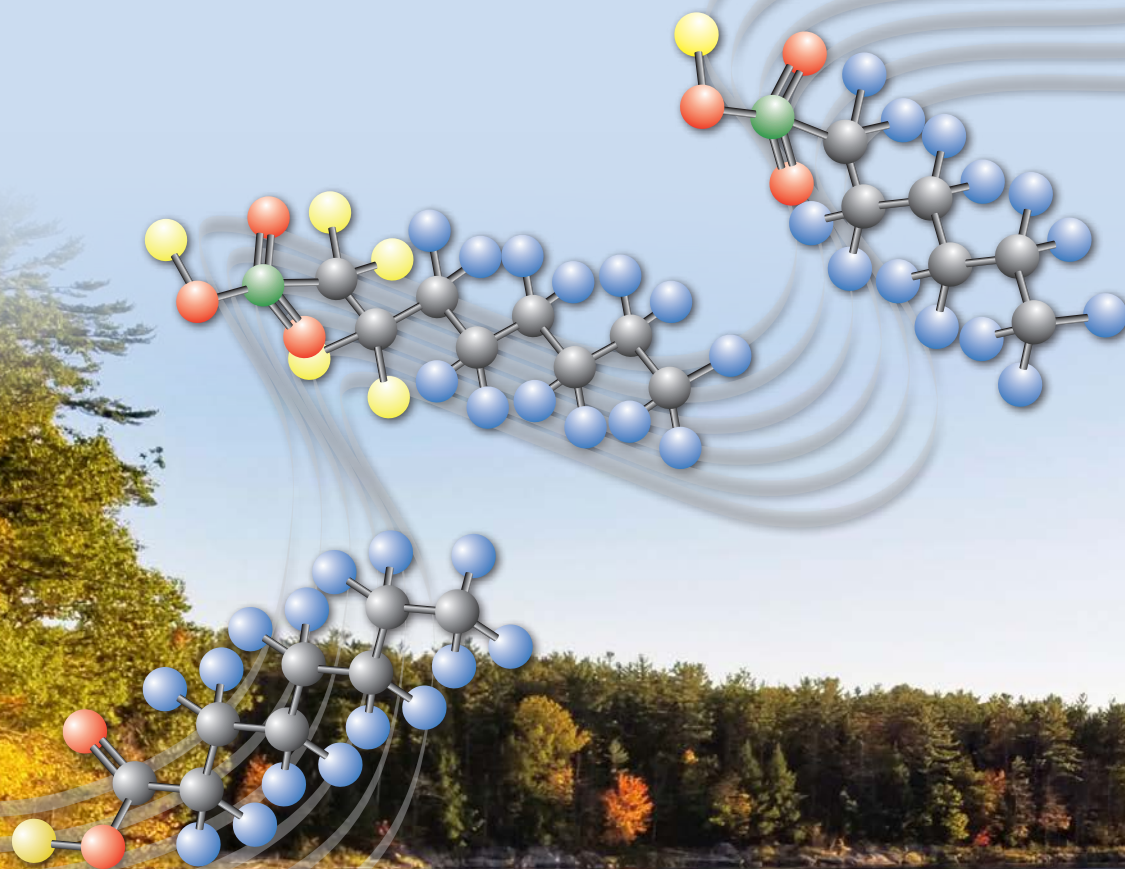


Integrated Science for the Study of Perfluoroalkyl and Polyfluoroalkyl Substances (PFAS) in the Environment

A Strategic Science Vision for the U.S. Geological Survey



Circular 1490

Cover. The Androscoggin River in Maine during fall. Photograph by Rena Kalmon, U.S. Geological Survey. PFAS molecule graphic created by Susan L. Meacham, U.S. Geological Survey.

Back cover. A tidally restricted wetland in the Herring River Estuary, Cape Cod, Massachusetts. Photograph by Jennifer O'Keefe-Suttles, U.S. Geological Survey.

Title page. Water drop hanging from a leaf. Photograph from www.pixabay.com. PFAS molecule graphic created by Susan L. Meacham, U.S. Geological Survey.

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U.S. Department of the Interior
U.S. Geological Survey

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Conversion Factors

International System of Units to U.S. customary units

Multiply	By	To obtain
liter (L)	0.2642	gallon (gal)
nanogram (ng)	3.527×10^{-11}	ounce, avoirdupois (oz) [water]

Abbreviations

CDC	Centers for Disease Control and Prevention
DOD	U.S. Department of Defense
EPA	U.S. Environmental Protection Agency
EOF	extractable organofluorine
HACCP	hazard analysis and critical control point
LC–MS/MS	liquid chromatography-tandem mass spectrometry
MRL	minimal risk level
NAPL	non-aqueous-phase liquid
NDAA	National Defense Authorization Act [“for Fiscal Year 2020” in this report]
NIEHS	National Institute of Environmental Health Sciences
NWIS	National Water Information System
NWQL	National Water-Quality Laboratory
NGWQN	National Groundwater Quality Network
PBPK	physiologically based pharmacokinetic
PFAA	perfluoroalkyl acid
PFAS	perfluoroalkyl and polyfluoroalkyl substances
PFBS	perfluorobutane sulfonate
PFHpA	perfluoroheptanoate
PFHxS:	perfluorohexane sulfonate
PFNA	perfluorononanoate
PFOA	perfluorooctanoate
PFOS	perfluorooctane sulfonate
QTOF	quadrupole time of flight
SPARROW	spatially referenced regression on watershed attributes
TOP	total oxidizable precursor
USGS	U.S. Geological Survey

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Executive Summary

Overview

Concerns related to perfluoroalkyl and polyfluoroalkyl substances (PFAS) in sources of drinking water and in natural and engineered environments have captured national attention over the last few decades. Recent legislation such as the National Defense Authorization Act for Fiscal Year 2020 (NDAA; Public Law 116–92, 133 Stat. 1198), which directs the U.S. Geological Survey (USGS) to carry out several activities related to PFAS, indicates that the study of PFAS is of importance to the U.S. Congress. In addition, topics related to PFAS are of great interest to a variety of external stakeholders, as demonstrated by ongoing Federal and State actions related to standards or guidelines for PFAS in drinking water or other environmental media (Longworth, 2020; Post, 2020).

This report provides an overview of the science gaps that exist in the fields of study related to PFAS that are relevant to the USGS mission and identifies opportunities where the USGS can help address these gaps on the basis of the agency's capabilities and expertise. This document is intentionally composed to enable a flexible implementation of the science, which ensures the scope of scientific studies is commensurate with resources, stakeholder priorities, and other considerations. The integrated science activities envisioned in this document can be designed to address science needs at local, regional, and national scales and varying timeframes as stakeholders are engaged and their needs evolve. In this way, the vision has a broad scientific scope and is not intended to address the specific requirements of any current or pending legislation or regulatory action. Rather, this document is an information resource for USGS scientists who are prioritizing and planning research related to PFAS and may be useful for developing partnerships with other scientists, agencies, and stakeholders.

Vision for an Integrated Science Approach to the Study of PFAS in the Environment

An integrated science approach that encompasses both living and nonliving components of ecological systems will provide stakeholders with the understanding, tools, and data they need to study PFAS in the environment and support a range of decisions that identify, mitigate, or prevent hazards related to PFAS. The USGS can build on a broad range of interdisciplinary, transdisciplinary, and external expertise and nationally consistent laboratory and field capabilities to support needed data collection and research. Studies focused on the life cycle of PFAS could provide a framework and actionable information for identifying and rectifying the most significant factors that may lead to hazards related to PFAS.



Photograph from www.pixabay.com

Capabilities

The USGS has analytical capabilities, national groundwater-quality and surface-water-quality networks, and longstanding partnerships with the following: (1) drinking-water and wastewater industries, (2) other Federal agencies (for example, U.S. Environmental Protection Agency, National Institutes of Health, Centers for Disease Control and Prevention, Department of Defense), and other Department of Interior bureaus, (3) State agencies, (4) Tribal Nations, (5) academic institutions, and (6) a range of local, regional, and national decision makers. The USGS workforce includes geologists, hydrologists, chemists, numerical modelers, programmers, statisticians, geographers, biologists, microbiologists, ecologists, wildlife toxicologists, pathologists, and epidemiologists, among others. Therefore, the execution of integrated science within a nationally consistent framework and oversight of field and laboratory protocols and approaches is a strength of the USGS.

The involvement of multiple Federal agencies, each with their own strengths, is necessary to tackle the multifaceted issues pertaining to PFAS. For example, the U.S. Environmental Protection Agency is engaged in monitoring the presence of PFAS in sources of drinking water, has provided non-enforceable health-based advisories for a limited number of PFAS, and has indicated its intent to initiate the process to evaluate the need for enforceable drinking-water-concentration limits for perfluorooctanoate (PFOA) and perfluorooctane sulfonate (PFOS) (U.S. Environmental Protection Agency, 2019a).

Because the USGS is a nonregulatory agency that provides scientific information to the public, the design and implementation of its research on PFAS can broaden and enhance national databases and the understanding of scientific processes. Therefore, USGS research opportunities to increase our understandings of PFAS and provide actionable information for a range of decision makers and researchers include study of (1) a broader range of PFAS and their precursors beyond those currently under investigation by regulatory agencies, (2) the fate and transport properties of PFAS in a range



of environmental settings, (3) the environmental pathways that expose humans and biota to PFAS, (4) the national-scale occurrence of PFAS in water resources and in the tissues of aquatic and terrestrial wildlife, (5) the bioaccumulation and trophic transfer of PFAS, and (6) the ecological hazards and toxicities resulting from exposures to PFAS.

The nationally consistent capabilities and field and laboratory protocols in USGS science centers across the United States create opportunities to integrate scientific and technical expertise from many natural-science disciplines such as geology, hydrology, chemistry, microbiology, ecology, and toxicology. These capabilities are highlighted in this document as the underpinnings of crosscutting science opportunities, identified through literature reviews and gap analyses, for the study of PFAS.

Fiscal Support

This vision document identifies short-term (1 to 2 years) science opportunities related to the study of PFAS that the USGS could address using existing resources as well as

long-term (3 or more years) science opportunities. The science gaps and approaches presented here can be scoped up or down depending on priorities at the time of implementation.

Science Opportunities That the USGS Could Address

The science opportunities identified herein are integral to the strategic vision for the USGS's study of PFAS and represent priorities for USGS scientists who are planning PFAS research. They are intentionally independent of scale and scope; thus, integrated science activities aligned with these priorities can be designed to address local, regional, and national scales and varying timeframes as stakeholder needs change. The major scientific opportunities for USGS identified through literature reviews and gap analyses are summarized below and are presented as short-term and long-term opportunities for each of seven key individual science topics that can incorporate the study of PFAS. The integration of these topics is summarized as well. These opportunities are listed in table ES.1 and described in individual sections.



Table ES.1. Scalable science opportunities for studying PFAS determined through literature reviews and gap analyses.

[ng/L, nanogram per liter; PFAA, perfluoroalkyl acid; PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS; U.S. Geological Survey; <, less than]

Science opportunities that could be addressed by USGS capabilities, by chapter or section	Short term (1–2 years)	Long term (3+ years)
2.1. Sampling protocols and analytical methods		
Aqueous analytical methods that are suitable for a variety of matrices (surface water, groundwater, and so on)	Yes	No
Standardized field sampling protocols for water and other matrices	Yes	No
Extraction and analytical method(s) for biological tissues	No	Yes
Extraction and analytical method(s) for sediment or soil	Yes	No
Low-detection-limit (<1–5 ng/L) aqueous analytical methods that are suitable for a variety of low-concentration samples (drinking water, and so on)	Yes	No
Analytical method(s) for nonhuman plasma	No	Yes
Sampling protocol and analysis method implementing the total oxidizable precursor assay to estimate PFAA precursor concentrations	No	Yes
Extractable organic fluorine sampling protocol and analysis method for water to screen large numbers of samples for PFAS and nontarget methods to identify unique structures of PFAS	Yes	Yes
Development of methods to facilitate onsite rapid detection of PFAS compounds, such as sensors for PFAS surrogates or proxies reflecting strength of PFAS sources	Yes	Yes
Development of passive samplers for aqueous sampling of PFAS	No	Yes
2.2. Environmental sources and source apportionment		
Develop models and identify data for quantifying or assessing source contributions of PFAS to watersheds and aquifers due to municipal and other wastewater effluents (source apportionment)	No	Yes
Develop models and identify data for quantifying or assessing source contributions of PFAS to watersheds and aquifers due to runoff and leaching from agricultural practices, including municipal biosolids applications (source apportionment)	No	Yes
Quantification of the relative environmental contributions of the above and other sources such as atmospheric deposition (source apportionment) using data and models	No	Yes
2.3. Environmental occurrence		
National evaluation of the occurrence of PFAS, co-contaminants, water-quality parameters, and explanatory factors in ambient water resources ¹	Yes	Yes
National evaluation of the occurrence of PFAS, co-contaminants, water-quality parameters, and explanatory factors in water resources used for drinking water and (or) recreation	No	Yes
National targeted reconnaissance of PFAS in streams and aquifers where water resources are used to supply drinking water and sources of PFAS are known or suspected	Yes	Yes
Modeling to predict PFAS concentrations in unmonitored locations in the future and for evaluation of spatial and temporal trends in composition and concentrations of PFAS	No	Yes
National evaluation of PFAS and related co-contaminants in soils (including those in agricultural, forested, urban, and suburban settings)	No	Yes
National evaluation of PFAS and related co-contaminants in biota (including a range of tissue and plasma)	No	Yes
Comprehensive list detailing the most frequently detected PFAS in the environment	Yes	Yes
National maps showing occurrence of PFAS in water resources, soils, atmospheric deposition, and biota to inform management actions and decision making	Yes	Yes
2.4. Environmental fate and transport		
A database of properties, reactions, and equations for quantitative prediction of transport using chemical reactions (reactive transport)	Yes	Yes
Solid-to-water and air-to-water sorption of PFAS under a variety of hydrobiogeochemical conditions	Yes	Yes
Field studies of PFAS to validate laboratory experiments	Yes	Yes
Abiotic and biotic mechanisms, transformation rates, and transformation products of PFAS under a variety of hydrobiogeochemical conditions	No	Yes
Reactive transport models and other decision tools for estimating transport of PFAS plumes from sources to receptors in space and time	No	Yes
Enhanced understanding of ecological pathways that support movement of PFAS in and through biota, food webs, and so on	No	Yes

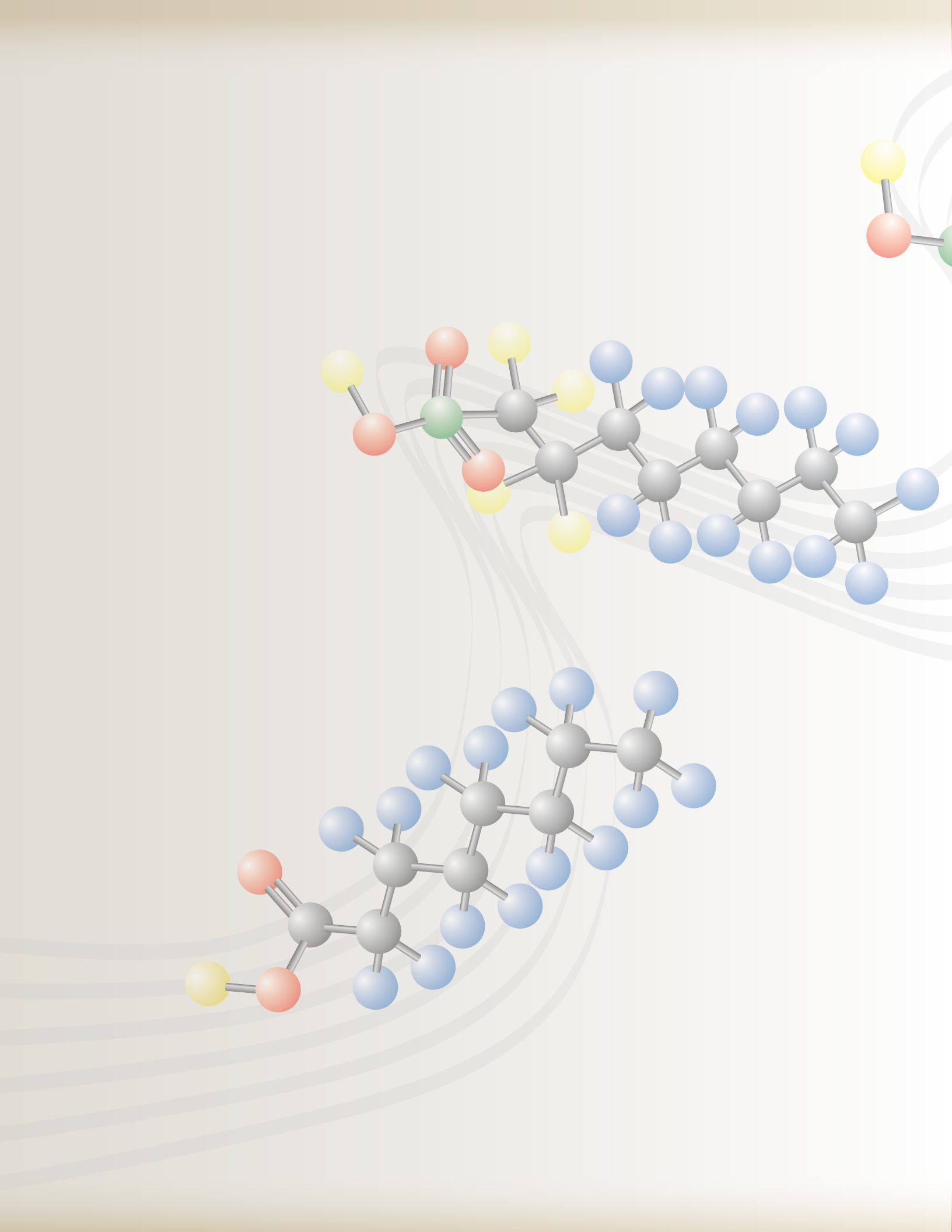
Table ES.1. Scalable science opportunities for studying PFAS determined through literature reviews and gap analyses.—Continued

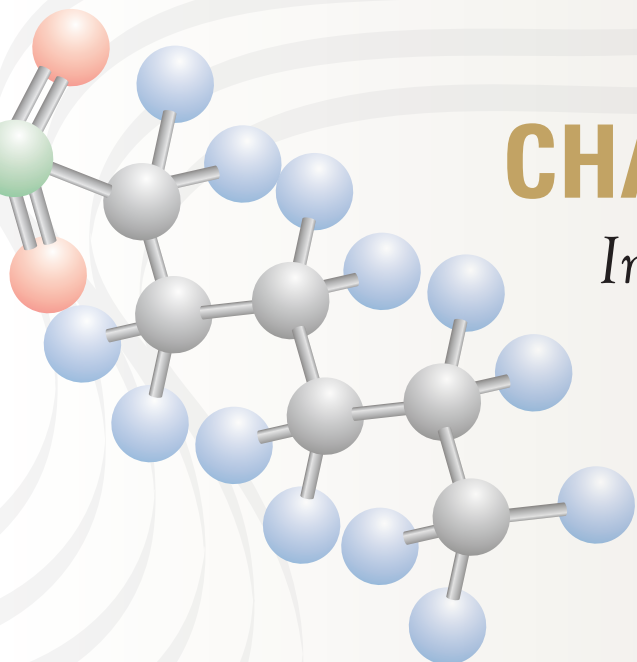
[ng/L, nanogram per liter; PFAA, perfluoroalkyl acid; PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS, U.S. Geological Survey; <, less than]

Science opportunities that could be addressed by USGS capabilities, by chapter or section	Short term (1–2 years)	Long term (3+ years)
2.5. Human and wildlife exposure routes		
Systematic evaluation of human exposure to PFAS in water for human consumption or ingestion (publicly supplied, privately supplied, bottled, and so on)	Yes	Yes
Assessment(s) of the relative importance of routes or mechanisms (inhalation, ingestion, sorption, and so on) and matrices or vectors (air, water, food, dust, soil, sediment, built environment, and so on) that expose humans to PFAS, performed in collaboration with public-health partners	No	Yes
Field evaluation(s) of exposure to PFAS in targeted aquatic and terrestrial wildlife and important exposure routes across locations, life-cycle stages, populations, and food webs	No	Yes
2.6. Bioaccumulation and biomagnification		
Quantification of bioaccumulation kinetics of PFAS in aquatic and terrestrial wildlife	Yes	Yes
Pharmacokinetic and pharmacodynamic studies to determine distribution of PFAS within aquatic and terrestrial wildlife	No	Yes
Determination of critical body residues (relation between uptake, bioaccumulation, and toxicity) within aquatic and terrestrial wildlife	No	Yes
Development and testing of models to predict bioaccumulation of PFAS in aquatic and terrestrial wildlife	No	Yes
Assessment of bioaccumulation, trophic transfer, and biomagnification across food webs	No	Yes
2.7. Ecotoxicology		
Toxicology studies focusing on chronic exposures, sublethal endpoints, and sensitive species	Yes	Yes
Molecular and biochemical toxicology to determine mechanisms in aquatic and terrestrial wildlife	No	Yes
Toxicology studies examining PFAS that co-occur with other contaminants	No	Yes
Microcosm- or mesocosm-level studies that emulate field conditions	No	Yes
3. Vision for integrated science		
Improved understanding of conceptual and other models and decision-support tools that provide actionable information for prediction, prevention, and mitigation of environmental hazards related to human exposure to PFAS through comprehensive evaluation and prioritization of sources, source apportionment, fate and transport, occurrence, and exposures	No	Yes
Improved understanding of conceptual and other models and decision-support tools that provide actionable information for prediction, prevention, and mitigation of environmental risk of exposure to PFAS in ecosystems through comprehensive evaluation and prioritization of sources, source apportionment, fate and transport, occurrence, exposures, and toxicity	No	Yes

¹As used here, “ambient water resources” are those resources necessary to maintain fish, wildlife, and other ecological needs. This term is distinct from the water resources used for public recreation or drinking water.







CHAPTER ONE

Introduction

Perfluoroalkyl and polyfluoroalkyl substances (PFAS) were first used around the 1940s and are a class of anthropogenic chemicals consisting of more than 4,000 unique compounds (Wang, DeWitt, and others, 2017; Organisation for Economic Cooperation and Development, 2018). Definitions and abbreviations of PFAS used herein are provided in sidebar 1. The fluorinated chain portion of PFAS is resistant to chemical and thermal breakdown and imparts stain and water-resistance properties, making PFAS useful for a variety of commercial applications but also persistent in the environment. Many PFAS are surfactants and can be a constituent of aqueous film-forming foams used to fight hydrocarbon fires. PFAS have been used in nonstick coatings for consumer products (water-repellent fabrics, food packaging, nonstick cooking surfaces) and in industrial activities including metal plating and fluoropolymer and plastic production, among others (Interstate Technology Regulatory Council, 2017).

Sidebar 1—PFAS Terminology

PFAS This term is used to describe all perfluoroalkyl and polyfluoroalkyl substances and broadly encompasses the more than 4,000 compounds known to exist within the PFAS class.

PFAAs This term refers to perfluoroalkyl acids such as perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA), which are two of the most widely recognized PFAAs and the subject of current EPA drinking-water health advisories. PFAAs are fully fluorinated (that is, there is no hydrogen attached to carbon in the carbon chain). Although there are several PFAA structures, references to PFAAs in this document refer specifically to perfluoroalkyl carboxylates (such as PFOA) and (or) perfluoroalkyl sulfonates (such as PFOS), which have been the primary subject of research on PFAS and are measured in routine laboratory analysis. PFAAs are frequently referred to as “legacy” or “terminal” PFAAs because of their long history of use, their resistance to transformation into another compound, and their persistence in the environment. Specific PFAAs discussed within this document include the following:

- perfluorobutane sulfonate (PFBS)
- perfluoroheptanoate (PFHpA)
- perfluorohexane sulfonate (PFHxS)
- perfluorononanoate (PFNA)
- perfluorooctane sulfonate (PFOS)
- perfluorooctanoate (PFOA)

Polyfluoroalkyl substances This term describes PFAS that are partially fluorinated. Some polyfluoroalkyl substances can break down in the environment to form terminal PFAAs and are referred to as PFAA precursors (see next definition).

PFAA precursors This term describes compounds that can transform into terminal PFAAs that are typically resistant to further transformation in the environment.



Sources of PFAS to the external environment include (1) wastewater effluent, (2) landfill leachate, (3) biosolids (the solid materials remaining after treatment of sewage) that are applied onto the landscape, (4) aqueous film-forming foam (used to fight hydrocarbon-fueled fires) released to the environment, (5) consumer products used outdoors (for example, ski waxes), and (6) PFAS released by production and manufacturing facilities (Interstate Technology Regulatory Council, 2017). Because of the wide variety of uses, PFAS have been found in many environments and organisms globally, including in atmospheric particulate matter (Lin and others, 2020) and in tissues and blood from polar bears in the Arctic (Smithwick and others, 2005; Spaan and others, 2020). Human exposure to PFAS primarily occurs through ingestion of drinking water and food and through inhalation of air and atmospheric particulates (including both household and outdoor dusts; Sunderland and others, 2019; De Silva and others, 2021).

Most PFAS research to date has focused on perfluoroalkyl acids (PFAAs) such as PFOS and PFOA (sidebar 1). PFAA precursor compounds are PFAS that can transform to PFAAs under both abiotic and biotic conditions (Houtz and others, 2013; Mejia-Avendaño and others, 2016). Exposures to PFAS are a concern because of their documented adverse effects on the immune system, lipid regulation, liver function, reproductive system, physical development, and thyroid function in wildlife and humans (Lau and others, 2004; Fuentes and others, 2007; Abbott and others, 2009; Behr and others, 2020).

