10 Site Characterization

The PFAS Team developed a [Production, Uses, Sources, and Site Characterization](#) training video with content related to this section.

The intent of this section is not to present general site characterization principles, but to highlight unique considerations or examples for this family of emerging contaminants. It is assumed that site characterization will follow all applicable state and federal (CERCLA or RCRA) guidelines. The general principles of site characterization are similar for PFAS as for any contaminant, in that the physical setting, release specifics, proximity to receptors, and fate and transport characteristics will determine the sampling locations and requirements. Because of the toxicity, persistence, mobility, ubiquity, the large number of compounds in this family of chemicals, the variability and uncertainty of specific compounds and their criteria being regulated, and the emerging nature of PFAS, it is necessary to consider specific concerns in PFAS site characterization efforts.

Section Number	Topic
10.1	[Site Characterization Issues Relevant to PFAS](#)
10.2	[Initial Steps](#)
10.3	[Site Investigation](#)
10.4	[Data Analysis and Interpretation](#)
10.5	[Source Identification](#)

Exposure to PFAS can occur through a variety of transport pathways involving all environmental media, as is described in [Section 5](#). Because ingestion of water is deemed a major route of exposure in humans, and the emerging nature of PFAS as contaminants of concern, regulatory interest has in the past several years been centered on this pathway. In turn, this focus has led to an increased emphasis on investigation of the connection between drinking water sources and groundwater, including direct use of groundwater as drinking water and connections between surface water and groundwater. Because of this regulatory and investigatory focus, this section places more emphasis on characterization of groundwater plumes than characterization of other media. Although groundwater may have in the past been more commonly the initial regulatory and investigatory focus, regulatory focus is broadening to other media such as surface water and biota and as a site-specific characterization process advances data are generally required from one or more other media including soil, sediment, surface water, stormwater, air, biota, or other media depending upon the nature, duration, and time of the release.

The guidelines below include general considerations for the most common types of PFAS sites.

10.1 Site Characterization Issues Relevant to PFAS

Historical investigations may have missed the potential for PFAS contamination at a site because, until recently, these chemicals were not regulated, were not considered a health or environmental concern, or PFAS sampling and analytical procedures may not have been available. As a result, PFAS plumes had years to develop and migrate without detection or characterization. Comparing a site timeline (for example, processes, layout, chemical use, and release history, and fire training and/or firefighting events when AFFF was used) with the timeline of PFAS development and use, and existing drinking water data (for example, UCMR3) can be helpful in evaluating the types and potential occurrences of PFAS releases. Once a potential source has been identified, a site investigation would step out from the source to characterize the nature and distribution of the release. However, if a PFAS site is like one of the many without an identified source ([ATSDR 2021](#)), an understanding of the site timeline or a general understanding of potential PFAS use may not be available. For sites without a known source release, the investigation approach starts with a review of available site information.

The following are some important considerations that are specific to PFAS sites.

10.1.1 Evolving Science and Regulations

State of the science: Understanding of many aspects of PFAS, such as toxicology and behavior in the environment, is changing rapidly. This may require reevaluation of earlier assumptions and conclusions throughout the site characterization process.

Analytical methodologies: Analytical methodologies continue to be developed and improved. Specific attention must be paid to a wide variety of factors, such as analytical methods, detection/reporting limits, and parameter lists that are continuing to expand. See Section 11.2, Analytical Methods/Techniques, for more details.

Sampling methodologies: Questions exist regarding cross-contamination potential due to the presence of PFAS in consumer products; many regulatory agencies require a precautionary approach to sampling prohibiting the use of materials that may be treated with PFAS. See Section 11.1, Sampling, for more details.

Regulatory environment: The regulatory environment remains in flux, with changing regulatory limits, sampling procedures, and compounds of interest. Investigators must remain vigilant to identify impacts to the site characterization. See Section 8, Basis of Regulations, for more details.

10.1.2 Source, Fate, and Transport Properties

Sources: PFAS sources are discussed in Section 2.6, PFAS Releases to the Environment, and AFFF releases are discussed in more detail in Section 3.3, Mechanisms for Release to the Environment. There are also "secondary sources," such as PFAS concentrating into one portion of a plume (for example, groundwater into surface water) that then acts as a source to further groundwater contamination.

Further, because of the widespread use of PFAS-containing products, there may be multiple locations that act as a source of PFAS at a site. In addition, PFAS are often detected at low levels in samples from locations without any apparent or nearby sources. In those instances, there may be a need to evaluate the site-specific anthropogenic background concentrations and determine their contribution to PFAS concentrations in environmental media at a site. See, for example, Strynar et al. (2012).

Pathways: PFAS may be present or migrate via pathways that are not often encountered with other compounds. For example, PFAS may be present in groundwater at a site via air deposition and no direct on-site release.

Complex transitions between media: The behavior of PFAS in the environment may deviate greatly from typical contaminants. Transitions between media may be complex because of specific characteristics of these compounds. For example, PFAS may disperse more upon reaching the water table than is typical for most other compounds, or a groundwater plume discharging into a surface water body may infiltrate into groundwater elsewhere, with contamination in the surface water acting as a secondary source. See Sections 5 and 6 for additional detail.

> **Secondary Sources**
>
> Sources created through movement of contaminated media into an area that was previously uncontaminated (for example, contaminated water from irrigation wells or reuse and application of biosolids) or an area where physical or chemical processes have concentrated PFAS, resulting in an additional source (for example, multi-media interfaces; see Sections 5 and 6).

Partitioning: Because of their physical and chemical properties and the variability of those properties, certain PFAS may partition from water through different mechanisms (including hydrophobic effects, electrostatic interactions, and interfacial behaviors) to other media or forms, including air, micelles, foam, solids, NAPL, and interfaces between these phases. Phase partitioning is discussed in more detail in Section 5.2 and as appropriate in several subsections in this section.

Site-Specific Anthropogenic Background

> Concentrations of PFAS present in environmental media at the site that are not the result of or influenced by site activities or releases.

10.2 Initial Steps

A comprehensive site preliminary assessment commonly starts with developing an understanding of potential PFAS uses in the area, history of the site operations that potentially used the chemicals, air deposition patterns where PFAS may have been produced or processed (for example, manufacturer with PFAS emissions), and the regional geologic and hydrologic framework as it relates to contaminant transport to surface waters or drinking water wells. Following the preliminary assessment, a series of site investigations may be required at a sufficient resolution to capture the effects of the heterogeneities that direct contaminant distribution, fate and transport, and remediation effectiveness. However, there may be a need to prioritize the evaluation of certain exposure pathways (for example, drinking water wells) during the beginning investigations to quickly assess potential human exposures and because of constraints on resources and schedule.

When historical PFAS releases occur upgradient of drinking water sources, drinking water sampling may be the first indication that there is a problem. In areas where there is a concern that a PFAS source may be present, it is common to identify and sample nearby drinking water sources (for example, groundwater and surface water) to determine if PFAS are present in potable water sources and evaluate the potential exposure to human receptors. This approach is a policy for the Department of Defense (USDOD 2014). In cases where sources are not well defined, reconnaissance sampling may be useful to inform the development of the CSM and site investigation. In these instances, drinking water source sampling has preceded typical site investigation work. Prior to further site characterization, proper notification to consumers and evaluating options to reduce or eliminate PFAS exposures, including alternative drinking water sources, may be required.

