

Sorption of Anionic, Zwitterionic, and Cationic Per- and Polyfluorinated Alkyl Substances to Soil and Sediment

KRISTA BARZEN-HANSON¹, MARKUS KLEBER², JENNIFER FIELD³

¹Department of Chemistry, Oregon State University, Corvallis, OR, 97331, United States,
barzenhk@onid.oregonstate.edu

²Department of Crop and Soil Science, Oregon State University, Corvallis, OR, 97331, United States,
markus.kleber@oregonstate.edu

³Department of Environmental and Molecular Toxicology, Oregon State University, Corvallis, OR, 97331, United States,
jennifer.field@oregonstate.edu

Routine discharge of aqueous film-forming foam (AFFF) at U.S. military bases during fire-fighter training resulted in elevated concentrations of per- and polyfluorinated alkyl substances (PFASs) in the groundwater. Newly-identified anionic, zwitterionic, and cationic PFASs plus the fluorotelomer sulfonic acids (FtSAs) present in AFFF formulations are not characterized with respect to their sorption (partitioning) behavior and subsurface transport. The sorption of anionic FtSAs, zwitterionic fluorotelomer sulfonamido betaines (FtSABs), and the cationic fluorotelomer sulfonamido amines (FtSaAms) were investigated using the National Foam AFFF formulation approved for use by the United States military and a commercial reference material containing the three PFAS classes. Batch sorption experiments were conducted using solutions comprised of 0.5 mM calcium chloride and National Foam AFFF with initial concentrations ranging from 1,000 ng/L up to 138,000,000 ng/L, the latter of which represents the AFFF concentration (3% AFFF in water) actually applied to hydrocarbon-based fuel fires. Analysis of the aqueous fraction by liquid chromatography tandem mass spectrometry after 24 h of shaking resulted in partial depletion of the anionic FtSAs and zwitterionic FtSABs and complete depletion of the cationic FtSaAms from solution. Plots of the PFAS concentration sorbed to soil against the equilibrium PFAS concentration in the aqueous phase were nonlinear for the anionic FtSAs and zwitterionic FtSABs over concentration ranges from 1,000 to 250,000 ng/L and from 1,000 ng/L – 138,000,000 ng/L. Organic carbon-water partition coefficients (log K_{oc}) ranged from 2.9 to 4.2 for the anionic 8:2 FtSA and zwitterionic 6:2 and 8:2 FtSABs, respectively. Preliminary data indicates that for zwitterionic FtSABs, each additional CF₂ group contributes 0.32 log units to the measured log K_{oc} values. The influence of organic carbon, cation exchange capacity, and pH on the sorption of the FtSAs, FtSABs, and FtSaAms to various soils and sediments under a narrower concentration range (1,000-250,000 ng/L) using National Foam AFFF or the commercial reference material will be discussed. The determination of partition coefficients and their dependence on organic carbon and cation exchange capacity will aid in the development of models to predict the behavior of the anionic FtSAs, zwitterionic FtSABs, and cationic FtSaAms in soil and subsurface environments.