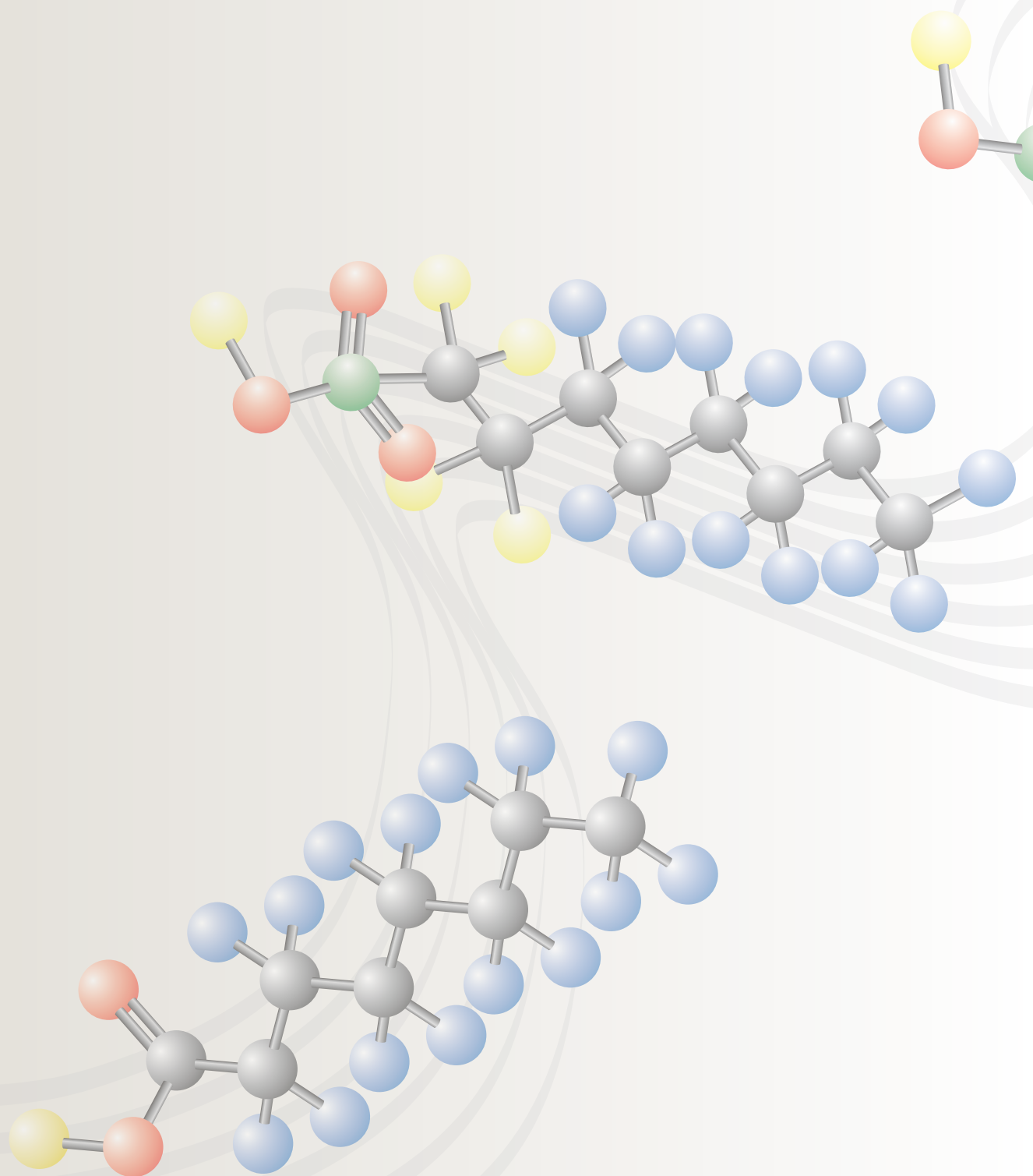
In 2016, the U.S. Environmental Protection Agency (EPA) introduced the current non-enforceable lifetime-human-health advisory for drinking water (the level below which it is anticipated that all people will be protected from adverse health effects from a lifetime of exposure to these compounds though drinking water), which is set at 70 nanograms per liter (ng/L) for the combined concentrations of PFOS and PFOA, two legacy PFAAs of recognized human-health concern. The 2019 EPA PFAS Action Plan indicated the agency's intent to initiate steps to evaluate whether maximum contaminant levels (the highest level of a contaminant that is allowed in drinking water) for PFOA and PFOS are needed (EPA, 2019a). The Centers for Disease Control and Prevention (CDC) and the Agency for Toxic Substances and Disease Registry developed minimal risk levels (MRLs) for four PFAS compounds (Agency for Toxic Substances and Disease Registry, 2018). These MRLs were stated as dosages, which convert to concentrations in drinking water ranging from 52 to 517 ng/L for adults and 14 to 140 ng/L for children, assuming an average adult's or child's weight and water consumption (Agency for Toxic Substances and Disease Registry, 2018). Many States have enacted or proposed maximum contaminant levels or guidance values for select PFAS, some of which are lower than the concentrations in the EPA's lifetime-human-health advisory for drinking water (Longworth, 2020; Post, 2020).

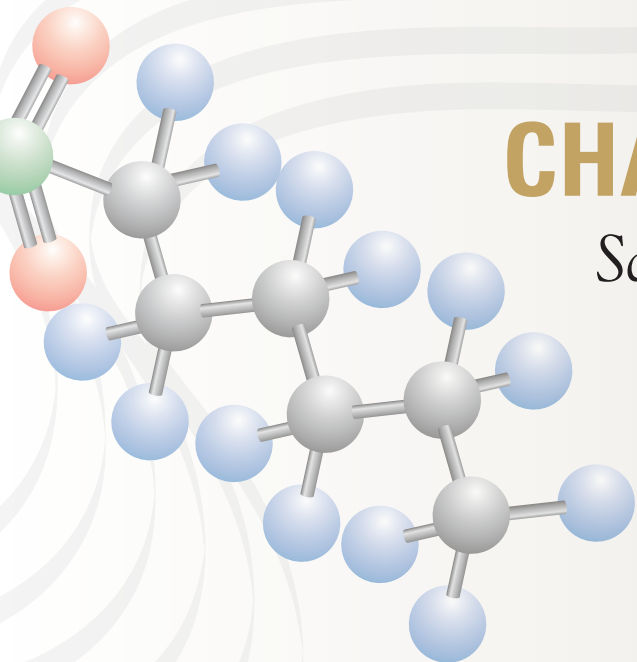
The widespread occurrence of PFAS in the environment compounded with a multitude of sources in the built environment (consumer products, air, dust, food, food packaging, and so on) requires detailed knowledge of complex human exposure routes to effectively design management strategies to protect human health. Studies quantifying exposure from various sources have identified food, drinking water, air, and dust as major contributors to the burden of PFAS in humans (Haug and others, 2011; Hu and others, 2019; De Silva and others, 2021). Additional work on exposure routes considering life stage, lifestyle, regional location, and other factors is needed to fully understand the complexity of human exposure.

The ecological effects of PFAS on aquatic and terrestrial organisms are highly dependent on exposure routes, species sensitivity to PFAS, and bioaccumulation and trophic transfer of PFAS. Although numerous studies on the ecotoxicity of PFAS have been conducted for aquatic organisms, terrestrial invertebrates and plants, and mammals (Interstate Technology Regulatory Council, 2020), there are few ecological guideline values and currently no Federal ecological criteria or guideline values in the United States.

The increasing scientific and public awareness of the widespread distribution of PFAS in U.S. drinking-water supplies and aquatic habitats has raised many public-health and resource-management issues that USGS science can help inform. There are a number of external drivers that support and inform the direction of USGS science related to PFAS. Such drivers include actions taken by Congress or the U.S. Department of the Interior and the needs of USGS stakeholders and partners. For example, the National Defense Authorization Act for Fiscal Year 2020 (NDAA; Public Law 116–92; 133 Stat. 1198) highlights several activities related to PFAS that USGS could support, such as establishing a performance standard (laboratory analytical method) to detect PFAS compounds and carrying out nationwide sampling for PFAS in a variety of water, soil, and other media such as fish tissue.

The focus of this document's vision is to identify existing data and science gaps related to the study of PFAS and determine how USGS capabilities can help address those gaps. Although there are areas of overlap between the NDAA and the science gaps laid out in this USGS strategic science vision document, this document identifies additional data gaps that go well beyond those outlined in the NDAA. The contamination of and potential adverse ecological effects on the environment by PFAS are complex problems best addressed using an integrated science approach, which provides a hydrogeology-, geochemistry- and ecotoxicology-based context at the watershed, regional, and national scales. This document provides a strategic vision for an integrated science approach to the study of PFAS at the USGS.





CHAPTER TWO

Science Needs, Data Gaps, and Opportunities for PFAS Monitoring, Assessment, and Research Activities

2.1. Sampling Protocols and Analytical Methods

2.1.1. State of the Science

Standardized protocols for collecting environmental samples to analyze for PFAS are not yet available. Guidance documents are available, however, and they describe the materials and techniques considered to reflect current best practices. For example, the U.S. Department of Defense (DOD) published a document about selecting the proper sampling vessel and other considerations when sampling for PFAS (Department of Defense, 2017).

With the exception of selected laboratories, analytical methods to date have primarily concentrated on a limited number of PFAS (usually around 24–40 substances), and analyses are typically completed using liquid chromatography-tandem mass spectrometry (LC–MS/MS). As of August 2021, there were two published methods available from the EPA: Methods 537.1 and 533, which focus on the quantification of a total of 29 PFAS in drinking water (Shoemaker and Tettenhorst, 2018; Rosenblum and Wendelken, 2019). Alternatively, EPA Method 8327 quantifies PFAS in surface water, groundwater, and wastewater by external standard calibration (EPA, 2019b). However, the quantification of PFAS is more reliably achieved using isotope dilution or internal standard quantitation (EPA Methods 537.1 and 533) instead of quantification by external standard calibration (EPA Method 8327) because internal standards are better able to account for matrix interference and variability introduced during sample preparation and analysis (EPA, 2021a). The EPA, in collaboration with the DOD, recently (August 2021) released Draft Method 1633 for the analysis of PFAS in aqueous, solid, biosolid, and tissue

samples using isotope dilution or extracted internal standard quantification (EPA, 2021a). Single-laboratory validation has not yet been completed for Draft Method 1633, and this method will not be finalized until multi-laboratory validation is complete. In a partial response to this gap in formalized methods, the USGS has completed the validation of and is in the documentation and method-approval stages for an aqueous direct-injection isotope-dilution method that is expected to measure concentrations of approximately 34 PFAS and could be suitable for analyzing wastewater, surface water, and groundwater. This type of analysis is currently being offered by USGS as a custom method (J. McCoy, U.S. Geological Survey, written commun., 2020). Contract and academic laboratories have developed nonstandardized methods for measuring PFAS in solid and biological matrices in the absence of a published EPA method (prior to the availability of Draft Method 1633).

Nontarget methods (methods that allow for identification of both known and unknown compounds) using high-resolution mass-spectrometry instrumentation (such as ion trap or quadrupole time-of-flight [QTOF] mass analyzers) have become popular because of their ability to identify and detect emerging compounds, such as those created as replacements for PFOS and PFOA (Barzen-Hanson and others, 2017b; McCord and Strynar, 2019). Nontarget methods do not quantify compounds for which no available standards are available, although semiquantitative approaches for estimating concentrations of identified compounds have been proposed (Song and others, 2020).

There are other techniques that differ from nontarget analysis; however, although they cannot distinguish individual molecules, they can be used to estimate concentrations of unquantified PFAS. The total oxidizable precursor (TOP) assay oxidizes PFAA precursors into individual PFAAs that can be quantified by LC–MS/MS as described above; the TOP assay has been used increasingly in recent years (Houtz and Sedlak, 2012; Houtz and others, 2013). The TOP assay produces a total estimated molar precursor concentration and provides some insight into the molar mass of precursors that can be broken down to PFAAs naturally in the environment. The precursor concentrations from the TOP assay are an estimate because some precursors may not be transformed and standardized targeted methods may not capture all transformation products (Zhang, Hopkins, and others, 2019). More broadly, there are research methods that measure the total extractable organofluorine (EOF; Miyake and others, 2007; Yeung and others, 2008; Spaan and others, 2020) and total fluorine (Ritter and others, 2017; Schaidler and others, 2017; Koch and others, 2019; Tokranov and others, 2019) in samples. These methods can be used to estimate total concentrations of PFAS in solid and aqueous matrices.

New extraction techniques for sediment and soil have been developed. Sediment extraction protocols were primarily developed for legacy PFAAs (anionic PFAS); therefore, they frequently employ an alkaline methanol extraction, which is inefficient at extracting all PFAS and may result in the transformation of PFAA precursors (McGuire and others, 2014; Munoz and others, 2018). Newer methods have been developed that target a wider range of PFAS compounds. For example, methanol with ammonium acetate was found to optimize the extraction of 86 PFAS compounds from sediment (Munoz and others, 2018).

Additionally, more cost effective and potentially field deployable methods of screening for PFAS are under development. For example, Australia's Cooperative Research Centre for Contamination Assessment and Remediation of the Environment has produced an anion surfactant test kit (astkCARE) that uses a colorimetric indicator to detect surfactants (Cooperative Research Centre for Contamination Assessment and Remediation of the Environment, 2020). This technology is applicable to PFAS because many of them are surfactants, but the detection limit is 10,000 ng/L (for total anion surfactants), and interference by other surfactants is problematic; however, this technology could be used as a screening tool for severe contamination. An electrochemical method utilizing bubble nucleation for detection of PFAS has been developed with a high specificity to PFOS and PFOA; the detection limits are 30,000 ng/L without preconcentration and 70 ng/L with preconcentration (Ranaweera and others, 2019). The recent development of an electrochemical method for quantifying PFOS at concentrations as low as 1 picomole per liter (0.5 ng/L PFOS) in simple aqueous matrices (Cheng and others, 2020) illustrates the potential for the future development of probes or sensors. Passive samplers (predeployed devices)

have also been investigated for collecting time-integrated aqueous and atmospheric samples. For aqueous sampling, the polar organic chemical integrative sampler has been tested primarily with legacy PFAAs (anionic PFAS), whereas polyurethane foam and sorbent-impregnated polyurethane foams have been used for particle-phase atmospheric sampling (Lai and others, 2019).

2.1.2. Science Gaps

2.1.2.1. Sampling and Extraction Protocols

Protocols for environmental sampling are needed by researchers, Federal and State agencies, and others. The USGS is expected to develop nationally consistent field-sampling protocols for PFAS for inclusion in the USGS National Field Manual (U.S. Geological Survey, 2018). Nationally consistent sampling protocols are critical to allow for the meaningful comparison of data collected across the country by multiple personnel, but no standardized sampling protocol currently exists. Small differences, such as collecting variable sample volumes or using different types of containers, can have major ramifications for detection limits and sample recovery (for example, loss of PFAS to container walls).

Although there is some information on field and laboratory materials (containers, aluminum foil, nitrile gloves, plastic bags, and so on) that have been tested and determined to be free of PFAS (Rodowa and others, 2020), no comprehensive comparison of materials has been conducted to determine which specific items are optimal for reducing contamination and providing a representative sample (through spike recovery tests). Beyond the legacy PFAA class, it is not generally known if or how extensively a sample's integrity is affected by phenomena such as sorption of PFAS to the sampling equipment, volatilization losses, transformation of PFAS after collection, and subsampling biases caused by sorption of PFAS to both container-to-water and air-to-water interfaces. Extraction protocols for sediment and biological tissues require extensive research to ensure the best possible recovery of PFAS compounds.

Validations of passive samplers to estimate concentrations of PFAS in the environment are currently needed, particularly for sampling the aqueous phase (Lai and others, 2019). Kinetic studies assessing the uptake and loss of PFAS and studies designed to address issues of flow, temperature, fouling, and so on, are important in the development of effective passive samplers. Studies also are needed to assess the feasibility of sampling PFAS beyond the typical legacy PFAAs by using passive samplers (Lai and others, 2019).

2.1.2.2. Analytical Methods

Standardized, validated laboratory methods to measure the expansive class of PFAS in solids, biota, water, blood, aqueous film-forming foam, air, food, and other matrices are needed to create reproducible datasets with the same analytes

and detection limits for comparison across studies. New standards are needed to quantify the range of PFAS identified in the environment and allow targeted LC–MS/MS and gas chromatography–tandem mass spectrometry methods to be expanded. Both EOF and TOP methods need to be further developed and standardized for environmental and biological samples. Techniques to streamline nontarget analyses to identify new PFAS are needed. Finally, new cost-effective, field-applicable screening methods are required to support broad surveys over space and time to identify areas contaminated by PFAS for subsequent targeted analyses using more costly methods, such as LC–MS/MS. Additionally, new technologies for quantitative detection and analysis in the laboratory are necessary. In particular, analytical methods capable of total organic fluorine analysis at environmental concentrations without extraction or preconcentration steps would be a significant contribution to the field.

Although detection and reporting limits may vary according to a study's needs, developing the capability to quantify targeted PFAS at very low levels (less than or equal to 1 ng/L) in drinking water is a high priority and may be necessary for studies of other types of water. This capability is especially important given the low concentration limits that are increasingly specified by States and are based on health-centric approaches (Post, 2020). It is vital that the reporting limits are substantially lower than health benchmarks; otherwise, the concentrations of PFAS may exceed the health benchmark(s) but may not be reported as being detected (EPA, 1989; Toccalino and others, 2010). Currently, the detection limits for drinking-water analytical methods from the EPA (537.1 and 533) are typically in the range of 1 to 10 ng/L. However, detection and reporting limits of at least an order of magnitude lower are needed, particularly to detect the legacy class of PFAAs, because advisory levels are already less than 10 ng/L for some States (Longworth, 2020; Post, 2020).

2.1.2.3. Quality Control

Although it is not necessary for every laboratory to follow the same protocol, it is important that the data produced by Federal agencies are compatible. Currently, direct comparisons of data from Federal PFAS laboratories using split samples and other laboratory validation techniques are limited. For laboratories that do not use published methods, the documentation of quality assurance and quality control is often limited.

2.1.3. USGS Capabilities and Expertise

The USGS has the capability to address many of the above gaps, particularly those related to sampling and analyzing water, sediment, soil, and biota. The USGS has a long history of developing sampling protocols, which are documented in the “National Field Manual for the Collection of Water-Quality Data” (U.S. Geological Survey, 2018), and producing quality-controlled data that document the concentrations of a large variety of constituents in water.

Research methods for sediment or biota extraction and analysis, TOP assay implementation, and other methods can be developed by or in collaboration with others (academic institutions, other Federal agencies, and so on), then validated and adopted by the USGS. To develop the needed analytical methods, the USGS can access the skills of research scientists at various laboratories located across the country. These laboratories routinely determine water quality and perform organic chemistry, geochemistry analyses, isotope analyses and more. Many of these laboratories already have the appropriate instrumentation for quantitative PFAS analysis. PFAS water analysis is already available as an internal custom method at the National Water Quality Laboratory (NWQL) in Colorado (J. McCoy, U.S. Geological Survey, written commun., 2020). The new PFAS laboratory at the Eastern Ecological Science Center Leetown Research Laboratory is expected to develop methods for the analysis of nonhuman plasma and biological tissues (T. O’Connell, U.S. Geological Survey, oral commun., 2021).

Several USGS laboratories already possess QTOF or other high-resolution mass spectrometry capabilities for nontarget analysis that are currently used for research and exploratory work and may be available for studies on PFAS. The development and expansion of nontarget-data-postprocessing capabilities would allow for additional high-resolution mass spectrometry sample analyses at larger scales. The passive sampling of aqueous media is an area where the USGS could expand its work. Preliminary research on passive samplers includes (1) the development of sampling for and analysis of PFAS using polar organic chemical integrative sampler technology (U.S. Geological Survey, 2020) and (2) the use of regenerated cellulose dialysis membranes (Imbrigiotta and Fiore, 2021). The examination of next-generation water-quality sensors in selected basins as part of the Next Generation Water Observing Systems is expected to present an opportunity to examine potential proxies (surrogates) for inferring the presence of and estimating the concentrations of PFAS, especially concentrations above regulatory or health advisory limits. Finally, the USGS is expected to investigate instrumentation that allows for EOF analysis, which could provide a bulk concentration estimate of all extractable organic PFAS without the identification of individual compounds.

It is imperative that the USGS work with other Federal partners, such as the EPA and DOD, to ensure standardized sampling, measurement, and quality-control methods to maximize consistency and reproducibility across agencies, with the recognition that Federal agencies will need some flexibility to tailor methods to meet their needs. The USGS is currently participating in the interagency PFAS Technical Working Group, which provides an avenue to exchange updated information on the development, progress, and advancement of PFAS research methods. Additional collaboration and interlaboratory method testing and development with academic institutions and the private sector are required to keep USGS research on PFAS relevant and responsive.

2.1.4. USGS Science Opportunities

2.1.4.1. Short-Term Opportunities

The USGS is expected to develop a nationally consistent protocol for the collection of groundwater and surface-water samples for PFAS analysis and also is expected to publish this protocol in the USGS National Field Manual for the Collection of Water-Quality Data (U.S. Geological Survey, 2018). The sampling protocol is expected to be validated for a targeted analyte list that aligns with the aqueous direct-injection isotope-dilution analytical method that is available as a custom method at the NWQL (J. McCoy, U.S. Geological Survey, written commun., 2020). The aqueous analytical method may be suitable for surface water, groundwater, and wastewater and currently contains 34 PFAS compounds. The new USGS sampling protocols and analytical methods for PFAS are also expected to meet the requirements of the NDAA, which requires the USGS, in consultation with the EPA, to establish a performance standard for detecting as many environmentally relevant, highly fluorinated compounds as possible using validated analytical methods. The act also authorizes the USGS to develop a training program that focuses on the appropriate method of collecting and analyzing samples for highly fluorinated compounds (Public Law 116–92, 133 Stat. 1198).

Following the completion of an approved and published aqueous direct-injection isotope dilution method, the NWQL is expected to develop a new method for analyzing aqueous samples to achieve lower detection limits and improve sample cleanup for complex matrices using an online solid-phase-extraction system (table 1); the initial testing of this method is already underway. Standard operating procedures for laboratories are expected to be written for both fish plasma analysis and implementation of the TOP assay for aqueous samples; the initial testing of these methods has already begun at the NWQL. Laboratory standard operating procedures are also expected to be developed for the extraction and analysis of biological tissues and sediment or soil by adapting methods such as those published by the EPA (2021a).

2.1.4.2. Long-Term Opportunities

The USGS could invest in the development of an EOF sampling protocol and analysis method to allow for an estimate of the total concentration of PFAS in environmental samples. The USGS expects to use a combustion ion chromatograph for the purpose of organic fluorine analysis. Depending on how quickly a method is developed, EOF analysis could be available in the short term. The USGS could follow the development of novel methods for the rapid identification of PFAS in water so that they could be tested in field applications. These methods could include (1) the implementation of sensors for target PFAS and surrogates (such as anionic surfactants) or (2) the development of sets of measurements that could be used as proxies for identifying where PFAS are likely to be present at concentrations above health advisory guidelines. The USGS could also invest in the development of passive samplers for low-cost time-integrated sampling.



Table 1. Scalable science opportunities, determined through literature reviews and gap analyses, that support the study of sampling protocols and analytical methods related to PFAS (section 2.1).

[ng/L, nanogram per liter; PFAA, perfluoroalkyl acid; PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS, U.S. Geological Survey; <, less than]

Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
Aqueous analytical methods that are suitable for a variety of matrices (surface water, groundwater, and so on)	Yes	No
Standardized field sampling protocols for water and other matrices	Yes	No
Extraction and analytical method(s) for biological tissues	No	Yes
Extraction and analytical method(s) for sediment or soil	Yes	No
Low-detection-limit (<1–5 ng/L) aqueous analytical methods that are suitable for a variety of low-concentration samples (drinking water, and so on)	Yes	No
Analytical method(s) for nonhuman plasma	No	Yes
Sampling protocol and analysis method implementing the total oxidizable precursor assay to estimate PFAA precursor concentrations	No	Yes
Extractable organic fluorine sampling protocol and analysis method for water to screen large numbers of samples for PFAS and nontarget methods to identify unique structures of PFAS	Yes	Yes
Development of methods to facilitate rapid onsite detection of PFAS compounds, such as sensors for PFAS surrogates or proxies reflecting strength of PFAS sources	Yes	Yes
Development of passive samplers for aqueous sampling of PFAS	No	Yes

2.2. Environmental Sources and Source Apportionment

2.2.1. State of the Science

The sources of PFAS to the environment include wastewater effluent, stormwater runoff, biosolids application, landfill and septic system leachate, aqueous film-forming foam releases, industry releases, and releases from the use of consumer products (Venkatesan and Halden, 2013; Anderson and others, 2016; Houtz and others, 2016; Lang and others, 2017; Weber and others, 2017; McCord and Strynar, 2019; Masoner and others, 2020). PFAS can be released into the atmosphere, the unsaturated zone, groundwater, surface water, or the oceans. There are several studies on global emission inventories for legacy PFAAs (Wang and others, 2014; Wang, Boucher, and others, 2017). Although the emissions of many PFAS remain unquantified, several studies have been conducted on contamination by PFAS in the environment that provide information on the spatial distribution and concentrations of PFAS. For example, a summary of contamination by PFAS resulting from releases of aqueous film-forming foam in areas on U.S. Air Force bases other than fire-training areas is provided by Anderson and others (2016). Additionally, an analysis of PFAS in biosolids sampled from 94 wastewater treatment facilities across 32 States and the District of Columbia (Venkatesan and Halden, 2013) provides insight into the widespread nature of PFAS in biosolids. Additional information on sources of PFAS is expected to become available in the future. The EPA's PFAS action plan details a short-term goal of compiling information on the sources of PFAS using

a mapping tool (EPA, 2019a). The NDAA directed that 172 PFAS be added to the EPA toxics release inventory; adding the additional PFAS is expected to aid in providing data on the releases of those PFAS compounds. Such information on the sources of the release of PFAS into the environment is needed to inform future monitoring activities and to support environmental modeling.