10.2.1 Initial Conceptual Site Model

CSMs are useful tools for the presentation and evaluation of site characteristics, releases, contaminant fate and transport, and exposure pathways. Generalized CSMs are presented in Figures 9-1, 9-2, and 9-3. The CSMs present most known and potential PFAS source areas, transport mechanisms, and pathways on a simplified physical setting. The CSMs also illustrate exposure routes and receptors. CSM development is an iterative process over the project life cycle with information obtained during site investigation, remedy design, and remedy implementation and optimization. Similar to the USEPA's data quality objectives (DQOs), it relies on a systematic objectives-based site characterization process (ITRC 2015). The CSM for a PFAS site is developed with information on PFAS sources and releases (whether occurring on site or off site from groundwater, surface water, sediment, or air), site characterization, pathways, and potential receptors.

Some specific challenges related to identifying the nature and extent of impacts for CSM development for PFAS sites are described in the following sections.

10.2.1.1 Surface Water Body Secondary Sources

Because certain PFAS are mobile and resistant to breakdown in the environment, there have been cases of surface water creating very large dilute groundwater plumes through recharge (ATSDR 2008). Infiltration of PFAS along the course of surface water systems, including tidal zones, may result in widespread secondary sources to groundwater, further enlarging the contamination area (Ju et al. 2008). A study assessing PFAS concentrations in river and groundwater from several locations found that concentrations and trends in groundwater were generally similar to those observed in surface water, suggesting the aquifer was contaminated with the same source as the surface water (Sharma et al. 2016). Areas with high hydraulic conductivity allow for the rapid spreading of PFAS over large areas. However, even in lower permeability geologic deposits, PFAS contamination is a problem because the combination of long groundwater residence times and persistence of most PFAS results in a long-time presence of these compounds in water resources (Banzhaf et al. 2017). In situations where PFAS-contaminated surface water is recharging groundwater, investigation of the potentially impacted groundwater should be conducted to fully characterize site-related contamination. Complicating surface water being a secondary source is that PFAS have been shown to concentrate at the surface water-air interface (Ju et al. 2008). PFAS contamination may also concentrate in naturally occurring surface water foam (due to an affinity to organic material in the foam and the higher PFAS concentrations at the surface water-air interface where the foam is formed). Therefore, site characterization must consider whether or not surface water bodies are the most downgradient extent of contamination.

10.2.1.2 Receptor Identification

Identification of potential ecological and human receptors as part of development of the CSM first includes identification of potential exposure pathways (for example, PFAS migration in groundwater to downgradient drinking water wells, creating human exposure to PFAS; or water containing PFAS entering surface water bodies, creating aquatic life exposure to PFAS). See Section 9 for additional information on receptor identification in the context of risk-based evaluations for PFAS.

10.3 Site Investigation

This section highlights some important considerations for site investigation that are relevant for PFAS. The general principles of site investigation are similar for PFAS as for any chemicals.

10.3.1 Development of Site Investigation Work Plan

PFAS investigation work plans should take into consideration the information provided in this guidance document (for example, Sections 2, 4, 5, 6, 9, and 11), including items such as sampling procedures and equipment to prevent cross-contamination, analytical methods and compounds to be reported, geographically variable and changing regulatory requirements and criteria, and site-specific environmental setting. From a general perspective the work plan will depend on the type of PFAS source and subsequent transport via various media. Attention should be paid to potential upgradient or nearby sources and potential secondary sources from irrigation, sludge, or biosolid application, the use of soils not recognized to be contaminated, and other anthropogenic factors affecting fate and transport of PFAS-contaminated media, such as discharge from landfills or wastewater treatment plants (WWTPs).

10.3.1.1 Geologic and Hydrogeologic Investigation

Evaluation of the geologic and hydrogeologic framework associated with the site is critical, and sometimes that framework may need to be addressed on a regional basis, as the PFAS impacts may extend significant distances from the site.

In development of a work plan, consideration should be given to obtaining adequate information to allow for applying Environmental Sequence Stratigraphy (ESS) or a similar assessment. ESS is an emerging best practice for understanding the geologic framework and related subsurface contaminant transport pathways, both regionally and underlying a site. The ESS approach is presented in USEPA Groundwater Issue Paper "Best Practices for Environmental Site Management: A Practical Guide for Applying Environmental Sequence Stratigraphy to Improve Conceptual Site Models" (USEPA 2017). The amount of information to be collected to complete an adequate assessment is a site-specific determination based on many factors such as complexity of stratigraphic and lithologic variability, project objectives, and available budget. High resolution site characterization (HRSC) techniques are normally appropriate to obtain adequate subsurface information (for example, grain size and permeability) to complete stratigraphic assessments (see https://clu-in.org/characterization/technologies/hrsc/index.cfm for more information on HRSC). ITRC has guidance on implementing advanced site characterization tools (see https://asct-1.itrcweb.org/).

Geochemical parameters that may be pertinent to potential PFAS migration and possible remedies also require consideration during the investigation. The understanding of soil type (possibly including f_{oc} surface charge, exchange capacity, grain size, minerology, and water content) and groundwater chemistry (possibly including cation concentrations or the ionic strength of aqueous solutions, oxidation-reduction conditions, and pH) at the site is needed to assess transformation, partitioning (including desorption), and migration in groundwater or soil. These and other geochemical data can be used to assess the viability of PFAS remedy options should remediation be necessary. For example, the groundwater's general chemistry, including cations, anions, total dissolved solids, and fouling parameters (for example, iron, manganese, hardness, biofoulants), as well as other organic compounds in groundwater, may have a significant impact on the selection, design, and implementation of potential groundwater remedies.

10.3.1.2 PFAS-Specific Tools for Site Screening or Characterization

Investigative techniques to characterize source soils and determine the three-dimensional extent of soil and groundwater contamination should be considered. High-resolution site characterization techniques beyond those that provide lithologic or hydrologic information and are *specific* to PFAS are currently limited because reliable analytical procedures that are cost-effective and can be used for field screening are not readily available. However, analytical procedures that can be used in a mobile laboratory and achieve ng/L detection limits are becoming more available. Use of a mobile laboratory can be expensive and is cost-effective only in specific situations when a sufficient number of samples can be collected in a short time period to keep the mobile laboratory at or near its capacity. Use of a mobile laboratory and the quick turnaround of results they provide allow for adaptive selection of additional sampling locations for delineation or other objectives. One of the main drawbacks associated with current field-screening methods is the inconsistency of results related to varying soil types and compositions. Other field-screening methodologies have either been tried or are in the research and development phase, including ion selective electrodes to quantify PFOS and a mobile field-screening unit for PFOS and PFOA, both of

which are attempting quantification to ng/L levels ([Deeb 2016](#)). Another method in the development stage is a synergistic approach for the targeted affinity-based capture of PFOS using a porous sorbent probe that may be able to obtain a detection limit for PFOS in water at about 0.5 ng/L ([Cheng et al. 2020](#)). Batelle, through the Pacific Northwest National Laboratory, has patented a version of this electrochemical sensor and is licensing its use ([Battelle 2021](#)). Rodriguez et al. ([2020](#)) provided a review of PFAS-detecting sensors and expected future direction for sensors.

