Derivation of PFAS Ecological Screening Values

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ACRYONMS AND ABBREVIATIONS

6:2 FTS	6:2 fluorotelomer sulfonate
ACR	acute-to-chronic ratio
AFFF	aqueous film-forming foam
Argonne	Argonne National Laboratory
ATSDR	Agency for Toxic Substances and Disease Registry
AUF	area use factor
BAF	bioaccumulation factor
BCF	bioconcentration factor
BMD	benchmark dose
BMF	biomagnification factor
BSAF	biota-sediment accumulation factor
BW	bodyweight
CCC	continuous concentration criterion
CCTE	Center for Computational Toxicology and Exposures
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act of 1980
CF2	carbon difluoride fragment
CMC	critical micelle concentration
d	day
DCPH	Defense Centers for Public Health
dg	data gap
DOC	dissolved organic carbon
DOD	U.S. Department of Defense
dw	dry weight
EC10	effect concentration affecting 10% of population
EC20	effect concentration affecting 20% of population
EC25	effect concentration affecting 25% of population
EC50	effect concentration affecting 50% of population
Eco-SSL	Ecological Soil Screening Level
ECOTOX	Ecological Toxicology Knowledgebase
EPA	U.S. Environmental Protection Agency
EqP	equilibrium partitioning model
ERA	Ecological Risk Assessment
ESV	ecological screening value
FACR	final acute-chronic ratio
FAV	final acute value
FCV	final chronic value
FIR	food ingestion rates

f_{oc}	fraction organic carbon
FPV	final plant value
GLI	Great Lakes Initiative
GLWQI	Great Lakes Water Quality Initiative
GMAV	genus mean acute value
GLTED	Great Lakes Toxicology and Ecology Division
HC5	hazardous concentration protective of 95% of test species
HQ	hazard quotient
IC25	inhibition concentration affecting 25% of population
IRP	Installation Restoration Program
K_d	distribution constant
kg	kilogram
K_{oc}	distribution constant water organic carbon
K_{ow}	distribution constant octanol water
K_p	partition constant
L	liter
LC50	lethal concentration to 50% of population
LD50	lethal dose to 50% of population
Li	lithium
LOAEC	lowest observed adverse effect concentration
LOAEL	lowest observed adverse effect level
MATC	maximum acceptable threshold concentration
MCC	maximum concentration criterion
mg	milligram
na	not available/not applicable
NOAEC	no observed adverse effect concentration
NOAEL	no observed adverse effect level
OC	organic carbon
PFAS	per- and polyfluorinated alky substances
PFBA	perfluorobutanoic acid
PFBS	perfluorobutanesulfonic acid
PFCAs	perfluorocarboxylic acids
PFDA	perfluorodecanoic acid
PFHxA	perfluorohexanoic acid
PFHxS	perfluorohexanesulfonic acid
PFNA	perfluorononanoic acid
PFOA	perfluorooctanoic acid
PFOS	perfluorooctanesulfonic acid
PFPeA	perfluoropentanoic acid

PFSAs	perfluorosulfonic acids
PFTrDA	perfluorotridecanoic acid
PNEC	predicted no-effect concentration
SAF	secondary acute factor
SARC	secondary acute -to chronic ratio
SAV	secondary acute value
SCC	secondary chronic criteria
SCV	secondary chronic value
SFACR	secondary final acute to chronic ratio
SMACR	species mean acute to chronic ratio
SMAV	species mean acute value
SMC	secondary maximum criteria
SMCV	species mean chronic value
SPM	suspended particulate matter
SQB	sediment quality benchmark
SUF	seasonal use factor
TD	test dose
TL	trophic level
TOC	total organic carbon
TRV	toxicity reference value
UF	uncertainty factor
UF_A	uncertainty factors for inter-taxon extrapolation
UF_L	uncertainty factors for extrapolating across endpoints
UF_S	uncertainty factors for extrapolation across exposure durations
µg	microgram
WQB	water quality benchmark
WV	wildlife value
ww	wet weight

EXECUTIVE SUMMARY

ES.1 Introduction

This report presents ecological screening values (ESVs) that have been developed to support screening-level ecological risk assessments at Air Force, Navy, Army, and other U.S. Department of Defense (DOD) sites where per- and polyfluorinated alkyl substances (PFAS) have been detected in soils and surface waters. These ESVs, developed for a study set of eight PFAS compounds, represent PFAS concentrations in soil and surface water at or below which chronically exposed biota are not expected to be adversely affected and ecological impacts are unlikely. These ESVs support the screening level steps (Steps 1 and 2 of eight steps) of U.S. Environmental Protection Agency's (EPA's) Ecological Risk Assessment Guidance for Superfund (EPA 1997), and may be applied at sites undergoing investigation for the historic release or disposal of PFAS, including those associated with the use of aqueous film-forming foam (AFFF), within DOD environmental restoration programs to identify whether PFAS levels pose potential unacceptable ecological risks. Sites that exceed ESVs may require further investigation in a baseline ecological risk assessment, which in turn may support risk-management decisions and actions to reduce risks. These ESVs are solely for use in conducting screening-level ecological risk assessments and are *not* recommended or intended for use as default cleanup values (EPA 2018).

This report is an update of an original report completed in September 2021. ESVs presented in this report have been updated with toxicological studies added to EPA's ECOTOX knowledgebase since March 2020, the nominal date of the studies included in the earlier report, and through the March 2023 ECOTOX quarterly update.

ES.2 Scope and Methods

This report describes the derivation of PFAS ESVs for the following media and receptors:

- Soils for invertebrates;
- Soils for plants;
- Soils for avian and mammalian wildlife;
- Surface water for freshwater and marine aquatic biota; and
- Surface water for aquatic-dependent avian and mammalian wildlife.

The PFAS ESVs were developed in coordination and consultation with an interagency team of subject-matter experts from across the DOD services through the DOD Tri-Services Environmental Risk Assessment Work Group. Several ecological risk assessors and environmental scientists from the EPA Ecological Risk Assessment Forum and program offices provided technical input and advice throughout this effort. This included staff from the EPA Office of Land and Emergency Management's Office of Superfund Remediation and Technology Innovation and Federal Facilities Restoration and Reuse Office; Office of Water;

Office of Chemical Safety and Pollution Prevention; Office of Research and Development; and EPA Regions.

The soil ESVs were derived by following the approach in EPA's Guidance for Developing Ecological Soil Screening Levels (the Eco-SSL guidance) (EPA 2005), while derivation of the surface water ESVs followed the approach in EPA's *Guidelines for Developing Numerical Water Quality Criteria for the Protection of Aquatic Organisms and Their Uses* (Stephen et al. 1985) and the EPA Great Lakes Water Quality Initiative *Final Water Quality Guidance for the Great Lakes System* (EPA 1995a, b, c), referred to here as the Great Lakes Water Quality Initiative (GLWQI) or simply GLI guidance.

The Air Force identified eight PFAS compounds in consultation with the Interagency Team for ESV development (Table ES-1). The study set is composed of homologs of carboxylic acids of 4 to 10 perfluorinated carbons and homologs of sulfonic acids of 4 to 8 perfluorinated carbons. The eight PFAS are among the most prevalent of 15 PFAS identified in various environmental media at military installations with historic use of AFFF (Anderson et al. 2016) and have a sufficient number of available toxicity studies for the development of ESVs.

TABLE ES-1 PFAS Compounds Included in the Literature Search for ESV Development

PFAS Abbreviation and Compound Names	International Union of Pure and Applied Chemistry Nomenclature	Chemical Abstracts Service Registry Number
	Carboxylic acids	
PFBA, perfluorobutanoic acid	2,2,3,3,4,4,4-heptafluorobutanoic acid	375-22-4
PFHxA, perfluorohexanoic acid	2,2,3,3,4,4,5,5,6,6,6-undecafluorohexanoic acid	307-24-4
PFOA, perfluorooctanoic acid	2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid	335-67-1
PFNA, perfluorononanoic acid	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluorononanoic acid	375-95-1
PFDA, perfluorodecanoic acid	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-nonadecafluorodecanoic acid	335-76-2
	Sulfonic acids	
PFBS, perfluorobutanesulfonic acid	1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonic acid	375-73-5
PFHxS, perfluorohexanesulfonic acid	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexane-1-sulfonic acid	355-46-4
PFOS, perfluorooctanesulfonic acid	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane-1-sulfonic acid	1763-23-1

ES.3 Toxicity Literature Identification and Extraction

ES.3.1 Data Sources

The data used to develop the PFAS ESVs come from publicly available scientific publications, as identified primarily through targeted searches of the Ecological Toxicology Knowledgebase (ECOTOX), and the Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profile for PFAS (ATSDR 2018). ECOTOX curates peer-reviewed literature on the effects of toxic substances on aquatic and terrestrial organisms, found through online searches of scientific databases from 1970 onward, and is updated quarterly to biannually. The most recent ECOTOX searches conducted for this effort were in March 2023.

ECOTOX searches were conducted on all available forms of the eight-PFAS study set, including the protonated and anionic forms, as well as all salt forms listed in the search menu. The searches included all terrestrial and aquatic biota, and all endpoints for ecologically relevant effects, specifically effects on reproduction, mortality, growth, and development. Adverse effects on populations can be inferred from measures related to impaired reproduction, growth, and survival. EPA's GLI guidance prioritizes effects on survival, growth, and reproduction for aquatic life for use in criteria development (Stephen et al. 1985; EPA 1995a), while EPA's Technical Support Document for Wildlife Criteria for the GLWQI defines acceptable endpoints for criteria derivation as those that affect reproductive or development success, viability, growth, or any other endpoint that is related to population dynamics (EPA 1995c). EPA's Ecological Soil Screening Level (Eco-SSL, EPA 2005) guidance similarly relies on effects on reproduction, growth, and mortality in the derivation of toxicity reference values (TRVs) for birds and mammals. In addition, EPA's Ecological Risk Assessment Guidance focuses on receptor populations of plants and animals, as measured by effects on reproduction, growth, and survival, as well as on effects on habitats and sensitive environments for screening-level assessments under the Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA; EPA 1997). Thus, ECOTOX searches did not include other effects such as physiological, cellular, biochemical/molecular, or behavioral effects, due to the difficulty of clearly and directly relating these effects to mortality, reproduction, growth, and development.

ES.3.2 Literature Review

A total of 420 aquatic and terrestrial studies on the effects of PFAS were identified for the eight PFAS targeted for ESV development (Table ES-1). Studies of aquatic organisms (309) were identified almost entirely from ECOTOX. Studies of terrestrial organisms (111) were identified from ECOTOX, ATSDR (2018) (mammals only), and as cited in other studies and reports. PFOS and PFOA were by far the most studied PFAS. Studies initially identified as potentially suitable for PFAS ESV development were acquired and screened against 12 exclusion criteria and 10 acceptance criteria, which were modified from the Eco-SSL criteria (EPA 2005). Applying the rejection and acceptance criteria to the 420 studies resulted in the retention of 282 studies: 203 aquatic studies and 79 terrestrial studies. Study rejection rates were 34% for aquatic studies and 29% for terrestrial studies (Table ES-2).

TABLE ES-2 Numbers of Accepted and Rejected Studies

No. Studies	Aquatic Studies	Terrestrial Studies
Total	309	111
Accepted	203	79
Rejected	106	32
Rejected	34%	29%

Finally, in the original September 2021 study, under supplemental scope and at the request of Navy members of the Tri-Services Environmental Risk Assessment Work Group, we performed a literature search for PFAS sediment toxicity studies with the assistance of EPA's Center for Computational Toxicology and Exposures (CCTE), Great Lakes Toxicology and Ecology Division. This search found no reports of direct measurements of PFAS toxicity in bulk sediment. Thus, it was not possible to derive sediment ESVs from direct toxicity measurements in bulk sediments. Details and results of this search and accompanying evaluation of PFAS toxicity in sediments are presented in Chapter 4. This part of the study has not been updated in the current report.

ES.4 ESV Derivations

ES.4.1 Terrestrial Plants, Invertebrates, Birds, and Mammals

Derivation of soil ESVs for terrestrial plants, invertebrates, birds, and mammals generally followed the Eco-SSL guidance (EPA 2005). Only direct exposure studies conducted in soil were accepted for plant and invertebrate derivations. Only feeding studies were accepted for birds and mammals. Plant studies included several food crop species, such as wheat, alfalfa, and pak choi, while the invertebrate studies were dominated by investigations using earthworms. Soil ESVs were computed as the geometric mean of the selected toxicity values for the studied species. Most plant studies reported effects on growth or germination, while the invertebrate studies reported effects on growth, reproduction, and mortality.

Soil ESVs for birds and mammals were derived for effects on species considered to be representative of the prevailing species composition for most geographic areas. Exposure estimates to PFAS in soils for representative species employed a food chain model, which accounted for ingestion of impacted soil and consumption of biota exposed to PFAS in soil. Concentrations of PFAS in the tissues of prey were estimated using a hierarchical decision process described in the Eco-SSL guidance (EPA 2005).

Toxicity reference values (TRVs) reported for laboratory test species were used to estimate the effects of estimated food chain exposures on representative bird and mammal species. Where available, we adopted values developed by the Defense Centers for Public Health (DCPH), which were developed in parallel with this effort. For other PFAS, we followed the technical guidance developed by DCPH (USACHPPM 2000) and EPA's GLI guidance (EPA 1995b, c) to develop TRVs. Uncertainty factors were applied in this development to account for interspecies differences and other extrapolations involved in the derivation.

