PFAS Signature®: A Forensic Tool to Differentiate AFFF and Non-AFFF PFAS Sources

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Background/Objectives. Per- and polyfluoroalkyl substances (PFAS) are widely used for many commercial and industrial applications, including in AFFF, oil and gas industry, manufacturing facilities, chrome plating operations, etc. Given PFAS are ubiquitously present in the environment, understanding the distinct chemical signatures of different sources is very important. As the number of PFAS-contaminated sites identified globally are on the rise, the need for a chemical forensic approach to understand the fate and tracking the PFAS sources has grown in the past decade. It is very challenging to delineate different sources using commonly used analytical techniques. Using a combination of high-resolution mass spectrometry techniques and machine learning tools, Battelle has developed a chemical forensic technique, PFAS Signature®, for PFAS source differentiation and tracking.

Approach/Activities. PFAS Signature® is a forensic approach based on the composition trends of different PFAS from various contamination scenarios to find correlation between PFAS profiles and their sources. All samples were analyzed using high-resolution mass spectrometry techniques (ultra-performance liquid chromatography coupled to a quadrupole time-of-flight [QTOF] mass spectrometry) in combination with PFAS targeted analysis. A library of suspects was developed, which is a structure-based library containing over 500 PFAS compounds to investigate the precursor and metabolites of a wide range of PFAS from different sources, both AFFF and non-AFFF. Data generated by QTOF are being investigated using both suspect screening and non-targeted methods. Multivariate statistical analysis was performed on the filtered data to correlate the PFAS profiles to the respective sources.

Results/Lessons Learned. Results have shown that using the PFAS Signature® approach, we were able to correlate the sources of some of the samples collected from contaminated sites. Statistical analysis of features filtered using mass defect and the suspect library showed good correlation between the data. The presentation will discuss case studies on the application of PFAS Signature® at different AFFF-impacted sites. The data collected on a broad range of analytes using a combination of high-resolution mass spectrometry techniques and advanced machine learning tools along with multiple lines of evidence provide information to identify PFAS source attribution and help manage contaminated sites.