10.3.2 Nature of PFAS Sources

The nature of primary and secondary PFAS sources at a site will largely determine the extent of PFAS contamination at the site. Multiple factors may contribute to the nature of PFAS sources at a site. Key factors related to secondary sources to consider in development of a work plan include:

- Leaching from the vadose zone to the saturated zone: PFAS present in unsaturated soils are subject to downward leaching during precipitation or irrigation events that promote desorption of soil-bound contaminant mass ([Sepulvado et al. 2011](#); [Ahrens and Bundshuh 2014](#); [Milinovic et al. 2015](#); [Guo, Zeng, and Brusseau 2020](#)).
- Back-diffusion: PFAS dissolved in groundwater that accumulated in lower permeability silt/clay layers below the water table may diffuse into the higher permeability zones due to changing relative concentrations ([Section 5.3.1](#)).
- Desorption: PFAS resulting from desorption from solids in the vadose or saturated zones and resolubilizing in porewater or groundwater could occur when adsorption (that is, partitioning) is reversible ([Milinovic et al. 2015](#)); such desorption would have the effect of sustaining PFAS concentrations in porewater or groundwater.
- Nonaqueous phase liquids (NAPL) dissolution: PFAS entrained in NAPL in the subsurface may be associated with releases of chlorinated solvents and/or petroleum hydrocarbons.
- Other sources: Given the widespread use of some PFAS, additional sources upgradient or within a plume may be contributing to PFAS concentrations at a site. Site-specific anthropogenic background may be a contributing factor.
- Atmospheric deposition: PFAS are sometimes associated with stack or other air-emission sources and may contribute to regional PFAS concentrations.
- Overland runoff: Runoff and stormwater conveyance systems can impact surface water locations downstream of the actual source or groundwater along the course of the conveyance system.
- Groundwater seepage into surface water or surface water seepage into groundwater: Groundwater elevations surrounding surface water bodies (that is, gaining or losing) may influence the extent of a plume. Seepage rates and directions may change seasonally, with extreme weather events, or during periods of drought or precipitation.
- Subsurface features, including utility lines: Preferential pathways may result from subsurface features. For example, flow may seep into or out of nonwatertight sewer lines based upon groundwater elevations relative to the utility. The bedding material of a subsurface line may also convey groundwater.
- Multicomponent mixtures: At some sites, numerous PFAS may be present in one or more source zones. Mixtures may be present for several reasons, including, but not limited to, the following: multiple sources, varying time frames, and a mixture of compounds introduced during production (Sections [5](#) and [10.5](#)).
- Precursors: Delineating, as practicable, the extent of precursors that may degrade to PFSAs and PFCAs will help the investigator understand sources and potential long-term concentrations.

10.3.3 Extent of PFAS

As with other chemicals, a site investigation for PFAS relies upon understanding the extent of sources as well as the extent of contaminant transport. A PFAS release can be localized or highly extensive, both horizontally and vertically. Some PFAS may be highly mobile in groundwater. In addition, PFAS plumes may have had years to develop, as discussed above. Therefore, PFAS plumes may be larger than expected. At some sites, more mobile shorter chain PFAS have been observed to extend relatively farther in groundwater than longer chain PFAS due to less retardation in groundwater. The partitioning behavior of PFAS is discussed in [Section 5.2](#).

Another factor in the extent of PFAS at mature sites is prior remediation intended to address other contaminants. For example, groundwater pump and treat systems designed and operating to address other contaminants may have partially captured PFAS or their discharge may have spread PFAS. Other remediation methods such as oxidation may result in a change in the relative concentrations of individual PFAS.

Depending upon site-specific conditions, several pathways need to be considered to assess potential upgradient sources.

PFAS migration in air from industrial or commercial sources can influence soil or groundwater a great distance from larger sources (Section 6.1), for example, see Barton (2010) and Shin et al. (2011). Data from urban soils and groundwater indicate that for sites near metropolitan areas, there may be measurable contributions of PFAS from other sources, unrelated to site-specific sources, see the site-specific anthropogenic background text box in Section 10.1.3 and Xiao et al. (2015).

Comingling of contaminants has a potential to impact PFAS extent. For example, for PFAS sites associated with industry, fire training, or emergency response that have a chlorinated solvent or other NAPL source, investigators need to consider potential effects on PFAS in the subsurface and related data collection requirements. Laboratory studies have demonstrated that sorption or partitioning of PFAAs may increase in the presence of trichloroethene DNAPL in bench-scale tests (McKenzie et al. 2016). Conceptual modeling of published PFAS data suggests that NAPL-water partitioning and NAPL-water interface interactions may significantly increase retardation of some PFAS in source zones (Brusseau 2018; Brusseau 2019; Brusseau et al. 2019, 2019; Costanza, Abriola, and Pennell 2020; Lyu and Brusseau 2020; Schaeffer et al. 2019; Silva, Šimůnek, and McCray 2020; Sima and Jaffe 2021). These enhanced attenuation processes are discussed in Section 5.2.4.1 (partitioning to air/water interfaces) and Section 5.2.5 (NAPL-water interface). This research suggests that if PFAS and NAPL are present in media that make effective source treatment unlikely—for example, in low-permeability soils or fractured rock—that fraction will represent a long-term contributor to groundwater plume persistence. At older sites where in situ (for example, oxidation) or pump and treat methods have been employed to reduce NAPL source areas prior to awareness of PFAS, those remedies may complicate characterization and distribution of PFAS. Depending upon the method employed, mobilization of some PFAS may have changed following treatment, and remedial actions may affect distribution and relative concentrations of individual PFAS (McKenzie et al. 2016; McGuire et al. 2014).

10.4 Data Analysis and Interpretation

There are a number of approaches, methods, and tools available for analyzing and interpreting site characterization data from a wide range of contaminated sites. Examples of approaches, methods, and tools that may be relevant to PFAS sites are described below.

10.4.1 Retardation Coefficients and Travel Time

It may be helpful to estimate retardation coefficients for PFAS to evaluate contaminant-specific velocity and travel time in groundwater, particularly for longer PFAS plumes. As discussed in Section 5.2.3, a linear sorption isotherm is typically assumed for PFAS sorption to organic matter in soil, and sorption coefficients. The Physical and Chemical Properties Table (Table 4-1) provided as a separate Excel file presents a range of available organic carbon partitioning coefficients for environmentally relevant PFAS.

However, as noted in Section 5.2, while common PFAS appear to be appropriately defined by linear sorption relative to organic carbon concentration when sufficient organic carbon is present, the current state-of-science supports Koc being reported in relatively broad ranges on a compound-specific basis. Section 4.2.9 presents a discussion of potential limitations in using K_{oc} values as a predictor of sorption and PFAS mobility. It is also important to note that other geochemical factors (for example, pH, presence of polyvalent cations, and electrostatic processes) may also impact PFAS sorption to solid phases (Section 5.2.3). Due to the uncertainty regarding Koc, it may be appropriate to evaluate transport of an individual PFAS using a range of partitioning coefficients to account for uncertainties in this parameter. In addition, empirical estimation of site-specific K_{oc} values in different areas of a site (for example, source zone versus downgradient plume) may be necessary if quantification of the retardation coefficient is important to its characterization.

For example, McGuire et al. (2014) described the calculation of site-specific K_{oc} values for various PFCAs and PFSAs at an AFFF-impacted site. These site-specific K_{oc} values were calculated based on seven pairs of co-located groundwater and soil samples, and fraction of organic carbon (f_{oc}) measurements at each sampling location. The soil samples were collected near or at the water table, which was about 4.6–6.1 m below ground surface. McGuire et al. (2014) found that there was a range of between one and three orders of magnitude in site-specific K_{oc} values for the PFAAs analyzed. This may reflect the enhanced sorption of PFAS that occurs at the NAPL-water or air-water interface (Brusseau 2018). There may be smaller ranges in K_{oc} values for PFAAs at greater depths below the water table and downgradient of a source zone (where NAPL is not present). When using this type of site-specific K_{oc} analysis method, it is also important that the groundwater samples be representative of conditions where the point soil samples are collected.