Given the many sources of PFAS in the environment, there is significant interest in source apportionment (quantifying the contribution of various sources of PFAS to the environment). Source apportionment can be achieved using receptor models, which rely on measurements of the composition of PFAS in environmental samples. Receptors in these models can be environmental (such as a surface-water body or a wild-life preserve) or ecological (such as fish, birds, or humans). Unique or characteristic compositions can help receptor models identify and differentiate complex sources of PFAS. These receptor models can therefore benefit from distinctive compositions of PFAS that arise from changes in the industrial use and production of PFAS over time, the introduction of new PFAS compounds to the market, and the presence of isomers (same chemical formula but different structures) in environmental samples. The feasibility of determining source apportionment using receptor models or other statistical methods has been demonstrated by several studies (Zhang, Lohmann, and others, 2016; Qi and others, 2017; Li and others, 2020). Zhang, Lohmann, and others (2016) used principal component analysis and hierarchical clustering coupled with geospatial analysis to identify sources of PFAS in surface waters. Another approach to source apportionment is to develop mechanistic models or mass balance models. For example, global models for selected PFAS have been simulated using

the mass balance model, Global Distribution Model for Persistent Organic Pollutants (GloboPOP), to incorporate emission estimates of direct sources of PFAS (Armitage and others, 2006; Wania, 2007).

2.2.2. Science Gaps

Although global emission inventories already exist for selected PFAS (Wang and others, 2014; Organisation for Economic Cooperation and Development, 2015; Wang, Boucher, and others, 2017), the locations, magnitudes (point versus non-point sources), composition, and temporal trends of releases to the environment are largely unknown on a regional or national scale. There is no national inventory of PFAS discharged to the environment through wastewater effluent in the United States, and the loading of PFAS through biosolids has not been determined at a regional scale. There is also a lack of data on the spatial and temporal variability in the concentration and composition of PFAS associated with wastewater effluent and biosolids. Finally, the use and production of PFAS generated as replacements for PFOS and PFOA are not well quantified.

A continued analysis of compositions of major sources of PFAS to the environment is needed to support source apportionment techniques. Source apportionment receptor models do not typically account for the aging process of PFAS in the environment (Qi and others, 2017). For example, the initial composition of aqueous film-forming foam may include a large fraction of PFAA precursors that can transform abiotically and biotically in the environment to intermediate precursors and (or) terminal PFAAs (Houtz and others, 2013; Harding-Marjanovic and others, 2015), resulting in a compositional profile that differs from that of the original aqueous film-forming foam. Similarly, compounds with shorter chain lengths (and branched isomers) experience less retention to solid surfaces than compounds with longer chain lengths and therefore are more mobile in the environment; PFAS with long

chain lengths are not expected to migrate as quickly from their sources compared to those with short chain lengths.

In addition to receptor models, advances are needed in mechanistic models to determine source apportionment. The additional 172 compounds added to the EPA toxics release inventory as a result of the NDAA and the expected EPA map of PFAS sources (EPA, 2019a) may enable mechanistic models to predict environmental concentrations of PFAS and determine source apportionment before impacts to human health or ecosystems occur. Such models are needed to provide decision makers with scientifically defensible information to protect water resources (Focazio and others, 2002), but currently the models are limited.

2.2.3. USGS Capabilities and Expertise

The USGS has investigated wastewater treatment plants, fire training areas, and landfill leachate as sources of PFAS to the environment (Weber and others, 2017; Masoner and others, 2020). These types of assessments can provide the basis for developing source apportionment techniques. The USGS has experience in geospatial analysis and statistical and mechanistic modeling, which lend themselves to identifying potential sources of PFAS and the natural or anthropogenic factors driving the occurrence and distribution of PFAS in the environment. Using these tools, the USGS could quantify the source contributions of PFAS in industrial waste, wastewater effluents, runoff, leaching from biosolids, atmospheric deposition, and other sources of PFAS to watersheds and aquifers. For example, the USGS's spatially referenced regression on watershed attributes (SPARROW) models can predict contaminant loading to water bodies by using occurrence data, knowledge of contaminant sources, and hydrogeological information (Saad and Preston, undated). SPARROW models are also capable of tracking contaminants downstream from a source and can keep track of sources such as septic systems



and wastewater treatment plants along downstream reaches. SPARROW models were used for a source apportionment study on nutrients in Tennessee streams (Hoos and others, 2019) and to create a mapping tool to calculate the impact of multiple wastewater treatment plant discharges into the Shenandoah River watershed (Kandel and others, 2017). Bayesian mass-balance mixed models have also been developed to determine the fractional contribution of the dominant sources of nitrate to groundwater (Ransom and others, 2016). Models developed for nutrients, including the SPARROW and Bayesian mass-balance mixed models, have the potential to be used for modeling the source apportionment of PFAS on a regional scale if the source and occurrence data are sufficient.

2.2.4. USGS Science Opportunities

2.2.4.1. Short-Term Opportunities

In collaboration with States and other Federal agencies, including the EPA and DOD, the USGS is expected to identify and inventory known or potential sites where PFAS are released by using geospatial data on manufacturing, locations of wastewater treatment plants, landfills, biosolids application, and similar information.

2.2.4.2. Long-Term Opportunities

Using data obtained in the short-term activities, the USGS could quantify the source contributions of PFAS from industrial facilities, wastewater effluents, runoff, atmospheric deposition, and leaching from biosolids applied to the land surface within watersheds and above aquifers (table 2). The USGS could also pursue process-based science pertaining to the sources of PFAS (biosolids, fire training areas, and so on) to understand the conditions that are conducive to leaching, the mobility of different PFAS compounds, and the compositional effects of PFAS as they age in the environment (see also section 2.4). The information gained from such studies could be used for source apportionment research, which could be achieved through the development of receptor, mechanistic, and statistical models and the use of statistical techniques such



Table 2. Scalable science opportunities, determined through literature reviews and gap analyses, that support the study of environmental sources and source apportionment of PFAS (section 2.2).

[PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS; U.S. Geological Survey]

Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
Develop models and identify data for quantifying or assessing source contributions of PFAS to watersheds and aquifers due to municipal and other wastewater effluents (source apportionment)	No	Yes
Develop models and identify data for quantifying or assessing source contributions of PFAS to watersheds and aquifers due to runoff and leaching from agricultural practices including municipal biosolids applications (source apportionment)	No	Yes
Quantification of the relative environmental contributions of the above, and other sources such as atmospheric deposition (source apportionment) using data and models	No	Yes

as principal component analysis and hierarchical clustering. For source apportionment to be successful, extensive occurrence data across space and time are needed (as described in section 2.3). The data must be of sufficient quality, preferably generated using a single sampling and analysis protocol (as outlined in section 2.1). The development of these models and the subsequent quantification of source contributions (verified by sample collection and analyses) could then be used to evaluate mitigation scenarios and create decision-making tools for water resource managers.

2.3. Environmental Occurrence

2.3.1. State of the Science

Monitoring the occurrence of PFAS is vital because of its long history of use in the United States and the unknown distribution of environmental releases over space and time. Between 2013 and 2015, the EPA monitored six PFAS (perfluorobutane sulfonate [PFBS], perfluoroheptanoate [PFHpA], perfluorohexane sulfonate [PFHxS], perfluorononanoate [PFNA], PFOA, and PFOS) through the third unregulated contaminant monitoring rule, which required monitoring of the six compounds in all public water supplies serving more than 10,000 people, and selected water supplies serving fewer than 10,000 people (EPA, 2016a). These data generally had high reporting limits (up to 90 ng/L) and, therefore, the monitored water supplies may have contained PFAS below these reporting limits but at concentrations that are above some human health benchmarks (Post, 2020). Several statewide efforts to collect water samples are ongoing. For example, Michigan and Vermont, among others, recently began testing public water

supplies using methods with lower reporting limits that are relevant to human health (Michigan Department of Environment, 2019; Vermont Agency of Natural Resources, 2019).

The USGS has sampled for more than 482 organic (including 10 PFAS) and more than 19 inorganic constituents in regulated publicly supplied and unregulated privately supplied drinking water at the point of use (tapwater) in selected regions of the United States (Bradley and others, 2018, 2020a). The USGS sampled more than 500 domestic, monitoring, and public-supply wells in the National Groundwater Quality Network (NGWQN; Lindsey and others, 2018) throughout the United States for 24 PFAS and is expected to continue this sampling at least into 2021. Millions of people rely on these sampled groundwater resources for drinking water (Maupin, 2018). However, more sampling is needed for national coverage. The data from sampled wells can provide an understanding of PFAS in groundwater used for private supply in important aquifers and a rigorous framework for evaluating PFAS in groundwater used for public supply.

In addition to water, PFAS have been detected in the air, soil or sediment, biosolids, and biota. PFAS have been found in air samples collected from various locations, including near manufacturing and waste management facilities (Ahrens and others, 2011b; Galloway and others, 2020), within indoor environments (Langer and others, 2010), and in remote regions (Ahrens and others, 2011a). PFAS also have been detected in extracts of soils and sediments from sites where aqueous film-forming foam was applied (McGuire and others, 2014; Anderson and others, 2016; Weber and others, 2017), in other sites with direct sources of PFAS (Sepulvado and others, 2011), and in remote areas (Rankin and others, 2016). Vermont has completed a study of background soil concentrations



(Vermont Agency of Natural Resources, 2019), one of the few large-scale studies of PFAS in soils. The National Water Quality Monitoring Council's Water Quality Portal provides public access to data about PFAS in water, biota (such as fish tissue), sediment, and soil samples by drawing from the USGS National Water Information System (NWIS), EPA Storage and Retrieval (STORET) Data Warehouse, and the U.S. Department of Agriculture Sustaining the Earth's Watersheds—Agricultural Research Database System (STEWARDS; National Water Quality Monitoring Council, undated). There is also increasing concern over biosolids application as a source of PFAS to the environment (Sepulvado and others, 2011; Venkatesan and Halden, 2013; Navarro and others, 2017). Because there is such widespread distribution of PFAS in the environment, PFAS have been frequently found in plants (Blaine and others, 2014; Zhang and others, 2015), fish (Fair and others, 2019), mammals (Dassuncao and others, 2019; Spaan and others, 2020), and other biota (Kannan and others, 2005).

2.3.2. Science Gaps

A systematic evaluation of the occurrence of PFAS in the Nation's water resources is needed to provide information on the nature and distribution of the sources of PFAS (for example, source apportionment, section 2.2), to support assessments of resource vulnerability, and to guide research directions on the fate, transport, and reduction of exposures. Such an evaluation should be based on nationally consistent analytical methods and sample collection protocols coupled with a list of likely co-contaminants, a comprehensive set of inorganic solutes, and other water-quality parameters. The trends in concentrations of PFAS in groundwater and surface water over time (seasonal and decadal) are unknown. The EPA third unregulated contaminant monitoring rule program did not test private drinking water supplies and tested only a small fraction of public tapwater supplies serving populations under 10,000 people. Approximately 30 percent of the U.S. population relies on private drinking water and small public drinking-water systems (serving less than 10,000 people; Hu and others, 2016); therefore, these water resources need to be evaluated. Similarly, the quality of raw (untreated) and finished drinking water would need to be compared to evaluate drinking-water quality (Boone and others, 2019; Bradley and others, 2020a). Understanding the spatial distribution of PFAS in groundwater is needed because of the decades-long transport times from source areas to drinking water supplies in many parts of the country. In addition to the spatial distribution of PFAS, knowledge of their distribution with depth in the subsurface is needed because the limited mixing and stratified hydrogeologic and biogeochemical zonation in soils and groundwater are expected to result in more heterogeneous concentrations of PFAS than in surface water. Because it will not be feasible to sample all of the Nation's water resources continuously, models are needed for predictive interpolation and extrapolation of PFAS occurrence.

National evaluations of PFAS in soils and biota are needed. To date, there have been no widescale, comprehensive

efforts to understand soil concentrations of PFAS across a variety of soil types and land-use settings, making determinations of ambient concentrations difficult. Although there have been many studies of biota (particularly fish, given human consumption), comparisons between studies are often difficult because of their different sampling and analysis methodologies, necessitating a coordinated national study with consistent, validated sampling, storage, and analysis protocols. Additionally, monitoring air quality, quantifying wet and dry atmospheric deposition of PFAS, and collecting data on PFAS distribution between air, aerosols, and dust are necessary to determine expected ambient background concentrations. Finally, a compilation of existing data for all matrices and from all agencies investigating PFAS has not been undertaken and could provide information on where data gaps exist.

2.3.3. USGS Capabilities and Expertise

The USGS is able to address the need for a national, systematic evaluation of PFAS and co-occurring contaminants in water resources, solids (soil, sediment, dust, and so on), and biota. Addressing this need would also help to meet the requirements of the NDAA, which requires the USGS to carry out nationwide sampling to determine the concentration of highly fluorinated compounds in estuaries, lakes, streams, springs, wells, wetlands, rivers, aquifers, and soil using the validated sampling and analysis protocols (performance standard) being developed by USGS.

The USGS's NGWQN targets groundwater, whereas the National Water Quality Network (U.S. Geological Survey, 2021) targets surface water, including large coastal rivers, large inland rivers, and small streams indicative of urban and agricultural land uses, and reference sites across the United States. Pesticides, major ions, nutrients, and trace metals can be sampled by both networks. The NGWQN also samples for radionuclides and age-dating tracers. This full suite of water-quality parameters can be paired with data on land use, soil type, geology, vegetation, geomorphology, and population to maximize information gained by data interpretation.

The USGS can develop sampling protocols and analytical methods (detection limits) that are standardized and whose quality is systematically controlled across all sites, thus allowing data to be compared across States and through time. The USGS can also work with EPA to prioritize existing sites and jointly cover all necessary monitoring. The NGWQN has already included PFAS in recent sample collection activities. Additionally, many USGS water science centers are already engaged in local monitoring of (1) PFAS in surface water and groundwater and (2) local sites known to have been affected by releases of PFAS. These monitoring and sampling activities can contribute data to national datasets, including available datasets maintained by other Federal agencies (for example, DOD) and statewide monitoring programs.

The USGS can make use of its expertise to create models for predicting concentrations of PFAS. Recently, machine-learning methods were used by the USGS to predict the occurrence or concentration of select contaminants across

and throughout principal aquifers of the United States that are important sources of drinking water (Nolan and others, 2015; Ayotte and others, 2016; Ransom and others, 2017; Lombard and others, 2021). These machine-learning models can incorporate both existing datasets (from USGS and from partners such as DOD, EPA, and State agencies) and the output from previously existing, process-based models and geostatistical models developed from empirical observations. These models can be used to constrain predictions by point-source proximity and hydrogeologic conditions that control the behavior of contaminants in the subsurface (Fienen and others, 2018; Starn and Belitz, 2018).

The USGS can also conduct national-scale soil sampling and analysis as demonstrated by a survey of national-scale soil geochemistry and mineralogy (Gustavsson and others, 2001; Eberl and Smith, 2009; Caritat and others, 2017; Smith and others, 2019; U.S. Geological Survey, 2019). This type of assessment could be used to determine PFAS concentrations and co-contaminants in soil.

Various research facilities across the USGS specialize in the study of fish, avian species, mussels, plants, and mammals. Studies have focused on concentrations of PFAS found in the tissues of tree swallows (Custer and others, 2017; Custer and others, 2019). Ongoing studies are focused on PFAS found in the tissues of fish in the Great Lakes, Chesapeake Bay, and other water bodies.



The USGS could incorporate PFAS and other contaminants of emerging concern into a reassessment of the national Biomonitoring of Environmental Status and Trends network (U.S. Geological Survey, undated), which monitored primarily legacy contaminants in the environment and their relation to effects in fish (Schmitt and Dethloff, 2000; Hinck and others, 2004).

Finally, data on PFAS in the atmosphere could be provided by the USGS's involvement in the multipartner National Atmospheric Deposition Program (U.S. Geological Survey, undated b), which monitors the atmospheric deposition of mercury and other constituents.

2.3.4. USGS Science Opportunities

2.3.4.1. Short-Term Opportunities

The USGS is expected to complete local studies for its cooperators that are already underway. The NGWQN is expected to evaluate data on PFAS in groundwater obtained from sampling efforts conducted during 2017–2021. The USGS is also expected to begin a national reconnaissance of PFAS in streams and aquifers that are sources of drinking water in areas where the sources are known or suspected (table 3). Finally, the USGS is expected to start producing maps showing occurrences of PFAS in water resources and begin developing lists of the most frequently detected PFAS compounds.

2.3.4.2. Long-Term Opportunities

The USGS could implement a national evaluation of PFAS in the Nation's water resources (including water used for raw and treated drinking water and recreation) to provide a thorough understanding of its occurrence (table 3). A national evaluation of occurrence would include a study of co-contaminants, water-quality parameters, and other parameters that can inform controls on distribution, such as isotopes for age dating. In addition to a broad, nontargeted effort to evaluate ambient concentrations of PFAS in water resources, the USGS could conduct a targeted effort to evaluate the concentrations of PFAS in streams and aquifers where its sources are known or suspected (table 3). The USGS could also evaluate trends in the Nation's aquifers over time and conduct modeling studies to inform the source apportionment discussed in section 2.2 and predict occurrences and concentrations of PFAS.

The USGS could also conduct a national evaluation of PFAS and co-contaminants in soils and biota (table 3), which would benefit from the recommended analytical methods developed in section 2.1. The coordination of water, soil, and biota sampling with consistent sampling and analytical methodology could result in a comprehensive national occurrence dataset. The occurrence data obtained for PFAS in water resources, soils, and biota could be mapped and continuously updated as additional information comes available.

Table 3. Scalable science opportunities, determined through literature reviews and gap analyses, that support studies about environmental occurrences of PFAS (section 2.3).

[PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS; U.S. Geological Survey]

Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
National evaluation of the occurrence of PFAS, co-contaminants, water-quality parameters, and explanatory factors in ambient water resources ¹	Yes	Yes
National evaluation of the occurrence of PFAS, co-contaminants, water-quality parameters, and explanatory factors in water resources used for drinking water and (or) recreation	No	Yes
National targeted reconnaissance of PFAS in streams and aquifers where water resources are used to supply drinking water and sources of PFAS are known or suspected	Yes	Yes
Modeling to predict PFAS concentrations in unmonitored locations in the future and for evaluation of trends in PFAS composition and concentrations over space and time	No	Yes
National evaluation of PFAS and related co-contaminants in soils (including those in agricultural, forested, urban, and suburban settings)	No	Yes
National evaluation of PFAS and related co-contaminants in biota (including a range of tissue and plasma)	No	Yes
Comprehensive list detailing the most frequently detected PFAS in the environment	Yes	Yes
National maps showing occurrences of PFAS in water resources, soils, atmospheric deposition, and biota to inform management actions and decision making	Yes	Yes

¹As used here, “ambient water resources” are those resources necessary to maintain fish, wildlife, and other ecological needs. This term is distinct from the water resources used for public recreation or drinking water.

2.4. Environmental Fate and Transport

2.4.1. State of the Science

2.4.1.1. Introduction

To best understand the environmental fate and transport of PFAS, a basic understanding of the terms is needed. The term “transport” refers to the movement of PFAS in the environment. PFAS are typically transported by water or air. The rate of transport of PFAS in water is affected by sorption, which involves the transfer of a compound from the mobile aqueous phase to an immobile solid phase or other interface, such as an immiscible liquid phase or the air-to-water interface, if present. The more extensively a specific PFAS compound sorbs, the lower its concentration in the mobile phase will be and, therefore, the lower its mobility will be in surface water and groundwater. Understanding sorption mechanisms related to PFAS is an area of active research. PFAS that have a larger number of perfluorinated carbons are typically less mobile than PFAS with a smaller number of perfluorinated carbons (Higgins and Luthy, 2006). Further, PFAS with negative charges (anionic) are thought to be more mobile than PFAS with positive, neutral, or both positive and negative charges (Place and Field, 2012). The extent of sorption—and therefore mobility—is influenced by the physical and chemical composition of the water and the soils or sediments.

The term “fate” refers to the ultimate destiny of PFAS molecules. Because the precursors to PFAA (such as N-methyl perfluorooctane sulfonamidoacetate) can transform, their fate is often linked to the transformation of one specific PFAS compound into another either in place or during transport through the atmosphere, surface water, unsaturated zone, or groundwater. For example, PFAS that are PFAA precursors may transform to PFAAs, which may have different sorption properties and different mobilities than those of the PFAA precursors. Transformations of precursors to PFAAs may increase the concentrations of regulated PFAAs at the expense of precursors, which are currently not regulated. Both sorption and transformation result in a decrease in the concentration of a targeted PFAS during transport, but sorption leaves the compound intact so that it could remobilize in response to changes in conditions. Reactive transport models can synthesize comprehensive datasets into fate-and-transport models that can be used to test site-specific conceptual models of processes that affect PFAS during movement from source areas to receptors. This section will discuss both the sorption and transformation of PFAS.

2.4.1.2. Fate and Transport

Polyfluoroalkyl substances can be susceptible to degradation, particularly at positions in the molecules of PFAS where the carbon atoms are not fully fluorinated. The breakdown products of polyfluoroalkyl substances can be PFAAs, which are generally thought to be resistant to further transformation.

Microbial activity can rapidly break down some PFAA precursors, and some transformation products are more persistent PFAA precursors than their parent compound (Liu and Mejia Avendaño, 2013; Harding-Marjanovic and others, 2015; Mejia Avendaño and Liu, 2015; Mejia-Avendaño and others, 2016). PFAA precursors can experience microbial transformations under (1) aerobic conditions (oxygen is present; Harding-Marjanovic and others, 2015; Mejia Avendaño and Liu, 2015; Mejia-Avendaño and others, 2016; Zhang, Lu, and others, 2016), (2) anaerobic conditions (oxygen is effectively absent; Zhang and others, 2013; Zhang, Lu, and others, 2016), and (3) abiotic conditions (hydrolysis and indirect photolysis; Plumlee and others, 2009; Washington and Jenkins, 2015). Recent work indicates that the breakdown, including partial defluorination, of terminal PFAAs such as PFOS can be mediated by the *Acidimicrobium* sp. strain A6 in iron-rich soils under anaerobic, iron-reducing conditions where the pH is less than 7 (Huang and Jaffé, 2019). It is not clear if this process can be exploited for mitigation and remediation or if conditions in the environment are suitable or extensive enough to cause significant decreases in concentrations of PFAS.

As surfactants, PFAS have an affinity for accumulating at interfaces, including solid-to-water, air-to-water, and interfaces between water and immiscible, non-aqueous-phase liquids (NAPLs). Generally, the extent of sorption is greater for PFAAs with longer chain lengths than for those with shorter chain lengths (Wang, DeWitt, and others, 2017; Lyu and others, 2018), and sorption can be affected by the charge and structure of the PFAS compound. The organic carbon content, protein content, anion exchange capacity, and iron oxide content are among important properties of soils and sediments controlling sorption. The pH value of a solution and the concentrations of multivalent cations (Ca^{2+} , Mg^{2+}) can also influence the sorption of PFAS (Higgins and Luthy, 2006; Wang and others, 2015; Campos Pereira and others, 2018; Li and others, 2018; Li and others, 2019).

Studies conducted with selected PFAA precursor compounds found sorption could not be predicted on the basis of soil properties (such as organic carbon) that can influence the sorption of PFAAs (Barzen-Hanson and others, 2017a; Xiao and others, 2019). Other processes including volatilization, sorption at the air-to-water interface, sorption at the water-to-NAPL interface in source areas, and competitive or synergistic interactions between surfactants have all been found to influence the sorption of PFAS (Guelfo and Higgins, 2013; Brusseau, 2018; Lyu and others, 2018; Costanza and others, 2019). PFAS can also be emitted to the atmosphere and transported in the gaseous phase or with aerosols (Young and others, 2007). The transformation of precursors through atmospheric oxidation is also likely to be a source of PFAAs to the environment (Young and others, 2007).

2.4.1.3. Modeling

Reactive-transport models predict how and where a compound will migrate over time and are based on knowledge about (1) water-flow directions and rates and (2) the chemical

reactions involving the compound of interest in the environment. Well-constrained reactive-transport models help identify the most critical information (such as source history, composition, and sorption parameters) required to predict the evolution of a compound's plume (Ma and others, 2014). Information about the degradation of PFAS, such as the half-lives of their transformation reactions (Liu and Liu, 2016), can be incorporated into reactive-transport models (Prommer and others, 2019). Similarly, the sorption parameters for PFAS obtained from laboratory and field experiments can be incorporated into models to help better predict future concentrations of PFAS.

Few studies exist that attempt to incorporate what is known about the sorption and transformation of PFAS to simulate fate and transport. A simulation of concentrations of PFOA in the vicinity of an industrial facility on the Ohio River incorporated their transport through air (to their eventual deposition), river water, and groundwater and required adjusting the coefficient describing sorption onto aquifer sediments to match that of the concentrations observed in drinking-water wells (Shin and others, 2011). There were several uncertainties in this study, including the lack of available information on historical water-pumping rates (Shin and others, 2011). A reactive-transport model incorporating multiple sorption processes (including sorption on sediment grains, sorption at the air-to-water interface, and sorption at the water-to-NAPL interface) was used to simulate the transport of PFOA or PFOS in laboratory column experiments (Brusseau, 2020). A PFOS-validated simplified-compartment model to predict the retention of PFAS in the environment has also been developed (Brusseau and others, 2019).

2.4.2. Science Gaps

2.4.2.1. Fate and Transport

Little is known about biotic and abiotic transformations of most of the more than 4,000 PFAS, including their transformation rates and products under the full range of biogeochemical conditions observed in field settings. The percentage of those transformations accounted for by biotic versus abiotic processes is not known. It is not clear if conditions in the

environment are suitable or extensive enough for the defluorination of terminal PFAAs in the environment.

