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Bridging Data Gaps for Ecological Assessment of Perfluoroalkyl and Polyfluoroalkyl (PFAS) Substances

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Background/Objectives. Perfluoroalkyl and polyfluoroalkyl (PFAS) substances are increasingly recognized to pose an ecological hazard due to their ubiquity in the environment from a multitude of sources. Ongoing environmental releases to groundwater include manufacturing, spill sites, or training locations where PFAS aqueous firefighting foams (AFFF) are used. From groundwater, PFAS compounds can be transported to surface water resources and contact ecological receptors. Aquatic toxicity data are scarce for most PFAS compounds but recently published studies with Daphnia magna have reported data for several PFAS compounds that may inform selection of surrogate values for compounds lacking data. The objective for this effort is to develop a robust extrapolation approach to leverage available data for data-poor PFAS compounds with similar characteristics.

Approach/Activities. For this study, nine PFAS compounds were selected for this initial evaluation based on their known importance to Department of Defense sites associated with AFFF contamination, their occurrence in groundwater, and their presence on federal and state agency monitoring lists. Data were gathered for the compounds for fate and transport properties, physical-chemical properties, and aquatic toxicity. Based on modification of the Wang et al. (2012) framework for identification of toxicity surrogates, a weight of evidence approach was exercised for PFAS compounds to identify appropriate surrogates for data-poor compounds with similar structural and environmental fate properties. A tiered surrogate approach was necessary due to the limitations of traditional quantitative structure activity relationships for the C-F bond groups and the prominence of these bonds for PFAS toxicity. The process was designed to facilitate inferences regarding relative ecological hazard or mobility based on structure (e.g., chain length, functional group) for data-poor PFAS compounds, specifically perfluorohexane sulfonate (PFHxS).

Results/Lessons Learned. Four structurally similar compounds were identified for PFHxS: perfluorohexanoic acid (PFHxA), perfluorobutane sulfonate (PFBS), perfluorooctane sulfonate (PFOS), and perfluorodecane sulfonate (PFBS). Of these potential surrogates, PFOS and PFDS were more structurally similar to PFHxS at 99.6% based on a ChemIDplus assessment. Fate and transport parameters aligned better with PFHxA and PFDS than PFOS; fate and transport parameters for PFBS were not available. When arraying PFAS compounds by carbon length using available ecotoxicity data, PFAS toxicity appeared to increase by carbon chain length. Sulfonic acid compounds appeared to be more toxic than carboxylic acids when chains were of equal length. Given these two conditions, PFOS was selected as a conservative surrogate for estimating PFHxS aquatic toxicity.