ES.4.2 Aquatic Life and Aquatic-Dependent Wildlife

Surface water PFAS ESVs for aquatic life were derived by following the two-tiered approach described in the GLI guidance (EPA 1995a, b, c). This methodology derives chronic exposure freshwater and marine ESVs using data from multiple taxonomic groupings (i.e., aquatic plants, invertebrates, and fish). The ESV Tier I methodology requires a specific level and type of data, as specified in the guidance. When sufficient data were not available to derive a Tier I ESV, the Tier II methodology was used. These derived ESVs represent surface water concentrations considered to be protective of 95% of tested aquatic genera chronically exposed.

A two-tiered methodology was also be used to develop ESVs for the protection of wildlife, based on the 1995 GLI Tier I and Tier II guidance for deriving water quality criteria to protect wildlife (EPA 1995b, c). Food-chain models were used to estimate PFAS exposures for three representative piscivorous birds (the belted kingfisher, the herring gull and osprey), two non-piscivorous birds (the mallard and the spotted sandpiper), and to two representative piscivorous mammals (the mink and the river otter). An avian wildlife value was computed as the geometric mean of the wildlife values derived for each of the avian receptor species; a mammal wildlife value was similarly calculated as the geometric mean of the individual mammal species wildlife values. The final aquatic-dependent wildlife ESV was the lower of the avian and mammal wildlife values.

ES.4.3 Investigation of Freshwater and Marine Sediments

In the absence of studies of PFAS toxicity in bulk sediments, use of an Equilibrium Partitioning model was considered as a possible means of deriving ESVs for sediments. An approach was explored that would substitute literature values of measured PFAS distribution constants for water/sediment organic carbon (K_{oc}) for partition coefficients conventionally used in the model. Although numerous measurements of K_{oc} values were found in the literature for single chemical experiments on a wide range of natural sediments, and linear or near-linear sorption isotherms have been reported for PFAS in sediments at low concentrations, we concluded that this preliminary investigation was informative yet the science is not yet mature enough to derive sediment ESVs.

In preparing this update we did not conduct a systematic search of the literature for studies of PFAS toxicities in sediments given their apparent scarcity in informal searches and the low likelihood of the availability of a sufficient number of studies to develop ESVs without

having to rely on an equilibrium partitioning model. To address this data gap, DoD has funded significant research on marine aquatic toxicity and bioaccumulation that is currently underway. Information on these efforts is available at the following link: https://serdp-estcp.org/page/f7ad705d-e8ef-11ec-9685-026db1cbe810.

ES.5 Summary of Results

Derived soil and surface water PFAS ESVs are presented in Table ES-3. Sufficient data were available to develop an ESV for PFOS for each of the eight soil and surface water receptor categories. However, limited available toxicity data for the other PFAS limited ESV development for PFOA and PFBS to six of the receptor categories, and to four or three receptor categories for the remaining PFAS. It was only possible to derive saltwater ESVs for marine aquatic life for PFOA and PFOS.

TABLE ES-3 Summary of Results and Data Gaps for PFAS Soil and Surface Water ESVs

	Soil ESVs (mg/kg)				Surface Water ESVs (µg/L)[d]			
					Freshwater			Marine
PFAS	Terrestrial Plants	Terrestrial Invertebrates	Terrestrial Mammals[e]	Terrestrial Birds[e]	Aquatic Life[b]	Aquatic-Dependent Mammals[c,e]	Aquatic-Dependent Birds[e]	Aquatic Life[b]
PFBA	—[a]	—	2.98	—	75.7	119	—	
PFHxA	—	—	6.20	—	33.8	544	—	
PFOA	101	77.8	3.84	—	**109**	47.6	—	3.16
PFNA	—	10	0.0242	—	16.9	0.116	—	
PFDA	—	—	0.0677	—	3.44	0.0937	—	
PFBS	—	100	0.817	15.8	446	209	2,783	
PFHxS	—	10	0.145	—	94.2	14.1	—	
PFOS	17.3	57.6	0.0040	0.0386	**4.85**	0.0167	0.487	1.44

[a] Dash (—) indicates a data gap – data not available.

[b] Chronic ESV values; PFOA and PFOS are Tier I ESVs (bold); the remaining are Tier II ESVs.

[c] The lower of the aquatic-dependent mammal or bird value is selected as the Aquatic-Dependent Wildlife ESV.

[d] The surface water values should only be used when the water column is relatively quiescent and sediments at the site are relatively undisturbed: the derived ESVs do not consider the antagonistic, additive or synergistic effects of other PFAS or other aquatic contaminants in combination with individual PFAS chemicals.

[e] Interspecies uncertainty factors were used to derive screening levels; see Sections 3.6.2 and 3.6.4.

ES.6 References

Anderson, R.H., G.C. Long, R.C. Porter, and J.K. Anderson. 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* 150: 678–685.

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1 INTRODUCTION

This report presents ecological screening values (ESVs) that have been developed to support screening-level ecological risk assessments at Air Force or other U.S. Department of Defense (DOD) sites where per- and polyfluorinated alkyl substances (PFAS) release or disposal have been detected in soils, sediments, and surface waters. These ESVs support the screening level steps (Steps 1 and 2 of eight steps) of the U.S. Environmental Protection Agency's (EPA's) Ecological Risk Assessment Guidance for Superfund (EPA 1997), and may be applied at sites undergoing investigation for the historic release or disposal of PFAS, including those associated with the use of aqueous film-forming foam (AFFF), within DOD environmental restoration programs. ESVs represent environmental concentration at or below which chronically exposed biota are not expected to be adversely affected and ecological impacts are unlikely. When used in support of the Installation Restoration Program (IRP), these ESVs may be applied at PFAS sites to identify whether detected concentrations of the PFAS are present at levels not expected to result in unacceptable ecological impacts. Exceeding an ESV does not indicate that unacceptable impacts will necessarily occur, but requires further investigation (e.g., further ecological risk assessment) within the IRP. The IRP cleanup process closely follows the requirements of the National Contingency Plan developed by the EPA in response to the enactment of the Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA), as amended by the Superfund Amendments and Reauthorization Act of 1986 (42 USC 9601 et seq.).

The PFAS ESVs were developed in coordination and consultation with an Interagency Team of subject-matter experts from across the DOD services through the DOD Tri-Services Environmental Risk Assessment Work Group. Several ecological risk assessors and environmental scientists from the EPA Ecological Risk Assessment Forum and program offices provided technical input and advice throughout this effort. They included staff from the EPA Office of Land and Emergency Management's Office of Superfund Remediation and Technology Innovation and Federal Facilities Restoration and Reuse Office; Office of Water; Office of Chemical Safety and Pollution Prevention; Office of Research and Development; and EPA Regions.

The derivation of ESVs for PFAS in soils follows the EPA Guidance for Developing Ecological Soil Screening Levels (the Eco-SSL guidance) (EPA 2005). The derivation of ESVs for PFAS in surface waters follows the EPA *Guidelines for Developing Numerical Water Quality Criteria for the Protection of Aquatic Organisms and Their Uses* (Stephen et al. 1985), later adopted as the EPA Final Water Quality Guidance for the Great Lakes System (40 CFR 60 No. 56), referred to here as the Great Lakes Water Quality Initiative (GLWQI) guidance, or simply the GLI guidance. Details of the Eco-SSL and GLI guidance are presented in Appendix A.

The derived ESVs presented in this report are solely for use in conducting screening-level ecological risk assessments and are *not* intended for use as cleanup values (EPA 2018). In addition, it is recognized for surface water ESVs that States have water-quality standards for aquatic life protection that may be lower than the ESVs calculated in this report. Therefore, if States have proposed or published final soil or water quality standards for PFAS, these values

should be reviewed and considered for possible incorporation into the ecological risk assessment process.

This report describes the derivation of PFAS ESVs for the following media and receptors:

- Soils for invertebrates;
- Soils for plants;
- Soils for avian and mammalian wildlife;
- Surface water for aquatic species; and
- Surface water for aquatic-dependent avian and mammalian wildlife.

1.1 PFAS Study Set

The Air Force identified eight PFAS compounds, with input from the Interagency Team for development of ESVs (Table 1-1). The study set is composed of homologs of perfluorinated carboxylic acids of 4 to 10 carbons and homologs of perfluorinated sulfonic acids of 4 to 8 carbons. This study set would be generally reflective of sites where so-called legacy PFOS AFFF was released. The eight PFAS are among the most prevalent of 15 PFAS identified in environmental media at military installations with historic use of AFFF (Anderson et al. 2016).

TABLE 1-1 PFAS Compounds for ESV Development

PFAS Abbreviation and Compound Names	International Union of Pure and Applied Chemistry Nomenclature	Chemical Abstracts Service Registry Number
	Carboxylic acids	
PFBA, perfluorobutanoic acid	2,2,3,3,4,4,4-heptafluorobutanoic acid	375-22-4
PFHxA, perfluorohexanoic acid	2,2,3,3,4,4,5,5,6,6,6-undecafluorohexanoic acid	307-24-4
PFOA, perfluorooctanoic acid	2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctanoic acid	335-67-1
PFNA, perfluorononanoic acid	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluorononanoic acid	375-95-1
PFDA, perfluorodecanoic acid	2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-nonadecafluorodecanoic acid	335-76-2
	Sulfonic acids	
PFBS, perfluorobutanesulfonic acid	1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulfonic acid	375-73-5
PFHxS, perfluorohexanesulfonic acid	1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexane-1-sulfonic acid	355-46-4
PFOS, perfluorooctanesulfonic acid	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluorooctane-1-sulfonic acid	1763-23-1

1.2 Literature Sources and Literature Search

The primary literature source used to identify studies and datasets for the development of the ESVs was the EPA's Ecotoxicology Knowledgebase (ECOTOX; available at https://cfpub.epa.gov/ecotox/). ECOTOX was created and is maintained by the EPA's Center for Computational Toxicology and Exposure's (CCTE's) Great Lakes Toxicology and Ecology Division (GLTED). ECOTOX consists primarily of peer-reviewed literature on the effects of toxic substances on aquatic and terrestrial organisms, found through online searches of scientific databases from 1970 onward, and is updated quarterly to biannually. The most recent ECOTOX searches conducted for this effort were in March 2023. CCTE systematically reviews individual scientific publications against numerous criteria in deciding whether to accept the publication into ECOTOX. The acceptance criteria relate primarily to whether a given study documents key elements of exposure (e.g., chemical name, dose, duration, and pathway) and the experimental design (e.g., controls and replicates).

Searches of ECOTOX were performed by selecting search parameters for toxicological effects and endpoints of interest for the PFAS substances in the study set. Searches were conducted on all available forms of the eight-PFAS study set, including the protonated and anionic forms, as well as all salt forms listed in the search menu. For example, ECOTOX identifies six forms of PFOS: the acid and anion, plus the K, Li, Na, and tetraethyl-ammonium salts. The PFOA entry includes three forms: the acid, anion, and Na salt. The searches included all terrestrial and aquatic biota, and all effects endpoints (e.g., NOECs, LOECs, EC50, and LC50).[1] Because of their inherent variability in environmental conditions, field studies were excluded. Searches were performed for studies that evaluated ecologically relevant effects, specifically effects on reproduction, mortality, growth, and development. Adverse effects on populations can be inferred from measures related to impaired reproduction, growth, and survival. ECOTOX searches did not include other effects, such as physiological, cellular, biochemical/molecular, or behavioral effects, due to the difficulty of clearly and directly relating these effects to mortality, reproduction, growth, and development. Table 1-2 lists the ECOTOX search criteria used for developing the PFAS ESVs. Finally, we performed a literature search for PFAS sediment toxicity studies with the assistance of EPA's CCTE, GLTED. This search found no reports of direct measurements of PFAS toxicity in bulk sediment. Details and results of this search are presented in Chapter 4.

[1] NOEC = no observed effect concentration; LOEC = lowest observed effect concentration; EC50 = concentration at which 50% of exposed organisms are affected; LC50 = concentration at which 50% of exposed organisms do not survive.

TABLE 1-2 ECOTOX Database Search Criteria for PFAS ESV Development

ECOTOX Parameters	ECOTOX Search Categories
Chemicals	Perfluorooctane sulfonates and acids (PFOS/PFOA)
All Effects	Growth (developmental, growth, morphological), mortality, reproduction, population
All Endpoints	Lethal concentration (LC_{xx})/lethal dose (LD_{xx}); effective concentration (EC_{xx})/effective dose (ED_{xx}); LOEC; lowest observed effect level (LOEL); maximum acceptable toxicant concentration (MATC); NOEC; no observed effect level (NOEL)
All Species	Kingdom: animals and plants (both)
All Test Conditions	Test location: laboratory Exposure media: water (freshwater, saltwater); soil (all categories); no substrate Exposure Type: Diet; environmental; not reported; flow through; intermittent; renewal; static Any Control Types: All ECOTOX Control Types and ECOTOX Historical Control Types Any Chemical Analysis: Any (measured, unmeasured, reported, not reported)
Any Control Types	Any Independently Compiled Data: (all)

1.3 Summary of ESV Derivation Methods

The methods used to derive soil and surface water ESVs are described in detail in Appendix A. The following sections provide a brief summary of the methods.

1.3.1 Terrestrial Plants and Invertebrates

For terrestrial plants and invertebrates, studies of direct exposure in soils were used to account for exposure to PFAS in soils via several routes. For soil invertebrates, exposure would occur by direct contact with, and/or ingestion of, impacted soils. For plants, exposure would occur primarily by root uptake. Effects endpoints considered for ESV development were increased mortality, reduced reproductive success, and reduced growth. PFAS ESVs for terrestrial plants and soil invertebrates were derived by following the approach in EPA's Eco-SSL guidance (EPA 2005). Only direct studies conducted in soil were accepted for these derivations (i.e., no hydroponic studies were considered). Plant studies included several food crop species, such as wheat, alfalfa and pak choi, while the invertebrate studies were dominated by investigations using earthworms. Toxicity values reported in studies were selected in the

preference order EC_{20} > MATC[2] > EC_{10}. Soil ESVs were computed as the geometric mean of the selected toxicity values for the studied species.