The influences of soil or sediment composition (such as its organic carbon content and mineralogy) and aqueous-phase composition (such as its dissolved organic carbon composition and concentration, ionic composition, and pH) on the sorption of PFAS to solid interfaces needs further quantitative analysis. The mechanisms of sorption are complex and appear to

depend on the specific compound and characteristics of the system (Zhang, Zhang, and others, 2019). Studies of sorption have thus far been primarily under aerobic conditions. Under anaerobic conditions, reductive dissolution of manganese and iron oxyhydroxides in sediments or the generation of sulfides possibly affect the sorption properties of sediments and thus possibly affect sorption mechanisms. The impact of co-contaminants, such as other hydrophobic organic compounds, on sorption is poorly understood. It is not clear whether sorption observed in controlled laboratory settings applies to sorption as it occurs in field settings. The role of biological activity on the sorption of PFAS (for example, the sorption of PFAS to sediment biofilms) has not been investigated in the context of the sediment-to-water interface. The role

of adsorption at the air-to-water interface on the transport of PFAS is not fully understood, although recent work suggests it is important (Brusseau, 2018; Lyu and others, 2018; Costanza and others, 2019; Li and others, 2019). In addition, air-to-water and sediment-to-water partitioning for the large number of compounds outside of the typically studied legacy PFAAs must be understood for model parameterization and to assess whether sorption at these interfaces exerts an important control on their movement through soils and sediments. Finally, there is a fundamental need for comprehensive, integrated field studies on the fate and transport of PFAS from their real-world source areas to receptors. Field studies are needed to evaluate the usefulness of laboratory-derived conceptual and quantitative models of sorption, transformations, and biological activity at the solid-to-water and air-to-water interfaces for predicting the transport of PFAS and their exposures in real-world settings. Field studies also are needed to help identify processes about which little or nothing is known but which



may affect the movement of PFAS through soils, sediments, and aquifers.

2.4.2.2. Modeling

Despite the widespread application of reactive-transport models to describe the fate and transport of many contaminants, there have been few instances of applying such models to PFAS. A database of sorption and transformation processes and parameters is needed for modeling, as described above. Field-scale observations are needed to identify the critical processes controlling the fate and transport of PFAS and to develop site-specific models describing the rate and extent of these processes over the relevant range of chemical conditions and sediment properties at the plume scale. Reactive-transport models developed from these types of studies are needed to help identify the critical pieces of information required to predict the movement of PFAS from sources to receptors and provide tools to estimate the extent of contamination from PFAS and their concentrations where exposures may occur. Where experimental data on the properties of PFAS are unavailable, simulated computations using quantitative structure-activity relationships and quantum chemical calculations, which have been used to estimate acidity constants and other chemical properties of PFAS (Goss, 2008; Steinle-Darling and Reinhard, 2008), could be used to predict transformation pathways and persistence under natural attenuation conditions (absence of human intervention; Blotvogel and others, 2011; Tratnyek and others, 2017).

2.4.3. USGS Capabilities and Expertise

2.4.3.1. Fate and Transport

The USGS already has the capabilities and expertise to perform a combination of field and laboratory studies to address the science gaps identified in the descriptions above about the fate, transport, and modeling of PFAS in the environment. The processes controlling the fate and transport of PFAS have been studied since 2014 by a collaboration of multidisciplinary scientists from USGS and academic institutions (Weber and others, 2017). USGS personnel at other long-term research sites already have worked on PFAS and can make use of the knowledge gained from their years of prior hydro-geochemical research (Cleary and others, 2021; Imbrigiotta and Fiore, 2021). These field studies can be supplemented by laboratory studies within the USGS that are already set up to analyze concentrations of PFAS. The USGS can evaluate of the fate and transport of PFAS at sites that span different geochemical and hydrological environments across the Nation to improve the broad understanding of sorption and transformation processes. The existing specialized laboratories at USGS are already available to further the understanding of precursor and PFAA biotransformation rates, determined by studying microbial pathways. USGS laboratories that are already set up for partitioning experiments (including column experiments) can determine sediment-water distribution coefficients.

Partners could include academic researchers and other Federal researchers from agencies such as the DOD, the EPA, and the U.S. Department of Energy. For example, the EPA's PFAS action plan includes research to better understand fate-and-transport pathways of PFAS (EPA, 2019a).

2.4.3.2. Modeling

Groundwater and surface-water flow modeling has been an integral part of USGS activities for decades. Models that are relevant to the study of PFAS have mainly focused on (1) the flow within complex systems such as the unsaturated zone, fractured rock, karst, and (2) the exchange between groundwater and surface water. The capability exists to incorporate reactive processes such as sorption to air-to-water and solid-to-water interfaces, gas-phase partitioning, degradation rates of PFAA precursors, and the potential degradation of terminal PFAAs into existing USGS models such as PHREEQC (originally, pH-redox-equilibrium; Parkhurst and Webb, 2020). The USGS employs many scientists with modeling experience who could incorporate the unique PFAS chemistry into existing models.

2.4.4. USGS Science Opportunities

2.4.4.1. Short-Term Opportunities

A database is expected to be prepared for the prioritized PFAS compounds (table 4). The database would be used for geochemical modeling and would include their physical and chemical properties, the equations for describing reactive processes (transformations and sorption), and the associated parameter values from literature studies. The database would be updated as further studies are conducted within and outside the USGS to advance an understanding of controls on reactive transport. A list of field sites could be developed for conducting integrated field studies of the fate and transport of PFAS; these studies could also investigate the potential impacts of the fate and transport of PFAS on humans, and (or) aquatic and terrestrial organisms.

2.4.4.2. Long-Term Opportunities

The USGS could conduct long-term, integrated field research at one or more sites with appropriate characteristics so that the results could be extrapolated to regional and national scales. Field experiments and laboratory studies with site-specific materials over a range of aqueous chemical conditions relevant to the site could be undertaken to produce sorption and transformation parameters necessary for the development of reactive-transport models (table 4). Some key aspects of the fate and transport of PFAS that could be quantitatively investigated include (1) microbial-catalyzed transformations (rates and transformation products), (2) the impact of PFAS on microbial communities, (3) sorption to different microbial communities and cotransport in the colloidal phase, (4) sorption to sediments, (5) sorption at the air-to-water

Table 4. Scalable science opportunities, determined through literature reviews and gap analyses, that support the study of the environmental fate and transport of PFAS (section 2.4).

[PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS; U.S. Geological Survey]

Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
A database of properties, reactions, and equations for quantitative prediction of transport using chemical reactions (reactive transport)	Yes	Yes
Solid-to-water and air-to-water sorption of PFAS under a variety of hydrobiogeochemical conditions	Yes	Yes
Field studies of PFAS to validate laboratory experiments	Yes	Yes
Abiotic and biotic mechanisms, transformation rates and transformation products of PFAS under a variety of hydrobiogeochemical conditions	No	Yes
Reactive transport models and other decision tools for estimating transport of PFAS plumes from sources to receptors in space and time	No	Yes
Enhanced understanding of ecological pathways that support movement of PFAS in and through biota, food webs, and so on	No	Yes
Comprehensive list detailing the most frequently detected PFAS in the environment	Yes	Yes
National maps showing occurrences of PFAS in water resources, soils, atmospheric deposition, and biota to inform management actions and decision making	Yes	Yes

interface, (6) the influence of water and sediment chemistry on sorption of PFAS, and (7) the impact of co-contaminants on the fate and transport of PFAS (table 4). Equations and parameters from laboratory and field studies could then be used to parameterize reactive-transport models that may apply to a variety of sites. The modeling results could inform studies of potential impacts on human health, aquatic organisms, and terrestrial ecosystems by predicting spatial concentrations of PFAS.

and others, 2019). Although concentrations of PFAS in human plasma may be higher in areas with contaminated tapwater, the inhalation of dust and air and ingestion of food contaminated with PFAS appear to be significant additional exposure routes to humans (Haug and others, 2011).

Biomonitoring studies of wildlife and humans have documented the presence of PFAS in a variety of species and

2.5. Human and Wildlife Exposure Routes

2.5.1. State of the Science

There are many types of commercial sources, applications, and corresponding pathways of PFAS to the environment (see section 2.2.1). There are also many associated environmental exposure vectors or matrices, such as air, water, food, dust, soil, sediment, and the built environment (Johansson and others, 2014; Liu and others, 2014; Scheringer and others, 2014; Wang and others, 2014; Gebbink and others, 2015; Sunderland and others, 2019). Similarly, there are many mechanisms that expose humans and wildlife to PFAS, such as (1) the prenatal transplacental transfer of PFAS from a mother to her fetus (Beesoon and others, 2011; Kim and others, 2011; Winkens and others, 2017) and (2) all primary postnatal life-stage contaminant exposure routes, including ingestion, inhalation, or dermal contact (Houde and others, 2006; Houde and others, 2011; Hu and others, 2018; Hu and others, 2019; Sunderland and others, 2019). The contamination of drinking water by PFAS has become an issue of national concern; however, a recent study indicates that tapwater may only contribute about 20 percent of all PFAS found in human plasma (Hu

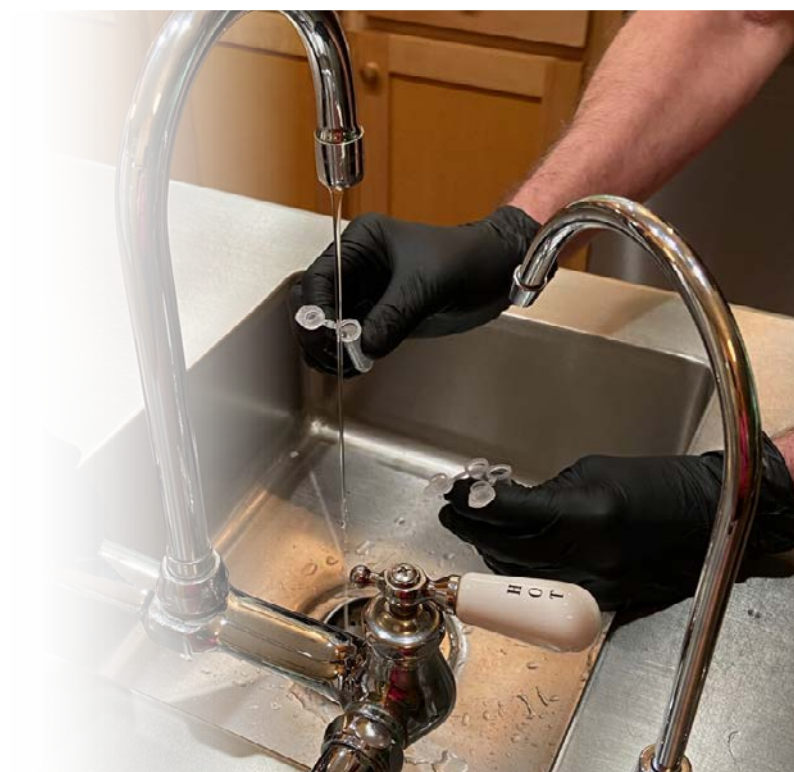


Table 5. Scalable science opportunities, determined through literature reviews and gap analyses, that support the study of human and wildlife exposure routes of PFAS (section 2.5).

[PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS; U.S. Geological Survey]

Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
Systematic evaluation of human exposure to PFAS in water for human consumption or ingestion (publicly supplied, privately supplied, bottled, and so on)	Yes	Yes
Assessment(s) of the relative importance of routes or mechanisms (inhalation, ingestion, sorption, and so on) and matrices or vectors (air, water, food, dust, soil, sediment, built environment, and so on) that expose humans to PFAS, performed in collaboration with public-health partners	No	Yes
Field evaluation(s) of exposure to PFAS in targeted aquatic and terrestrial wildlife and important exposure routes across locations, life-cycle stages, populations, and food webs	No	Yes

tissue types (Houde and others, 2006; Houde and others, 2011; Kannan, 2011; Custer and others, 2013; Roos and others, 2013; Gebbink and others, 2015; Dassuncao and others, 2017; Cui and others, 2018; Dassuncao and others, 2019; Lynch and others, 2019; Sunderland and others, 2019). Multiple studies have reported shifts in the presence of PFAS over time, including declines in the concentrations of individual legacy compounds such as PFOS and PFOA in human and wildlife tissues. However, persistent (and, in several cases, increasing) trends in total concentrations of PFAS in tissues indicate an extensive and continuously evolving exposure landscape, most notably related to replacement and emerging PFAS (Houde and others, 2006; Houde and others, 2011; Roos and others, 2013; Dassuncao and others, 2017; Olsen and others, 2017; Lynch and others, 2019; Sunderland and others, 2019).

2.5.2. Science Gaps

Previous studies have documented the diversity of exposure routes of PFAS to humans (Gebbink and others, 2015; Sunderland and others, 2019; De Silva and others, 2021). The relative importance of each exposure route across different locations, life-cycle stages, populations, and food webs, however, is poorly understood (Hu and others, 2018). An analogous but less well studied range of exposure routes exists for wildlife and agricultural animals, with poorly understood toxicological implications for environmental (wild) populations and for humans through consumption of wild-caught and farmed fish and animals (Houde and others, 2006; Houde and others, 2011; Ghisi and others, 2019; Sunderland and others, 2019). An improved understanding of (1) the exposure routes for the more than 4,000 PFAS in commercial use (Wang, DeWitt, and others, 2017) and (2) their relative importance across human and wildlife populations is a fundamental science and risk-management data gap (Houde and others, 2006; Houde and

others, 2011; Birnbaum and Grandjean, 2015; Grandjean and Clapp, 2015; Wang, DeWitt, and others, 2017; Grandjean, 2018; Hu and others, 2018; Sunderland and others, 2019; De Silva and others, 2021). The continued characterization and profiling of PFAS and co-occurring contaminants associated with various exposure routes and quantitative comparisons of contaminant exposure rates and loads are needed. Chemical identification techniques (see section 2.2.1) also need to be developed to support the study of the source apportionment of PFAS detected in samples of human and wildlife tissue. Both coordination within the USGS and external collaboration of the USGS with State and Federal public health and regulatory agencies, utility companies, and academic institutions are required to assess human-health risks from ingestion of contaminated drinking water and food and to identify and implement mitigation strategies.



2.5.3. USGS Capabilities and Expertise

Human exposures to PFAS and other contaminants through drinking water are particular concerns because of the greater susceptibility of sensitive subpopulations—including formula-fed infants, children, older adults, and those with compromised immune systems and chronic health conditions (EPA, 2021b,c). The USGS is well positioned to continue supporting human-health risk-assessment activities of public health agencies (such as the EPA or the National Institute of Environmental Health Sciences [NIEHS], which is part of the National Institutes of Health, and others) by characterizing mixture profiles, which include PFAS, in ambient drinking-water reservoirs and aquifers, at drinking-water treatment facilities, and at the point of use for tapwater (Bradley and others, 2018; Bradley and others, 2020a; Bradley and others, 2021). The USGS is also poised to contribute to the quantitative assessment of concentrations of PFAS associated with drinking-water consumption relative to other human exposure mechanisms, including through food and air. The USGS is also able to support the priorities of Federal and State environmental protection agencies (for example, the EPA, NIEHS, CDC, U.S. Fish and Wildlife Service, State agencies, and others) by characterizing the diverse exposure profiles of PFAS in surface water, groundwater, soil, sediment, wastewater effluent, biosolids, and air; and quantitatively assessing the relative concentrations of PFAS associated with different environmental settings and their ecological exposure mechanisms. The USGS can support Federal and State wildlife and natural-resource managers by assessing the relative importance of the exposure of wildlife to PFAS through water, food, air, dust, sediment, soils, biosolids, and so on, in collaboration with researchers who are assessing biomagnification and trophic transfer (see section 2.6). The USGS is also positioned to support research documenting trends in exposure over space and time in areas where data are lacking; however, this research would require the development of analytical methods for a variety of matrices, including human and wildlife tissue (see discussion of analytical methods in section 2.1).

2.5.4. USGS Science Opportunities

2.5.4.1. Short-Term Opportunities

The USGS is expected to continue to work with public health agencies, regulatory agencies, utility companies, and academic institutions to expand its research on tapwater that contains contaminant mixtures including PFAS (Bradley and others, 2018; Bradley and others, 2020a). These studies would target various regions and hydrologic settings to assess exposures to PFAS in sensitive subpopulations and determine which infrastructure-linked drivers may account for the exposure to PFAS by drinking tapwater (table 5).

2.5.4.2. Long-Term Opportunities

The USGS could contribute to and (as needed) initiate collaborative, multiagency or multi-institution research studies that would investigate the relative importance of human exposure to PFAS through (1) food and drinking water and (2) the built-environment including air, dust, soil, and sediment (table 5). For wildlife, USGS could initiate studies to investigate exposure routes and environmental controls of PFAS across locations, life-cycle stages, populations, and food webs.

2.6. Bioaccumulation and Biomagnification

2.6.1. State of the Science

The uptake of a chemical from the environment or through the diet and into the tissues of an organism is known as bioaccumulation. The bioaccumulation of PFAS in organisms has been studied using aquatic invertebrate, fish, avian, and mammalian models (Kudo and others, 2001; Gannon and others, 2011; Custer and others, 2017; Dassuncao and others, 2019; Langberg and others, 2019; Song and others, 2020). Bioconcentration is the partitioning of PFAS from exposure media such as water, sediment, or soil into organism tissue, whereas biomagnification of PFAS refers to the increase in accumulation that occurs as the chemical moves through a food chain. A recent review summarized the bioconcentration or biomagnification factors for 17 different PFAS in aquatic and terrestrial organisms (Conder and others, 2020); this study noted that data for compounds other than PFOA and PFOS were often limited. Traditional partitioning approaches, such as the use of a lipid-based partition models, for predicting tissue concentrations from environmental media are not supported by the properties and behavior of PFAS (for example, solubility and lack of consistent partitioning relations) and are therefore unreliable. For example, in fish there is significant variability in reported bioaccumulation factors and biota-sediment accumulation factors (Houde and others, 2006; Giesy and others, 2010). Laboratory and field bioaccumulation relations are often inconsistent, and laboratory-derived relations may underestimate bioaccumulation (Burkhard and others, 2012). Bioaccumulation models based on protein binding or phospholipid partitioning have been developed (Armitage and others, 2013; Ng and Hungerbühler, 2014) but will require additional development when the factors that control exposure, uptake, and elimination are better understood.

2.6.2. Science Gaps

The ability to accurately assess ecological risk from PFAS is limited by an incomplete understanding of exposure concentrations within an ecosystem and through food webs (Ankley and others, 2020). An understanding of why bioaccumulation and biota-sediment accumulation factors vary

across different studies is needed. Bioaccumulation information for less studied compounds that are frequently detected in the environment is also needed for fish, birds, and other aquatic biota consumed by fish, birds, and mammals. Controlled bioconcentration and bioaccumulation laboratory studies designed to determine the adsorption, distribution, metabolism, and elimination kinetic parameters for PFAS with different physicochemical properties are needed. These studies could cover a range of aquatic and terrestrial species with different life-history strategies (such as feeding mechanisms and lifespan) and probabilities of exposure to PFAS. Bioconcentration studies are needed that focus on aquatic species, such as fish, for which water is the primary initial route of exposure to PFAS; fish have great variability in bioconcentration rates and data are currently limited for many PFAS. In addition, studies of the bioaccumulation of PFAS from other media such as sediment or aquatic invertebrate food sources are needed for those PFAS that are relatively insoluble in water.

Bioconcentration and bioaccumulation models are needed because there are more than 4,000 PFAS, and there are significant challenges to assessing and predicting their bioaccumulation in aquatic and terrestrial organisms (Conder and others, 2008). The bioaccumulation of PFAS is not similar to that of nonpolar contaminants such as polycyclic aromatic hydrocarbons and polychlorinated biphenyls and thus requires different modeling variables and kinetic information to accurately model bioaccumulation in ecosystems (Bertin and others, 2016; Prosser and others, 2016). The lipid-based partition models typically used to predict the bioaccumulation of organic compounds do not accurately predict the bioaccumulation of PFAS. Those models are based on contaminants partitioning into neutral lipids, which are not the drivers for the bioaccumulation of PFAAs (Ng and Hungerbühler, 2014). Several studies have demonstrated that bioaccumulation in aquatic organisms should not be normalized to neutral lipid content because PFAS bind to amino acids, proteins, and lipoproteins (Higgins and others, 2007; Prosser and others, 2016). Therefore, bioconcentration and bioaccumulation models specific to PFAS are needed.

Pharmacokinetic and pharmacodynamic models are used to predict the distribution of chemicals within an organism and the organs in which PFAS are most likely to be found. The pharmacokinetic properties of PFOS and PFOA have been studied in mammalian models (Lau and others, 2007; Kim and others, 2016) and have shown that they are absorbed orally with limited elimination and they are distributed mainly to the serum, kidneys, and liver. These data are currently not available for most aquatic organisms and wildlife. Therefore, there is a need to conduct *in vitro* and *in vivo* studies to support the development of physiologically based pharmacokinetic (PBPK) models in these taxa.

The PBPK models can also be used to identify organs where toxicity may occur and help guide studies to determine the biochemical-level mechanisms of toxicity. Rate constants, used for PBPK models to determine the partitioning of PFAS

compounds from blood to organs, are dependent on diffusion across membranes, binding to membrane components, and binding to fatty acids in cytosol (Armitage and others, 2013; Ng and Hungerbühler, 2014). A more thorough understanding about the binding properties of PFAS, which may be accomplished through *in vitro* studies, is needed to parameterize and further develop PBPK models for fish, birds, and other wildlife.

2.6.3. USGS Capabilities and Expertise

The USGS is capable of conducting studies focusing on the bioaccumulation and biomagnification of PFAS in aquatic and terrestrial ecosystems. This research will require collaboration between biologists and analytical chemists to provide chemical analyses of PFAS in blood, serum, other biological fluids, and tissues (see section 2.1). The USGS maintains a variety of aquatic (fish, invertebrates) and terrestrial (avian) colonies at several locations that are available for *in vivo* studies that would support bioaccumulation and biomagnification research and PBPK model development. USGS scientists have experience conducting bioaccumulation and PBPK research, as exemplified by published studies on the bioaccumulation and biomagnification of PFAS in tree swallows and bioaccumulation of PFAS in great blue herons (Custer and others, 2013; Custer and others, 2019). USGS possesses a mobile laboratory that can be used to perform experiments on fish exposed to water contaminated by PFAS to better understand bioaccumulation and exposure effects. Finally, USGS scientists have the expertise to conduct field studies to examine the uptake of PFAS and its potential effects on birds.

2.6.4. USGS Science Opportunities

2.6.4.1. Short-Term Opportunities

The USGS could develop chemical-specific bioconcentration and bioaccumulation rate constants and pharmacokinetic parameters for use in predictive bioaccumulation models (table 6). Pharmacokinetic parameters, such as protein binding, can be determined using *in vitro* approaches. These parameters would inform the development of bioaccumulation, toxicokinetic, and PBPK models that would be used to predict the uptake and internal distribution of PFAS in organisms.

2.6.4.2. Long-Term Opportunities

The USGS could develop (1) laboratory-based parameters describing the uptake and trophic transfer of PFAS within food webs and critical body residues and (2) models that are used to predict the bioaccumulation and PBPK of less studied PFAS or mixtures of PFAS (table 6). The USGS could partner with other agencies such as EPA and DOD to support the development of new models to predict the bioaccumulation of PFAS.

Table 6. Scalable PFAS science opportunities, determined through literature reviews and gap analyses, that support studies about the bioaccumulation and biomagnification of PFAS (section 2.6).

[PFAA, perfluoroalkyl acid; PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS; U.S. Geological Survey]

Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
Quantification of bioaccumulation kinetics of PFAS in aquatic and terrestrial wildlife	Yes	Yes
Pharmacokinetic and pharmacodynamic studies to determine distribution of PFAS within aquatic and terrestrial wildlife	No	Yes
Determination of critical body residues (relation between uptake, bioaccumulation, and toxicity) within aquatic and terrestrial wildlife	No	Yes
Development and testing of models to predict bioaccumulation of PFAS in aquatic and terrestrial wildlife	No	Yes
Assessment of bioaccumulation, trophic transfer, and biomagnification across food webs	No	Yes

2.7. Ecotoxicology

2.7.1. State of the Science

Ecotoxicology data are limited or do not exist for many PFAS, mixtures of PFAS, and mixtures of PFAS with co-occurring chemicals (Giesy and Kannan, 2002; Giesy and others, 2010; Naile and others, 2013). Some ecotoxicology data related to fish, birds, and mammals exist for a small number of PFAS, such as PFOS and PFOA (Beach and others, 2006). Toxicology studies on PFOS and PFOA have reported effects on survival and growth for aquatic invertebrates and fish; as a result, there are adequate data for the development of initial toxicity reference values (Conder and others, 2020). Data for other species such as amphibians, reptiles, mammalian wildlife, and birds are currently inadequate to derive toxicity reference values, although preliminary screening values have been proposed (Dykema, 2015). Adverse health outcomes linked to exposure to PFAS are limited and have been reported only for common laboratory species, including some fish, mice, and rats. Recent research indicated that exposures to PFBS at environmentally relevant concentrations adversely impacted fish reproduction and skewed the sex ratio (Chen and others, 2019).

2.7.2. Science Gaps

To date, ecotoxicological data have been reported for a limited number of PFAS (primarily PFOS and PFOA) using a small number of aquatic laboratory species (Conder and others, 2020). For most PFAS, a significant data gap exists where there are little to no ecotoxicity data and for less studied species that may be highly sensitive to PFAS (Ankley and others, 2020). Animals that have a potential susceptibility or sensitivity to PFAS and that are relevant to the management and protection activities of the Departments of the Interior and Defense (Conder and others, 2020) remain to be studied. Toxicity data are currently limited for many managed and protected amphibians, reptiles, mammalian wildlife, and

birds; these data are essential to predict potential effects on and support conservation management goals for those species (Ankley and others, 2020). In addition, data on sensitive species are needed to derive protective toxicity reference values. For example, the midge *Chironomus tentans* is more sensitive to PFOS than other taxa such as crustaceans and fish (MacDonald and others, 2004). Additional studies of sentinel invertebrates and insects, such as the mayfly, could be conducted to determine vulnerability and inform species sensitivity distributions. Ecotoxicity studies could also address data gaps regarding the roles of exposure routes (ingestion, contact, or inhalation), the duration of exposure (acute versus chronic; see section 2.5), and the links between adverse biological effects and levels of PFAS accumulated in tissues (critical body residues).

Understanding the physiological basis of PFAS toxicity is necessary to extrapolate across species and to PFAS that have not yet been tested. PFAS have been shown to affect thyroid function, fertility, development, metabolism, inflammation, immune function, and cognitive function in mammalian animal models used for human-health toxicity assessments (for an overview, see Sunderland and others, 2019). Molecular, biochemical, and cell-based tools and techniques are needed to (1) understand the mechanisms of chemicals (such as endocrine active substances) and (2) identify molecular endpoints that are linked through understood pathways to known adverse outcomes of PFAS at higher levels of biological organization, such as adverse effects of PFAS on the behavior, development, and immune system in fish and wildlife.