As another alternative to the use of K_{oc} values and the assumption of a linear sorption isotherm, in situ or ex situ studies may

be used to develop parameters for simulation of PFAS transport. Such studies could allow development of pseudo-constants to use in model simulations. For example, lysimeter studies were used to establish relative rates of transport of PFOA and shorter chained PFCAs, and PFSAs as compared with PFOS (Stahl et al. 2013).

Desorption of PFAS from solids in the vadose zone or below the water table could occur when partitioning is reversible; such desorption would have the effect of maintaining PFAS concentrations in porewater or groundwater. There is uncertainty regarding the extent to which sorption is irreversible and rate-limited versus an equilibrium process (Section 5.2.3). It may be important to characterize the extent and kinetics of desorption that may occur as a result of remedial activities at the site. Assuming equilibrium desorption may result in overestimation of PFAS removal during remediation activities (Sima and Jaffe 2021).

10.4.2 Mass Flux/Mass Discharge

Note that it may be challenging to estimate the relative mass flux contribution of multiple sources at some sites due to the low PFAS concentrations present in groundwater. In addition, it is important to consider the potential for increases in dissolved mass flux of some PFAS due to biotransformation reactions or desorption between transects.

ITRC (2010) presented a variety of methods available for estimating mass flux and mass discharge, including the use of transects of temporary or permanent monitoring wells across the width of a plume. Even simple methods such as the use of chemical isoconcentration figures to estimate mass discharge may be applicable for an initial order of magnitude estimate. Calibration of solute transport models is another method that may be used to estimate the mass discharge of PFAS from a source zone or at a point in a plume.

10.4.3 Contributions from Different Sources

The potential impact to a site from multiple sources, particularly in proximity to urban or developed locations, needs to be accounted for when assessing site data or identifying data gaps. Each source then needs to be assessed in terms of its specific contributions, and their relative importance or magnitude. Although there are no naturally occurring background levels of PFAS, it may be important to gain an understanding of the Site-specific anthropogenic background (see the text box in Section 10.1.3) concentrations that may be present at a site, as these can have significant implications for site characterization, assessing exposures, evaluating ecological and human health risks, and establishing site action and cleanup levels. Most states have guidance on how to establish site-specific background concentrations for their regulated contaminants.

Tools available to quantify relevant contributions from different types of sources are discussed below.

10.4.3.1 Atmospheric Deposition

Certain PFAS may be present in ambient air and may be elevated near sources such as landfills, WWTPs, fire training facilities, and manufacturing plants (Section 2.6). Many PFAS exhibit relatively low volatility; however, airborne transport of some PFAS can be a relevant migration pathway for some industrial releases. Sections 5.3.2 and 6.1 provide an overview of transport of aerosols and particulates via air. To assess relative contributions from atmospheric sources, air sampling for PFAS can be conducted. Additionally, air dispersion models, such as AERMOD or Industrial Source Complex (ISC3) Model, can be employed to estimate airborne PFAS concentrations and total wet and dry deposition rates at designated receptor locations. Examples where AERMOD could be beneficial during site characterization activities include sites with no obvious source area and sites in industrial areas with multiple potential sources of airborne PFAS. See Section 2.6 for additional details on the most typical PFAS source scenarios.

10.4.3.2 Vadose Zone Percolation

Recent research has illuminated the complexities of PFAS fate and transport in the vadose zone. PFAS surfactant properties can enhance or reduce PFAS sorption, in particular at high concentrations such as those encountered at release locations (Sections 5.2.2.2 and 5.2.3). For example, Guo, Zeng, and Brusseau (2020) conducted a sophisticated modeling study indicating that PFOS in the vadose zone at a hypothetical fire training site is primarily sorbed at the air-water interface and only 1–2% of PFOS is in the aqueous phase under the modeled conditions. This indicates that strong PFOS attenuation may occur in the vadose zone over time, although Guo, Zeng, and Brusseau (2020) showed that eventually there still may be discharge of PFOS to the underlying water table under their modeled conditions. This is consistent with high concentrations of PFOS observed at some fire training sites. The air-water interface may have important implications for vadose zone transport (Section 5.2.4). Therefore, model simulations of PFAS transport in the vadose zone should be performed with appropriate caveats.

For example, models such as USEPA's VLEACH (information and model available at https://www.epa.gov/water-research/vadose-zone-leaching-vleach), and Seview's Seasonal Soil (SESOIL) compartment model (information and model available at http://www.seview.com/aboutsesoil.htm) can simulate one-dimensional vertical transport in the vadose zone via diffusion, adsorption, volatilization, biodegradation, cation exchange, and/or hydrolysis. But these models do not include air-water interface interactions that are important to the vadose zone migration of PFAS, and these models have not been validated for use with PFAS. For these reasons, these models may not be appropriate for use with PFAS at this time. Most PFAS are resistant to biotic or abiotic degradation, and in general PFAS are far less volatile than many other contaminants. However, it is noted that certain PFAS are volatile, for example, the FTOHs (Section 4.2.3 and Table 4-1). With the exception of the few volatile PFAS, the most important vadose zone processes to model are the physical transport processes.

Analytical leaching methods such as Synthetic Precipitation Leaching Procedure (SPLP) [SW-846 Method 1312 (USEPA 2014)] and the Toxicity Characteristic Leaching Procedure (TCLP) [SW-846 Method 1311 (USEPA 2014)] may provide insight into the leachability of PFAS from vadose zone materials. The TCLP is designed to determine the mobility of both organic and inorganic analytes present in liquid, solid, and multiphasic wastes for waste characterization purposes (USEPA 2014). The SPLP is designed to determine the mobility of both organic and inorganic analytes present in liquids, soils, and waste to evaluate the potential of contaminants to leach into groundwater (USEPA 2014). Therefore, the SPLP is typically used for soils in site characterization contaminant leaching studies and allows for less acidic extraction fluids (simulating exposure to acid rain) than the TCLP test (simulating exposure in a landfill) so it can better represent environmental conditions expected to be encountered at a site.

USEPA has also developed a Leaching Environmental Assessment Framework (LEAF). LEAF is a leaching evaluation framework consisting of four leaching tests (SW-846 Methods 1313, 1314, 1315, and 1316), a data management tool, and approaches for estimating constituent releases from solid materials (USEPA 2019). The four leaching tests discussed have been validated for inorganic constituents, but the methods and/or framework may be helpful when evaluating leaching of PFAS in the environment.

Optimizing LEAF leaching tests for use with PFAS is one component of an in-progress SERDP-ESTCP sponsored study: Development and Validation of Novel Techniques to Assess Leaching and Mobility of Per- and Polyfluoroalkyl Substances (PFAS) in Impacted Media, ER-1126 (SERDP-ESTCP 2021). The project overview states that the study has the overarching goal of developing a framework for evaluation and prediction of the release of PFAS from AFFF-impacted media. Identified specific objectives include: 1) development of a standard leaching assessment methodology for AFFF-impacted media; 2) utilization of approaches including high resolution mass spectrometry (HRMS), mid-infrared spectroscopy (MIR), and chemometrics to evaluate and develop a predictive model of PFAS sorption and desorption to AFFF-impacted media; and 3) comparison of results of laboratory testing to leaching and mobility under field-relevant conditions to develop an approach for translation of bench-scale test results to site-scale implications.

Stahl et al. (2013) completed a study evaluating the behavior of PFOA and PFOS in soil and the carryover from soil to plants. Plant samples and percolated water collected by a lysimeter were analyzed for PFOA and PFOS throughout a period of 5 years. PFOA was found to pass through the soil much more quickly than PFOS, and of the original mass applied, 96.88% of the PFOA and 99.98% of the PFOS were still present in the soil after a period of 5 years. Plants were found to have accumulated 0.001% of the PFOA and 0.004% of the PFOS. Loss through the soil through leachate was reported to be 3.12% for PFOA and 0.013% for PFOS.

