SESSION

Tools and Approaches to Quantify PFAS Fate and Transport in Subsurface Environments

WEDNESDAY 20 SEPTEMBER

14.30 – 17.00 CEST (Central European Summer Time)

Opening

14:30 Welcome from SERDP-ESTCP International and Remtech Europe
Marvin Unger (SERDP-ESTCP) Marco Falconi (ISPRA, Remtech Europe)

Presentations

14:35

- "PFAS Leaching at AFFF-Impacted Sites: Insight into Soil-to-Groundwater Ratios" by Dr. Charles Schaefer (ESTCP Project ER20-5088)
- "PFAS Bioaccumulation in Freshwater Fish " by Dr. Christopher Salice (SERDP Project ER19-1193)
- "Development and Validation of Novel Techniques to Assess Leaching and Mobility of PFAS in Impacted Media" by Dr. Jennifer Guelfo (SERDP Project ER20-1126)
- "In Silico Estimation of PFAS Properties" by Dr. Paul Tratnyek (SERDP Project ER20-1481)

16:50 Questions and Answers
Marvin Unger (SERDP-ESTCP) Marco Falconi (ISPRA, Remtech Europe)

17:00 End of the training

Register yourself in the Google form https://forms.gle/jSoBkMZXg9gpZbbQA

"PFAS Leaching at AFFF-Impacted Sites: Insight into Soil-to-Groundwater Ratios" by Dr. Charles Schaefer (ESTCP Project ER20-5088)

This ongoing ESTCP project supports the DoD's efforts to understand the risks associated with the leaching of PFAS from soils that have been impacted with AFFF. Specifically, this research explores the relationship between PFAS concentrations measured in unsaturated soils and PFAS concentrations in mobile porewater that could potentially migrate to underlying groundwater, with the ultimate goal of facilitating site management. The roles of both kinetics and phase equilibria are examined using a field-based approach that uses porous cup suction lysimeters coupled with bench-scale testing on AFFF-impacted soils. This research focuses on assessing the practical limits of lysimetry at AFFF source areas with varying characteristics and developing approaches for selecting appropriate soil cleanup criteria. This presentation investigates the nature of the PFAS in porewater and discusses potential impacts to conceptual site models.

Dr. Charles Schaefer is the Director of CDM Smith's Research and Testing Laboratory in Bellevue, Washington. He has over 25 years of experience in evaluating the fate, transport and treatment of organic contaminants in water, soil and fractured rock. Dr. Schaefer has served as a principal or co-principal investigator for research projects funded by SERDP, ESTCP, the Air Force Civil Engineering Center, the Navy Environmental Sustainability Development to Integration Program and the Water Research Foundation. He has authored over 90 peer-reviewed publications and has been awarded the SERDP/ESTCP Project of the Year three times as either a principal investigator or co-principal investigator. In addition, Dr. Schaefer has served as the technical lead on several site investigation and remedial efforts supporting state, municipal, industrial and federal clients. He received his undergraduate and doctoral degrees in chemical and biochemical engineering from Rutgers University.

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"PFAS Bioaccumulation in Freshwater Fish" by **Dr. Christopher Salice** ***(SERDP Project ER19-1193)***

Aquatic systems are often sinks for PFAS contamination. Freshwater fish can accumulate PFAS when exposed, which may result in ecological effects or fish consumption advisories. Moreover, fish are often the focus of PFAS monitoring and assessment programs. There are important gaps in our knowledge and understanding of PFAS bioaccumulation in fish. For example, there can be substantial variability in PFAS accumulation across fish species and studies and different PFAS. This presentation focuses on research to better understand how environmental, physiological and ecological factors may influence bioaccumulation of different PFAS in environmentally common yet understudied fish species. The project team found that data highlighting temporal, spatial, and species-specific differences in PFAS revealed several factors to consider for better understanding and predicting PFAS concentrations in fish tissues. In the future, a combination of laboratory, field and modeling efforts are likely to yield important insights and predictive tools.

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Dr. Christopher Salice is a professor in the department of biological sciences and director of the environmental science and studies program at Towson University in Towson, Maryland. Prior to moving to Towson, Dr. Salice was an associate professor in the department of environmental toxicology at Texas Tech University. Before entering academia, he was an ecological risk assessor with the U.S. Environmental Protection Agency (EPA) Office of Pesticide Programs and a toxicologist with the U.S. Army Public Health Center. His research has focused on understanding the effects and risk of anthropogenic chemicals to algae, birds, and reptiles. Since 2010, he has been working on ecotoxicity and ecological risk of PFAS, using field research, laboratory toxicity studies, and risk modeling. Dr. Salice's current SERDP projects include a focus on bioaccumulation of PFAS in fish and ecotoxicity of PFAS and PFAS-free foams to ecological receptors, especially reptiles. He received his doctoral degree in toxicology from the University of Maryland, Baltimore.