Toxicity studies to characterize the ecotoxicological properties of each individual PFAS compound are cost prohibitive. Thus, methods and models to predict the toxicity of a broader range of PFAS are needed. Currently there are several modeling approaches that have the potential to predict the toxicity of classes of PFAS and PFAS mixtures. The expansion or development of PFAS-specific models for ecotoxicological purposes could include (1) the EPA's Sequence Alignment To Predict Across Species Susceptibility (SeqAPass) model

(EPA, 2021d), which relies on the sequence and molecular structure of target proteins to predict the transferability or relevance across species; (2) the EPA's Web-Based Interspecies Correlation Estimation (WebICE) model (EPA, 2016b), which extrapolates mechanisms across different chemicals; and (3) data about adverse outcome pathways, which inform the cascade of adverse effects from the molecular level up to organism, population, and community levels.

2.7.3. USGS Capabilities and Expertise

USGS scientists have the laboratory and field experience necessary to conduct ecotoxicological studies of PFAS in a wide range of aquatic and terrestrial species (including invertebrate, fish, and avian species). Methods and approaches from previous and ongoing studies about other chemical compounds such as metals, pesticides, and industrial chemicals can be adapted to assess PFAS ecotoxicity. These capabilities exist at USGS facilities that already perform research on wildlife and the environment. Some facilities already maintain a wide range of invertebrate and fish species for aquatic toxicology studies and house avian species such as American kestrels that may be available for toxicity testing. The USGS also has expertise to conduct field studies to investigate exposure to PFAS. USGS researchers have studied the reproductive

success of ospreys in the Chesapeake Bay region in relation to multiple contaminant exposures, including PFAS (Rattner and others, 2004). More recently, USGS scientists investigated the exposure to and effects of PFAS in tree swallows at a contaminated site (Custer and others, 2019). The mobile toxicology laboratory is currently deployed and is performing experiments on fish exposed to water contaminated by PFAS. Ongoing field studies and physiological assessments are being conducted at contaminated sites, and laboratory studies are being conducted on the adverse biological effects resulting from exposure to PFAS in fish and wildlife species that can be translated to field populations.

2.7.4. USGS Science Opportunities

2.7.4.1. Short-Term Opportunities

The USGS could identify toxicity data for relevant sensitive species over a broad range of PFAS (table 7). Research focused on acute and chronic toxicity as well as sublethal endpoints (such as growth and reproduction) could provide data for population models. These data can be used by resource-management agencies to support risk-based decisions on the potential effects of PFAS on fish and wildlife.



Table 7. Scalable science opportunities, determined through literature reviews and gap analyses, that support studies about PFAS and ecotoxicology (section 2.7)

[PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS; U.S. Geological Survey].

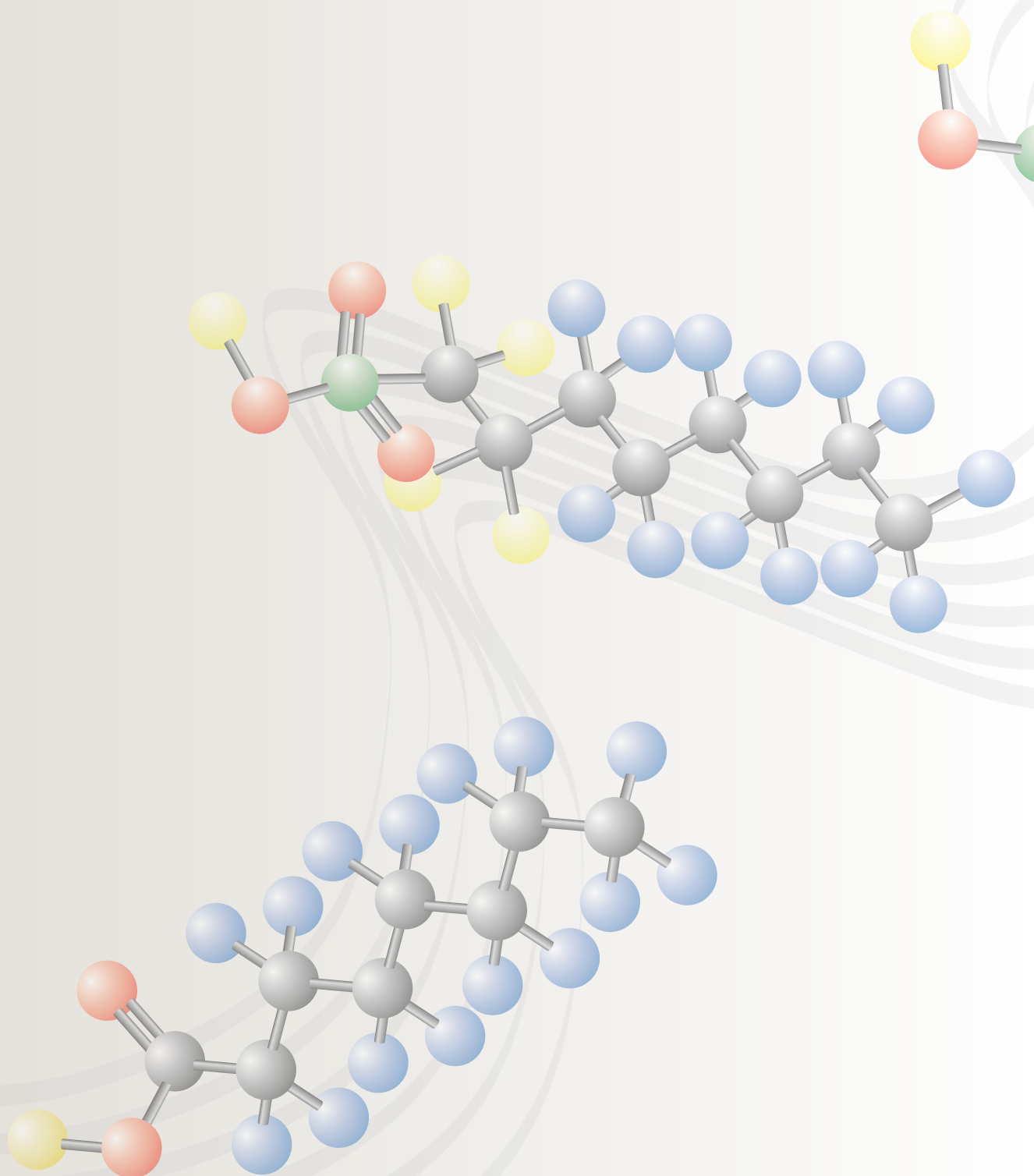
Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
Toxicology studies focusing on chronic exposures, sublethal endpoints, and sensitive species	Yes	Yes
Molecular and biochemical toxicology to determine mechanisms in aquatic and terrestrial wildlife	No	Yes
Toxicology studies examining PFAS that co-occur with other contaminants	No	Yes
Microcosm- or mesocosm-level studies that emulate field conditions	No	Yes

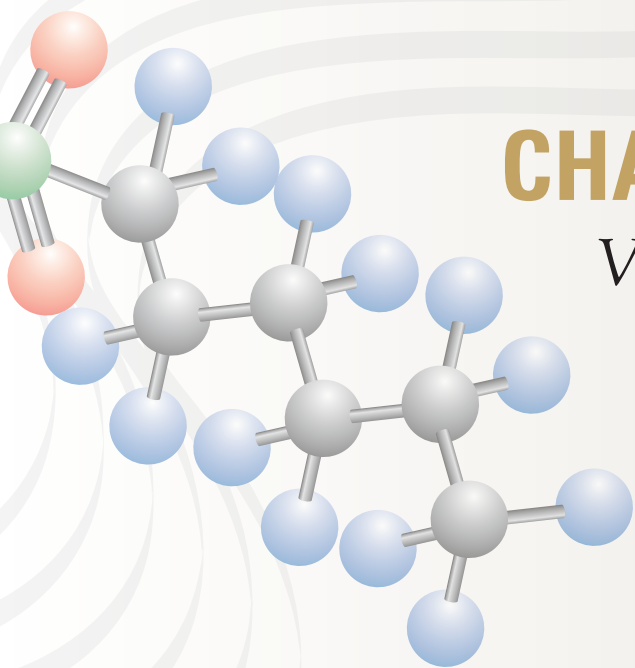
2.7.4.2. Long-Term Opportunities

The best approach to predict the effects from the diverse subclasses of PFAS needs to be identified. Data on the mechanisms of PFAS ecotoxicity could be generated to support extrapolations of toxicity across species. Where it is available, human toxicity data generated by others (outside of USGS) can be used to inform potential mechanisms and ecotoxicological effects. Conversely, there are opportunities where ecotoxicology studies can inform potential adverse effects in humans (Ankley and others, 2020). Laboratory toxicity data describing

the effects of (1) mixtures of different PFAS compounds or (2) mixtures of PFAS with non-PFAS compounds could be generated to support models used to predict toxicity for a wide range of PFAS across different species (table 7). Additional data from (1) microcosm- or mesocosm-level studies and (2) field studies would describe the relation between effects observed in the laboratory and those observed in the field; data at these various scales would be used to support resource-management decisions on the ecological risk of exposure and contamination by PFAS.







CHAPTER THREE

Vision for Integrated Science

3.1. Integrated Science at the USGS To Support Studies of PFAS

Scientists in the USGS have been engaged in integrated scientific studies on a variety of topics for several decades. These activities have largely been conducted collaboratively between a few colleagues across discipline boundaries and have resulted in many contributions to the scientific literature and body of knowledge (Kolpin and others, 2002; Bradley and others, 2020a; Bradley and others, 2020b). However, these grassroots approaches are not capable of taking advantage of the potential full range of expertise that could be realized if integrated science was more formally supported at the Bureau level and institutionalized as an ongoing science enterprise. Although a fully developed implementation plan and associated workflow for integrated scientific studies of PFAS is beyond the scope of this strategic science vision document, this vision can guide the next steps toward full implementation.

The conceptual approach to workflow and scientific studies related to PFAS in this document could be relevant for integrating other crosscutting science topics in USGS because it (1) builds on existing resources, expertise, and capabilities; (2) provides a framework for leveraged and shared resources across existing mission areas and programs; (3) highlights the science gaps that individually and together speak to the strengths of the USGS, such as the transfer of process-based understandings to various spatial and temporal scales, regional and national assessments, statistical and deterministic models, and research-method development; and (4) takes advantage of increased efficiencies and available expertise made possible with transdisciplinary collaboration.

The USGS workforce includes geologists, hydrologists, chemists, statisticians, modelers, geographers, biologists, ecologists, and toxicologists, among others. Therefore, conducting integrated science within a nationally consistent framework of field and laboratory protocols and approaches is a strength of the USGS. In this chapter, we build on the topical scope of the preceding individual chapters to provide a vision that strategically integrates those topics into a larger enterprise within the USGS. Accordingly, integrated science in this chapter strictly refers to the collaborative efforts of expert scientists and laboratory personnel across the USGS, drawing on their collective capabilities to answer science questions or test hypotheses related to PFAS in the environment and associated hazards (table 8).

Stakeholders who prevent, mitigate, remediate, or otherwise manage the hazards brought by exposures to environmental contaminants in either ecosystems or humans require comprehensive integrated science to understand key processes and data, including the source of the contaminant, its behavior in the environment, exposure pathways, and ecotoxicity (fig. 1). Although much knowledge is gained through scientific explorations of individual processes (as described in the preceding chapters), the full breadth of these understandings as an integrated science topic can often be overlooked in favor of more narrowly focused studies. Although this approach is common, it may sometimes fall short of providing the information needed to envision the entire scope of a scientific question and could misidentify opportunities to mitigate or remediate the most significant hazard, if one exists.

By contrast, the ability to envision the entire scope of a scientific question through the lens of integrated science could focus attention on areas where the most potential for health

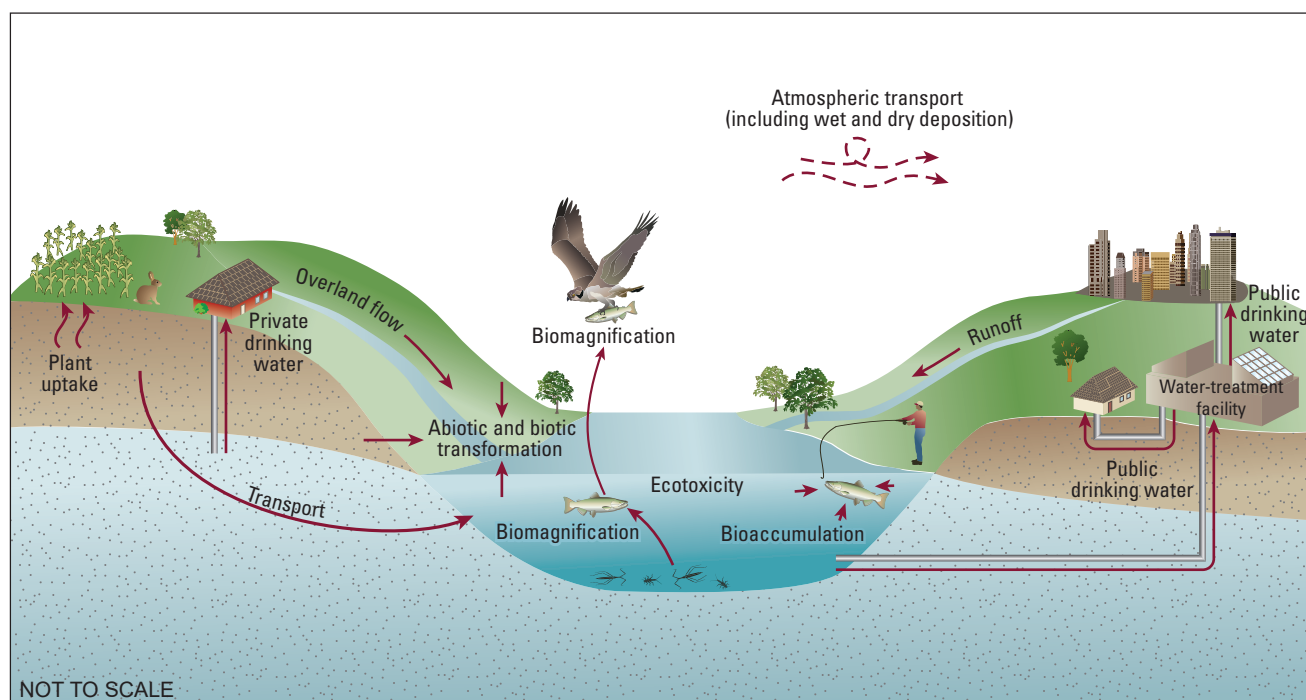
Table 8. Scalable science opportunities, determined through literature reviews and gap analyses, that support an integrated science approach to the study of perfluoroalkyl and polyfluoroalkyl substances (chapter 3).

[PFAS, perfluoroalkyl and polyfluoroalkyl substances; USGS, U.S. Geological Survey]

Science opportunities that could be addressed by USGS capabilities	Short term (1–2 years)	Long term (3+ years)
Improved understanding of conceptual and other models and decision-support tools that provide actionable information for prediction, prevention, and mitigation of environmental PFAS human-exposure hazard through comprehensive evaluation and prioritization of sources, source apportionment, fate and transport, occurrence, and exposures	No	Yes
Improved understanding of conceptual and other models and decision-support tools that provide actionable information for prediction, prevention, and mitigation of environmental PFAS risk to ecosystems through comprehensive evaluation and prioritization of sources, source apportionment, fate and transport, occurrence, exposures, and toxicity	No	Yes

and economic benefit coexists. For example, stakeholders have an incentive to invest resources to mitigate or remediate hazards when the toxicity of a contaminant is high and the contaminant is frequently present in the environment. Conversely, this incentive is minimized when (1) the toxicity of a contaminant is low, the contaminant is infrequently detected, or the contaminant is likely to be transformed or degraded in the environment to a harmless substance; or (2) people and aquatic or terrestrial organisms are unlikely to be exposed to harmful concentrations. In some cases, a contaminant may be

completely transformed through microbial or other degradation processes once it enters the environment and is rendered harmless before people and aquatic or terrestrial organisms are exposed; however, in other cases, a contaminant could be transformed by those same processes into something more harmful. Other factors such as the spatial (local, regional, national) and temporal (short or long term) aspects often drive the significance, if any, of hazards associated with an environmental contaminant.

**Figure 1.** Conceptual diagram showing the major mechanisms of the fate, transport, and exposure pathways of perfluoroalkyl and polyfluoroalkyl substances (PFAS) in the environment. Artwork courtesy of Jacqueline Olsen, U.S. Geological Survey.

3.2. Source-to-Receptor Integrated Science Paradigm

A source-to-receptor paradigm for integrated science can be conceptualized as a continuum of processes that begin at the source of an environmental contaminant and end at a receptor (fig. 2A). In this model, a receptor can be a cell, an organism, or a community. The intervening processes can include transport, transformation, exposure, and uptake of a contaminant. The source-to-receptor paradigm is an example of an integrated science process that leads to actionable information for stakeholder decisions at key points in the continuum determined to be the most important drivers of a contaminant hazard, if one exists.

When considering how the continuum may lead to actionable information, it may be instructive to view source-to-receptor continuums as analogous to the hazard analysis and critical control point (HACCP) model developed by the U.S. Food and Drug Administration (2018; see sidebar 2). A control point in a source-to-receptor continuum can be defined as an integrated scientific process(es) within the continuum. For example, the transformation of a contaminant in the environment can lead to exposure; however, the exposure itself may not be of consequence if microbial degradation leads to a nontoxic product. Thus, the scientific understanding of the transformation process would represent a critical control point in understanding how, or if, stakeholders choose to mitigate the source of the original contaminant (parent product). In this case, an understanding of the transformation process would provide actionable information for mitigation. Similarly, if exposure to a contaminant leads to bioaccumulation and (or) biomagnification with a serious toxic effect, a critical control point could be identified in the specific exposure pathway before biouptake of the contaminant can occur. Critical control points defined in this manner help decision makers (1) identify and prioritize actionable information, (2) prioritize further integrated scientific research, and (3) focus attention on the balance between economic and health effects.

With this conceptual model in mind (fig. 2), there are numerous possibilities to link individual or groups of processes together that would otherwise not be possible without integrated science (fig. 2B; table 8). Significantly, when providing actionable information and general understandings about the potential hazards of PFAS in the environment, there are likely to be different control points at different spatial or time scales across the Nation that will come into play. The variability in the source type and strength of the PFAS compound, the hydrogeologic settings of the affected watersheds and aquifers, the use of water or other natural resources that may be contaminated, the sensitivity and composition of affected species, and other factors may contribute to the complexity of each individual scientific process (control point). This approach can support planning and design considerations for research; such decisions include choosing whether a targeted monitoring or a random monitoring design is optimal, choosing whether laboratory research is more optimal

than field- or mesocosm-level research, and choosing how to tell the complete story of the life cycle of a contaminant, as exemplified by the USGS's existing approach to the study of several inorganic elements and compounds (Papp, 1994; Goonan, 2014).

Figure 2 illustrates how integrated science is based on many processes; therefore, it can provide flexibility to transfer a study's results, provide information at the spatial and temporal scales of the science question that is being asked or the hypothesis that needs to be tested, and be a road map in all phases of study planning, design, and execution. The strategic science vision described here can provide a useful starting point to guide USGS science managers in designing their own integrated science programs that address PFAS in the environment and thus serve the needs of their stakeholders at local, regional, or national levels. These unifying concepts can also be useful for building coalitions of research partners by providing clarity on roles and needed expertise.

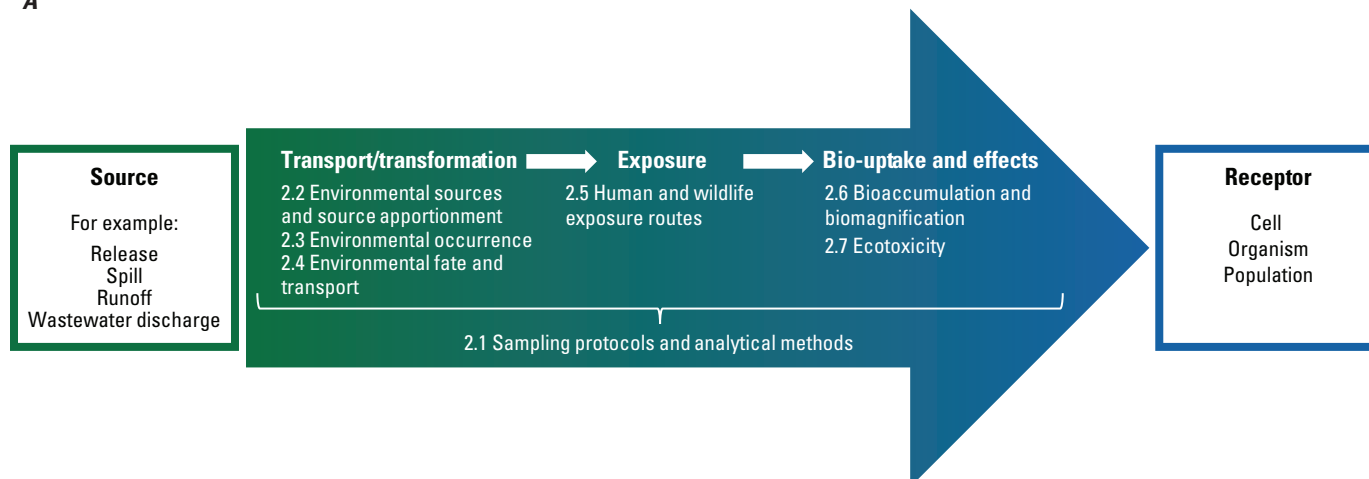
3.3. Conceptual Workflow for an Integrated Science Approach to Studying PFAS at the USGS

As noted above, the collaborative and integrated science efforts in USGS are often conducted at grassroots levels by individuals or small groups of scientists. Beyond the technical and scientific limitations inherent in these efforts, institutional impediments can limit the sharing of resources. Consequently, under current practices, it is more straightforward to partition and implement the science, rather than share resources, provide common review and oversight, and manage science between mission areas. These preferences can be rectified

Sidebar 2—Hazard Analysis and Critical Control Point (HACCP): An Example

The HACCP system provides actionable information by identifying where the most significant control point(s) exist along a continuum of processes that could lead to a hazard. HACCP is most commonly used by the food industry to provide effective hazard mitigation as resources move from farms to the consumer. As a simple example, if an HACCP analysis determines that harmful microbes are introduced in the grocery store but not at the other locations (the farm, the processing plant, or the distribution center) in the farm-to-consumer continuum, then it would follow that the grocery store is the critical control point where appropriate countermeasures can be focused to protect consumer health while simultaneously avoiding costly supply-chain disruptions. This simple example illustrates how decisions leading to the most effective and least impactful countermeasure could be missed without the full knowledge about and accounting for the continuum of processes leading to the hazard and critical control point.

A



B

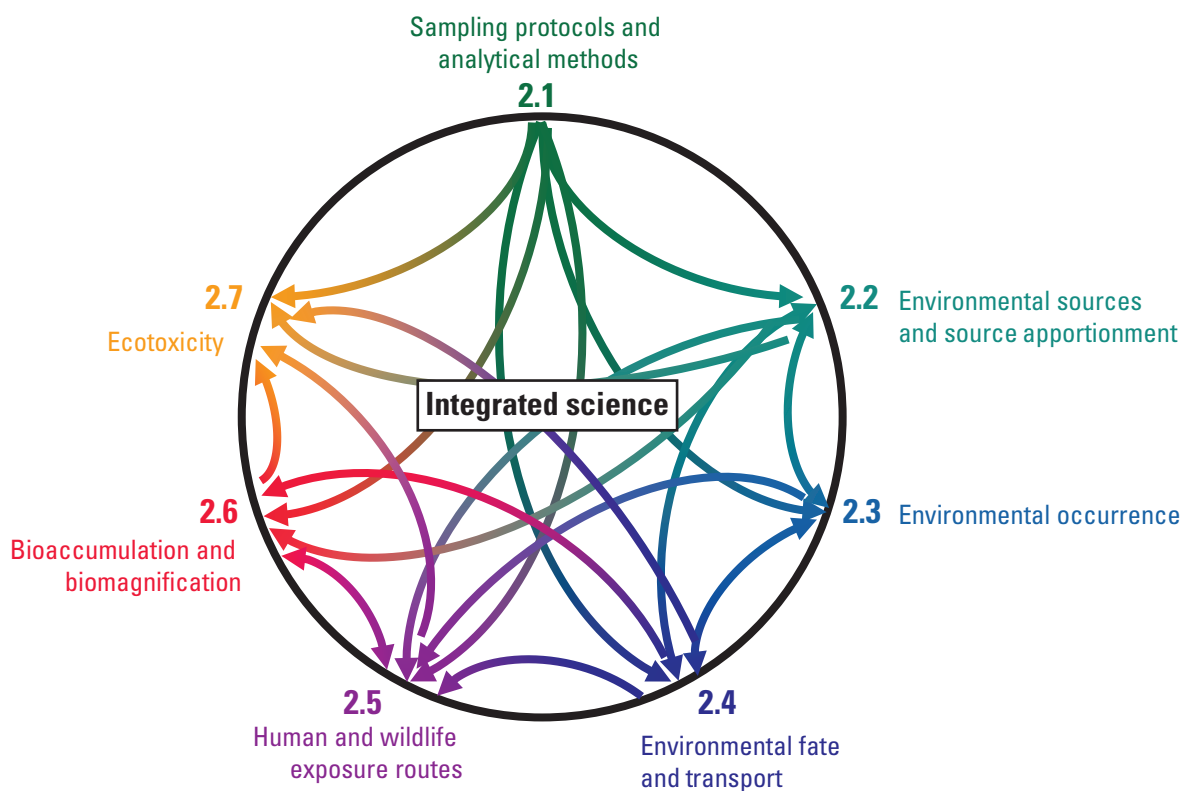


Figure 2. A, A source-to-receptor model for the study of the transport, exposure, and effects of perfluoroalkyl and polyfluoroalkyl substances (PFAS) in the environment is shown as a continuum of integrated science processes representing potentially critical control points where actionable information can be developed; the sections of chapter 2 are mapped on this continuum. B, The connections and interdependencies between the continuum of integrated science processes, described in the seven sections of chapter 2, are shown by the arrows.

through the implementation of a workflow model that has Bureau-level oversight and the support of shared and leveraged resources.

