A Technique for Determining Total Oxidizable Precursors (TOP) of Perfluoroalkyl Compounds

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Background/Objectives.
Perfluoroalkyl and polyfluoralkyl sustances (PFAS) have been manufactured and in use for many years. The many uses include surfactants used as processing aids and in aqueous film forming foams (AFFF), water repellant coatings in consumer products and as aids in several manufacturing processes. Over that time and due to variables in production processes like electrofluorination, many different chemistries of PFAS have been produced and used. In addition to the recalcitrant perfluorocarboxylic acids (PFCA) and perfluorosulfonic acids (PFSA), chemistries such as telomer sulfonates, telomer alcohols, sulfonamides and many others have been identified, Many of these compounds have not yet been fully characterized and therefore, analytical standards are typically not available. This presents a challenge for the accurate assessment of the total PFAS contamination at environmental sites.

Approach/Activities.
PFCAs and PFSAs enter the environment directly or via the transformation of precursor compounds. Many of the polyfluoro- and other chemistries, some of which are not completely characterized, function as precursors to PFCAs and PFSAs. The transformation to the terminal acids can be facilitated as described by Erika Houtz and David Sedlak (Environ. Sci. Technol. **46**, 9342-9349 (2012)). The oxidation process described yields an estimation of the total oxidizable precursors present in a given environmental sample. The process has been augmented in our laboratory by incorporating isotopically labelled compounds, in addition to those use in the course of the LC/MS/MS method, to monitor the oxidation efficiency and the overall process recovery, independent of the extraction/analysis process. The incorporation of these additional parameters allows the analyst to assess the “goodness” of the analytical product, but potentially more important, may allow one to optimize the reaction conditions to sample matrix types.

Results/Lessons Learned. The presentation will describe the rationalization for the compounds chosen and at what points in the process they are introduced. The validation data and application to several sample types will be presented along with suggestions for how the data might be used for field investigations and evaluations.