A follow-up to this leaching study was completed by Gassmann, Weidemann, and Stahl (2021). The study used 8 years of data from a lysimeter and MACRO—a one-dimensional, process-oriented, dual-permeability model for water flow and reactive solute transport in soil (information and model available at https://www.slu.se/en/Collaborative-Centres-and-Projects/SLU-centre-for-pesticides-in-the-environment/models/macro-52/). The study evaluated the ability of MACRO to simulate leaching and plant uptake of PFOA and PFOS using two adsorption concepts: a kinetic two-side sorption concept usually applied for pesticide leaching (scenario I) and the formation of what Gassmann, Weidemann, and Stahl (2021) called non-extractable residues (NER) (scenario II). NER are adsorbed PFAS that either do not leach or leach very slowly from soil. Leaching of PFOA and PFOS could be adequately simulated for scenario II, but scenario I was not able to reproduce sampled leaching concentrations (Gassmann, Weidemann, and Stahl 2021). Plant uptake was simulated well in the first year after contamination but was not simulated well in the following years (Gassmann, Weidemann, and Stahl 2021). The model results suggest that more than 90% of the original mass of PFOA and PFOS is present as NER after 8 years, which they concluded was a larger percentage of the mass compared with other studies (Gassmann, Weidemann and Stahl 2021). The authors also concluded that even though there are open questions and more

research is necessary, the study showed that it is possible to use an existing leaching model for the long-term simulation of PFOA and PFOS leaching in unsaturated soils and the short-term simulation of plant uptake. Furthermore, they concluded that even though not all environmental processes are yet understood, this model may already provide valuable information for groundwater protection and crop safety.

Given the complexity of predicting the mass discharge of PFAS from vadose soils to groundwater, along with modeling and leaching methods, direct measures of mass discharge, including the use of soil lysimeters, may be considered. Care should be taken when selecting an approach to assess PFAS leachability to ensure it is appropriate for the physical environmental setting and parameters that are present, and considers the end use of the data.

10.4.3.3 Back-Diffusion

When evaluating fate and transport of PFAS in a groundwater plume, including time frame for remediation of PFAS, matrix diffusion may be an important process to consider (Section 5.3.1). As such, the potential impacts of diffusion on PFAS persistence in natural soils are a topic of ongoing research. Diffusion coefficients for PFAS are generally uncertain but are in development using measurements and models (Pereira et al. 2014).

During the characterization of PFAS plumes, it may be beneficial to collect PFAS soil samples from the transmissive zone directly above a silt/clay layer, and at different depths into the silt/clay layer, to evaluate the potential for back-diffusion to be occurring presently or in the future if there is a decline in PFAS concentrations in the transmissive zone (see Parker, Cherry, and Chapman (2004) and Chapman and Parker (2005) for an example of this sampling approach).

Schaefer et al. (2019) calculated aqueous diffusivity values for nine PFAAs; however, prediction of the influence that back-diffusion will have on PFAS remediation timeframe remains uncertain because the back-diffusion of PFAS from low permeability materials involves desorption. As discussed above, PFAS desorption may be a rate-limited process and these rates have a high degree of uncertainty (Sima and Jaffe 2021). In addition, the irreversible fraction of PFAS in low permeability materials is uncertain at this time. Therefore, the uncertainty associated with modeling remediation timeframes of PFAS back-diffusion should be noted.

10.4.3.4 Upgradient Site Contributions

PFAS persistence in the environment and their use in a multitude of industrial processes and commercial products result in potential for nonsite-related inputs, similar to other mobile contaminants (Figures 9-1, 9-2 and 9-3). Assessment of potential upgradient site inputs is recommended. The very low health advisory criteria for groundwater only increase the potential importance of identifying what might otherwise be considered "minor" upgradient sources and may result in alternate source identification (Sections 10.3.2 and 10.5). As part of site investigation of an air deposition release, soil data can be statistically compared to background samples, evaluated for vertical stratification, and assessed for spatial distribution relative to the potential source. Groundwater data from the site may be compared to data from other locations using cluster analysis to assess whether there was evidence of other source terms, or if the site in question appeared to be the sole source.

> **Alternate Sources**
>
> Sources that may exist within, upgradient of, or near a site under investigation, that are distinct from the PFAS source being investigated.

10.4.4 Transformation Pathways and Rates

As discussed in Section 5.4, the transformation of precursors may result in increasing concentrations of PFAAs such as PFOS and PFOA along the flow path of a dissolved plume. Transformation reactions may occur due to aerobic biological or chemical oxidation. For example, McGuire et al. (2014) concluded that infusion of dissolved oxygen to bioremediate hydrocarbons downgradient of a former burn pit also likely caused the transformation of precursor compounds to PFAAs such as PFHxS. Some methods that may be used to assess the degree to which transformation is affecting PFAS plume extent and

stability include:

- plotting concentration isopleths for precursors and various PFAAs, for example, McGuire et al. (2014)
- use of the total oxidizable precursor (TOP) assay to identify whether precursors are present that may be available for transformation to PFAAs at a point in the plume (Section 11.2.2)
- assessment of ratios of precursor and daughter product species at monitoring wells situated along the centerline of a plume, or the ratio of various PFAAs in various portions of a plume. For example, McGuire et al. (2014) plotted an isopleth map for the ratio of PFHxS to PFOS to show that in areas where dissolved oxygen was injected this ratio was as high as 50, and in other areas where bioremediation was not conducted this ratio was less than 1.
- use of concentration trends along a plume centerline and quantitative methods described in USEPA (1998) to estimate precursor transformation rates
- groundwater modeling to demonstrate that the relative plume lengths of different PFAAs with different retardation coefficients can be explained only through the transformation of precursors, for example, McGuire et al. (2014).
- a literature review to identify potential precursor transformation mechanisms and evaluate whether site geochemistry and redox conditions are favorable for the occurrence of these mechanisms.

Another method that may be used to illustrate the occurrence of these transformations is radial diagrams. See the case study in Section 15.1.1.

Figure 10-1 shows three radial diagrams based on data from an AFFF release site (McGuire et al. 2014). Each radial diagram compares groundwater concentrations at a monitoring well within the oxygen infusion zone to concentrations at a well approximately 76 m upgradient. The radial diagram shown at the left of Figure 10-1 compares concentrations for five PFCAs between these two wells; the middle diagram shows concentrations from the TOP assay conducted using samples from each well; and the radial diagram on the right compares concentrations for four PFSAs.