For individual plant and invertebrate studies that conducted exposures using soil of different types or from different locations, the results for each soil were included in the ESV derivation. Most plant studies reported effects on growth or germination, while the invertebrate studies reported effects on growth, reproduction, and mortality. The soil PFAS ESVs derived for plants and invertebrates are presented in Chapter 3, and details of the derivations are presented in Appendix B.

1.3.2 Terrestrial Birds and Mammals

For terrestrial birds and mammals, it was assumed that exposure to PFAS in soils could occur via incidental ingestion of impacted soil and ingestion of impacted food (i.e., food-chain uptake). The effects endpoints considered in deriving the ESVs were increased mortality, reduced reproductive success, and reduced growth. The Eco-SSL guidance (EPA 2005) was similarly followed for the derivation of soil ESVs for terrestrial birds and mammals. Derivations of soil ESVs were based on effects on specified representative species, not on the specific species used in the exposure studies. The surrogate receptors selected to derive ESVs for terrestrial wildlife species were based on EPA guidance for developing ecological soil screening values (EPA 2005). As identified in that guidance, these surrogate species are considered as representatives for other terrestrial wildlife species within the same class (mammalian or avian), at the same trophic levels, and that have similar diets. Such specification of representative species allows ESVs for birds and mammals to be representative of prevailing species composition for most geographic areas.

Estimating exposures of representative species to PFAS in soils required the use of a food chain model that accounted for ingestion by representative species of PFAS-impacted soil and of prey items directly or indirectly exposed to PFAS in soil. The absorbed fraction from consumption of biota and the area use factor for impacted soils were each conservatively computed at 100%. Estimations of concentrations of PFAS in the tissues of prey items were estimated using a hierarchical decision process described in the Eco-SSL guidance (EPA 2005). Measured and modeled bioaccumulation factors (BAFs) were considered to estimate concentrations of PFAS in prey items eaten by the representative species of mammals and birds.

Chronic toxicity reference values (TRVs) for mammalian and avian species were derived as described in Appendix A after a review of available laboratory studies. TRVs were then used to estimate the effects on representative species from PFAS in soils via the food chain and to derive soil ESVs. In the derivation of TRVs, uncertainty factors were applied to the effects/no-effects doses identified for laboratory test species to account for extrapolations across species, for extrapolations from sub-chronic to exposures, for extrapolations from lowest observed adverse effect levels (LOAELs) to no observed adverse effects levels (NOAELs).

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[2] MATC = maximum acceptable toxicant concentration.

The derived soil PFAS ESVs for terrestrial birds and mammals are presented in Chapter 3. Details of their derivation are presented in Appendix C.

1.3.3 Aquatic Life

For aquatic biota, exposure to PFAS in surface waters is considered to occur primarily by direct uptake from the water column across body surfaces (e.g., gill membranes). The effects of such exposure include increased mortality, reduced reproduction, and reduced growth. Surface water PFAS ESVs for aquatic life were derived following the GLI guidance (EPA 1995a). Chronic freshwater and marine ESVs were derived using data from multiple taxonomic groupings (i.e., aquatic plants, invertebrates, and fish). The GLI Tier I methodology required toxicity values for genera in eight specified families. When these minimum data requirements were not met, the Tier II methodology was used to develop ESVs. This hierarchy follows EPA's 2018 guidance for developing surface water screening levels (EPA 2018). Tier II surface-water ESVs have greater levels of uncertainty than Tier I values, due to reduced data availability. The derived ESVs represent surface water concentrations considered to be protective of 95% of tested aquatic genera chronically exposed.

Surface-water PFAS ESVs for aquatic life are presented in Chapter 3. Details of the derivations are presented in Appendix D.

1.3.4 Aquatic-Dependent Wildlife

For aquatic-dependent birds and mammals (i.e., those that forage in aquatic environments or on aquatic biota), exposure to PFAS in surface waters was assumed to occur through the ingestion of PFAS residuals in water and food (i.e., food-chain uptake), with greatest concern for exposures that could reduce survival, reproductive success, and/or growth. As for aquatic biota, the methodology used to develop aquatic ESVs for the protection of wildlife followed the 1995 GLI Tier I and Tier II guidance for deriving water quality criteria to protect wildlife (EPA 1995b, c). These ESVs represent surface-water PFAS concentrations at or below which exposure of birds or mammals is not expected to result in unacceptable adverse impacts on growth, reproduction, or survival.

Derivation of these PFAS ESVs employed food-chain models to estimate exposures of birds and mammals via ingestion of PFAS residuals in water and prey items. Five avian and two mammalian species, considered to be representative surrogates of aquatic-dependent wildlife and with a high potential for PFAS exposure through the aquatic food web, were selected for ESV development. The aquatic wildlife surrogates used for ESV development were revised somewhat from those identified in the EPA GLI 1995 guidance for aquatic wildlife. Sections IV.A and IV.B of that guidance identify five representative wildlife species: mink, river otter, kingfisher, herring gull, and bald eagle. The bald eagle was replaced with the osprey, a more cosmopolitan species. Two additional avian surrogates were selected to represent waterfowl and shorebirds: the mallard and the spotted sandpiper. Among the three piscivorous species, the belted kingfisher is largely restricted to freshwater habitats, and the herring gull and osprey may forage in

freshwater and marine coastal habitats. The mallard and the spotted sandpiper are non-piscivorous freshwater species that may be exposed through the ingestion of sediment-dwelling invertebrates while foraging or, in the case of the mallard, through the consumption of aquatic vegetation. The two piscivorous mammal species, the mink and the river otter, also forage in freshwater and marine coastal habitats.

The derivation of the ESVs included estimates of PFAS ingestion that applied BAFs for food from different trophic levels, with the BAFs obtained from statistical summaries of published studies. The ESV derivation also required the availability of mammalian and avian TRVs representing chronic NOAELs in receptor species. A single set of mammalian and avian TRVs were derived for both terrestrial and aquatic-dependent wildlife. As noted above for terrestrial wildlife, the TRVs were derived with the application of uncertainty factors for extrapolations from NOAELs to LOAELs, for extrapolations from acute to chronic toxicities, and to account for interspecies variations between test and representative species (EPA 1995b,c).

Per the GLI guidance (EPA 1995b,c), wildlife values representing PFAS water concentrations at or below which exposure is not expected to result in unacceptable adverse effects were developed for each avian and mammal receptor, and the geometric mean of each receptor category was calculated to provide either an avian or mammalian wildlife value. Either Tier I or Tier II ESVs values were derived, depending on data availability. If sufficient data were available, Tier I PFAS ESVs were based on the lower of the avian and mammal wildlife values. If only an avian or a mammalian wildlife value could be calculated, the available value was the Tier II ESV. Tier I ESVs could only be derived for PFOS, PFBS, and PFHxA and Tier II ESVs were derived for the remaining five PFAS. These Tier I and II ESVs for aquatic-dependent wildlife are presented in Chapter 3. Details of their derivation are presented in Appendix E.

1.4 References

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2 TOXICITY DATA ACQUISTION, REVIEW AND EXTRACTION

The data used to develop the PFAS ESVs presented in this report come from publicly available scientific publications, as identified primarily through targeted searches of the ECOTOX database and the Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profile for PFAS (ATSDR 2018). Once this initial set of publications was identified, the individual studies were reviewed and vetted against a set of acceptance and rejection criteria that focused on the data quality needs for ESV development. The acquisition, review, and extraction of these data are described in the following sections.

2.1 Toxicity Data Acquisition

The majority of studies used to develop the PFAS ESVs were identified in a comprehensive ECOTOX searches conducted through the March 2023 update. ECOTOX searches, delimited to ecologically relevant effects, were exported to Microsoft Excel spreadsheets for aquatic and terrestrial studies. Only studies employing acceptable exposure types and media were selected for further evaluation against specific exclusion and acceptance criteria, as described below.

Studies of rats and mice are generally not included in ECOTOX, with a few exceptions, such as studies using the Norway rat. However, because rat and mice studies are relevant to screening value development for mammals, other sources, including the ATSDR Toxicological Profile for PFAS (ATSDR 2018), were reviewed to identify additional rodent studies for consideration in developing wildlife ESVs. Only rodent studies that used oral exposure routes and examined effects on growth, development, reproduction, or mortality—or in limited cases, more sensitive proximate effects, such as liver or immune function effects in studies identified by the DCPH—were evaluated (Johnson et al. 2021).

2.2 Application of Rejection and Acceptance Criteria

After the initial set of published studies were identified, the studies were acquired and screened according to Eco-SSL criteria (EPA 2005) modified for relevance to PFAS compounds (Appendix A). Each study underwent review for inclusion and acceptability for derivation of ESVs. Table 2-1 presents the study exclusion and acceptance criteria review form used to evaluate studies. For example, LC_{50} and EC_{50} endpoints were rejected for soil ESV development as insufficiently protective of terrestrial ecological receptors (EPA 2005). Similarly, unbounded NOAEL and LOAEL values are generally not acceptable for deriving ESVs in general, as they do not reliably identify a threshold of effects (i.e., a dose-response). Appendix F presents summary tables of accepted and rejected studies as well as the completed acceptance forms.

TABLE 2-1 Literature Evaluation Checklist Used for PFAS Studies Identified in ECOTOX

Study Exclusion Criteria	Y/N
Fate and transport of substance in the environment (only).	
Human or primate subjects.	
In vitro studies, including cell cultures and excised tissues.	
Methods for measuring contaminants.	
Only modeling results reported.	
No viable plant or animal present or tested.	
No effect was reported for a biological test species.	
Study is not the primary source or author states information is published in another source.	
Data developed only from quantitative-structure activity relationships.	
Data reported are not primary data.	
Adverse effects were not caused by a single chemical stressor.	
Assessment of toxicity in the field over a period of time.	
Study Acceptance Criteria	
The test species' scientific name, common name, variety, or strain is reported.	
The chemical form and concentration are reported.	
Nominal or measured dose or concentration is reported, or able to be calculated from information given.	
The duration of the exposure is reported.	
Study used a control(s).	
At least three treatment levels are used (i.e., control plus two chemical exposures).	
Control mortality (or other endpoint under investigation) is acceptable based on the species and endpoint under consideration.	
A calculated endpoint is reported (e.g., LC_{50}, LOEL, LOAEC, NOAEC, NOAEL EC_{10} and EC_{20}).	
Study effects are ecologically relevant endpoints related to growth, mortality, and reproduction.	
Administered doses are provided or can be calculated from the information provided in the study (wildlife only).	
ACCEPT/REJECT:	

2.3 Results of Literature Acceptance Review

2.3.1 Literature Identification and Acceptance/Rejection

A total of 420 aquatic and terrestrial studies on the effects of PFAS were identified for the eight PFAS targeted for ESV development (Table 2-2). Studies of aquatic organisms (309) were identified almost entirely from ECOTOX. Studies of terrestrial organisms (111) were identified from ECOTOX, ATSDR (2018), and as cited in other studies and reports, including those identified by AHPC (Johnson et al. 2021) in ongoing derivations of PFAS TRVs. PFOS and PFOA were by far the most studied PFAS.

TABLE 2-2 Numbers of Accepted and Rejected Studies

No. Studies	Aquatic Studies	Terrestrial Studies
Total	309	111
Accepted	203	79
Rejected	106	32
% Rejected	34%	29%

Applying the rejection and acceptance criteria identified in Table 2-1 to the 420 studies resulted in the retention of 282 studies: 203 aquatic studies and 79 terrestrial studies. Study rejection rates were 34% for aquatic studies and 29% for terrestrial studies (Table 2-2). For both terrestrial and aquatic studies, the primary reasons for rejection were: (1) only one treatment level was used; or (2) the studies measured but did not find statistically significant effects on growth, development, reproduction, or survival (i.e., studies for which no bounded toxicity data on ecologically relevant effects was obtained). Some terrestrial studies were also rejected because they reported only EC_{50} or LC_{50} values which are not considered protective of wildlife (EPA 2005). Although they were not disqualified, a substantial number of accepted studies did not report control mortality or only reported nominal PFAS concentrations. Candidate studies were reviewed for acceptance by a single reviewer. Specific issues identified by the reviewer were discussed among the Argonne team.

Tables listing accepted and rejected studies and completed evaluation sheets for all studies are presented in Appendix F.

2.3.2 Taxa Evaluated in the Accepted Studies

Table 2-3 presents the number of terrestrial and aquatic taxa in the accepted studies. Relatively few terrestrial species were studied, and those were dominated by studies of rats and mice. Most aquatic organisms studied were freshwater species. Fish, amphibians, crustaceans, and algae were the most frequently studied taxa across PFAS.

TABLE 2-3 Number of Studies by Major Taxa

Organism	PFOA	PFOS	Other PFAS
	Terrestrial		
Amphibian	1	1	1
Arthropod	3	4	0
Worms	7	5	1
Plants	6	4	0
Mammals	19	17	13

TABLE 2-3 (Cont.)

Organism	PFOA	PFOS	Other PFAS
Reptile	1		
Birds	1	7	2
	Freshwater		
Fish	37	69	30
Amphibians	8	10	5
Insects	4	6	5
Crustaceans	17	23	8
Molluscs	3	5	0
Worms	1	3	0
Planarian	3	3	0
Rotifers	4	5	1
Ciliate	0	0	0
Vascular Plants	1	4	1
Algae	10	12	7
	Marine		
Fish	2	5	3
Crustaceans	2	5	1
Molluscs	3	4	0
Echinoderms	2	3	0
Algae	3	2	1

2.3.2.1 PFOA Studies

Table 2-4 presents the number of terrestrial PFOA studies accepted for ESV development. Seven worm species and three insect species were evaluated in toxicity studies. One PFOA study was accepted for each an avian, amphibian, and reptile species. For plants, six plant studies were accepted. Twenty-two PFOA rat and mouse studies were accepted for screening level development.