To help ensure the success of integrated science activities at USGS to study PFAS, a collaborative workflow across mission areas could be identified, developed, and instituted. Although the specifics of governing this workflow are beyond the scope of this document, the critical elements of the workflow for integrated science activities (such as those envisioned here) would best include agreed-upon mechanisms for (1) developing shared technical requirements; (2) effective leveraging of program resources; (3) collaborative design and implementation of reimbursable work across individual science centers, where appropriate and possible; and (4) Bureau-level work plans, project reviews, and accountability. A communication and outreach plan to coordinate existing and new internal networks of web pages, social media, and other outlets is also important.

3.4. Conclusion

The work documented here and in related discussions by the writing team and other colleagues in the USGS has been instrumental in forming a concise strategic vision for conducting PFAS-related studies using an integrated science approach (see sidebar 3). The vision is focused on how USGS scientific expertise and capabilities can be used to address the key identified science gaps.

This strategic vision can guide the implementation of integrated science that provides actionable information to managers at the spatially and temporally appropriate scale of specific decisions, helps build coalitions of research partners, and is an information resource for others engaged in studies of PFAS in the environment. The integrated science activities guided by this vision can therefore be designed to address issues at local, regional, and national scales and at varying timeframes as stakeholder needs evolve. A source-to-receptor paradigm is presented as a guiding principle of science integration for monitoring, modeling, and forecasting processes that drive environmental hazards related to PFAS to ecosystems and the public. A conceptual workflow is provided as an example to support, review, and manage integrated science at the USGS.

Sidebar 3—Vision for an Integrated Science Approach to the Study of PFAS in the Environment

An integrated science approach that encompasses both living and nonliving components of ecological systems will provide stakeholders with the understanding, tools, and data they need to study PFAS in the environment and support a range of decisions that identify, mitigate, or prevent hazards related to PFAS. The USGS can build on a broad range of interdisciplinary, transdisciplinary, and external expertise and nationally consistent laboratory and field capabilities to support needed data collection and research. Studies related to PFAS are envisioned as occurring along a source-to-receptor integrated-science continuum that provides a framework and actionable information for identifying and rectifying the most significant factors that may lead to hazards related to PFAS.



References Cited

- Abbott, B.D., Wolf, C.J., Das, K.P., Zehr, R.D., Schmid, J.E., Lindstrom, A.B., Strynar, M.J., and Lau, C., 2009, Developmental toxicity of perfluorooctane sulfonate (PFOS) is not dependent on expression of peroxisome proliferator activated receptor- α (PPAR α) in the mouse: *Reproductive Toxicology*, v. 27, no. 3-4, p. 258–265, accessed September 26, 2021, at <https://doi.org/10.1016/j.reprotox.2008.05.061>.
- Agency for Toxic Substances and Disease Registry, 2018, ATSDR's minimal risk levels (MRLs) and environmental media evaluation guides (EMEGs) for PFAS: Agency for Toxic Substances and Disease Registry web page, accessed January 2, 2020, at https://www.atsdr.cdc.gov/pfas/mrl_pfas.html.
- Ahrens, L., Shoeib, M., Del Vento, S., Codling, G., and Halsall, C., 2011a, Polyfluoroalkyl compounds in the Canadian Arctic atmosphere: *Environmental Chemistry*, v. 8, no. 4, p. 399–406, accessed September 26, 2021, at <https://doi.org/10.1071/EN10131>.
- Ahrens, L., Shoeib, M., Harner, T., Lee, S.C., Guo, R., and Reiner, E.J., 2011b, Wastewater treatment plant and landfills as sources of polyfluoroalkyl compounds to the atmosphere: *Environmental Science & Technology*, v. 45, no. 19, p. 8098–8105, accessed September 26, 2021, at <https://doi.org/10.1021/es1036173>.
- Anderson, R.H., Long, G.C., Porter, R.C., and Anderson, J.K., 2016, Occurrence of select perfluoroalkyl substances at U.S. Air Force aqueous film-forming foam release sites other than fire-training areas—Field-validation of critical fate and transport properties: *Chemosphere*, v. 150, p. 678–685, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2016.01.014>.
- Ankley, G.T., Cureton, P., Hoke, R.A., Houde, M., Kumar, A., Kurias, J., Lanno, R., McCarthy, C., Newsted, J., Salice, C.J., Sample, B.E., Sepúlveda, M.S., Steevens, J., and Valsecchi, S., 2020, Assessing the ecological risks of per- and polyfluoroalkyl substances—Current state-of-the science and a proposed path forward: *Environmental Toxicology and Chemistry*, v. 40, no. 3, p. 565–605, accessed September 26, 2021, at <https://doi.org/10.1002/etc.4869>.
- Armitage, J., Cousins, I.T., Buck, R.C., Prevedouros, K., Russell, M.H., MacLeod, M., and Korzeniowski, S.H., 2006, Modeling global-scale fate and transport of perfluorooctanoate emitted from direct sources: *Environmental Science & Technology*, v. 40, no. 22, p. 6969–6975, accessed September 26, 2021, at <https://doi.org/10.1021/es0614870>.
- Armitage, J.M., Arnot, J.A., Wania, F., and Mackay, D., 2013, Development and evaluation of a mechanistic bioconcentration model for ionogenic organic chemicals in fish: *Environmental Toxicology and Chemistry*, v. 32, no. 1, p. 115–128, accessed September 26, 2021, at <https://doi.org/10.1002/etc.2020>.
- Ayotte, J.D., Nolan, B.T., and Gronberg, J.A., 2016, Predicting arsenic in drinking water wells of the Central Valley, California: *Environmental Science & Technology*, v. 50, no. 14, p. 7555–7563, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.6b01914>.
- Barzen-Hanson, K.A., Davis, S.E., Kleber, M., and Field, J.A., 2017a, Sorption of fluorotelomer sulfonates, fluorotelomer sulfonamido betaines, and a fluorotelomer sulfonamido amine in National Foam aqueous film-forming foam to soil: *Environmental Science & Technology*, v. 51, no. 21, p. 12394–12404, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.7b03452>.
- Barzen-Hanson, K.A., Roberts, S.C., Choyke, S., Oetjen, K., McAlees, A., Riddell, N., McCrindle, R., Ferguson, P.L., Higgins, C.P., and Field, J.A., 2017b, Discovery of 40 classes of per- and polyfluoroalkyl substances in historical aqueous film-forming foams (AFFFs) and AFFF-impacted groundwater: *Environmental Science & Technology*, v. 51, no. 4, p. 2047–2057, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.6b05843>.
- Beach, S.A., Newsted, J.L., Coady, K., and Giesy, J.P., 2006, Ecotoxicological evaluation of perfluorooctanesulfonate (PFOS), in Albert, L.A., Voogt, P. de, Gerba, C.P., Hutzinger, O., Knaak, J.B., Mayer, F.L., Morgan, D.P., Park, D.L., Tjeerdema, R.S., Whitacre, D.M., Yang, R.S.H., Ware, G.W., Nigg, H.N., Doerge, D.R., and Gunther, F.A., eds., *Reviews of Environmental Contamination and Toxicology*, v. 186 of *Reviews of Environmental Contamination and Toxicology—Continuation of Residue Reviews*: New York, Springer, p. 133–174. [Also available at https://doi.org/10.1007/0-387-32883-1_5].
- Beesoon, S., Webster, G.M., Shoeib, M., Harner, T., Ben-skin, J.P., and Martin, J.W., 2011, Isomer profiles of perfluorochemicals in matched maternal, cord, and house dust samples—Manufacturing sources and transplacental transfer: *Environmental Health Perspectives*, v. 119, no. 11, p. 1659–1664, accessed September 26, 2021, at <https://doi.org/10.1289/ehp.1003265>.
- Behr, A.-C., Plinsch, C., Braeuning, A., and Buhrke, T., 2020, Activation of human nuclear receptors by perfluoroalkylated substances (PFAS): *Toxicology in Vitro*, v. 62, article 104700, 6 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.tiv.2019.104700>.

- Bertin, D., Labadie, P., Ferrari, B.J.D., Sapin, A., Gar-ric, J., Geffard, O., Budzinski, H., and Babut, M., 2016, Potential exposure routes and accumulation kinetics for poly-and perfluorinated alkyl compounds for a freshwater amphipod—*Gammarus* spp. (Crustacea): *Chemosphere*, v. 155, p. 380–387, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2016.04.006>.
- Birnbaum, L.S., and Grandjean, P., 2015, Alternatives to PFASs—Perspectives on the science: *Environmental Health Perspectives*, v. 123, no. 5, p. A104–A105, accessed September 26, 2021, at <https://doi.org/10.1289/ehp.1509944>.
- Blaine, A.C., Rich, C.D., Sedlacko, E.M., Hundal, L.S., Kumar, K., Lau, C., Mills, M.A., Harris, K.M., and Higgins, C.P., 2014, Perfluoroalkyl acid distribution in various plant compartments of edible crops grown in biosolids-amended soils: *Environmental Science & Technology*, v. 48, no. 14, p. 7858–7865, accessed September 26, 2021, at <https://doi.org/10.1021/es500016s>.
- Blotvogel, J., Mayeno, A.N., Sale, T.C., and Borch, T., 2011, Prediction of contaminant persistence in aqueous phase—A quantum chemical approach: *Environmental Science & Technology*, v. 45, no. 6, p. 2236–2242, accessed September 26, 2021, at <https://doi.org/10.1021/es1028662>.
- Boone, J.S., Vigo, C., Boone, T., Byrne, C., Ferrario, J., Benson, R., Donohue, J., Simmons, J.E., Kolpin, D.W., Furlong, E.T., and Glassmeyer, S.T., 2019, Per- and polyfluoroalkyl substances in source and treated drinking waters of the United States: *Science of The Total Environment*, v. 653, p. 359–369, accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2018.10.245>.
- Bradley, P.M., Argos, M., Kolpin, D.W., Meppelink, S.M., Romanok, K.M., Smalling, K.L., Focazio, M.J., Allen, J.M., Dietze, J.E., Devito, M.J., Donovan, A.R., Evans, N., Givens, C.E., Gray, J.L., Higgins, C.P., Hladik, M.L., Iwanowicz, L.R., Journey, C.A., Lane, R.F., Laughrey, Z.R., Loftin, K.A., McCleskey, R.B., McDonough, C.A., Medlock-Kakaley, E., Meyer, M.T., Putz, A.R., Richardson, S.D., Stark, A.E., Weis, C.P., Wilson, V.S., and Zehraoui, A., 2020a, Mixed organic and inorganic tapwater exposures and potential effects in greater Chicago area, USA: *Science of The Total Environment*, v. 719, article 137236, 16 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2020.137236>.
- Bradley, P.M., Journey, C.A., Button, D.T., Carlisle, D.M., Huffman, B.J., Qi, S.L., Romanok, K.M., and Van Metre, P.C., 2020b, Multi-region assessment of pharmaceutical exposures and predicted effects in USA wadeable urban-gradient streams: *PLoS ONE*, v. 15, no. 1, article e0228214, 25 p., accessed September 26, 2021, at <https://doi.org/10.1371/journal.pone.0228214>.
- Bradley, P.M., Kolpin, D.W., Romanok, K.M., Smalling, K.L., Focazio, M.J., Brown, J.B., Cardon, M.C., Carpenter, K.D., Corsi, S.R., DeCicco, L.A., Dietze, J.E., Evans, N., Furlong, E.T., Givens, C.E., Gray, J.L., Griffin, D.W., Higgins, C.P., Hladik, M.L., Iwanowicz, L.R., Journey, C.A., Kuivila, K.M., Masoner, J.R., McDonough, C.A., Meyer, M.T., Orlando, J.L., Strynar, M.J., Weis, C.P., and Wilson, V.S., 2018, Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States: *Environmental Science & Technology*, v. 52, no. 23, p. 13972–13985, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.8b04622>.
- Bradley, P.M., LeBlanc, D.R., Romanok, K.M., Smalling, K.L., Focazio, M.J., Cardon, M.C., Clark, J.M., Conley, J.M., Evans, N., Givens, C.E., Gray, J.L., Gray, L.E., Hartig, P.C., Higgins, C.P., Hladik, M.L., Iwanowicz, L.R., Loftin, K.A., McCleskey, R.B., McDonough, C.A., Medlock-Kakaley, E.K., Weis, C.P., and Wilson, V.S., 2021, Public and private tapwater—Comparative analysis of contaminant exposure and potential risk, Cape Cod, Massachusetts, USA: *Environment International*, v. 152, article 106487, 14 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.envint.2021.106487>.
- Brusseau, M.L., 2018, Assessing the potential contributions of additional retention processes to PFAS retardation in the subsurface: *Science of The Total Environment*, v. 613–614, p. 176–185, accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2017.09.065>.
- Brusseau, M.L., 2020, Simulating PFAS transport influenced by rate-limited multi-process retention: *Water Research*, v. 168, article 115179, 11 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.watres.2019.115179>.
- Brusseau, M.L., Yan, N., Van Glubt, S., Wang, Y., Chen, W., Lyu, Y., Dungan, B., Carroll, K.C., and Holguin, F.O., 2019, Comprehensive retention model for PFAS transport in subsurface systems: *Water Research*, v. 148, p. 41–50, accessed September 26, 2021, at <https://doi.org/10.1016/j.watres.2018.10.035>.
- Burkhard, L.P., Arnot, J.A., Embry, M.R., Farley, K.J., Hoke, R.A., Kitano, M., Leslie, H.A., Lotufo, G.R., Parkerton, T.F., Sappington, K.G., Tomy, G.T., and Woodburn, K.B., 2012, Comparing laboratory and field measured bioaccumulation endpoints: *Integrated Environmental Assessment and Management*, v. 8, no. 1, p. 17–31, accessed September 26, 2021, at <https://doi.org/10.1002/ieam.260>.
- Campos Pereira, H., Ullberg, M., Kleja, D.B., Gustafsson, J.P., and Ahrens, L., 2018, Sorption of perfluoroalkyl substances (PFASs) to an organic soil horizon—Effect of cation composition and pH: *Chemosphere*, v. 207, p. 183–191, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2018.05.012>.

- Caritat, P. de, Reimann, C., Smith, D.B., and Wang, X., 2017, Chemical elements in the environment—Multi-element geochemical datasets from continental- to national-scale surveys on four continents: *Applied Geochemistry*, v. 89, p. 150–159, accessed September 26, 2021, at <https://doi.org/10.1016/j.apgeochem.2017.11.010>.
- Chen, L., Lam, J.C.W., Hu, C., Tsui, M.M.P., Lam, P.K.S., and Zhou, B., 2019, Perfluorobutanesulfonate exposure skews sex ratio in fish and transgenerationally impairs reproduction: *Environmental Science & Technology*, v. 53, no. 14, p. 8389–8397, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b01711>.
- Cheng, Y.H., Barpaga, D., Soltis, J.A., Shutthanandan, V., Kargupta, R., Han, K.S., McGrail, B.P., Motkuri, R.K., Basuray, S., and Chatterjee, S., 2020, Metal-organic framework-based microfluidic impedance sensor platform for ultrasensitive detection of perfluorooctanesulfonate: *ACS Applied Materials & Interfaces*, v. 12, no. 9, p. 10503–10514, accessed September 26, 2021, at <https://doi.org/10.1021/acsami.9b22445>.
- Cleary, R.S., Karnjanapiboonwong, A., Thompson, W.A., Lasee, S.J., Subbiah, S., Kauble, R.K., Andraski, B.J., and Anderson, T.A., 2021, Emerging and historical contaminants detected in desert rodents collected near a low-level radioactive waste site: *Environmental Toxicology and Chemistry*, v. 40, no. 3, p. 727–734, accessed September 25, 2021, at <https://doi.org/10.1002/etc.4715>.
- Conder, J., Arblaster, J., Larson, E., Brown, J., and Higgins, C., 2020, Guidance for assessing the ecological risks of PFASs to threatened and endangered species at aqueous film forming foam-impacted sites: Department of Defense Strategic Environmental Research and Development Program, project ER18-1614 guidance document, 181 p., accessed March 30, 2020, at <https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/ER18-1614>.
- Conder, J.M., Hoke, R.A., Wolf, W. de, Russell, M.H., and Buck, R.C., 2008, Are PFCAs bioaccumulative? A critical review and comparison with regulatory criteria and persistent lipophilic compounds: *Environmental Science & Technology*, v. 42, no. 4, p. 995–1003, accessed September 26, 2021, at <https://doi.org/10.1021/es070895g>.
- Cooperative Research Centre for Contamination Assessment and Remediation of the Environment [CTC CARE], 2020, astkCARE: Cooperative Research Centre for Contamination Assessment and Remediation of the Environment web page, accessed January 27, 2020, at <https://www.crccare.com/products-and-services/technologies/astkcare>.
- Costanza, J., Arshadi, M., Abriola, L.M., and Pennell, K.D., 2019, Accumulation of PFOA and PFOS at the air–water interface: *Environmental Science & Technology Letters*, v. 6, no. 6, p. 487–491, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.9b00355>.
- Cui, Q., Pan, Y., Zhang, H., Sheng, N., Wang, J., Guo, Y., and Dai, J., 2018, Occurrence and tissue distribution of novel perfluoroether carboxylic and sulfonic acids and legacy perfluoroalkyl substances in black-spotted frog (*Pelophylax nigromaculatus*): *Environmental Science & Technology*, v. 52, no. 3, p. 982–990, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.7b03662>.
- Custer, C.M., Custer, T.W., Delaney, R., Dummer, P.M., Schultz, S., and Karouna-Renier, N., 2019, Perfluoroalkyl contaminant exposure and effects in tree swallows nesting at Clarks Marsh, Oscoda, Michigan, USA: *Archives of Environmental Contamination and Toxicology*, v. 77, no. 1, p. 1–13, accessed September 26, 2021, at <https://doi.org/10.1007/s00244-019-00620-1>.
- Custer, T.W., Custer, C.M., Dummer, P.M., Goldberg, D., Franson, J.C., and Erickson, R.A., 2017, Organic contamination in tree swallow (*Tachycineta bicolor*) nestlings at United States and binational Great Lakes Areas of Concern: *Environmental Toxicology and Chemistry*, v. 36, no. 3, p. 735–748, accessed September 26, 2021, at <https://doi.org/10.1002/etc.3598>.
- Custer, T.W., Dummer, P.M., Custer, C.M., Wu, Q., Kannan, K., and Trowbridge, A., 2013, Perfluorinated compound concentrations in great blue heron eggs near St. Paul, Minnesota, USA, in 1993 and 2010–2011: *Environmental Toxicology and Chemistry*, v. 32, no. 5, p. 1077–1083, accessed September 26, 2021, at <https://doi.org/10.1002/etc.2146>.
- Dassuncao, C., Hu, X.C., Zhang, X., Bossi, R., Dam, M., Mikkelsen, B., and Sunderland, E.M., 2017, Temporal shifts in poly- and perfluoroalkyl substances (PFASs) in North Atlantic pilot whales indicate large contribution of atmospheric precursors: *Environmental Science & Technology*, v. 51, no. 8, p. 4512–4521, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.7b00293>.
- Dassuncao, C., Pickard, H., Pfohl, M., Tokranov, A.K., Li, M., Mikkelsen, B., Slitt, A., and Sunderland, E.M., 2019, Phospholipid levels predict the tissue distribution of poly- and perfluoroalkyl substances in a marine mammal: *Environmental Science & Technology Letters*, v. 6, no. 3, p. 119–125, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.9b00031>.

- De Silva, A.O., Armitage, J.M., Bruton, T.A., Dassuncao, C., Heiger-Bernays, W., Hu, X.C., Kärrman, A., Kelly, B., Ng, C., Robuck, A., Sun, M., Webster, T.F., and Sunderland, E.M., 2021, PFAS exposure pathways for humans and wildlife—A synthesis of current knowledge and key gaps in understanding: *Environmental Toxicology and Chemistry*, v. 40, no. 3, p. 631–657, accessed September 26, 2021, at <https://doi.org/10.1002/etc.4935>.
- Department of Defense, 2017, Bottle selection and other sampling considerations when sampling for per- and poly-fluoroalkyl substances (PFAS) (revision 1.2, July 2017): Department of Defense fact sheet, 2 p., accessed March 30, 2020, at <https://www.denix.osd.mil/edqw/home/what-s-new/unassigned/edqw-pfas-sampling-factsheet-rev-1-2-july-2017/>.
- Dykema, L.D., 2015, Measuring perfluorinated compounds in Michigan surface waters and fish—USEPA—Great Lakes Restoration Initiative Project final report: Michigan Department of Community Health, 54 p., accessed June 19, 2020, at https://www.michigan.gov/documents/mdch/MDCH_GL-00E01122-0_Final_Report_493494_7.pdf.
- Eberl, D.D., and Smith, D.B., 2009, Mineralogy of soils from two continental-scale transects across the United States and Canada and its relation to soil geochemistry and climate: *Applied Geochemistry*, v. 24, no. 8, p. 1394–1404, accessed September 26, 2021, at <https://doi.org/10.1016/j.apgeochem.2009.04.010>.
- Fair, P.A., Wolf, B., White, N.D., Arnott, S.A., Kannan, K., Karthikraj, R., and Vena, J.E., 2019, Perfluoroalkyl substances (PFASs) in edible fish species from Charleston Harbor and tributaries, South Carolina, United States—Exposure and risk assessment: *Environmental Research*, v. 171, p. 266–277, accessed September 26, 2021, at <https://doi.org/10.1016/j.envres.2019.01.021>.
- Fienen, M.N., Nolan, B.T., Kauffman, L.J., and Feinstein, D.T., 2018, Metamodeling for groundwater age forecasting in the Lake Michigan Basin: *Water Resources Research*, v. 54, no. 7, p. 4750–4766, accessed September 26, 2021, at <https://doi.org/10.1029/2017wr022387>.
- Focazio, M.J., Reilly, T.E., Rupert, M.G., and Helsel, D.R., 2002, Assessing ground-water vulnerability to contamination—Providing scientifically defensible information for decision makers: U.S. Geological Survey Circular 1224, 33 p., accessed March 30, 2020, at https://pubs.usgs.gov/circ/2002/circ1224/pdf/circ1224_ver1.pdf.
- Fuentes, S., Colomina, M.T., Vicens, P., Franco-Pons, N., and Domingo, J.L., 2007, Concurrent exposure to perfluorooctane sulfonate and restraint stress during pregnancy in mice—Effects on postnatal development and behavior of the offspring: *Toxicological Sciences*, v. 98, no. 2, p. 589–598, accessed September 26, 2021, at <https://doi.org/10.1093/toxsci/kfm121>.
- Galloway, J.E., Moreno, A.V.P., Lindstrom, A.B., Strynar, M.J., Newton, S., May, A.A., and Weavers, L.K., 2020, Evidence of air dispersion—HFPO—DA and PFOA in Ohio and West Virginia surface water and soil near a fluoropolymer production facility: *Environmental Science & Technology*, v. 54, no. 12, p. 7175–7184, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b07384>.
- Gannon, S.A., Johnson, T., Nabb, D.L., Serex, T.L., Buck, R.C., and Loveless, S.E., 2011, Absorption, distribution, metabolism, and excretion of [1-¹⁴C]-perfluorohexanoate ([¹⁴C]-PFHx) in rats and mice: *Toxicology*, v. 283, no. 1, p. 55–62, accessed September 26, 2021, at <https://doi.org/10.1016/j.tox.2011.02.004>.
- Gebbink, W.A., Berger, U., and Cousins, I.T., 2015, Estimating human exposure to PFOS isomers and PFCA homologues—The relative importance of direct and indirect (precursor) exposure: *Environment International*, v. 74, p. 160–169, accessed September 26, 2021, at <https://doi.org/10.1016/j.envint.2014.10.013>.
- Ghisi, R., Vamerali, T., and Manzetti, S., 2019, Accumulation of perfluorinated alkyl substances (PFAS) in agricultural plants—A review: *Environmental Research*, v. 169, p. 326–341, accessed September 26, 2021, at <https://doi.org/10.1016/j.envres.2018.10.023>.
- Giesy, J.P., and Kannan, K., 2002, Peer reviewed—Perfluorochemical surfactants in the environment: *Environmental Science & Technology*, v. 36, no. 7, p. 146A–152A, accessed September 26, 2021, at <https://doi.org/10.1021/es022253t>.
- Giesy, J.P., Naile, J.E., Khim, J.S., Jones, P.D., and Newsted, J.L., 2010, Aquatic toxicology of perfluorinated chemicals, in Whitacre, D.M., ed., *Reviews of Environmental Contamination and Toxicology*, v. 202: New York, Springer, p. 1–52, accessed September 26, 2021, at https://doi.org/10.1007/978-1-4419-1157-5_1.
- Goonan, T.G., 2014, The lifecycle of silver in the United States in 2009: U.S. Geological Survey Scientific Investigations Report 2013–5178, 17 p., accessed October 13, 2021, at <http://pubs.er.usgs.gov/publication/sir20135178>.
- Goss, K.-U., 2008, The pK_a values of PFOA and other highly fluorinated carboxylic acids: *Environmental Science & Technology*, v. 42, no. 2, p. 456–458, accessed September 26, 2021, at <https://doi.org/10.1021/es702192c>.