These radial diagrams illustrate that oxygen infusion into groundwater likely stimulated the production of mainly PFHxA, PFPeA, PFHxS, and PFBS. The middle radial diagram shows that the difference in TOP assay results between the upgradient well and the well in the oxygen infusion zone does not explain the large PFAAs concentration increases that were observed at the well in the oxygen infusion zone. The TOP assay results were low at both wells throughout the area. This suggests that desorption and subsequent transformation of precursors were occurring within the oxygen infusion zone. These radial diagrams are also useful for evaluating relative concentrations of various PFAAs at each monitoring well. The use of radial diagrams for additional types of trend analysis is discussed further in Section 10.4.7.
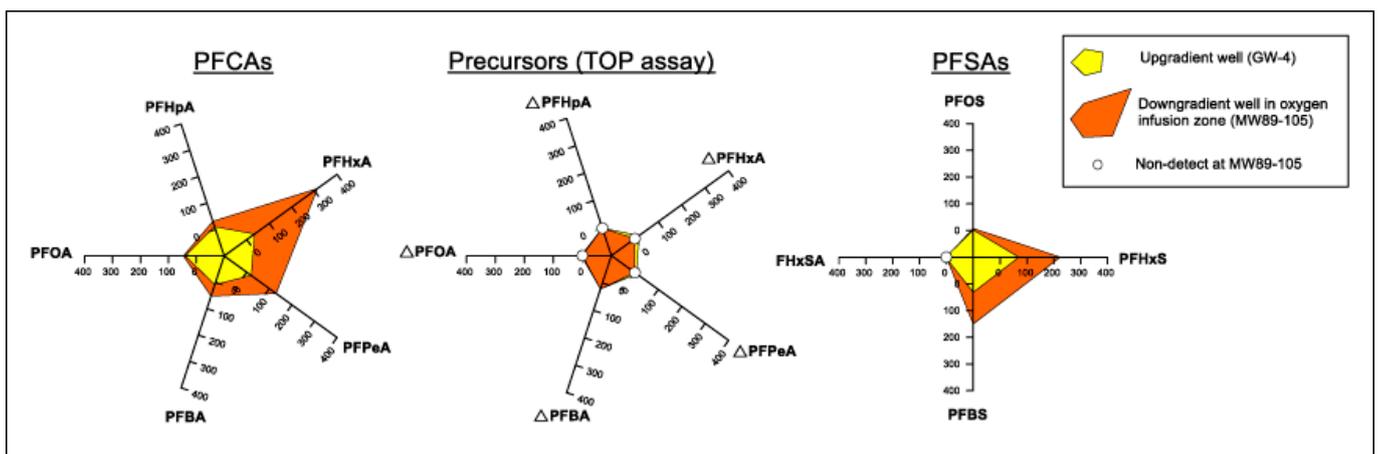

Figure 10-1. Radial diagrams showing the production of various PFAAs in the vicinity of an oxygen infusion zone at an AFFF release site remediated for hydrocarbons in groundwater.
Source: G. Carey, Porewater Solutions. Used with permission.

10.4.5 Assessing Plume Stability

In addition to evaluating potential transformations to PFAAs, it may be necessary to evaluate PFAS plume stability – whether the plume is stable, receding, or expanding. Many PFAS plumes are long-lived and mobile. Methods for evaluating plume stability include qualitative evaluations of temporal plume trends or statistical evaluations such as Mann-Kendall (ITRC 2013;

ITRC 2016; AFCEC 2012; USEPA 2009).

Data uncertainties may have a greater than usual impact on plume stability evaluations because of the low concentrations assessed. Biotransformation of precursors may also have an impact on plume stability evaluations. As such, more frequent or longer duration monitoring may be required to confirm trends or plume stability.

10.4.6 Modeling PFAS Fate and Transport

Some modeling of PFAS fate and transport has been conducted recently (McGuire et al. 2014; Barr 2017; Carey et al. 2019; Guo, Zeng, and Brusseau 2020; Persson and Andersson 2016; Gassmann, Weidemann, and Stahl 2021). Sima and Jaffe

(2021) provide a critical review of applicable transport processes, modeling approaches, and potential limitations and uncertainty associated with modeling PFAS transport. Modeling the fate and transport of PFAS may have significant uncertainty contributed by precursor concentrations, transformation pathways, and biodegradation rates. In addition, desorption kinetics of PFAS are not currently well understood (Sima and Jaffe 2021). Although modeling of PFAS transport may be appropriate under certain conditions, the uncertainty of PFAS transport simulations requires that the results be qualified. Site-specific data are important for evaluating some potential model input parameters such as K_{oc}, which can exhibit significant spatial variation. This is particularly true in source zones, the vadose zones, and at or near the water table. There are situations where modeling of PFAS transport may not be appropriate due to a lack of site-specific input parameters.

10.4.7 Visualization Methods

One of the challenges associated with characterization of PFAS sites is the analysis of trends for a number of PFAS constituents that may be sampled in soil and groundwater, and then the communication of the results of these analyses to a less technical audience. Typical site characterization visualization methods such as plume maps, cross-sections, fence diagrams, 3D models may be used to depict the horizontal and vertical extent of PFAS plumes. Several other visualization methods may be helpful when analyzing PFAS data, including:

- bar charts that show the relative concentrations of individual PFAS constituents at each location to help evaluate PFAS composition trends in soil and groundwater (for example, figures 6 and 7 of 7 Field (2017), Figure 15-1)
- radial diagrams to illustrate:
    - transformations of precursors to PFCAs and/or PFSAs along a flow path (for example, see Section 15.1.1)
    - relative concentrations of constituents at each sample location to assist with source fingerprinting and to identify potential risk drivers in different parts of a plume
    - locations of potential hot spots
    - general extent of a PFAS plume.

Case study examples of these different methods are discussed in Section 15.1.

10.5 Source Identification

Source identification can be one of the challenges of PFAS investigations. The field of PFAS forensics is in its nascent stages. Researchers are still conducting studies to more fully understand the fate and transport of PFAS in the environment, and they continue to evaluate tools to investigate changes in PFAS composition for the purposes of source attribution. Benotti et al. (2020) have suggested a tiered approach for characterizing the PFAS signatures associated with source materials and have suggested that some or all aspects of this approach may be useful when evaluating PFAS contamination in soil or water samples. However, until more details on the chemical composition of source materials is available, and until researchers understand the full scope of forensic information that may help elucidate sources, the best approach for associating or dissociating environmental contamination from one or more sources is to compare PFAS information in a soil or water sample to similar information from the site-specific source area/s. An overview of PFAS source identification analyses can be found in Dorrance, Kellogg, and Love (2017).

To that end, any site-specific investigation begins with a careful review of available records. In a best-case scenario, such records may directly link a source to environmental contamination without significant contribution from any other potential sources. More often than not, source attribution of PFAS contamination is more complicated. Groundwater plumes of PFAS contamination are heterogeneous due to weathering and differential rates of subsurface transport between PFAS. Care must be taken not to attribute changes associated with fate and transport to different sources. If there are two or more likely

sources contributing to mixed contaminant plumes, the challenge becomes greater still. In addition, atmospheric transport and deposition of some PFAS could be considered (Ahrens, Rakovic, et al. 2016; Davis et al. 2007; Galloway et al. 2020).

The following sections describe some of the source identification tools that may be used or considered for use in identifying sources of PFAS.

10.5.1 Source Identification Tools

Chemical fingerprinting involves the evaluation of the relative proportions of different substances in a mixture to link contaminants in the environment to one or more known or suspected sources (see the text box in Section 10.4.3.4). The data from available analytical methods can be evaluated using various graphical, statistical, or geospatial techniques. These methods have been commonly used for petroleum and chlorinated compound source identification and can potentially be applied to PFAS, because the release of PFAS into the environment generally involves the release of a complex mixture of substances, including different subclasses of PFAS. The following sections describe some of the forensic information that may be useful to evaluate sources, as well as some tools for comparing samples within a data set.

10.5.1.1 Manufacturing Signatures

PFAAs (PFCAs and PFSAs) can be produced as a mixture of homologues of different chain lengths depending on the various manufacturing process(es) used (Section 2.2). PFAAs produced by electrochemical fluorination (ECF) can include both even and odd chain-length homologues. PFAAs produced by fluorotelomerization contain mostly even chain-length homologues. However, transformation of some of the fluorotelomer precursors results in the formation of odd chain length PFCAs (Prevedouros et al. 2006; Dasu, Liu, and Lee 2012; Liu and Mejia Avendano 2013). Most commercial laboratories can report PFCA homologues ranging from C4 to C14 and select PFSA homologues between C4 and C12. USEPA (2009) published PFCA profiles in various commercial products that showed different patterns of PFCA chain lengths. Chemical fingerprinting for source identification may be useful for PFAS sites; however, changes in raw materials and processes over time, as well as environmental fractionation, must be taken into account.

