longitudinal mixing in beds of finite length, numerical values. Chem. Engin. Sci., 17, 229-243.

Lunkenheimer, K., Prescher, D., Hirte, R., Geggel, K. 2015. Adsorption properties of surface chemically pure sodium perfluoro-n-alkanoates at the air/water interface: counterion effects within homologous series of 1:1 ionic surfactants. Langmuir 31, 970-981.

Lunkenheimer, K., Geggel, K., and Prescher, D. 2017. Role of counterion in the adsorption behavior of 1:1 ionic surfactants at fluid interfaces-- Adsorption properties of alkali perfluoro-n-octanoates at the air/water interface. Langmuir 33, 10216–10224.