"Development and Validation of Novel Techniques to Assess Leaching and Mobility of PFAS in Impacted Media" by Dr. Jennifer Guelfo (SERDP Project ER20-1126)

To effectively prioritize sites impacted by PFAS for further investigation and/or remediation, standardized tools are needed to rapidly assess PFAS retention, leaching and transport from the source zone to downgradient regions. Standard leaching methods in EPA SW-846, known as the Leaching Environmental Assessment Framework (LEAF; EPA Methods 1313–1316), were originally developed for inorganic constituents and need to be optimized and validated for PFAS. To meet these needs, a primary objective of ER20-1126 is to develop a standard leaching assessment methodology for aqueous film forming foam (AFFF)-impacted media. Methods 1313, 1314 and 1316 have been optimized and demonstrated using four AFFF-impacted soils. This presentation will compare these three methods, discuss approaches to optimizing them for PFAS, and compare the method results and replicability. Consistency between the LEAF methods implemented on AFFF-impacted soils were similar to what has been observed in prior studies for inorganic constituents. Future work will evaluate LEAF estimates of PFAS leaching and mobility to PFAS releases (i.e., leaching source terms) observed in the field.

Dr. Jennifer Guelfo is an Assistant Professor and an Edward and Linda Faculty Fellow in the Civil, Environmental and Construction Engineering Department at Texas Tech University. She joined Texas Tech University in 2018 following a postdoctoral appointment in the Brown University School of Engineering. For the past 13 years, her research has focused primarily on PFAS occurrence, fate and transport. In addition to academia, she also has a combination of consulting and industry experience, and she uses this background to inform policy and bridge gaps between research and practice.

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Dr. Guelfo has a bachelor's degree in geology from the College of Charleston, a master's degree in environmental science and engineering from the Colorado School of Mines (CSM), and a doctoral degree in hydrologic science and engineering from CSM.

"In Silico Estimation of PFAS Properties" by ***Dr. Paul Tratnyek (SERDP Project ER20-1481)***

The environmental fate, effects, and remediation of chemical contaminants are determined by their properties, such as phase partitioning coefficients, reaction rate constants, and toxicities. For emerging contaminant families—such as in sensitive munitions compounds (ISMs) and per- and polyfluoroalkyl substances (PFAS)—these property data tend to be lacking. Therefore, methods are needed to estimate these properties using statistical correlations (i.e., quantitative structure-activity relationships [QSARs]) and/or chemical structure theory. This presentation will focus on the development of such methods to provide estimates of physico-chemical properties for most PFAS. These methods have two major benefits in addition to property prediction. First, they are very effective for assessing the quality of existing data. Second, they can be a powerful tool for diagnosis of underlying processes (e.g., modes of toxicity). However, the prediction of properties of PFAS presents special challenges. They are usually present as cations and/or anions, whereas most prediction methods work well only for neutral compounds, and carbon-fluorine bonds are not well represented in prediction models for chemical transformations. To overcome the former challenge, the project team developed a way to estimate partition coefficients for anions from data for the neutral forms. This method requires pKa's for PFAS, which we can estimate from fully in silico calculations.

Dr. Paul G. Tratnyek is a professor in the School of Public Health at the Oregon Health & Science University in Portland, Oregon. Dr. Tratnyek has served as a National Research Council (NRC) Postdoctoral Fellow at the U.S. EPA Laboratory in Athens, GA and as a Research Associate at the Swiss Federal Institute for Water Resources and Water Pollution Control (EAWAG). He joined the faculty in the department of environmental science and engineering at the Oregon Graduate Institute (OGI) where he became involved in OGI's Center for Groundwater Research and the University Consortium Solvents-In-Groundwater research program based at the University of Waterloo where he became involved in research on zerovalent iron (ZVI) for remediation of contaminated groundwater. Since then, Dr. Tratnyek's areas of research have expanded to include most aspects of

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in situ chemical reduction and oxidation, including some of the earliest work on abiotic reduction of contaminants and the largest body of high-impact research on ZVI. Much of this work has targeted chlorinated solvents and explosives, but also applies to emerging and recalcitrant contaminants like 1,2,3-trichloropropane and PFAS. A cross-cutting theme in most of Dr. Tratnyek's work is the use of correlation analysis to develop predictive models for contaminant fate determining properties. He received his doctoral degree in applied chemistry from the Colorado School of Mines.