The accepted aquatic PFOA studies primarily evaluated freshwater taxa, with fish, amphibians, crustacean, and algae as the primary species groups tested (Table 2-5). Marine studies also evaluated a variety of taxa (13 species) of crustaceans, mollusks, echinoderms, fish, and algae.

TABLE 2-4 Accepted Terrestrial PFOA Studies by Species

Species	No. of Studies
Worms	
Aporrectodea caliginosa[a]	1
Caenorhabditis elegans	1
Eisenia fetida[a]	4
Eisenia andrei	1
Insects	
Folsomia candida	1
Drosophila sp.[a]	1
Lobella sokamensis	1
Reptiles	
Eremias argus[a]	1
Amphibians	
Ambystoma tigrinum	1
Birds	
Coturnix japonica[a]	1
Mammals	
Laboratory rat and mouse	19
Plants	
Brassica chinensis[a]	1
Cucumis sativus[a]	1
Oryza sativa[a]	1
Sorghum bicolor[a]	1
Triticum aestivum[a]	1
Vigna radiata[a]	1
[a] Non-native species to North America	

TABLE 2-5 Accepted Aquatic PFOA Studies by Species

Organism	No. of Studies
Freshwater	
Amphibians	
Ambystoma jeffersonianum	1
Ambystoma tigrinum	2
Anaxyrus americanus	2
Bufo gargarizans[a]	1
Hyla versicolor	1

TABLE 2-5 (Cont.)	
Organism	No. of Studies
Rana catesbeiana	3
Rana sylvatica	1
Rana pipiens	2
Xenopus sp.[a]	1
Fish	
Carassius auratus[a]	1
Danio rerio[a]	23
Lepomis macrochirus	1
Oncorhynchus mykiss	3
Oreochromis niloticus[a]	1
Oryzias latipes[a]	3
Pimephales promelas	4
Pseudorasbora parva[a]	1
Crustaceans	
Chydorus sphaericus	2
Cyclops sp.	2
Daphnia magna	13
Hyalella Azteca	1
Macrobrachium nipponense[a]	1
Moina macrocopa[a]	1
Neocardina denticulate[a]	1
Zooplankton community (multiple species)	2
Planaria	
Dugesia japonica[a]	4
Mollusks	
Anodonta woodiana[a]	1
Cipangopaludina cathayensis[a]	1
Lampsilis siliquoidea	1
Ligumia recta	1
Worms	
Limnodrilus hoffmeisteri	1
Plants	
Lemna gibba	0
Algae	
Chlamydomonas reinhardtii	1
Chlorella sp.	4
Isochrysis galbana[a]	1
Pseudokirchneriella subcapitata[a]	4
Selenastrum capricornutum	1

TABLE 2-5 (Cont.)	
Organism	No. of Studies
Rotifer	
Rotifera spp.	2
Brachionus calyciflorus[a]	2
Insects	
Chironomus plumosus	1
Chironomus dilutus	1
Chironomus riparius	1
Chironomus tentans	1
Marine	
Fish	
Psetta maxima[a]	1
Coryphaena hippurus	1
Crustaceans	
Siriella armata[a]	1
Americamysis bahia	1
Molluscs	
Mytilus galloprovincialis[a]	2
Perna viridis[a]	1
Algae	
Chlorella vulgaris	1
Geitlerinema amphibium[a]	1
Isochrysis galbana[a]	1
Pyrocystis lunula[a]	1
Skeletonema marinoi	1
Echinoderm	
Paracentrotus lividus[a]	1
Strongylocentrotus purpuratus	1
[a] Non-native species.	

2.3.2.2 PFOS Studies

For PFOS, a relatively small number of terrestrial studies identified in the ECOTOX searches were determined to be acceptable for ESV development. These studies examined toxic effects on six species of arthropods, two species of worms, one amphibian, and seven species of plants (Table 2-6). For wildlife, studies of three bird species were accepted for ESV development (Table 2-7). There were 19 studies of laboratory mammals including rats and mice, primarily identified from ATSDR (2018) determined to be acceptable for ESV development.

TABLE 2-6 Accepted Terrestrial Invertebrate and Plant PFOS Studies by Species

Species	No. of Studies
Arthropods	
Apis sp.	2
Blattella germanica[a]	1
Bombus terrestris[a]	1
Drosophila hydei	1
Folsomia candida	1
Oppia nitens	1
Worms	
Eisenia fetida[a]	4
Aporrectodea caliginosa[a]	1
Amphibians	
Ambystoma tigrinum	1
Plants	
Allium cepa	1
Brassica chinensis[a]	1
Lactuca sativa[a]	3
Linum usitatissimum[a]	1
Lolium perenne[a]	1
Lycopersicon esculentum[a]	1
Medicago saliva[a]	1

[a] Non-native species.

TABLE 2-7 Accepted Bird and Mammal PFOS Studies by Species

Species	No. of Studies
Birds	
Colinus virginianus	4
Coturnix japonica[a]	2
Anas platyrhynchos	3
Mammals	
Laboratory rat and mouse	17

[a] Non-native species.

As with PFOA studies, aquatic PFOS studies primarily evaluated freshwater taxa, with studies of over 61 species accepted (Table 2-8). The greatest number of studies were of *Danio rerio* (a non-native species to North America) and *Daphnia magna*. Of the marine studies accepted, 13 species were evaluated across crustacean, fish, mollusk, echinoderm, and microalgal taxa.

TABLE 2-8 Accepted Aquatic Biota PFOS Studies by Species

Organism	No. of Studies
Freshwater	
Amphibians	
Anaxyrus americanus	
Bufo gargarizans[a]	1
Ambystoma jeffersonianum	1
Ambystoma texanum	1
Ambystoma tigrinum	1
Hyla versicolor	1
Rana pipiens	4
Rana catesbeiana	3
Rana clamitans	1
Rana sylvatica	1
Silurana tropicalis[a]	1
Xenopus sp.[a]	1
Xenopus laevis	1
Fish	
Carassius aratus[a]	1
Catostomus commersoni	1
Cyprinus carpio[a]	1
Danio rerio	49
Notropis hudsonius	1
Oncorhynchus mykiss	4
Oreochromis niloticus[a]	1
Oryzias latipes[a]	1
Pseudorasbora parva[a]	1
Pimephales promelas	7
Semotilus atromaculatus	1
Xiphophorus helleri	1
Crustaceans	
Astacus leptodactylus Eschscholtz[a]	1
Ceriodaphnia dubia	1
Daphnia magna	15
Daphnia pulicaria	1
Daphnia carinata[a]	1
Hyella azteca	2

TABLE 2-8 (Cont.)

Organism	No. of Studies
Macrophthalmus japonicus[a]	1
Neocaridina denticulate[a]	1
Zooplankton community	1
Mollusks	
Anodonta woodiana[a]	1
Cipangopaludina cathayensis[a]	1
Lampsilis siliquoidea	1
Ligumia recta	1
Physa acuta[a]	1
Unio ravoisieri[a]	1
Unio complamatus[a]	1
Worms	
Limnodrilus hoffmeisteri	3
Plants	
Lemna gibba	3
Myriophyllum sibiricum	1
M. spicatum[a]	1
Algae	
Chlorella vulgaris	2
Chlorella pyrenoidosa	1
Navicula pelliculosa[a]	1
Pseudokirchneriella subcapitata[a]	2
Scenedesmus obliquus	2
Selenastrum capricornutum	2
Scenedesmus quadricauda	1
Planarian	
Dugesia japonica[a]	3
Rotifer	
Rotifera sp.	2
Brachionus calyciflorus[a]	2
Insects	
Chironomus dilutus	2
Chironomus plumosus	1
Chironomus riparius	1
Chironomus tentans	1
Enallagma cyathigerum	1

TABLE 2-8 (Cont.)

Organism	No. of Studies
Marine	
Fish	
Psetta maxima[a]	1
Oryzias melastigma[a]	4
Crustaceans	
Americamysis bahia	1
Gammarus insensibilis[a]	1
Mysidopsis bahia	2
Siriella armata[a]	1
Mollusks	
Crassostrea virginica	1
Perna viridis[a]	1
Mytilus galloprovincialis[a]	2
Algae	
Isochrysis galbana[a]	1
Pyrocystis lunula[a]	1
Echinoderm	
Paracentrotus lividus[a]	2
Strongylocentrotus purpuratus	1

[a] Non-native species.

2.3.2.3 Other PFAS Studies

Qualifying studies for the remaining six PFAS are shown in Table 2-9. The studies evaluated an amphibian, an earthworm, laboratory rats and mice, bobwhite, and mallard. The accepted aquatic studies were almost all of freshwater organisms (Table 2-9). The studies included seven species of amphibians, five species of algae, four species each of crustaceans and fish, and one species each of rotifer and aquatic plant.

TABLE 2-9 Accepted PFBS, PFHxS, PFBA, PFDA, PFHxA, and PFNA Studies by Species						
Organism	PFBS	PFHxS	PFBA	PFDA	PFHxA	PFNA
Terrestrial Species						
Amphibians						
Ambystoma tigrinum	0	1	0	0	0	0
Worms						
Eisenia fetida[a]	1	1	0	0	0	1
Mammals						
Rat	2	1	0	0	0	0
Mice	1	2	1	2	1	5
Birds						
Bobwhite	1	0	0	0	1	0
Mallard	1	0	0	0	0	0
Aquatic Species						
Organism	PFBS	PFHxS	PFBA	PFDA	PFHxA	PFNA
Fish						
Danio rerio[a]	7	3	3	3	4	8
Lepomis macrochirus	1	0	0	0	0	0
Oryzias malastigma (saltwater)[a]	3	0	0	0	0	0
Pimephales promelas	1	1	0	0	0	0
Amphibians						
Ambystoma jeffersonianum	0	1	0	0	0	0
Ambystoma texanum	0	1	0	0	0	0
Lithobates pipiens	0	1	0	0	0	0
Rana catesbeiana	0	2	0	0	0	0
Rana clamitans	0	1	0	0	0	0
Rana pipiens	0	3	0	0	0	0
Rana sylvatica	0	1	0	0	0	0
Crustaceans						
Chydorus sphaericus	0	0	1	1	0	1
Daphnia magna	2	0	3	2	1	3
Daphnia pulicaria	0	0	0	0	0	0
Mysidopsis bahia (saltwater)	1	0	0	0	0	0
Rotifers						
Brachionus calyciflorus[a]	0	0	1	0	1	0
Insects						
Chironomus riparius	1	0	0	0	0	0

TABLE 2-9 Accepted PFBS, PFHxS, PFBA, PFDA, PFHxA, and PFNA Studies by Species (cont.)						
Plants						
Lemna gibba	0	0	1	1	0	1
Algae						
Chlorella vulgaris (saltwater)	0	0	0	0	1	1
Geitlerinema amphibium[a] *(saltwater)*	0	0	0	0	1	1
Pseudokirchneriella subcapitata[a]	3	0	2	2	1	1
Scenedesmus obliquus	2	0	0	0	0	0
Skeletonema marinoi[a] *(saltwater)*	0	0	0	0	1	1
[a] Non-native species.						

2.4 References

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3 DERIVATION OF PFAS ECOLOGICAL SCREENING VALUES

This section presents a summary of soil and surface-water PFAS ESVs derived using the methodology summarized in Chapter 1 and described in detail in Appendix A. The ESVs were derived using the toxicity values extracted from accepted studies, as described in Chapter 2. Accepted and rejected studies are listed and review forms provided in Appendix F. Appendix G includes tables summarizing the basis of changes in ESVs from the 2021 report to this 2024 update.

3.1 Soil ESVs for Plants and Invertebrates

The PFAS ESVs for plants and soil invertebrates were derived from selected toxicity values in qualifying studies. Studies in both natural and artificial soil were considered. Because of the limited number of available studies, studies were not selected on the basis of expected bioavailability based on the soil's organic carbon (OC) content, and all studies were included that passed the acceptance criteria review. The available studies used a variety of soil types with varying OC content and sorption characteristics. Only studies involving direct exposure of plants or invertebrates in soil were selected (i.e., studies that used unimpacted soils spiked with single compounds of PFAS). Because spiked soils tend to exhibit higher bioavailability in general than do aged soils (Schuler et al. 2003), the resultant derived ESVs would be conservative.

In accordance with the Eco-SSL guidance (EPA 2005), derivation of the PFAS ESVs used the following hierarchy of toxicity values from a given study: EC_{20} > MATC > EC_{10}. Plants used in studies were primarily crop plants, including corn, wheat, and pak choi. For studies that tested soils from multiple locations or of multiple types, all results were included separately in ESV derivations. Soil invertebrate ESV derivations relied heavily on earthworm studies but included one PFOS study using oribatid mites and springtails (Collembola). ESVs for PFNA, PFBS, and PFHxS were derived from the same single study on earthworms. The ESVs for terrestrial plants and invertebrates were calculated as the geometric mean of the toxicity values selected from qualifying studies. Table 3-1 presents the soil PFAS ESVs for terrestrial plants and soil invertebrates. These values represent PFAS soil concentrations at or below which exposure to plants and soil invertebrates is not expected to pose unacceptable ecological risks. Details of the analyses are presented in Appendix B.

TABLE 3-1 Soil PFAS ESVs for Terrestrial Plant and Soil Invertebrates

PFAS	Plant ESV (mg/kg)	Soil Invertebrate ESV (mg/kg)
PFBA	—[a]	—
PFHxA	—	—
PFOA	101	77.8
PFNA	—	10
PFDA	—	—
PFBS	—	100
PFHxS	—	10
PFOS	17.3	57.6

[a] Dashes indicate a data gap; insufficient data available to derive an ESV.