Laboratories generally report the concentration of a given PFAA as the total of the branched and linear forms; however, the concentration of the linear form and an estimated concentration for the branched form can be reported independently. The concentration of branched form must be estimated because standards do not yet exist for most branched-chain PFAA (Section 11.2.1). Benskin (2011) used the absence of branched PFCA isomers in dated sediment cores of two lakes to support the conclusion that oxidation of FTOH was the major atmospheric source of PFCAs in the lakes and not direct transport of PFOA. Fredriksson (2016) used isomer profiles along with homologue patterns to assess the sources of PFAS in avian eggs. The potential for environmental fractionation must be taken into account when evaluating isomer profiles because linear and branched-chain isomers have different physical and biological properties, adsorption, and bioaccumulation (Fredriksson 2016; Miralles-Marco and Harrad 2015). Other examples of isomer analysis for PFAS source identification include Shi et al. (2015), Benskin, DeSilva, and Martin (2010), and Karrman et al. (2011).

Chiral fingerprinting through enantiospecific isomer differentiation is a potential method for source identification, although its use is still under development. Asher et al. (2012) applied this method to identify PFAS sources to an aquatic foodweb. However, they noted several limitations and assumptions when using this method for PFAS source identification.

10.5.1.2 Visual Representations of Data

It is common to show representations of measured PFAS in figures or graphs to give the reader a visual sense for relative abundance. Two common graphs for representing PFAS data are bar graphs and radar plots. If one is considering the role of concentration, then it is helpful to plot PFAS concentrations on the axes. However, if one is considering the patterns of data, then it is helpful to plot relative abundance, or the concentration of each PFAS divided by the sum of all measured PFAS, on the axes. It is also suggested to group subclasses of PFAS together and order them by perfluorinated alkyl chain length. For example, PFCAs ordered from the shortest to longest perfluorinated alkyl chain length, followed by PFSAs ordered from the shortest to longest perfluorinated alkyl chain length, followed by fluorotelomer sulfonates ordered from the shortest to longest perfluorinated alkyl chain length allows the viewer to compare changes in compositional patterns both within and between different subclasses of PFAS to assess changes that may occur due to environmental fate and transport. When showing data in this fashion, it is common to report estimated concentrations or J-flagged values and use the value of zero (0) for nondetects. A comparison of PFAS signatures between two samples (Sample A and Sample B) using either bar graphs (Figure 10-2) or radar plots (Figure 10-3) is shown below.
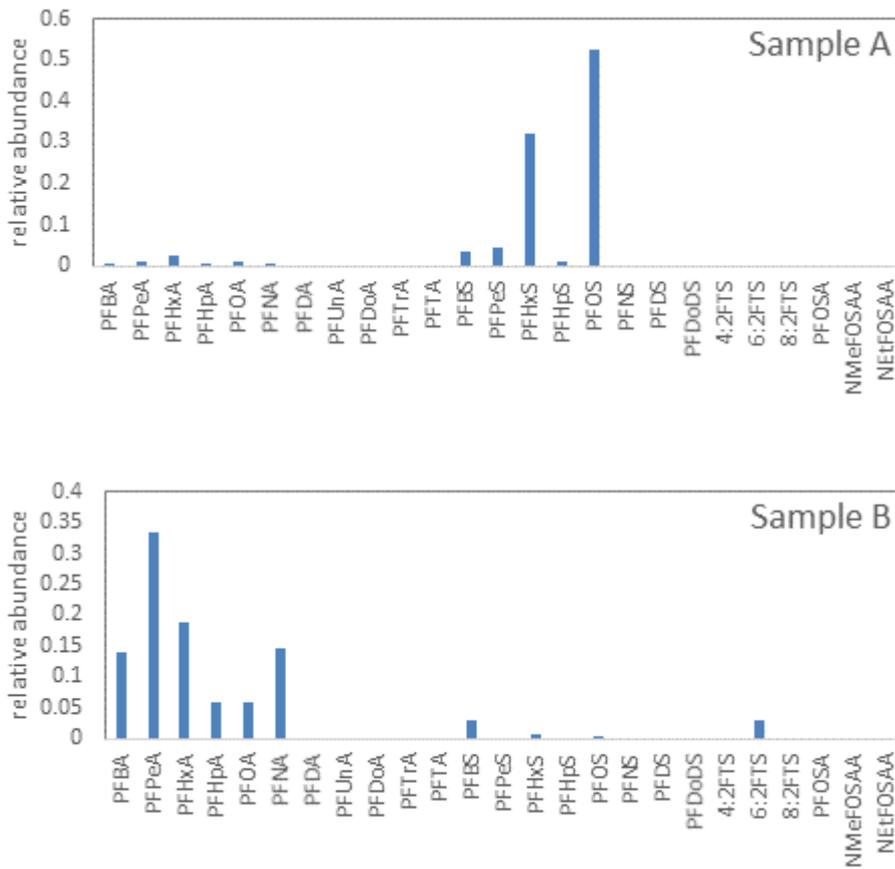
Figure 10-2. Comparison of PFAS signatures in Sample A and B using bar graphs. The concentration of each PFAS has been divided by the sum of all measured PFAS to represent the relative abundance of PFAS in each sample.

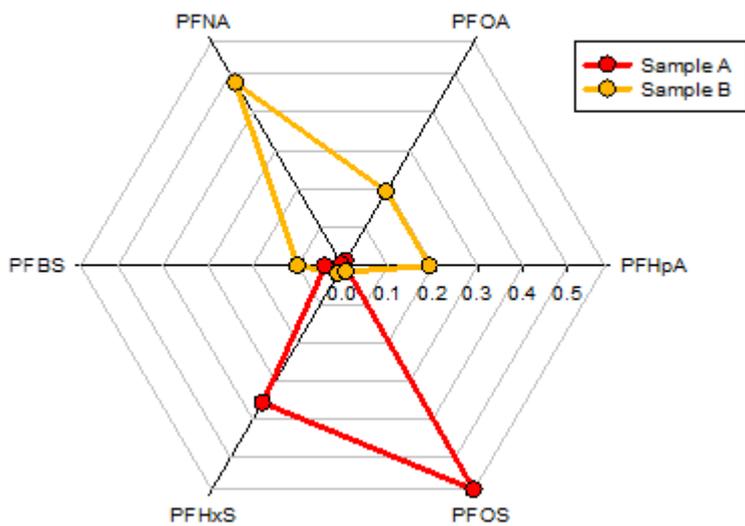*Source: M. Benotti, NewFields. Used with permission.*

Figure 10-3. Comparison of PFAS signatures in Sample A and B using radar plots. The concentration of each PFAS has been divided by the sum of all measured PFAS to represent the relative abundance of PFAS in each sample.

Source: M. Benotti, NewFields. Used with permission.

10.5.1.3 Diagnostic Ratios

In some applications of PFAS forensics, it may be beneficial to show similarities or differences between sample signatures using relative abundances of one or more PFAS or diagnostic ratios, or double ratio plots. Without a comprehensive library of PFAS source materials, such ratios should be site-specific, and should be selected to query the data for a site-specific question and to show similarity or differences between contamination throughout the site and those in known or purported source area/s. Examples of factors that may help identify suitable diagnostic ratios include the relative abundance of PFCAs, PFSAs, or FTSs, the ratio of PFCAs to PFSAs (or more specifically the ratio of PFOA to PFOS), the ratio of even-numbered to odd-numbered PFCAs, the relative abundance of linear to branched isomers of selected PFAS, and others. Table 10-1 shows some example diagnostic ratios for PFAS in Sample A and Sample B above.