- Grandjean, P., 2018, Delayed discovery, dissemination, and decisions on intervention in environmental health—A case study on immunotoxicity of perfluorinated alkylate substances: *Environmental Health*, v. 17, no. 1, article 62, 6 p., accessed September 26, 2021, at <https://doi.org/10.1186/s12940-018-0405-y>.
- Grandjean, P., and Clapp, R., 2015, Perfluorinated alkyl substances—Emerging insights into health risks: *New Solutions*, v. 25, no. 2, p. 147–163, accessed September 26, 2021, at <https://doi.org/10.1177/1048291115590506>.
- Guelfo, J.L., and Higgins, C.P., 2013, Subsurface transport potential of perfluoroalkyl acids at aqueous film-forming foam (AFFF)-impacted sites: *Environmental Science & Technology*, v. 47, no. 9, p. 4164–4171, accessed September 26, 2021, at <https://doi.org/10.1021/es3048043>.
- Gustavsson, N., Bølviken, B., Smith, D.B., and Severson, R.C., 2001, Geochemical landscapes of the conterminous United States—New map presentations for 22 elements: U.S. Geological Survey Professional Paper 1648, 46 p., accessed July 1, 2020, at <http://pubs.er.usgs.gov/publication/pp1648>.
- Harding-Marjanovic, K.C., Houtz, E.F., Yi, S., Field, J.A., Sedlak, D.L., and Alvarez-Cohen, L., 2015, Aerobic biotransformation of fluorotelomer thioether amido sulfonate (Lodyne) in AFFF-amended microcosms: *Environmental Science & Technology*, v. 49, no. 13, p. 7666–7674, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.5b01219>.
- Haug, L.S., Huber, S., Becher, G., and Thomsen, C., 2011, Characterisation of human exposure pathways to perfluorinated compounds—Comparing exposure estimates with biomarkers of exposure: *Environment International*, v. 37, no. 4, p. 687–693, accessed September 26, 2021, at <https://doi.org/10.1016/j.envint.2011.01.011>.
- Higgins, C.P., and Luthy, R.G., 2006, Sorption of perfluorinated surfactants on sediments: *Environmental Science & Technology*, v. 40, no. 23, p. 7251–7256, accessed September 26, 2021, at <https://doi.org/10.1021/es061000n>.
- Higgins, C.P., McLeod, P.B., MacManus-Spencer, L.A., and Luthy, R.G., 2007, Bioaccumulation of perfluorochemicals in sediments by the aquatic oligochaete *Lumbriculus variegatus*: *Environmental Science & Technology*, v. 41, no. 13, p. 4600–4606, accessed September 26, 2021, at <https://doi.org/10.1021/es062792o>.
- Hinck, J.E., Schmitt, C.J., Bartish, T.M., Denslow, N.D., Blazer, V., Anderson, P.J., Coyle, J.J., Dethloff, G.M., and Tillitt, D.E., 2004, Biomonitoring of Environmental Status and Trends (BEST) Program—Environmental contaminants and their effects on fish in the Columbia River Basin: U.S. Geological Survey Scientific Investigations Report 2004–5154, 126 p., accessed June 18, 2020, at <http://pubs.er.usgs.gov/publication/sir20045154>.
- Hoos, A.B., Wang, S.H., and Schwarz, G.E., 2019, Adapting a regional water-quality model for local application—A case study for Tennessee, USA: *Environmental Modelling & Software*, v. 115, p. 187–199, accessed September 26, 2021, at <https://doi.org/10.1016/j.envsoft.2019.01.001>.
- Houde, M., De Silva, A.O., Muir, D.C.G., and Letcher, R.J., 2011, Monitoring of perfluorinated compounds in aquatic biota—An updated review: *Environmental Science & Technology*, v. 45, no. 19, p. 7962–7973, accessed September 26, 2021, at <https://doi.org/10.1021/es104326w>.
- Houde, M., Martin, J.W., Letcher, R.J., Solomon, K.R., and Muir, D.C.G., 2006, Biological monitoring of polyfluoroalkyl substances—A review: *Environmental Science & Technology*, v. 40, no. 11, p. 3463–3473, accessed September 26, 2021, at <https://doi.org/10.1021/es052580b>.
- Houtz, E.F., Higgins, C.P., Field, J.A., and Sedlak, D.L., 2013, Persistence of perfluoroalkyl acid precursors in AFFF-impacted groundwater and soil: *Environmental Science & Technology*, v. 47, no. 15, p. 8187–8195, accessed September 26, 2021, at <https://doi.org/10.1021/es4018877>.
- Houtz, E.F., and Sedlak, D.L., 2012, Oxidative conversion as a means of detecting precursors to perfluoroalkyl acids in urban runoff: *Environmental Science & Technology*, v. 46, no. 17, p. 9342–9349, accessed September 26, 2021, at <https://doi.org/10.1021/es302274g>.
- Houtz, E.F., Sutton, R., Park, J.-S., and Sedlak, M., 2016, Poly- and perfluoroalkyl substances in wastewater—Significance of unknown precursors, manufacturing shifts, and likely AFFF impacts: *Water Research*, v. 95, p. 142–149, accessed September 26, 2021, at <https://doi.org/10.1016/j.watres.2016.02.055>.
- Hu, X.C., Andrews, D.Q., Lindstrom, A.B., Bruton, T.A., Schaider, L.A., Grandjean, P., Lohmann, R., Carignan, C.C., Blum, A., Balan, S.A., Higgins, C.P., and Sunderland, E.M., 2016, Detection of poly- and perfluoroalkyl substances (PFASs) in U.S. drinking water linked to industrial sites, military fire training areas, and wastewater treatment plants: *Environmental Science & Technology Letters*, v. 3, no. 10, p. 344–350, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.6b00260>.

- Hu, X.C., Dassuncao, C., Zhang, X., Grandjean, P., Weihe, P., Webster, G.M., Nielsen, F., and Sunderland, E.M., 2018, Can profiles of poly- and perfluoroalkyl substances (PFASs) in human serum provide information on major exposure sources?: *Environmental Health*, v. 17, article 11, 15 p., accessed September 26, 2021, at <https://doi.org/10.1186/s12940-018-0355-4>.
- Hu, X.C., Tokranov, A.K., Liddie, J., Zhang, X., Grandjean, P., Hart, J.E., Laden, F., Sun, Q., Yeung, L.W.Y., and Sunderland, E.M., 2019, Tap water contributions to plasma concentrations of poly- and perfluoroalkyl substances (PFAS) in a nationwide prospective cohort of U.S. women: *Environmental Health Perspectives*, v. 127, no. 6, article 067006, 11 p., accessed September 26, 2021, at <https://doi.org/10.1289/EHP4093>.
- Huang, S., and Jaffé, P.R., 2019, Defluorination of perfluorooctanoic acid (PFOA) and perfluorooctane sulfonate (PFOS) by *Acidimicrobium* sp. strain A6: *Environmental Science & Technology*, v. 53, no. 19, p. 11410–11419, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b04047>.
- Imbrigiotta, T.E., and Fiore, A.R., 2021, Distribution of chlorinated volatile organic compounds and per- and polyfluoroalkyl substances in monitoring wells at the former Naval Air Warfare Center, West Trenton, New Jersey, 2014–17: U.S. Geological Survey Open-File Report 2020–1105, 107 p., accessed September 25, 2021, at <https://doi.org/10.3133/ofr20201105>.
- Interstate Technology Regulatory Council, 2017, History and use of per- and polyfluoroalkyl substances (PFAS): Interstate Technology Regulatory Council Fact Sheet, accessed March 30, 2020, at https://pfas-1.itrcweb.org/fact_sheets_page/PFAS_Fact_Sheet_History_and_Use_April2020.pdf.
- Interstate Technology Regulatory Council, 2020, Human and ecological health effects of select PFAS: Interstate Technology Regulatory Council web page, accessed June 10, 2020, at <https://pfas-1.itrcweb.org/7-human-and-ecological-health-effects-of-select-pfas/>.
- Johansson, J.H., Berger, U., Vestergren, R., Cousins, I.T., Bignert, A., Glynn, A., and Darnerud, P.O., 2014, Temporal trends (1999–2010) of perfluoroalkyl acids in commonly consumed food items: *Environmental Pollution*, v. 188, p. 102–108, accessed September 26, 2021, at <https://doi.org/10.1016/j.envpol.2014.01.026>.
- Kandel, C.M., Rapp, J.L., and Barber, L.B., 2017, Shenandoah River accumulated wastewater ratio mapper: U.S. Geological Survey web page, accessed March 28, 2020, at <https://va.water.usgs.gov/webmap/shenmap/>.
- Kannan, K., 2011, Perfluoroalkyl and polyfluoroalkyl substances—Current and future perspectives: *Environmental Chemistry*, v. 8, no. 4, p. 333–338, accessed September 26, 2021, at <https://doi.org/10.1071/EN11053>.
- Kannan, K., Tao, L., Sinclair, E., Pastva, S.D., Jude, D.J., and Giesy, J.P., 2005, Perfluorinated compounds in aquatic organisms at various trophic levels in a Great Lakes food chain: *Archives of Environmental Contamination and Toxicology*, v. 48, no. 4, p. 559–566, accessed September 26, 2021, at <https://doi.org/10.1007/s00244-004-0133-x>.
- Kim, S., Choi, K., Ji, K., Seo, J., Kho, Y., Park, J., Kim, S., Park, S., Hwang, I., Jeon, J., Yang, H., and Giesy, J.P., 2011, Trans-placental transfer of thirteen perfluorinated compounds and relations with fetal thyroid hormones: *Environmental Science & Technology*, v. 45, no. 17, p. 7465–7472, accessed September 26, 2021, at <https://doi.org/10.1021/es202408a>.
- Kim, S.-J., Heo, S.-H., Lee, D.-S., Hwang, I.G., Lee, Y.-B., and Cho, H.-Y., 2016, Gender differences in pharmacokinetics and tissue distribution of 3 perfluoroalkyl and polyfluoroalkyl substances in rats: *Food and Chemical Toxicology*, v. 97, p. 243–255, accessed September 26, 2021, at <https://doi.org/10.1016/j.fct.2016.09.017>.
- Koch, A., Aro, R., Wang, T., and Yeung, L.W.Y., 2019, Towards a comprehensive analytical workflow for the chemical characterisation of organofluorine in consumer products and environmental samples: *TrAC Trends in Analytical Chemistry*, v. 123, article 115423, 9 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.trac.2019.02.024>.
- Kolpin, D.W., Furlong, E.T., Meyer, M.T., Thurman, E.M., Zaugg, S.D., Barber, L.B., and Buxton, H.T., 2002, Pharmaceuticals, hormones, and other organic wastewater contaminants in U.S. streams, 1999–2000—A national reconnaissance: *Environmental Science & Technology*, v. 36, no. 6, p. 1202–1211, accessed September 26, 2021, at <https://doi.org/10.1021/es011055j>.
- Kudo, N., Suzuki, E., Katakura, M., Ohmori, K., Noshiro, R., and Kawashima, Y., 2001, Comparison of the elimination between perfluorinated fatty acids with different carbon chain length in rats: *Chemico-Biological Interactions*, v. 134, no. 2, p. 203–216, accessed September 26, 2021, at [https://doi.org/10.1016/S0009-2797\(01\)00155-7](https://doi.org/10.1016/S0009-2797(01)00155-7).
- Lai, F.Y., Rauert, C., Gobelius, L., and Ahrens, L., 2019, A critical review on passive sampling in air and water for per- and polyfluoroalkyl substances (PFASs): *TrAC Trends in Analytical Chemistry*, v. 121, article 115311, 14 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.trac.2018.11.009>.

- Lang, J.R., Allred, B.M., Field, J.A., Levis, J.W., and Barlaz, M.A., 2017, National estimate of per- and polyfluoroalkyl substance (PFAS) release to U.S. municipal landfill leachate: *Environmental Science & Technology*, v. 51, no. 4, p. 2197–2205, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.6b05005>.
- Langberg, H.A., Breedveld, G.D., Grønning, H.M., Kvennås, M., Jenssen, B.M., and Hale, S.E., 2019, Bioaccumulation of fluorotelomer sulfonates and perfluoroalkyl acids in marine organisms living in aqueous film-forming foam impacted waters: *Environmental Science & Technology*, v. 53, no. 18, p. 10951–10960, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b00927>.
- Langer, V., Dreyer, A., and Ebinghaus, R., 2010, Polyfluorinated compounds in residential and nonresidential indoor air: *Environmental Science & Technology*, v. 44, no. 21, p. 8075–8081, accessed September 26, 2021, at <https://doi.org/10.1021/es102384z>.
- Lau, C., Anitole, K., Hodes, C., Lai, D., Pfahles-Hutchens, A., and Seed, J., 2007, Perfluoroalkyl acids—A review of monitoring and toxicological findings: *Toxicological Sciences*, v. 99, no. 2, p. 366–394, accessed September 26, 2021, at <https://doi.org/10.1093/toxsci/kfm128>.
- Lau, C., Butenhoff, J.L., and Rogers, J.M., 2004, The developmental toxicity of perfluoroalkyl acids and their derivatives: *Toxicology and Applied Pharmacology*, v. 198, no. 2, p. 231–241, accessed September 26, 2021, at <https://doi.org/10.1016/j.taap.2003.11.031>.
- Li, F., Fang, X., Zhou, Z., Liao, X., Zou, J., Yuan, B., and Sun, W., 2019, Adsorption of perfluorinated acids onto soils—Kinetics, isotherms, and influences of soil properties: *Science of The Total Environment*, v. 649, p. 504–514, accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2018.08.209>.
- Li, Y., Feng, X., Zhou, J., and Zhu, L., 2020, Occurrence and source apportionment of novel and legacy poly/perfluoroalkyl substances in Hai River basin in China using receptor models and isomeric fingerprints: *Water Research*, v. 168, article 115145, 11 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.watres.2019.115145>.
- Li, Y., Oliver, D.P., and Kookana, R.S., 2018, A critical analysis of published data to discern the role of soil and sediment properties in determining sorption of per and polyfluoroalkyl substances (PFASs): *Science of The Total Environment*, v. 628–629, p. 110–120, accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2018.01.167>.
- Lin, H., Taniyasu, S., Yamazaki, E., Wei, S., Wang, X., Gai, N., Kim, J.H., Eun, H., Lam, P.K.S., and Yamashita, N., 2020, Per- and polyfluoroalkyl substances in the air particles of Asia—Levels, seasonality, and size-dependent distribution: *Environmental Science & Technology*, v. 54, no. 22, p. 14182–14191, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.0c03387>.
- Lindsey, B.D., Johnson, T.D., Privette, L.M., and Estes, N.J., 2018, Decadal changes in groundwater quality: U.S. Geological Survey web page, accessed December 2, 2021, at <https://nawqatrends.wim.usgs.gov/decadal/>.
- Liu, C., and Liu, J., 2016, Aerobic biotransformation of polyfluoroalkyl phosphate esters (PAPs) in soil: *Environmental Pollution*, v. 212, p. 230–237, accessed September 26, 2021, at <https://doi.org/10.1016/j.envpol.2016.01.069>.
- Liu, J., and Mejia Avendaño, S., 2013, Microbial degradation of polyfluoroalkyl chemicals in the environment—A review: *Environment International*, v. 61, p. 98–114, accessed September 26, 2021, at <https://doi.org/10.1016/j.envint.2013.08.022>.
- Liu, X., Guo, Z., Krebs, K.A., Pope, R.H., and Roache, N.F., 2014, Concentrations and trends of perfluorinated chemicals in potential indoor sources from 2007 through 2011 in the US: *Chemosphere*, v. 98, p. 51–57, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2013.10.001>.
- Lombard, M.A., Bryan, M.S., Jones, D.K., Bulka, C., Bradley, P.M., Backer, L.C., Focazio, M.J., Silverman, D.T., Toccalino, P., Argos, M., Gribble, M.O., and Ayotte, J.D., 2021, Machine learning models of arsenic in private wells throughout the conterminous United States as a tool for exposure assessment in human health studies: *Environmental Science & Technology*, v. 55, no. 8, p. 5012–5023, accessed November 2, 2021, at <https://doi.org/10.1021/acs.est.0c05239>.
- Longworth, S.G., 2020, Processes & considerations for setting state PFAS standards: The Environmental Council of the States, 36 p., accessed April 2, 2020, at <https://www.ecos.org/wp-content/uploads/2020/02/Standards-White-Paper-FINAL-February-2020.pdf>.
- Lynch, K.M., Fair, P.A., Houde, M., Muir, D.C.G., Kannan, K., Bossart, G.D., Bartell, S.M., and Gribble, M.O., 2019, Temporal trends in per- and polyfluoroalkyl substances in bottlenose dolphins (*Tursiops truncatus*) of Indian River Lagoon, Florida and Charleston, South Carolina: *Environmental Science & Technology*, v. 53, no. 24, p. 14194–14203, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b04585>.

- Lyu, Y., Brusseau, M.L., Chen, W., Yan, N., Fu, X., and Lin, X., 2018, Adsorption of PFOA at the air–water interface during transport in unsaturated porous media: *Environmental Science & Technology*, v. 52, no. 14, p. 7745–7753, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.8b02348>.
- Ma, R., Zheng, C., Liu, C., Greskowiak, J., Prommer, H., and Zachara, J.M., 2014, Assessment of controlling processes for field-scale uranium reactive transport under highly transient flow conditions: *Water Resources Research*, v. 50, no. 2, p. 1006–1024, accessed September 26, 2021, at <https://doi.org/10.1002/2013wr013835>.
- MacDonald, M.M., Warne, A.L., Stock, N.L., Mabury, S.A., Solomon, K.R., and Sibley, P.K., 2004, Toxicity of perfluorooctane sulfonic acid and perfluorooctanoic acid to *Chironomus tentans*: *Environmental Toxicology and Chemistry*, v. 23, no. 9, p. 2116–2123, accessed September 26, 2021, at <https://doi.org/10.1897/03-449>.
- Masoner, J.R., Kolpin, D.W., Cozzarelli, I.M., Smalling, K.L., Bolyard, S.C., Field, J.A., Furlong, E.T., Gray, J.L., Lozinski, D., Reinhart, D., Rodowa, A., and Bradley, P.M., 2020, Landfill leachate contributes per-/poly-fluoroalkyl substances (PFAS) and pharmaceuticals to municipal wastewater: *Environmental Science: Water Research & Technology*, v. 6, no. 5, p. 1300–1311, accessed September 26, 2021, at <https://doi.org/10.1039/D0EW00045K>.
- Maupin, M.A., 2018, Summary of estimated water use in the United States in 2015: U.S. Geological Survey Fact Sheet 2018–3035, 2 p., accessed October 15, 2021, at <http://pubs.er.usgs.gov/publication/fs20183035>.
- McCord, J., and Strynar, M., 2019, Identification of per- and polyfluoroalkyl substances in the Cape Fear River by high resolution mass spectrometry and nontargeted screening: *Environmental Science & Technology*, v. 53, no. 9, p. 4717–4727, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.8b06017>.
- McGuire, M.E., Schaefer, C., Richards, T., Backe, W.J., Field, J.A., Houtz, E., Sedlak, D.L., Guelfo, J.L., Wunsch, A., and Higgins, C.P., 2014, Evidence of remediation-induced alteration of subsurface poly- and perfluoroalkyl substance distribution at a former firefighter training area: *Environmental Science & Technology*, v. 48, no. 12, p. 6644–6652, accessed September 26, 2021, at <https://doi.org/10.1021/es5006187>.
- Mejia Avendaño, S., and Liu, J., 2015, Production of PFOS from aerobic soil biotransformation of two perfluoroalkyl sulfonamide derivatives: *Chemosphere*, v. 119, p. 1084–1090, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2014.09.059>.
- Mejia-Avendaño, S., Vo Duy, S., Sauvé, S., and Liu, J., 2016, Generation of perfluoroalkyl acids from aerobic biotransformation of quaternary ammonium polyfluoroalkyl surfactants: *Environmental Science & Technology*, v. 50, no. 18, p. 9923–9932, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.6b00140>.
- Michigan Department of Environment, Great Lakes, and Energy, 2019, Statewide testing initiative: Michigan Department of Environment, Great Lakes, and Energy, Michigan PFAS Action Response Team web page, accessed November 22, 2019, at https://www.michigan.gov/pfasresponse/0,9038,7-365-86510_87918-464299--,00.html.
- Miyake, Y., Yamashita, N., Rostkowski, P., So, M.K., Taniyasu, S., Lam, P.K.S., and Kannan, K., 2007, Determination of trace levels of total fluorine in water using combustion ion chromatography for fluorine—A mass balance approach to determine individual perfluorinated chemicals in water: *Journal of Chromatography A*, v. 1143, no. 1–2, p. 98–104, accessed September 26, 2021, at <https://doi.org/10.1016/j.chroma.2006.12.071>.
- Munoz, G., Ray, P., Mejia-Avendaño, S., Vo Duy, S., Tien Do, D., Liu, J., and Sauvé, S., 2018, Optimization of extraction methods for comprehensive profiling of perfluoroalkyl and polyfluoroalkyl substances in firefighting foam impacted soils: *Analytica Chimica Acta*, v. 1034, p. 74–84, accessed September 26, 2021, at <https://doi.org/10.1016/j.aca.2018.06.046>.
- Naile, J.E., Khim, J.S., Hong, S., Park, J., Kwon, B.-O., Ryu, J.S., Hwang, J.H., Jones, P.D., and Giesy, J.P., 2013, Distributions and bioconcentration characteristics of perfluorinated compounds in environmental samples collected from the west coast of Korea: *Chemosphere*, v. 90, no. 2, p. 387–394, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2012.07.033>.
- National Water Quality Monitoring Council, undated, Water Quality Data: National Water Quality Monitoring Council database, accessed November 11, 2020, at <https://www.waterqualitydata.us/portal/>.
- Navarro, I., de la Torre, A., Sanz, P., Porcel, M.Á., Pro, J., Carbonell, G., and Martínez, M. de los Á., 2017, Uptake of perfluoroalkyl substances and halogenated flame retardants by crop plants grown in biosolids-amended soils: *Environmental Research*, v. 152, p. 199–206, accessed September 26, 2021, at <https://doi.org/10.1016/j.envres.2016.10.018>.
- Ng, C.A., and Hungerbühler, K., 2014, Bioaccumulation of perfluorinated alkyl acids—Observations and models: *Environmental Science & Technology*, v. 48, no. 9, p. 4637–4648, accessed September 26, 2021, at <https://doi.org/10.1021/es404008g>.