Plant ESVs could only be derived for two PFAS in our study set, PFOS and PFOA, which provided at least one value each for perfluorosufonic acids (PFSAs) and perfluorocarboxylic acids (PFCAs). Soil invertebrate ESVs were derived for five PFAS. The resultant PFAS ESVs covering both groups fell within a range of 10–101 mg PFAS/kg of soil.

3.2 Soil ESVs for Wildlife

The derivation of soil ESVs for the protection of birds and mammals followed the Eco-SSL guidance (EPA 2005) except in the derivation of TRVs, as described in Appendix A. Where available, we adopted TRVs derived by the Defense Centers for Public Health (DCPH), which were developed in parallel with this effort (Johnson et al. 2021). For other PFAS, we followed DCPH guidance (USACHPPM 2000) and EPA's GLI wildlife guidance (EPA 1995b,c) to develop TRVs. Toxicity values were taken from selected studies measuring effects on growth, development, reproduction, and mortality in feeding studies as identified in Appendix C. Chronic NOAEL TRVs were derived from test doses identified in laboratory studies after applying uncertainty factors to account for interspecies extrapolation, for extrapolation from sub-chronic to chronic exposure durations, and for extrapolation from LOAELs to NOAELs as appropriate. The chronic NOAEL TRVs were used to calculate ESVs via a food-chain model as soil concentrations that would not result in a dose to surrogate receptor species exceeding the TRV.

Appendix C presents the input values used in the derivation of soil PFAS ESVs for birds and mammals, including the basis for deriving TRVs, following the methods presented in Appendix A. Table 3-2 presents the soil PFAS ESVs developed for birds and mammals based upon the use of surrogate receptor species.

TABLE 3-2 Soil PFAS ESVs (mg/kg) for Terrestrial Birds and Mammals[a,b]

	Mammalian ESVs			Avian ESVs		
PFAS	Mammalian Herbivore (Meadow Vole)	Mammalian Ground Invertivore (Short-tailed Shrew)	Mammalian Carnivore (Long-tailed Weasel)	Avian Granivore (Mourning Dove)	Avian Ground Invertivore (American Woodcock)	Avian Carnivore (Red-tailed Hawk)
PFBA	6.23	**2.98**	32.3	—[c]	—	—
PFHxA	12.8	**6.20**	18.4	—	—	—
PFOA	141	**3.84**	12.9	—	—	—
PFNA	0.209	**0.0242**	0.153	—	—	—
PFDA	1.17	**0.0677**	0.553	—	—	—
PFBS	16.7	**0.817**	39.1	148	**15.8**	2,820
PFHxS	10.7	**0.145**	5.27	—	—	—
PFOS	0.495	**0.0040**	0.010	0.988	**0.0386**	0.384

[a] Bolded values are the selected ESVs for either mammalian or avian classes, the lowest values among feeding classes.
[b] Interspecies uncertainty factors were used to derive screening levels; see Section 3.6.2.
[c] Dashes indicate a data gap; insufficient data were available to derive an ESV.

To capture a range of exposure pathways via food chains originating in soil, mammalian ESVs were derived for a representative herbivore, a ground-dwelling invertivore, and a carnivore (Table 3-2). Soil ESVs were determined as the lowest values among the mammalian and avian feeding types, respectively. Mammalian values were lowest for all PFAS for the short-tailed shrew, a ground-dwelling invertivore, and higher for the meadow vole, an herbivore, and the long-tailed weasel, a carnivore. The PFAS mammalian ESVs ranged over 3 orders of magnitude for the shrew across the PFAS study set, with ESVs generally having lowest values (greater sensitivity) for longer chain PFCAs and PFSAs. Due to the limited number of mammalian and bird studies available for PFAS other than PFOA and PFOS, ESVs for these PFAS have greater uncertainty than those for PFOA and PFOS.

Avian ESVs for soil could only be derived for PFBS and PFOS (Table 3-2) due to the general lack of avian toxicity studies for the other PFAS, including PFOA, which otherwise has a rich dataset. Avian ESVs for both PFAS were lowest for the American woodcock, a ground invertivore, and ranged over a range of 5 orders of magnitude for this small dataset. See Appendix C.

3.3 Surface Water ESVs for Aquatic Life

3.3.1 Freshwater ESVs for Aquatic Life

The derivation of ESVs for PFAS in surface waters follows the EPA *Guidelines for Developing Numerical Water Quality Criteria for the Protection of Aquatic Organisms and Their Uses* (Stephen et al. 1985), later adopted as the EPA Final Water Quality Guidance for the Great Lakes System (EPA 1995a). These are referred to as the GLWQI guidance, or simply the GLI guidance. Details of the Eco-SSL and GLI guidance are presented in Appendix A, while Appendix D presents the details of the ESV development for aquatic life.

Although GLI methods derive aquatic values for both acute and chronic exposure scenarios, only values for chronic exposures are presented here. Following the GLI methodology, species-sensitivity distributions were developed to identify PFAS water concentrations considered protective of an estimated 95% of tested aquatic taxa chronically exposed as ESVs for aquatic life.

As described in Appendix A (Section A.5.1.2), within Tier I there are two approaches to derive the chronic ESV (1) by using a sensitivity distribution when there is chronic data for all eight data requirements or (2) by dividing the final acute value (FAV) by a final acute–chronic ratio (FACR) when there is not chronic data for all eight data requirements, but there is acute data for all eight data requirements. The second approach using FACRs was used in the derivation of ESVs for all PFAS because of greater data availability for acute studies than for chronic studies, especially for PFAS other than PFOA and PFOS.

Tier II values were derived when fewer than eight data requirements were met with either acute or chronic data. Because Tier II values are adjusted using an uncertainty factor to account for fewer taxa, the derived Tier II ESVs have greater uncertainty than Tier I ESVs. Freshwater Tier I values were derived for PFOA and PFOS. Tier II values were derived for the other six PFAS in the study set, because the eight data requirements were not met for developing Tier I values.

Table 3-3 presents the Tier I and Tier II freshwater PFAS ESVs derived for chronic exposures. The table also presents the number of taxonomic families for which toxicity data was drawn in meeting the data requirements for the derivation of Tier I or Tier II values. Also shown are surface water HC5 concentrations computed from no-observed-adverse effect concentrations (NOAECs) for PFOA and PFOS for purposes of comparison. As seen in the table, PFAS aquatic ESVs tend to decrease with increasing length of the fluorinated carbon chain, except for PFOA, which is higher than its neighboring PFCAs. This apparent deviation may be a consequence of the reduced uncertainty of the PFOA Tier I value compared to the Tier II values of the other PFCAs, which were based on far fewer taxonomic families, and which may be more conservative (lower) after the application of uncertainty factors for fewer taxa per the GLI methodology.

TABLE 3-3 Freshwater Chronic Exposure ESVs (µg/L) for Aquatic Life

PFAS	No. Tier I Taxonomic Data Requirements Met[a]	Tier I ESV[b]	Tier II ESV[b]	HC5[c]	Draft WQC[d]
PFBA	4	—	75.7	—	
PFHxA	2	—	33.8	—	
PFOA	8	109	—	156	94
PFNA	3	—	16.9	—	
PFDA	4	—	3.44	—	
PFBS	2	—	446	—	
PFHxS	2	—	94.2	—	
PFOS	8	4.85	—	0.31	8.4

[a] Number of Tier I taxonomic data requirements met with available toxicity data per GLI guidance; a minimum of eight are needed for Tier I ESV development; a varying secondary acute factor is applied in deriving Tier II values when fewer than eight data requirements are met (Appendix A, Table A-5.2).

[b] Tier I and Tier II values were derived from acute LC_{50} and EC_{50} values for the most sensitive effect in a given study using an ACR to convert to chronic ESVs, as sufficient numbers of chronic studies were not available to derive ESVs directly from species sensitivity distributions from chronic studies.

[c] HC5 values were derived from acute, sub-chronic, and chronic NOAEC values for the most sensitive effect from a given study.

[d] EPA's draft Water Quality criteria for chronic exposures (EPA 2022a,b).

The HC5 values for PFOA and PFOS in Table 3-3 similarly represent a surface-water concentration predicted to have no detrimental ecological effects on 95% of tested aquatic species. As such, the HC5 values provide a point of comparison for the Tier I and Tier II ESVs, arriving at the 95% protection level based on NOAEC endpoints as opposed to the EC_{50}/LC_{50} endpoints used to derive the Tier I and II ESVs. While the latter were converted to chronic exposure ESVs through the application of FACRs, HC5s were derived directly from exposure durations ranging from acute to chronic in order to maximize the data set and capture as many life-stages as possible in test species (see Appendix D). The PFOA HC5 is roughly 50% greater than the Tier I ESV and the PFOS HC5 is about a factor of 16 lower than the PFOS Tier I ESV. The latter result may be because HC5s were derived from NOAECs, which, while in most cases were bounded by LOAECs, may be well below levels of effects, or to the possibility that the NOAEC studies covered more sensitive life stages or effects than did the acute effects studies underlying the Tier I/II values. Conversely, it is possible that the estimate of the PFOS Tier I value from acute studies using ACRs to compute chronic toxicity levels was insufficiently conservative.

For PFOS, examining the genus NOAEC values contributing to the HC5 value (0.31 µg/L) finds three genera that had NOAEC values below the Tier I ESV (4.85 µg/L). The recently reported NOAEC for mayfly (*Neocloeon*) had the lowest value at 0.21 ug/L (Soucek et al. 2023, supporting information), and the genus geomean for two species of midge (*Chironomus*) and for the fatmucket clam (*Lampsilis*) had genus geomean values of 3.11 and 4.5 µg/L, respectively (Appendix D, Table D.3.2.2). These three values weighed heavily in the derivation of the HC5.

Thus, this comparison finds that the PFOS Tier I ESV of 4.85 µg/L, derived from acute effects, may be somewhat unprotective of the most sensitive aquatic test species as determined by NOAEC values, such as the mayfly, which is not inconsistent with the ESV's 95% species protection level.

Conversely, for the PFOA ESV, no genera that had NOAEC values below the ESV of 109 ug/L. The closest genus geomean NOAECs were for the rotifer (*Brachionus*) (177 µg/L), the Northern leopard frog/Bullfrog (*Lithobates*) (262 ug/L), and the American toad (*Anaxyrus*) (307 ug/L) contributing to an HC5 value of 156 µg/L (Appendix D), Table D.3.1.2. Thus, the ESV for PFOA appears to be protective of even the most sensitive test species as determined by NOAEC values.

The right-hand column of Table 3-3 presents EPA's currently published draft Water Quality Criteria (WQC) for PFOA and PFOS (EPA 2022a,b). These values were derived using the same general GLI methodology as used here, except that values were derived from chronic exposure studies directly, rather than using acute studies and extrapolating to chronic exposures using ACRs, as was done here. The draft WQC value for PFOA is similar to the HC5 value derived here, while the value for PFOS was somewhat higher than the HC5. However, the draft WQC did not include the recent results for the mayfly, which will likely lower the WQC value for PFOS in the final WQC when published. Practitioners may wish to choose or evaluate for potential use at sites EPA's WQC, when available and finalized, as ESVs for PFOA and PFOS. The Tier II ESVs in Table 3-3 would be used for the remaining six PFAS in the study set.

3.3.2 Saltwater ESVs for Marine Aquatic Life

The saltwater PFAS ESVs for aquatic life (Table 3-4) were also derived following the two-tier GLI guidance methodology (EPA 1995a). The methods are described in Appendix A, while Appendix D identifies the studies and toxicity values that were used to develop the marine ESVs. Because of the limited availability of toxicity data for marine biota, it was only possible to derive Tier II ESVs for PFOA and PFOS. No other PFAS in the study set had marine studies available for the derivation of ESVs.

TABLE 3-4 Saltwater Chronic Exposure ESVs (µg/L) for Aquatic Life

PFAS	No. Tier I Taxonomic Data Requirements Met[a]	Saltwater Tier II ESV
PFOA	5	3.16
PFOS	5	1.44

[a] Number of taxonomic classes of marine life in the toxicity data set out of 8; used for computing a Secondary Acute Factor.

3.4 ESVs for Aquatic-Dependent Wildlife

The derivation of surface-water ESVs for the protection of aquatic-dependent birds and mammals followed the GLI guidance (EPA 1995b,c). The methods are described in detail in Appendix A. Table 3-5 presents the wildlife values derived for mammals and birds, using two representative aquatic-dependent mammalian species and five representative aquatic-dependent avian species. When both mammalian and avian wildlife values could be derived, a Tier I final ESV was the lower of the avian and mammal values. If only one wildlife value was available, that value was the final Tier II ESV. Appendix E presents the details of the derivation of these ESVs. Sufficient data were only available to derive avian wildlife values for PFBS and PFOS, while sufficient, but limited data in many cases, were available to derive mammal wildlife values for all eight PFAS.

TABLE 3-5 Freshwater ESVs (µg/L) for Aquatic-Dependent Wildlife[a,b]

	Aquatic-Dependent Wildlife ESV (µg/L)		
PFAS	Mammal Wildlife Value	Avian Wildlife Value	Final ESV[a]
PFBA	119	—[c]	119
PFHxA	544	—	544
PFOA	47.6	—	47.6
PFNA	0.116	—	0.116
PFDA	0.0937	—	0.0937
PFBS	209	2,783	209
PFHxS	14.1	—	14.1
PFOS	0.0167	0.487	0.0167

[a] The lower of the mammal or bird value is selected as the final aquatic-dependent wildlife ESV.
[b] Interspecies uncertainty factors were used to derive screening levels; see Section 3.6.4.
[c] Dashes indicate a data gap; insufficient data available to derive an ESV.