Table 10-1. Example diagnostic ratios to compare PFAS signatures of Sample A and Sample B.

	Sample A	Sample B
relative abundance of PFCAs	0.062	0.93
relative abundance of PFSAs	0.94	0.041
relative abundance of FTSs	0	0.029
PFCAs/PFSAs	0.066	22
PFOA/PFOS	0.0217	13

10.5.1.4 Multivariate Statistical Tools Such as Principal Component Analysis (PCA)

PFAS data sets, including TOP assay data, are amenable to a variety of multivariate numerical data analysis techniques that provide a means to categorize PFAS compositional data. The advantages of multivariate numerical methods are that they provide a convenient means to analyze large data sets and reduce the output into relatively straightforward graphical output that describes the most important factors affecting chemical variability throughout the data set. Principal component analysis (PCA) is a multivariate statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components. In other words, it identifies and graphically shows the most important features of data that describe similarities and differences between sample chemistries within a data set. The investigator can use this tool to identify samples that have similar or different PFAS signatures and what changes are driving those differences. Changes in PFAS patterns may be attributable to changes associated with fate and transport, or there may be changes that can be explained only by additional sources. Figure 10-4 presents an example PCA scores plot, which demonstrates the similarity or dissimilarly of PFAS signatures between all samples in a data set.
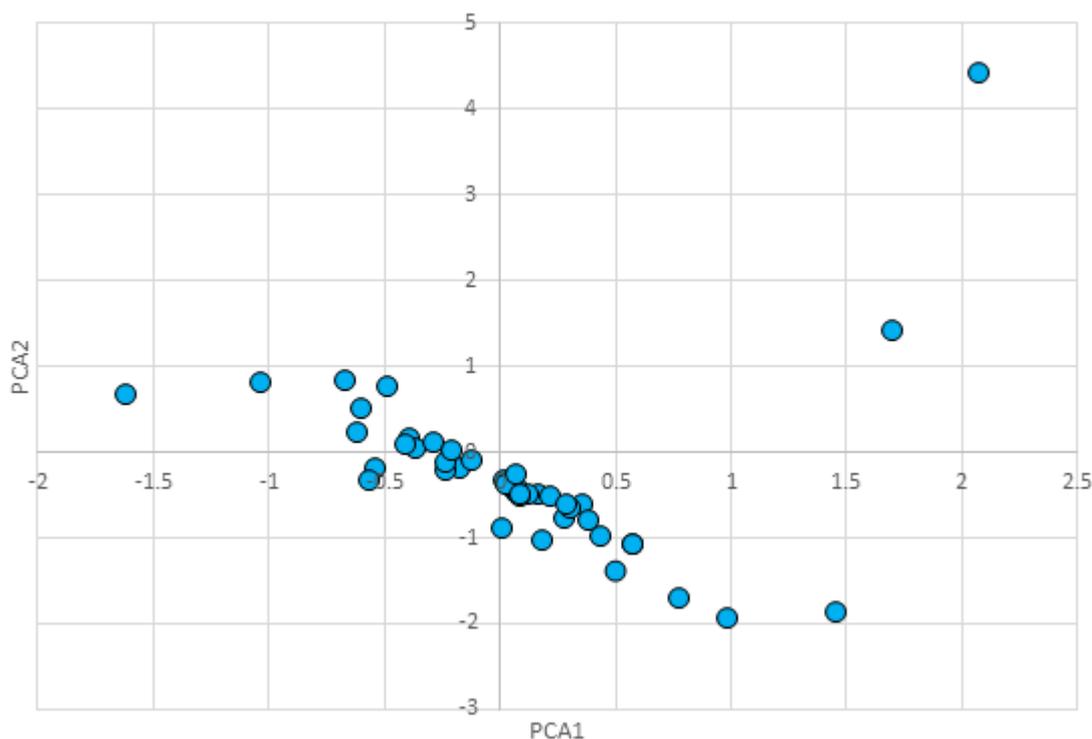
Figure 10-4. PCA scores plot of the analysis of a PFAS data set. Each circle represents the pattern of PFAS contamination of an individual sample. Samples that plot close together have similar PFAS signatures. Samples that plot apart have dissimilar PFAS signatures.

Source: M. Benotti, NewFields. Used with permission.

Examples of chemical fingerprinting for PFAS source identification can be found for wastewater treatment plants (Clara et al. 2008), differentiating AFFF sources (KEMI 2015; Hatton, Holton, and DiGuiseppi 2018; see also Section 3.5), landfills (Lang et al. 2017; Xiao et al. 2012), surface water (Xie et al. 2013), sediment (Qi et al. 2016), and groundwater (Yao et al. 2014). Multivariate statistical analyses (that is, PCA, cluster analysis, and unmixing models) and geospatial analysis have been used extensively to distinguish PFAS sources. Guelfo (2017) emphasized the importance of geospatial distribution of PFAS for source identification. Qi et al. (2016) used PCA–multiple linear regression, positive matrix factorization, and unmix models to identify four PFAS sources (textile treatment, fluoropolymer processing aid/fluororesin coating, textile treatment/metal plating, and precious metals). Zhang et al. (2016) used PCA, hierarchical clustering, and geospatial analysis to determine sources in the northeast United States, and Lu et al. (2017) used factor analysis to classify three categories of PFAS in impacted groundwater. Pan et al. (2014) used PCA in water and sediment samples to distinguish between rural/agricultural and urban/industrial sources.

10.5.1.5 High Resolution Mass Spectrometry (HRMS)

High resolution mass spectroscopic methods using quadrupole time-of-flight mass spectrometry (qTOF/MS) can be used to determine both the chemical formula and structure of unknown PFAS in source materials (see Section 11.2.2.5 for further information on qTOF/MS) (Newton et al. 2017; Moschet et al. 2017; Barzen-Hanson et al. 2017; Battelle 2020; Washington et al. 2020; Getzinger, Higgins, and Ferguson 2021; Guelfo et al. 2021). PFAS suspect screening libraries have been developed to include broader lists of PFAS analytes found across many different PFAS sources (Newton et al. 2017; Moschet et al. 2017; Barzen-Hanson et al. 2017; Getzinger, Higgins, and Ferguson 2021). Because analytical standards are not available for most PFAS included under this extended list of analytes, often these analytical tools are used for qualitative/semiqualitative analysis. These methods have the potential to greatly increase the number of identified PFAS, including precursors and the transformation products, and hence provide more accurate source identification (Washington et al. 2020, Getzinger, Higgins, and Ferguson et al. 2021; Guelfo et al. 2021).

10.5.2 Challenges and Reasonable Expectations

Important factors when considering source identification for PFAS include:

- *data quality*, where care must be taken to ensure that analytical results from different time periods, different methods, or different labs are comparable, as older data sets may provide incomplete information when compared to more recent data
- *target PFAS list*, where a reduced compound list may prevent full differentiation between sources. Linear versus branched (isomer) distinction may also be important.
- *temporal effect*, where an understanding of historical production, use, and release of PFAS becomes important, as is an understanding of differences between samples due to weathering processes that may be interpreted as different sources
- *spatial effect* of long-distance air deposition versus local sources
- *sample collection procedures* to ensure there is no cross-contamination from other sources during sampling
- *weight of evidence* based on multiple lines of inquiry.

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