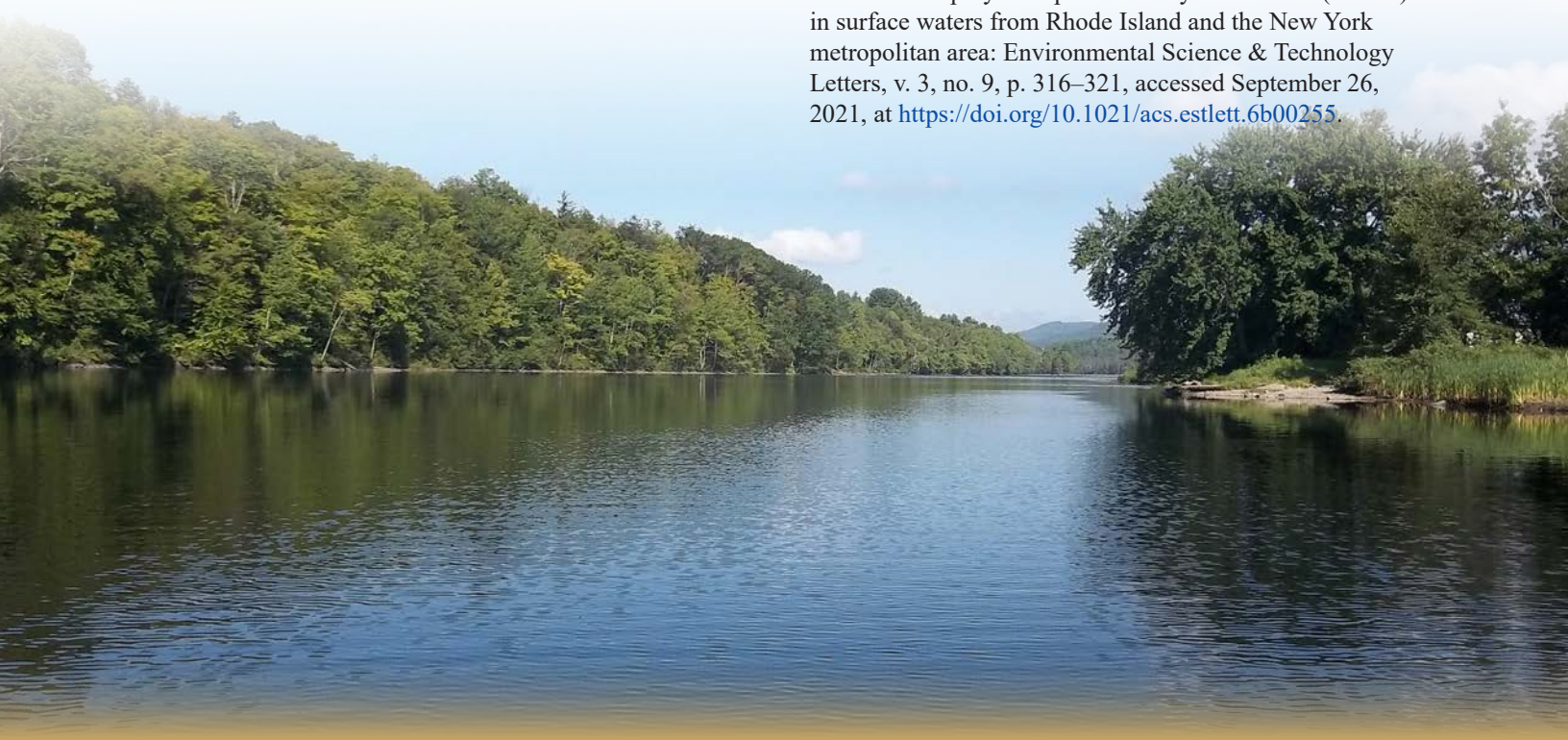
- Nolan, B.T., Fienen, M.N., and Lorenz, D.L., 2015, A statistical learning framework for groundwater nitrate models of the Central Valley, California, USA: *Journal of Hydrology*, v. 531, p. 902–911, accessed September 26, 2021, at <https://doi.org/10.1016/j.jhydrol.2015.10.025>.
- Olsen, G.W., Mair, D.C., Lange, C.C., Harrington, L.M., Church, T.R., Goldberg, C.L., Herron, R.M., Hanna, H., Nobiletti, J.B., Rios, J.A., Reagen, W.K., and Ley, C.A., 2017, Per- and polyfluoroalkyl substances (PFAS) in American Red Cross adult blood donors, 2000–2015: *Environmental Research*, v. 157, p. 87–95, accessed September 26, 2021, at <https://doi.org/10.1016/j.envres.2017.05.013>.
- Organisation for Economic Cooperation and Development, 2015, Working towards a global emission inventory of PFASs—Focus on PFCAs; Status quo and the way forward: Organisation for Economic Cooperation and Development Environment, Health and Safety Publication Series on Risk Management No. 30, accessed March 30, 2020, at <http://www.oecd.org/chemicalsafety/Working%20Towards%20a%20Global%20Emission%20Inventory%20of%20PFAS.pdf>.
- Organisation for Economic Cooperation and Development, 2018, Toward a new comprehensive global database of per- and polyfluoroalkyl substances (PFASs)—Summary report on updating the OECD 2007 list of per- and polyfluoroalkyl substances (PFASs): Organisation for Economic Cooperation and Development Environment, Health and Safety Publication Series on Risk Management No. 39, accessed March 30, 2020, at [http://www.oecd.org/official-documents/publicdisplaydocumentpdf/?cote=ENV-JM-MONO\(2018\)7&doclanguage=en](http://www.oecd.org/official-documents/publicdisplaydocumentpdf/?cote=ENV-JM-MONO(2018)7&doclanguage=en).
- Papp, J.F., 1994, Chromium life cycle study: U.S. Bureau of Mines Information Circular 9411, 94 p., accessed October 13, 2021, at <http://pubs.er.usgs.gov/publication/70005356>.
- Parkhurst, D.L., and Webb, R.M.T., 2020, PHREEQC version 3: U.S. Geological Survey web page, accessed January 30, 2020, at <https://www.usgs.gov/software/phreeqc-version-3>.
- Place, B.J., and Field, J.A., 2012, Identification of novel fluorochemicals in aqueous film-forming foams used by the US military: *Environmental Science & Technology*, v. 46, no. 13, p. 7120–7127, accessed September 26, 2021, at <https://doi.org/10.1021/es301465n>.
- Plumlee, M.H., McNeill, K., and Reinhard, M., 2009, Indirect photolysis of perfluorochemicals—Hydroxyl radical-initiated oxidation of N-ethyl perfluorooctane sulfonamido acetate (N-EtFOSAA) and other perfluoroalkanesulfonamides: *Environmental Science & Technology*, v. 43, no. 10, p. 3662–3668, accessed September 26, 2021, at <https://doi.org/10.1021/es803411w>.
- Post, G.B., 2020, Recent US State and Federal drinking water guidelines for per- and polyfluoroalkyl substances: *Environmental Toxicology and Chemistry*, v. 40, no. 3, p. 550–563, accessed September 26, 2021, at <https://doi.org/10.1002/etc.4863>.
- Prommer, H., Sun, J., and Kocar, B.D., 2019, Using reactive transport models to quantify and predict groundwater quality: *Elements*, v. 15, no. 2, p. 87–92, accessed September 26, 2021, at <https://doi.org/10.2138/gselements.15.2.87>.
- Prosser, R., Mahon, K., Sibley, P.K., Poirier, D., and Watson-Leung, T., 2016, Bioaccumulation of perfluorinated carboxylates and sulfonates and polychlorinated biphenyls in laboratory-cultured *Hexagenia* spp., *Lumbriculus variegatus* and *Pimephales promelas* from field-collected sediments: *Science of The Total Environment*, v. 543, p. 715–726, accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2015.11.062>.
- Qi, Y., He, Z., Huo, S., Zhang, J., Xi, B., and Hu, S., 2017, Source apportionment of perfluoroalkyl substances in surface sediments from lakes in Jiangsu Province, China—Comparison of three receptor models: *Journal of Environmental Sciences*, v. 57, p. 321–328, accessed September 26, 2021, at <https://doi.org/10.1016/j.jes.2016.12.007>.
- Ranaweera, R., Ghafari, C., and Luo, L., 2019, Bubble-nucleation-based method for the selective and sensitive electrochemical detection of surfactants: *Analytical Chemistry*, v. 91, no. 12, p. 7744–7748, accessed September 26, 2021, at <https://doi.org/10.1021/acs.analchem.9b01060>.
- Rankin, K., Mabury, S.A., Jenkins, T.M., and Washington, J.W., 2016, A North American and global survey of perfluoroalkyl substances in surface soils—Distribution patterns and mode of occurrence: *Chemosphere*, v. 161, p. 333–341, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2016.06.109>.
- Ransom, K.M., Grote, M.N., Deinhart, A., Eppich, G., Kendall, C., Sanborn, M.E., Souders, A.K., Wimpenny, J., Yin, Q.-z., Young, M., and Harter, T., 2016, Bayesian nitrate source apportionment to individual groundwater wells in the Central Valley by use of elemental and isotopic tracers: *Water Resources Research*, v. 52, no. 7, p. 5577–5597, accessed September 26, 2021, at <https://doi.org/10.1002/2015WR018523>.
- Ransom, K.M., Nolan, B.T., Traum, J.A., Faunt, C.C., Bell, A.M., Gronberg, J.M., Wheeler, D.C., Rosecrans, C.Z., Jurgens, B., Schwarz, G.E., Belitz, K., Eberts, S.M., Kourakos, G., and Harter, T., 2017, A hybrid machine learning model to predict and visualize nitrate concentration throughout the Central Valley aquifer, California, USA: *Science of The Total Environment*, v. 601–602, p. 1160–1172, accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2017.05.192>.

- Rattner, B.A., McGowan, P.C., Golden, N.H., Hatfield, J.S., Toschik, P.C., Lukei, R.F., Jr., Hale, R.C., Schmitz-Afonso, I., and Rice, C.P., 2004, Contaminant exposure and reproductive success of ospreys (*Pandion haliaetus*) nesting in Chesapeake Bay regions of concern: *Archives of Environmental Contamination and Toxicology*, v. 47, no. 1, p. 126–140, accessed September 26, 2021, at <https://doi.org/10.1007/s00244-003-3160-0>.
- Ritter, E.E., Dickinson, M.E., Harron, J.P., Lunderberg, D.M., DeYoung, P.A., Robel, A.E., Field, J.A., and Peaslee, G.F., 2017, PIGE as a screening tool for per- and polyfluorinated substances in papers and textiles: *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms*, v. 407, p. 47–54, accessed September 26, 2021, at <https://doi.org/10.1016/j.nimb.2017.05.052>.
- Rodowa, A.E., Christie, E., Sedlak, J., Peaslee, G.F., Bogdan, D., DiGuseppi, B., and Field, J.A., 2020, Field sampling materials unlikely source of contamination for perfluoroalkyl and polyfluoroalkyl substances in field samples: *Environmental Science & Technology Letters*, v. 7, no. 3, p. 156–163, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.0c00036>.
- Roos, A., Berger, U., Järnberg, U., Dijk, J. van, and Bignert, A., 2013, Increasing concentrations of perfluoroalkyl acids in Scandinavian otters (*Lutra lutra*) between 1972 and 2011—A new threat to the otter population?: *Environmental Science & Technology*, v. 47, no. 20, p. 11757–11765, accessed September 26, 2021, at <https://doi.org/10.1021/es401485t>.
- Rosenblum, L., and Wendelken, S.C., 2019, Method 533—Determination of per- and polyfluoroalkyl substances in drinking water by isotope dilution anion exchange solid phase extraction and liquid chromatography/tandem mass spectrometry: U.S. Environmental Protection Agency Document 815-B-19-020, 52 p., accessed March 30, 2020, at <https://www.epa.gov/sites/production/files/2019-12/documents/method-533-815b19020.pdf>.
- Saad, D.A., and Preston, S.T., [undated], SPARROW modeling—Estimating nutrient, sediment, and dissolved solids transport: U.S. Geological Survey web page, accessed January 27, 2020, at https://www.usgs.gov/mission-areas/water-resources/science/sparrow-modeling-estimating-nutrient-sediment-and-dissolved?qt-science_center_objects=0#qt-science_center_objects.
- Schaidter, L.A., Balan, S.A., Blum, A., Andrews, D.Q., Strynar, M.J., Dickinson, M.E., Lunderberg, D.M., Lang, J.R., and Peaslee, G.F., 2017, Fluorinated compounds in U.S. fast food packaging: *Environmental Science & Technology Letters*, v. 4, no. 3, p. 105–111, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.6b00435>.
- Scheringer, M., Trier, X., Cousins, I.T., de Voogt, P., Fletcher, T., Wang, Z., and Webster, T.F., 2014, Helsingør Statement on poly- and perfluorinated alkyl substances (PFASs): *Chemosphere*, v. 114, p. 337–339, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2014.05.044>.
- Schmitt, C.J., and Dethloff, G.M., eds., 2000, *Biomonitoring of Environmental Status and Trends (BEST) Program—Selected methods for monitoring chemical contaminants and their effects in aquatic ecosystems*: U.S. Geological Survey Information and Technology Report USGS/BDS/ITR–2000-0005, 96 p., accessed June 18, 2020, at <http://pubs.er.usgs.gov/publication/itr000005>.
- Sepulvado, J.G., Blaine, A.C., Hundal, L.S., and Higgins, C.P., 2011, Occurrence and fate of perfluorochemicals in soil following the land application of municipal biosolids: *Environmental Science & Technology*, v. 45, no. 19, p. 8106–8112, accessed September 26, 2021, at <https://doi.org/10.1021/es103903d>.
- Shin, H.-M., Vieira, V.M., Ryan, P.B., Detwiler, R., Sanders, B., Steenland, K., and Bartell, S.M., 2011, Environmental fate and transport modeling for perfluorooctanoic acid emitted from the Washington Works facility in West Virginia: *Environmental Science & Technology*, v. 45, no. 4, p. 1435–1442, accessed September 26, 2021, at <https://doi.org/10.1021/es102769t>.
- Shoemaker, J.A., and Tetttenhorst, D.R., 2018, Method 537.1—Determination of selected per- and polyfluorinated alkyl substances in drinking water by solid phase extraction and liquid chromatography/tandem mass spectrometry (LC/MS/MS): U.S. Environmental Protection Agency Document EPA/600/R–18/352, accessed March 30, 2020, at https://cfpub.epa.gov/si/si_public_record_Report.cfm?dirEntryId=343042&Lab=NERL.
- Smith, D.B., Solano, F., Woodruff, L.G., Cannon, W.F., and Ellefsen, K.J., 2019, Geochemical and mineralogical maps, with interpretation, for soils of the conterminous United States: U.S. Geological Survey Scientific Investigations Report 2017–5118, accessed June 12, 2020, at <http://pubs.er.usgs.gov/publication/sir20175118>.
- Smithwick, M., Mabury, S.A., Solomon, K.R., Sonne, C., Martin, J.W., Born, E.W., Dietz, R., Derocher, A.E., Letcher, R.J., Evans, T.J., Gabrielsen, G.W., Nagy, J., Stirling, I., Taylor, M.K., and Muir, D.C.G., 2005, Circumpolar study of perfluoroalkyl contaminants in polar bears (*Ursus maritimus*): *Environmental Science & Technology*, v. 39, no. 15, p. 5517–5523, accessed September 26, 2021, at <https://doi.org/10.1021/es048309w>.

- Song, X., Vestergren, R., Shi, Y., and Cai, Y., 2020, A matrix-correction approach to estimate the bioaccumulation potential of emerging PFASs: *Environmental Science & Technology*, v. 54, no. 2, p. 1005–1013, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b04906>.
- Spaan, K.M., Noordenburg, C. van, Plassmann, M.M., Schultes, L., Shaw, S., Berger, M., Heide-Jørgensen, M.P., Rosing-Asvid, A., Granquist, S.M., Dietz, R., Sonne, C., Rigét, F., Roos, A., and Benskin, J.P., 2020, Fluorine mass balance and suspect screening in marine mammals from the Northern Hemisphere: *Environmental Science & Technology*, v. 54, no. 7, p. 4046–4058, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b06773>.
- Starn, J.J., and Belitz, K., 2018, Regionalization of groundwater residence time using metamodeling: *Water Resources Research*, v. 54, no. 9, p. 6357–6373, accessed September 26, 2021, at <https://doi.org/10.1029/2017wr021531>.
- Steinle-Darling, E., and Reinhard, M., 2008, Nanofiltration for trace organic contaminant removal—Structure, solution, and membrane fouling effects on the rejection of perfluorochemicals: *Environmental Science & Technology*, v. 42, no. 14, p. 5292–5297, accessed September 26, 2021, at <https://doi.org/10.1021/es703207s>.
- Sunderland, E.M., Hu, X.C., Dassuncao, C., Tokranov, A.K., Wagner, C.C., and Allen, J.G., 2019, A review of the pathways of human exposure to poly- and perfluoroalkyl substances (PFASs) and present understanding of health effects: *Journal of Exposure Science and Environmental Epidemiology*, v. 29, no. 2, p. 131–147, accessed September 26, 2021, at <https://doi.org/10.1038/s41370-018-0094-1>.
- Toccalino, P.L., Norman, J.E., and Hitt, K.J., 2010, Quality of source water from public-supply wells in the United States, 1993–2007: U.S. Geological Survey Scientific Investigations Report 2010–5024, 126 p., accessed June 17, 2020, at <http://pubs.er.usgs.gov/publication/sir20105024>.
- Tokranov, A.K., Nishizawa, N., Amadei, C.A., Zenobio, J.E., Pickard, H.M., Allen, J.G., Vecitis, C.D., and Sunderland, E.M., 2019, How do we measure poly- and perfluoroalkyl substances (PFASs) at the surface of consumer products?: *Environmental Science & Technology Letters*, v. 6, no. 1, p. 38–43, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.8b00600>.
- Tratnyek, P.G., Bylaska, E.J., and Weber, E.J., 2017, In silico environmental chemical science—Properties and processes from statistical and computational modelling: *Environmental Science: Processes & Impacts*, v. 19, no. 3, p. 188–202, accessed September 26, 2021, at <https://doi.org/10.1039/C7EM00053G>.
- U.S. Environmental Protection Agency [EPA], 1989, Human health evaluation manual (part A), interim final, v. 1 of Risk assessment guidance for superfund: U.S. Environmental Protection Agency Document EPA/540/1-89/002, accessed June 17, 2020, at https://www.epa.gov/sites/production/files/2015-09/documents/rags_a.pdf.
- U.S. Environmental Protection Agency [EPA], [2016]a, Third unregulated contaminant monitoring rule: U.S. Environmental Protection Agency web page, accessed November 22, 2019, at <https://www.epa.gov/dwucmr/third-unregulated-contaminant-monitoring-rule>.
- U.S. Environmental Protection Agency [EPA], [2016]b, Interspecies correlation estimation: U.S. Environmental Protection Agency web page, accessed December 2, 2021, at <https://www3.epa.gov/webice/>.
- U.S. Environmental Protection Agency [EPA], 2019a, EPA's per- and polyfluoroalkyl substances (PFAS) action plan: U.S. Environmental Protection Agency Document EPA 823R18004, 72 p., accessed March 30, 2020, at https://www.epa.gov/sites/production/files/2019-02/documents/pfas_action_plan_021319_508compliant_1.pdf.
- U.S. Environmental Protection Agency [EPA], 2019b, Method 8327—Per- and polyfluoroalkyl substances (PFAS) using external standard calibration and multiple reaction monitoring (MRM) liquid chromatography/tandem mass spectrometry (LC/MS/MS): U.S. Environmental Protection Agency [Document], 58 p., accessed March 30, 2020, at https://www.epa.gov/sites/production/files/2019-06/documents/proposed_method_8327_procedure.pdf. [Update VII to third edition of EPA publication SW-846, “Test methods for evaluating solid waste, physical/chemical methods”]
- U.S. Environmental Protection Agency [EPA], 2021a, Draft method 1633—Analysis of per- and polyfluoroalkyl substances (PFAS) in aqueous, solid, biosolids, and tissue samples by LC–MS/MS: U.S. Environmental Protection Agency Document EPA 821–D–21–001, 65 p., accessed September 13, 2021, at https://www.epa.gov/system/files/documents/2021-09/method_1633_draft_aug-2021.pdf.
- U.S. Environmental Protection Agency [EPA], 2021b, How EPA regulates drinking water contaminants: U.S. Environmental Protection Agency web page, accessed September 26, 2021, at <https://www.epa.gov/dwregdev/how-epa-regulates-drinking-water-contaminants>.
- U.S. Environmental Protection Agency [EPA], 2021c, National primary drinking water regulations: U.S. Environmental Protection Agency web page, accessed September 26, 2021, at <https://www.epa.gov/ground-water-and-drinking-water/national-primary-drinking-water-regulations>.

- U.S. Environmental Protection Agency [EPA], 2021d, Sequence alignment to predict across species susceptibility (SeqAPASS): U.S. Environmental Protection Agency web page, accessed December 2, 2021, at <https://seqapass.epa.gov/seqapass/info.xhtml>.
- U.S. Food and Drug Administration, 2018, Hazard Analysis Critical Control Point (HACCP): U.S. Food and Drug Administration web page, accessed May 28, 2021, at <https://www.fda.gov/food/guidance-regulation-food-and-dietary-supplements/hazard-analysis-critical-control-point-haccp>.
- U.S. Geological Survey, 2018, General introduction for the “National Field Manual for the Collection of Water-Quality Data” (ver. 1.1, June 2018): U.S. Geological Survey Techniques and Methods, book 9, chap. A0, 4 p., accessed March 15, 2020, at <http://pubs.er.usgs.gov/publication/tm9A0>. [Supersedes USGS Techniques and Methods, book 9, chap. A0, version 1.0.]
- U.S. Geological Survey, [2019], Application of the national-scale soil geochemical and mineralogical data for the conterminous U.S.: U.S. Geological Survey web page, accessed June 19, 2020, at <https://www.usgs.gov/energy-and-minerals/mineral-resources-program/science/application-national-scale-soil-geochemical>. [Page moved at time of publication to <https://www.usgs.gov/centers/geology%2C-energy-%26amp%3Bamp%3B-minerals-science-center/science/application-national-scale-soil>.]
- U.S. Geological Survey, [2020], Passive sampling using SPMDs and POCIS: U.S. Geological Survey web page, accessed March 10, 2020, at https://www.usgs.gov/centers/cerc/science/passive-sampling-using-spm-ds-and-pocis?qt-science_center_objects=0#qt-science_center_objects.
- U.S. Geological Survey, [2021], Tracking water quality in U.S. streams and rivers—USGS National Water Quality Network data, water-quality loads, and trends: U.S. Geological Survey web page, accessed December 2, 2021, at <https://nrtwq.usgs.gov/nwqn/>.
- U.S. Geological Survey, [undated]a, Biomonitoring of environmental status and trends (BEST) large rivers monitoring network (LRMN): U.S. Geological Survey web page, accessed June 19, 2020, at <https://www.cerc.usgs.gov/data/best/search/>.
- U.S. Geological Survey, [undated]b, National Atmospheric Deposition Program (NADP): U.S. Geological Survey web page, accessed December 2, 2021, at <https://www.usgs.gov/mission-areas/water-resources/science/national-atmospheric-deposition-program-nadp/>.
- Venkatesan, A.K., and Halden, R.U., 2013, National inventory of perfluoroalkyl substances in archived U.S. biosolids from the 2001 EPA National Sewage Sludge Survey: *Journal of Hazardous Materials*, v. 252–253, p. 413–418, accessed September 26, 2021, at <https://doi.org/10.1016/j.jhazmat.2013.03.016>.
- Vermont Agency of Natural Resources, 2019, Per and polyfluoroalkyl substances (PFAS) statewide sampling plan: Vermont Agency of Natural Resources [report], 22 p., accessed March 30, 2020, at https://anrweb.vt.gov/PublicDocs/DEC/PFOA/2019%20Statewide%20Sampling%20Plan/PFAS%20sampling%20plan%2007162019_Final.pdf.
- Wang, F., Shih, K., Ma, R., and Li, X.-y., 2015, Influence of cations on the partition behavior of perfluoroheptanoate (PFHpA) and perfluorohexanesulfonate (PFHxS) on wastewater sludge: *Chemosphere*, v. 131, p. 178–183, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2015.03.024>.
- Wang, Z., Boucher, J.M., Scheringer, M., Cousins, I.T., and Hungerbühler, K., 2017, Toward a comprehensive global emission inventory of C4–C10 perfluoroalkanesulfonic acids (PFASs) and related precursors—Focus on the life cycle of C8-based products and ongoing industrial transition: *Environmental Science & Technology*, v. 51, no. 8, p. 4482–4493, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.6b06191>.
- Wang, Z., Cousins, I.T., Scheringer, M., Buck, R.C., and Hungerbühler, K., 2014, Global emission inventories for C4–C14 perfluoroalkyl carboxylic acid (PFCA) homologues from 1951 to 2030, part I—Production and emissions from quantifiable sources: *Environment International*, v. 70, p. 62–75, accessed September 26, 2021, at <https://doi.org/10.1016/j.envint.2014.04.013>.
- Wang, Z., DeWitt, J.C., Higgins, C.P., and Cousins, I.T., 2017, A never-ending story of per- and polyfluoroalkyl substances (PFASs): *Environmental Science & Technology*, v. 51, no. 5, p. 2508–2518. [Also available at <https://doi.org/10.1021/acs.est.6b04806>.]
- Wania, F., 2007, A global mass balance analysis of the source of perfluorocarboxylic acids in the Arctic Ocean: *Environmental Science & Technology*, v. 41, no. 13, p. 4529–4535, accessed September 26, 2021, at <https://doi.org/10.1021/es070124c>.
- Washington, J.W., and Jenkins, T.M., 2015, Abiotic hydrolysis of fluorotelomer-based polymers as a source of perfluorocarboxylates at the global scale: *Environmental Science & Technology*, v. 49, no. 24, p. 14129–14135, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.5b03686>.

- Weber, A.K., Barber, L.B., LeBlanc, D.R., Sunderland, E.M., and Vecitis, C.D., 2017, Geochemical and hydrologic factors controlling subsurface transport of poly- and perfluoroalkyl substances, Cape Cod, Massachusetts: *Environmental Science & Technology*, v. 51, no. 8, p. 4269–4279, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.6b05573>.
- Winkens, K., Vestergren, R., Berger, U., and Cousins, I.T., 2017, Early life exposure to per- and polyfluoroalkyl substances (PFASs)—A critical review: *Emerging Contaminants*, v. 3, no. 2, p. 55–68, accessed September 26, 2021, at <https://doi.org/10.1016/j.emcon.2017.05.001>.
- Xiao, F., Jin, B., Golovko, S.A., Golovko, M.Y., and Xing, B., 2019, Sorption and desorption mechanisms of cationic and zwitterionic per- and polyfluoroalkyl substances in natural soils—Thermodynamics and hysteresis: *Environmental Science & Technology*, v. 53, no. 20, p. 11818–11827, accessed September 26, 2021, at <https://doi.org/10.1021/acs.est.9b05379>.
- Yeung, L.W.Y., Miyake, Y., Taniyasu, S., Wang, Y., Yu, H., So, M.K., Jiang, G., Wu, Y., Li, J., Giesy, J.P., Yamashita, N., and Lam, P.K.S., 2008, Perfluorinated compounds and total and extractable organic fluorine in human blood samples from China: *Environmental Science & Technology*, v. 42, no. 21, p. 8140–8145, accessed September 26, 2021, at <https://doi.org/10.1021/es800631n>.
- Young, C.J., Furdui, V.I., Franklin, J., Koerner, R.M., Muir, D.C.G., and Mabury, S.A., 2007, Perfluorinated acids in arctic snow—New evidence for atmospheric formation: *Environmental Science & Technology*, v. 41, no. 10, p. 3455–3461, accessed September 26, 2021, at <https://doi.org/10.1021/es0626234>.
- Zhang, C., Hopkins, Z.R., McCord, J., Strynar, M.J., and Knappe, D.R.U., 2019, Fate of per- and polyfluoroalkyl ether acids in the total oxidizable precursor assay and implications for the analysis of impacted water: *Environmental Science & Technology Letters*, v. 6, no. 11, p. 662–668, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.9b00525>.
- Zhang, D.Q., Zhang, W.L., and Liang, Y.N., 2019, Adsorption of perfluoroalkyl and polyfluoroalkyl substances (PFASs) from aqueous solution—A review: *Science of The Total Environment*, v. 694, article 133606, 17 p., accessed September 26, 2021, at <https://doi.org/10.1016/j.scitotenv.2019.133606>.
- Zhang, H., Liu, W., He, X., Wang, Y., and Zhang, Q., 2015, Uptake of perfluoroalkyl acids in the leaves of coniferous and deciduous broad-leaved trees: *Environmental Toxicology and Chemistry*, v. 34, no. 7, p. 1499–1504, accessed September 26, 2021, at <https://doi.org/10.1002/etc.2968>.
- Zhang, S., Lu, X., Wang, N., and Buck, R.C., 2016, Biotransformation potential of 6:2 fluorotelomer sulfonate (6:2 FTSA) in aerobic and anaerobic sediment: *Chemosphere*, v. 154, p. 224–230, accessed September 26, 2021, at <https://doi.org/10.1016/j.chemosphere.2016.03.062>.
- Zhang, S., Szostek, B., McCausland, P.K., Wolstenholme, B.W., Lu, X., Wang, N., and Buck, R.C., 2013, 6:2 and 8:2 fluorotelomer alcohol anaerobic biotransformation in digester sludge from a WWTP under methanogenic conditions: *Environmental Science & Technology*, v. 47, no. 9, p. 4227–4235, accessed September 26, 2021, at <https://doi.org/10.1021/es4000824>.
- Zhang, X., Lohmann, R., Dassuncao, C., Hu, X.C., Weber, A.K., Vecitis, C.D., and Sunderland, E.M., 2016, Source attribution of poly- and perfluoroalkyl substances (PFASs) in surface waters from Rhode Island and the New York metropolitan area: *Environmental Science & Technology Letters*, v. 3, no. 9, p. 316–321, accessed September 26, 2021, at <https://doi.org/10.1021/acs.estlett.6b00255>.



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