For PFBA, PFHxA, PFOA, PFNA, PFDA and PFHxS, only mammalian wildlife values were available, which determined the Tier II ESV for aquatic wildlife for these PFAS. For PFBS and PFOS, the lower mammalian values determined the Tier I wildlife value, which were lower than the respective avian values. Mammalian values were at sub-ppb levels for PFNA, PFDA, and PFOS, largely because of relatively high bioaccumulation factors (BAFs) for fish, which was a major factor in determining exposures in receptor species, combined with relatively low TRVs for these PFAS. These trends in BAFs and TRVs have been previously associated with increasing carbon number in PFAS. See Appendix E for the inputs and derivation of ESVs for aquatic-dependent wildlife.

3.5 Summary of Results and Data Gaps

Table 3-6 presents all the PFAS ESVs that were developed for aquatic and terrestrial biota and identifies data gaps where development of ESVs was not possible. Toxicity data were limited for most PFAS except PFOA and PFOS, and the data that existed were often restricted to relatively few test biota. Data were particularly limited for terrestrial plants, birds, and marine biota. Bird toxicity data necessary to derive both soil and water ESVs were lacking for all but PFBS and PFOS, while terrestrial plant and marine aquatic life data were available for only PFOA and PFOS. Studies of terrestrial invertebrates were almost entirely on earthworms, which may or may not be a good surrogate representative species for all soil invertebrate species. Many of the freshwater aquatic studies used to derive aquatic ESVs included test biota that are not native to North America, such as zebrafish, Asiatic frog, and oriental river prawn.

TABLE 3-6 Summary of Results and Data Gaps for PFAS Soil and Surface Water ESVs

	Soil ESVs (mg/kg)				Surface Water ESVs (µg/L)[a]			
					Freshwater			Marine
PFAS	Terrestrial Plants	Terrestrial Invertebrates	Terrestrial Mammals	Terrestrial Birds	Aquatic Life[b]	Aquatic-Dependent Mammals[c]	Aquatic-Dependent Birds	Aquatic Life[b]
PFBA	—[d]	—	2.98	—	75.7	119	—	
PFHxA	—	—	6.20	—	33.8	544	—	
PFOA	101	77.8	3.84	—	109	47.6	—	3.16
PFNA	—	10	0.0242	—	16.9	0.116	—	
PFDA	—	—	0.0677	—	3.44	0.0937	—	
PFBS	—	100	0.817	15.8	446	209	2,783	
PFHxS	—	10	0.145	—	94.2	14.1	—	
PFOS	17.3	57.6	0.0040	0.0386	4.85	0.0167	0.487	1.44

[a] The surface-water values can only be used when the water column is relatively quiescent and sediments at the site are relatively undisturbed: the derived ESVs do not consider the antagonistic, additive, or synergistic effects of other PFAS or other aquatic contaminants in combination with individual PFAS chemicals.

[b] Chronic ESV values; PFOA and PFOS are Tier I ESVs; the remaining are Tier II ESVs.

[c] The lower of the aquatic-dependent mammal or bird value is selected as the aquatic-dependent wildlife ESV.

[d] Dashes indicate a data gap; data not available.

Table 3-7 further describes the nature of the data gaps affecting ESV development. Data gaps and needs are presented for soils, freshwater and sediments, and marine water and sediments. Data needs include toxicity studies for PFAS, especially beyond PFOA and PFOS, as well as needs for a range of taxa in which they are tested. In addition, data needs are identified for supporting food chain models used to develop ESVs for birds and mammals, including data on bioaccumulation factors (BAFs) and biomagnification factors (BMFs) for many PFAS.

TABLE 3-7 Data Gaps and Needs Identified during Development of Terrestrial and Aquatic PFAS ESVs[a]

ESV Receptor Category	Data Gap	Data Need
	Soil	
Terrestrial Plant	• Few wild plant studies	• Acute and chronic studies on more PFAS • Studies with additional species of wild plants • Studies including aging/weathering of PFAS in soils • Studies in more soil types
Terrestrial Invertebrate	• Few invertebrate studies	• Acute and chronic studies on invertebrates other than earthworm • Studies including aging/weathering of PFAS in soils • Studies in more soil types representing different properties that may impact bioavailability of PFAS.
Terrestrial Bird	• Few or no bird studies for most PFAS	• Toxicity studies on more PFAS • Studies on relevant bird species
Terrestrial Mammal	• Few if any studies on representative wildlife species; mouse and rat studies only, and not with native species	• Toxicity studies on more PFAS • Studies on representative wildlife species • Acute, sub-chronic, and chronic studies on native species to derive/validate TRV uncertainty factors
	Fresh Water and Sediment	
Aquatic Biota	• Limited toxicity data, especially for bulk sediment exposures	• Acute and chronic studies on more PFAS • Acute and chronic studies on more categories of biota, especially using native North American biota
Aquatic-Dependent Birds	• Total dose data • BAF, and BMF for food chain modeling	• Studies to develop PFAS-specific TRVs • Uptake studies to develop PFAS-specific BAF, and BMF values
Aquatic-Dependent Mammals	• Total dose data • BAF, and BMF for food chain modeling	• Studies to develop PFAS-specific TRVs • Uptake studies to develop PFAS-specific BAF, and BMF values
	Marine Water and Sediment	
Aquatic and Benthic Life	• Limited toxicity data for both water and bulk sediment exposures	• Acute and chronic studies on more PFAS • Acute and chronic studies on more categories of biota, especially native North American biota

[a] The identified data gaps apply to the individual study set PFAS and do not address the broader issues of PFAS mixtures, precursors, or co-contaminants, or toxicity additivity, synergism or antagonism.

3.6 Uncertainties in Developing the Terrestrial and Aquatic ESVs

Numerous uncertainties are associated with the derivation of the terrestrial and aquatic ESVs. The following discussion describes the uncertainties that may have the largest effect on the derived ESVs. Sources of major uncertainties are identified for each of the receptor categories for which ESVs were developed.

3.6.1 Terrestrial Plants and Invertebrates

In the derivation of soil ESVs for terrestrial plants, the greatest overall uncertainty was related to limited toxicity data, both with respect to the number, type, and variety of plants tested, and the number of PFAS with published toxicity values. Toxicity data were also very limited for invertebrates and included very little species diversity and few studies on PFAS other than PFOA and PFOS. The fact that ESVs for PFNA, PFBS, and PFHxS were derived from the same single study on earthworms exemplifies this uncertainty.

The plants used in the toxicity studies selected were dominated by commercial crop plants, which may not represent the sensitivity of native vegetation present at PFAS sites, while the invertebrate studies were dominated by investigations using a non-native earthworm (*Lumbricus terrestris*). Because the toxicity data is dominated by these earthworm studies, there is uncertainty as to how well these data reflect PFAS sensitivity of other, native, soil invertebrates. In addition, only a relatively small number of different soil types and locations are included in the available PFAS studies. Soil characteristics that may affect PFAS bioavailability were not consistently available, so the representativeness of the test soils in the studies used in ESV derivation is difficult to assess. The properties of the limited set of soils tested likely does not encompass the range of soils to which ESVs may be applied.

Limiting the plant and invertebrate studies to those that evaluated direct exposure in soil likely reduced uncertainty in the derived ESVs compared to terrestrial wildlife ESVs, which relied on modeling PFAS exposure from soil via the food chain. Conversely, the use of PFAS-spiked native or synthetic soils in plant and soil invertebrate studies may have introduced uncertainty related to bioavailability. Spiked soils that have not undergone an aging and weathering protocol prior to test species exposure have been reported to increase the bioavailability of contaminants to a greater extent than what would be commonly found in the environment (Schuler et al. 2003). This uncertainty would tend to make the soil ESVs more conservative.

3.6.2 Terrestrial Birds and Mammals

Deriving soil ESVs for birds and mammals involved food-chain modeling, which in the absence of site-specific information, utilized several conservative assumptions in inputs (e.g., diet comprised 100% of a single food item and BCFs at upper ends of ranges for prey items), leading to inherent uncertainties. In addition, PFAS toxicity data were very limited for birds and ecologically relevant mammals, which introduced an additional source of uncertainty.

A third major area of uncertainty is in the extrapolation of laboratory test doses for laboratory species to chronic TRVs for representative ESV species using uncertainty factors.

Food-chain modeling for estimating soil PFAS exposures of birds and mammals required several inputs related to the diet of each receptor species. These inputs included the composition of the diet (i.e., percentage of different food items), an estimated soil fraction of the diet (i.e., incidental soil ingestion), the estimated concentration of PFAS in each diet item, absorption of PFAS from consumed food, and the daily food ingestion rate. These inputs were based on values from the scientific literature, although some are adopted from species that are similar to the receptor species and others are estimated using allometric equations. Each of these aspects added to the uncertainty in the modeling results that were carried forward into the derived ESVs. The terms in the uptake models were selected to be conservative (i.e., likely to overestimate the ingested dose), including the use of values from the upper end of reported ranges for BCFs and soil fraction estimates and the use of a site use factor of 1 for all species.

Another uncertainty was related to the limited availability of toxicity data for terrestrial wildlife. To date, most of the dose data come from studies that use either a small set of test species or laboratory-based species that are rarely ecologically relevant species. For example, the dose data used to develop both the terrestrial and aquatic-dependent avian ESVs came primarily from studies on two species, bobwhite quail and mallard. These data were extrapolated to effect endpoints in a variety of native birds, including herbivorous and insectivorous species and birds of prey. In the case of mammals, most of the available PFAS dose data were derived from studies that used laboratory strains of mice and rats. Again, these results were then extrapolated to wild native mammalian wildlife in different trophic levels within the food chain.

To account for these uncertainties, uncertainty factors (UFs) were applied in the extrapolation of laboratory test doses in the derivation of TRVs for wildlife. Table C-3.2 in Appendix C presents UFs applied to derive TRVs from laboratory test doses. For TRVs adopted from DCPH, the total UFs used in their derivation are listed. UFs developed here followed GLI guidance (EPA 1995b,c), which includes UFs for extrapolating across taxa (UF_A), from sub-chronic-to-chronic exposure durations (UF_S), and from LOAEL-to-NOAEL endpoints (UF_L). For UF_A, a factor of 2 was applied for each taxonomic level the representative species was removed from the test species. For UF_S, a value of 5 was applied for extrapolating from sub-chronic to chronic exposures. No UF_L values were needed for the TRVs developed in this report. The wildlife TRVs derived using these UFs were used in the derivation of ESVs for both terrestrial and aquatic-dependent wildlife.

Use of interspecies UFs (UFAs) in TRV development may be controversial because differences in sensitivity between species are rarely quantified. Use of UFAs can complicate site-specific ecological risk assessments (ERAs) that include multiple receptors, where different UFAs are required for different wildlife receptors being evaluated. While the EPA's GLI guidance uses UFAs within a "critical studies" approach, EPA's EcoSSL guidance (EPA 2005) uses a "weight-of-evidence" approach in deriving TRVs, which does not use UFAs. The current study applies UFAs in deriving TRVs for PFAS following the GLI guidance. Their use within a critical studies approach may be reconsidered in site-specific ERAs and in the development of site-specific cleanup levels, as policies regarding the use of UFs can vary based on regulatory

policies and stakeholder directives. Table C-3.2 (Appendix C) provides the NOAELs, LOAELs, and benchmark dose low (BMDL) used to derive TRVs for terrestrial wildlife (see Test Dose column).

3.6.3 Aquatic Life

Uncertainty in the surface water ESVs for aquatic life was primarily associated with the limited availability of qualified toxicity data. Development of Tier I ESVs requires toxicity data for biota from at least eight specific families, and such data were available only for PFOA and PFOS. The availability of data for the other six PFAS was far lower, supporting only the development of Tier II ESVs. Further, the secondary acute factors (SAFs) used in deriving Tier II ESVs to account for the reduced representation of fewer tested families, ranging from 4.3 for seven families to 21.9 for a single family, have associated uncertainty, partly because they depend only on the number of available test genera, not on their makeup.

Some of the toxicity data used in the derivation of the aquatic ESVs comes from studies that used non-native species (e.g., zebrafish [*Danio rerio*], Asiatic toad [*Bufo gargarizans*], and the European physa [*Physella acuta*]), which adds uncertainty associated with the representativeness of such species to native North American aquatic fauna. Although it is not native to North America, in the absence of suitable data on native cyprinids, the zebrafish was accepted as representative. The zebrafish is in the family Cyprinidae, to which all our native minnows (including the fathead minnow, a commonly used toxicity test organism), shiners, and dace belong. In addition, the zebrafish has a life history similar to that of many of our native cyprinids, occurring in similar habitats. However, because Danio was frequently among the four most sensitive species driving ESV values (Appendix D), the absence of a North American cyprinid, which might be more sensitive than Danio, contributes to the overall uncertainty of the aquatic ESV.

Further uncertainties were related to the use of acute exposure studies to derive aquatic ESVs for chronic exposures using an acute-to-chronic ratio (ACR). This study used the provisional ACRs identified in EPA's draft WQC reports for PFOA and PFOS (EPA 2022a,b) and applied these to other PFCAs and PFSAs, respectively. The development of these ACRs depended on the availability of studies on species that include both acute and chronic PFAS exposures, which were limited to PFOA and PFOS, thus requiring the application of these values across their respective PFAS classes. In the development of the provisional ACR of 207.5 for PFOA, EPA notes the caveat that the species mean ACRs (SMACRs) that contributed to this value covered a range of greater than 100, which would not normally be acceptable for deriving an overall ACR under the GLI guidelines, which requires a range of no greater than 10 (EPA 2022a). Similarly, EPA noted that its provisional ACR for PFOS of 122.2 was also based on SMARCs with a range exceeding a factor of 10 and with no relationship between ACR and species mean acute value (SMAV), which again would not normally be acceptable under the GLI guidelines (EPA 2022b). Thus, the use of these provisional ACRs includes the attendant uncertainty associated with exceeding these GLI guidelines.

3.6.4 Aquatic-Dependent Wildlife

The derivation of PFAS ESVs for aquatic-dependent birds and mammals involved many of the same types of uncertainties as described above for the derivation of soil ESVs for terrestrial wildlife, specifically the use of food chain modeling, the availability of receptor-specific PFAS toxicity data for receptor families, and the extrapolations involved in deriving TRVs for representative species from tests on laboratory species. Food-chain modeling uncertainties were also associated with a greater complexity of exposure pathways, a typically greater number of trophic levels, and the availability of PFAS-specific BMFs for modeling trophic transfer.

In particular, the BAFs used for modeling, while median values of published values (Burkhard 2021), spanned several orders of magnitude, both across PFAS and across species (Appendix E). Because of this variability, the development of site-specific values may be an important focus of data collection efforts supporting baseline ecological risk assessments at sites to reduce this uncertainty.

Uncertainties accrued in deriving TRVs related to the multiple uncertainty factors to account for extrapolating across taxa, from sub-chronic to chronic exposures, and from LOAEL to NOAEL concentrations, as described in Section 3.6.2, above. These uncertainty factors ranged from 1 to 8 for each of the three extrapolations, and their specific values were strongly dependent on professional judgement. The derivation of the PFAS ESVs for aquatic-dependent wildlife employed total uncertainty factors ranging from 1 to 40, depending on the receptor species and the species from which the dose data were obtained (see Appendix E, Table E-4). The wildlife TRVs derived using these UFs were used in the derivation of ESVs for both terrestrial and aquatic-dependent wildlife.

Use of interspecies UFAs in TRV development may be controversial because differences in sensitivity between species are rarely quantified. Use of UFAs can complicate site-specific ERAs that include multiple receptors, where different UFAs are required for different wildlife receptors being evaluated. While the EPA's GLI guidance uses UFAs within a "critical studies" approach, EPA's EcoSSL guidance (EPA 2005) uses a "weight-of-evidence" approach in deriving TRVs, which does not use UFAs. The current study applies UFAs in deriving TRVs for PFAS following the GLI guidance. Their use within a critical studies approach may be reconsidered in site-specific ERAs and in the development of site-specific cleanup levels, as policies regarding the use of UFs can vary based on regulatory policies and stakeholder directives. Tables E.5-1 through E.5-8 (Appendix E) provide the NOAELs, LOAELs, and BMDLs used to derive TRVs for aquatic-dependent wildlife.

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4 SEDIMENT INVESTIGATIONS

4.1 Introduction

This study was not able to derive ESVs for sediments for the effects of PFAS on benthic life. An extensive search of the published literature found no studies reporting toxicity values for benthic organisms directly exposed to single PFAS compounds in bulk sediments. In the absence of direct studies, we explored the possibility of deriving sediment ESVs from those derived for aquatic life by applying an equilibrium partitioning (EqP) model using empirical measurements of partition coefficients for PFAS in water and sediments for a multitude of natural sediments. Although this approach appeared promising, we concluded that our preliminary effort would produce results prematurely with unacceptable levels of uncertainty. However, the effort did produce useful insights into the approach, while revealing sources of method uncertainty and associated data gaps, which are examined below.

PFAS occur in sediments as a result of a variety of mechanisms, including their migration to sediments from the water column, which in turn may receive atmospheric inputs, even when sediments do not directly receive inputs from releases. The presence of PFAS in sediments presents risks of potential adverse effects on benthic life.

A search of the literature to identify studies of direct exposures of benthic life to PFAS-impacted sediments found no such laboratory studies and only a handful of field studies, which focused on occurrence and uptake of PFAS mixtures and which could not support the development of ESVs for single PFAS chemicals. A description of the search and the search results are presented Section 4.2.

Section 4.3 explores a proposed alternative employing an EqP model (EPA 1993; Jones et al. 1997; Brooke et al. 2004) to derive sediment screening values. The EqP model assumes that benthic organisms are exposed to PFAS via pore water in equilibrium with sediments, and that the sensitivities of benthic species and water column species are similar. Jones et al. (1997) accepts that these and other major assumptions hold true for purposes of using EqP modeling for deriving sediment ecological toxicity benchmarks for nonionic organic contaminants in CERCLA applications.

A remaining question is whether EqP modeling is similarly applicable to the ionic PFAS acids. There are a limited number of studies with measured sediment-water distribution constants (K_d values) for PFAS or observations of linear sorption isotherms at low PFAS concentration (low-to-sub parts per million), suggesting that substituting K_d for the partition coefficient K_p, in the EqP model could be a valid approach for deriving sediment ESVs for PFAS. The EqP model and issues related to its use for deriving sediment screening values for PFAS are explored in greater detail below.

4.2 Search for In-Sediment Toxicity Studies

The ECOTOX knowledgebase was searched to identify any studies employing direct exposure of individual benthic species to single PFAS chemicals in a controlled laboratory experiment. No such studies were found, nor were any studies of any sort involving controlled direct sediment PFAS exposures. In forward searches of ECOTOX using the public-facing interface, "sediment" is not a selectable matrix, nor do any subcategories under the medium "soil" include aquatic sediments. Searches were conducted selecting "all test conditions" and "any exposure media," and the outputs were reviewed for exposures to sediment or pore water. No studies were found.

A more expansive effort was conducted for us in August 2019 by EPA's CCTE, GLTED, which maintains ECOTOX. GLTED conducts literature searches of several abstract services (Agricola, Biosys, Proquest, etc.) to identify prospective papers to curate in ECOTOX and reviews a far greater number of papers than are ultimately accepted into the Knowledgebase. Using the results from a literature search conducted in April of 2019, a total of 8,181 references were identified as having PFAS information in them, but data from only about 400 of them were curated in ECOTOX.

Using the data analytical tool of Swift-Review (available at https://www.sciome.com/swift-review/), GLTED investigators searched all 8,181 references using custom evidence stream filters with the following terms: '"sediment" AND "toxicity"' and '"sediment" AND "effects."' The evidence stream filtering identified 64 references with those terms, but review of those titles and abstracts found no studies of direct exposures of PFAS in sediments in controlled laboratory settings that were usable for deriving sediment screening values. Several subsequent broad chemical searches have been conducted (quarterly for those 8 PFAS structures addressed in this document and biannually for >400 PFAS chemical structures) by GLTED, and similar efforts are underway to identify any potentially useful publications on sediment toxicity.

In addition to the above searches, a general internet search was conducted in October 2020 using popular search engines and similar search terms. No useful studies were identified. Finally, recently published studies in which predicted no-effect concentrations (PNECs) were reported were reviewed to identify any relevant sediment toxicity values (Giesy et al. 2010; Hoke et al. 2012; Qi et al. 2011; Salice et al. 2018; Valsecchi et al. 2017). No useful sediment studies were identified in the cited literature.

Searches did find a handful of recent field studies that measured PFAS concentrations in water, sediment, and sediment-dwelling biota at affected sites, but did not examine toxicity impacts on biota. Several studies did derive biota-sediment accumulation factors (BSAFs). The studies are summarized in the following paragraphs.

Schaanning et al. (2020) analyzed more than 30 PFAS in water, sediment, pore water, and two species of benthic organisms: an oligochaete (*Tubifex tubifex*) and a mussel (*Anodonta anatine*). The organisms were placed in sediments taken from an industrially impacted river site in Norway and from upstream, downstream, and a control site for 4 weeks. Tests were conducted in flow-through aquaria; PFAS concentrations in aquarium water, sediment, pore water, and the test organisms derived BSAFs, BCFs and sediment-pore water partition coefficients (K_d). Fluxes

of PFAS to overlying water were also determined. In the 4-week exposure, uptake of PFAS by the oligochaetes, which are exposed to whole body absorption in sediments, was far greater than uptake by the mussels, which have a hard shell and feed through a siphon extending into the overlying water. The condition of both species was reduced in the impacted sediments, but this was attributed to high levels of petrogenic hydrocarbons also present, and not to PFAS. The study was complicated by the presence of PFAS in upstream and control sites and in the unexposed test organisms.

Langberg et al. (2019) similarly conducted a field study of the marine environment around a military site, Bodo Air Station, in Norway where they analyzed up to 30 PFAS in stormwater, soil leachate, fjord water, marine sediments, marine invertebrates (snails and various crabs), and teleost fish collected from the impacted area. Comparisons of PFAS accumulation levels in species reflected differences in exposure routes and in the rates of depuration and/or enzymatic degradation as well as trophic biomagnification. A key finding of the study was the detection of elevated levels of 6:2 fluorotelomer sulfonate (6:2 FTS) in marine invertebrates, suggesting bioaccumulation, while little or no 6:2 FTS was detected in teleost fish (Atlantic cod), as noted in previous studies. PFAS concentrations in fjord water were below detection (0.5–3 ng/L total PFAS), except for PFBA. Likewise, all PFAS were close to or below the limit of quantification (0.1–0.2 µg/kg) at all but two locations. Perfluorpentanoic acid (PFPeA, 0.26 µg/kg) and PFOS (0.32 µg/kg) were detected at one site and PFOS (0.29 µg/kg) only at a second site of eight sites. Low concentrations in seawater and marine sediments were attributed to local geophysical conditions involving high winds favoring sea spay formation with transfer of PFAS to the atmosphere and currents favoring dilution in seawater.

Bertin et al. (2018) tested two hypothetical models of PFAS bioaccumulation by *Chironomus riparius*, a passive diffusion model, essentially a partition model, and a concentration-dependent model, which involves a saturable active transport uptake mechanism. Midge larvae were exposed to river sediments collected downstream of a fluorotelomer plant in France. Accumulation and elimination tests with *C. riparius* were run using field sediments and field sediments spiked with perfluorotridecanoic acid (PFTrDA), the highest level PFAS constituent found in the impacted sediments, with concentrations up to 1.67 ng/g dw. PFTrDA was also used as a model compound to test concentration dependency. *C. riparius* exhibited complete elimination of all PFAS within 42 hours. The kinetic data better supported the concentration-dependent model. However, measurement data for determining BSAFs for PFTrDA did not support this model. Low measured BSAF values for PFTrDA suggested that chironomids would not be a significant source of PFCAs to predators, such as fish.

Munksgaard et al. (2016) measured 13 PFAS including PFOS, PFOA, and PFHxS in aquatic sediments and several aquatic food species, including two snails, two mussels and a crayfish, in creeks and coastal waters in and around Darwin, in Northern Territory, Australia. PFAS concentrations at impacted sites were up to 2 orders of magnitude higher than at a reference site. Large variations in levels between and within sites indicated that PFAS are heterogeneously distributed within sediment and biota on relatively small scales. Estimated dietary intakes were found to be well below European food safety tolerable daily intake values, while sediment PFOS concentrations fell in the category of “good ecological health” when compared to Norwegian marine sediment criteria.

4.3 Equilibrium Partitioning Model

Applying the EqP model is a promising approach to deriving bulk sediment ESVs. The EPA has supported the use of EqP modeling for setting sediment ecotoxicity thresholds (EPA 1993, 2018), and has published ecotoxicity thresholds derived using the EqP method for 8 metals and 41 organics in sediments (normalized to 1% total organic carbon [TOC]) for use in screening contaminants at CERCLA sites (OSWER 1996). The U.K.'s Environment Agency, in its risk evaluation of PFOS in sediments, noted that in the absence of direct sediment toxicity information, the EqP method would be used for developing a PNEC for PFOS in sediment, and notes that a K_{ow} value would not be needed if a measured K_d was available (Brooke et al. 2004).

Jones et al. (1997), citing Adams (1987), addressed concerns that benthic organisms are exposed to contaminants via exposure routes other than ingestion of interstitial water, such as dermal absorption and ingestion of sediment particles. In an analysis of the feeding habits of freshwater benthic species, Adams (1987) concluded that these species were not sediment feeders, except for the oligochaetes (aquatic earthworms) and some chironomids that are both filter feeders and occasional sediment feeders. Conversely, marine burrowing species frequently ingest sediment.

The EPA (1993) has observed that exposures are correlated not to total sediment concentrations, but to porewater concentrations, noting that porewater ingestion is not necessarily the main route of exposure, as all exposure pathways are at the same chemical activity at equilibrium. Jones et al. (1997), citing Maughan (1993) in this regard, argue that if the organism is in equilibrium with the pore water, then the concentration in the pore water would reflect the sum of all exposure routes. Therefore, an organism that has accumulated contaminants, through feeding, at a higher concentration than the equilibrium with pore water, would reestablish the equilibrium by losing contaminants to the pore water. Consequently, PFAS pore water concentrations may be a reasonable basis for deriving sediment screening values for benthic organisms.

Sediment quality benchmarks (SQB) for bulk sediment, then, may be calculated from porewater concentrations using the EqP model, via the partition coefficient K_p between sediment and water. In this approach, porewater concentrations would be set equal to relevant water quality benchmarks (WQBs):

$$\text{SQB} = K_p \times \text{WQB}$$

The partitioning of nonionic chemicals between sediment particles and water depends on the partitioning of the chemical to the organic carbon (OC) fraction (f_{oc}) of the particles, referred to as the K_{oc}. The overall partition coefficient, K_p, is then the partition coefficient for OC in the sediment, K_{oc}, times the f_{oc}:

$$K_p = f_{oc} \times K_{oc}.$$

Jones et al. (1997) identified four major assumptions that must be met for implementing the EqP approach: (1) partitioning of the organic chemical between OC and interstitial water (porewater) is stable at equilibrium; (2) the sensitivities of benthic species and species tested to derive WQBs, predominantly water column species, are similar; (3) the levels of protection afforded by WQBs are appropriate for benthic organisms; and (4) exposures are similar regardless of feeding type or habitat (EPA 1993).

Further, EPA (1993) describes that EqP modeling is more reliable when $f_{oc} > 0.2\%$. At lower levels of OC, factors controlling second-order effects on partitioning (e.g., particle size, sorption to nonorganic mineral fractions) become relatively more important. With respect to strong sorption of polar organics, including PFAS, to mineral sites, EqP modeling would overestimate porewater concentrations of polar organics, which would result in conservative screening values for benthic exposures.

Major assumption (1) requires that sediments have not been recently disturbed and are in equilibrium with porewater, a condition that would be confirmed when applying sediment screening values. With respect to Major Assumptions (2) and (3), the EqP approach assumes that the WQBs, when applied to the interstitial water of sediments, protect infaunal organisms. The EPA (1993) considers sensitivities of benthic species to be sufficiently similar to those of water column species to tentatively permit the use of WQBs for the derivation of SQBs. The requirements of Major Assumption (4) with respect feeding type are addressed in the discussion above.

The EqP modeling approach can offer some advantages over the direct measuring of pore water approach (Jones et al. 1997). The former is independent of the dissolved organic carbon (DOC) concentration, while the latter requires that the DOC concentration and the DOC partition coefficient be known. This requirement arises from the fact that a substantial proportion of a chemical in pore water can be complexed with DOC, while it is the free and un-complexed component that is bioavailable and in equilibrium with the OC normalized sediment concentration.

4.4 Use of K_{oc} in the EqP for PFAS

For PFAS carboxylic and sulfonic acids, which are in dissociated anionic forms at environmental pH, a similar EqP approach can be applied by substituting the sorption distribution constant K_d for the partition constant K_p. This would be a valid substitution when sorption follows a linear or near-linear isotherm over the solution concentration of interest, and thus behaves in a linear manner similar to partitioning. Johnson et al. (2007) observed sorption on a variety of natural solids that could be acceptably fitted to linear, Langmuir, and Freundlich isotherms. Ahrens et al. (2011) also observed linear isotherms on marine sediments, as did Milinovic et al. (2015) for soils and peat. Higgins and Luthy (2006) observed sorption isotherms on natural sediments of varying iron oxide and OC content fitted to the Freundlich model, of the form:

$$C_{sed} = K_f(C_w)^n$$

Where:

C_{sed} = sediment concentration;
K_f = Freundlich constant;
C_w = water concentration at equilibrium; and
n = exponential term for nonlinearity.

They reported the value of *n* to range from 0.75 to 1, with an average of 0.9. A value of 1 indicates linearity. Guelfo and Higgins (2013) similarly found Freundlich *n* values of 0.7 to 1.1. Nonlinearity is generally attributed to heterogeneity in the strength of sorption sites. For anionic PFAS, it may also be attributed to electrostatic repulsion at high sorption levels (Higgins and Luthy 2007) or exceeding monolayer adsorption (Johnson et al. 2007). In the latter study, surface area normalized adsorption of PFOS was greatest for Ottawa sand, then high iron sand, kaolinite, and least for goethite. Adsorption appeared to approach saturation at aqueous concentrations nearing 8 ppm for both goethite and Ottawa sand, indicating the possibility of monolayer coverage. A similar flattening of sorption began to appear at 4 ppm PFOS on Lake Michigan sediment (f_{oc} = 2–3%). The sorption nonlinearities observed in these studies would be expected given the complex character of natural sorbents and the multiple forces involved in PFAS sorption. However, although the available data are limited, the relatively low level of nonlinearity observed, especially at low or sub-part-per-million aqueous concentrations, could be considered as satisfying the assumption of linearity or near-linearity.

Formation of micelles or hemimicelles could produce a discontinuity, resulting in a sharp increase in the sorption of PFAS. Such formation would occur at levels above the concentrations relevant to ESV development. Shinoda et al. (1972, as cited in Johnson et al. 2007) found that micelle formation depends on PFAS chain length, not on counterion concentration. For the potassium salts of PFCAs and PFSAs, Shinoda et al. (1972, as cited in Rayne and Forest 2009) reported a linear relationship between critical micelle formation concentration (CMC) and the number of carbons in the perfluoroalkyl chain: $\log_{10}$ CMC (mmol L^{-1}) = 5.46–0.588 × number of perfluoroalkyl carbons. The head group acid type had little effect on the CMC, with both *n*-PFNA and *n*-PFOS having approximately equivalent CMCs. Shinoda reported a CMC of 6.3 mM (3,200 mg/L) for PFOS and 8–9 mM (3,500 mg/L) for PFOA. Hemimicelle formation could occur at 0.1–1% of the CMC (Schwarzenbach et al. 2003, as cited in Johnson et al. 2007), or at 3.2–320 mg/L for PFOS. These concentrations are above the low- to sub-part-per-million levels relevant to PFAS aquatic screening criteria.

Further, several studies on a variety of river, lake, and ocean sediments show that sorption of PFAS acids correlates to various degrees to the organic content of the sediment, while normalizing K_d values to OC reduced variability in measured results (Higgins and Luthy 2006; Johnson et al. 2007; Kwadijk et al. 2010; Li et al. 2018). Researchers identified several mechanisms for interactions between PFAS and sediment OC, dominated by hydrophobic and electrostatic interactions (Higgins and Luthy 2006; Du et al. 2014; Li et al. 2018). Hydrophobic forces relate to the size of the water exclusion cavity produced by the hydrophobic tail of PFAS molecules, resulting in observed increases in K_{oc} with tail length. These forces drive PFAS molecules out of the aqueous phase and on to surfaces of OC, typically composed of humic substances. Hydrophobic forces dominate sorption of long-chain PFAS, while sorption of short-chain PFAS is controlled by electrostatic forces (Zhao et al. 2012). Electrostatic repulsion of

PFAS anions by negatively charged OC and some minerals such clays at neutral pH (Johnson et al. 2007) are overcome by the greater hydrophobic forces driving sorption of long-chain PFAS but reduce the net K_{oc} compared to what it would be for the neutral form. Electrostatic attraction has been noted on positively charged iron oxide and silicon oxide surfaces (Higgins and Luthy 2006; Johnson et al. 2007; Ferrey et al. 2012). These forces complicate sorption on sediments with low OC, prompting EPA's >0.2% OC requirement even for hydrophobic contaminants.

Several investigators have measured PFAS concentrations in suspended particulate matter (SPM), functionally similar to DOC, as well as in the associated dissolved and bulk sediment phases in both freshwater and marine environments (Liu et al. 2019; Ding et al. 2018; Nguyen et al. 2016; Zhao et al. 2016; Chen et al. 2015; Munoz et al. 2015; Aherns et al. 2010a,b). These measurements conducted on field samples afforded estimates of PFAS K_d values for partitioning between the dissolved phase and SPM, typically operationally defined by that captured on a 0.7-µm filter or similar size fraction. These measurements also determined the PFAS SPM mass fraction, the proportion PFAS mass in the respective dissolved and particulate phases. Since SPM typically has a very high f_{oc} and low mineral content compared to bulk sediment, it is a useful medium for investigating PFAS sorption to OC.

These investigations found PFAS sorption to OC in SPM to behave quite similarly to that observed in bulk phase sediment OC, with SPM K_d values similar in magnitude to bulk sediment K_{oc} values, reflecting the high OC of SPM, and increasing with fluorinated chain length. Importantly, these studies determined that long-chain PFAS predominantly occurred in the SPM and OC of bulk sediment phases, while short-chain PFAS occurred predominantly in the water dissolved phase. Further, the mass of SPM-sorbed PFAS could exceed the dissolved mass for long-chain PFAS (C > 9). These are important considerations for the distribution and transport of PFAS in aquatic systems, exposure routes for aquatic organisms, and bioaccumulation potential.

A phenomenon of potential importance in particulate sorption studies is known as the particle concentration effect (EPA 1993). Many experiments with nonionic organic substances employing particle suspensions have exhibited a decrease in the particle-water partition coefficients as particle concentration increased, with a decrease of as much as 2–3 orders of magnitude at high particle concentrations. However, it is not clear that this effect would apply to settled or undisturbed sediments for which few experiments have been conducted. EPA (1993) presents an empirical model for explicitly accounting for this effect for reversible sorption in suspensions. The cause of this effect is poorly understood, and it is not clear whether it is relevant to anionic PFAS; however, it is possible that this is distinct phenomenon and a common feature of suspended particle sorption. If the particle concentration effect does apply to bedded sediments with high particle concentrations, actual partition coefficients could be lower than those measured in suspension experiments and sediment screening values would be reduced accordingly (EPA 1993). Note that relatively good concordance has been observed among PFAS K_{oc} values measured for SPM and for bulk sediments in field studies and for spiked sediment suspensions in the laboratory, suggesting that empirically reported K_{oc} values could support deriving sediment screening values using an EqP model, with appropriate accounting for sediment variability and model uncertainty.

Here, we describe how sediment ESVs for PFAS might be derived by applying the EqP method described above. Such an application would use the herein-derived PFAS surface-water ESVs as WQBs to derive PFAS sediment ESVs. Setting the porewater concentration equal to the surface-water ESVs in equilibrium with sediment produces the sediment ESV via the distribution constant for sorption, K_d, which may be substituted for K_p in the EqP model, per the foregoing discussion. Measured K_{oc} values, normalized to 1% f_{oc}, produced a set of baseline K_d values on which the sediment ESVs were derived, as follows:

$$ESV_{sed} = PW_{ESV} \times K_d$$

$$PW_{ESV} = SW_{ESV}$$

$$K_d = K_{oc} \times f_{oc},$$

$$\text{thus for } f_{oc} = 1\%,$$

$$ESV_{sed} = SW_{ESV} \times K_{oc} \times 0.01 \qquad \text{(Eq. 1)}$$

Where:

ESV_{sed} = sediment ecological screening value;
PW_{ESV} = pore water ecological screening value;
SW_{ESV} = surface water ecological screening value;
K_d = pore water/sediment distribution constant;
K_{oc} = pore water/organic carbon distribution constant, and
f_{oc} = fraction organic carbon.

Sediment screening values would be computed using K_{oc} values using Equation (1), which normalizes K_d computed from K_{oc} to f_{oc} = 1%. In actual use, ESV_{sed} values would be adjusted to site-specific sediment f_{oc}.

Table 4-1 presents published K_{oc} values for the eight study PFAS. When reported, the CF_2 fragment value for the effect on log K_{oc} is noted, which has a typical value of about 0.6. We do not compute mean K_{oc} values for the study set PFAS because the current compilation is not exhaustive and often studies report multiple values, so weighting values for computing a mean is difficult.

Table 4-1 also shows theoretical log octanol-water partition coefficients (log K_{ow} values) of neutral form PFAS produced by the COMOtherm model (Wang et al. 2011). Because the PFAS acids are almost entirely in anionic form at environmental pH, these data are presented mainly to show a similar thermodynamically predicted CF_2 group factor of 0.6, while also showing that the modeled neutral form K_{ow} values are 2–3 orders of magnitude higher than empirical K_{oc} values, reflecting the repulsive effect of the anionic head group of PFAS by negatively charged OC.

TABLE 4-1 Published K_{oc} Values for PFAS

	Log K_{oc} (L/kg$_{oc}$)									
Paper	PFDA	PFNA	PFOA	PFHxA	PFBA	PFOS	PFHxS	PFBS	Log K_{oc}/CF_2	Source of Sediment
Higgins and Luthy 2006	2.76	2.39	2.06			2.57			0.55	5 U.S. river and lake sediments, f_{oc} = 0.56–9.7%
Guelfo and Higgins 2013			1.89		1.88				0.45, 0.46, 0.51	3 soil standards of various types, f_{oc} = 1.7–4.5%
Johnson et al. 2007[a]						2.4–2.6				Lake Michigan sediment, f_{oc} = 0.02–0.03 (2–3%)
Ahrens et al. 2011[b]			2.3–2.5			3.4–3.7				Marine sediments from 3 locations around Japan, f_{oc} = 0.03–1.6%
Ahrens et al. 2010a	3.6	2.4	1.9			3.8	3.6		PFCAs 0.52–0.75, PFSAs 0.71–0.76	Marine sediments from 3 locations around Japan
Chen et al. 2012[c]			2.5			3.54				High f_{oc} (7.1–27%) wastewater treatment plant sludge
Milinovic et al. 2015[d]			1.98			2.85		1.22	0.4	5 soils from the Iberian Peninsula, f_{oc} = 0.2–9.4%, Belarus peat, f_{oc} = 39%
Zhao et al. 2012	3.23, 2.78	2.50, 2.35	2.09, 2.17			2.97, 2.68	2.02, 2.14	1.75, 2.09		Haihe River in urban Tianjin, wetland protection area, f_{oc} = 4.2, 2.4%
Li et al. 2011	4.2, na	3.8, 3.4	3.7, 3.1	3.7, 3.1		4.3, 4.6			PFCAs 0.1–0.6	Fresh water, salty water sections of the Haihe River in China

TABLE 4-1 (Cont.)

	Log K_{oc} (L/kg$_{oc}$)									
Paper	PFDA	PFNA	PFOA	PFHxA	PFBA	PFOS	PFHxS	PFBS	Log K_{oc}/CF_2	Source of Sediment
Pico et al. 2012	3.74	3.56	2.98	2.62		3.58		2.79		Irrigation channels near Valencia, Spain, f_{oc} = 1.6–6.4%
Labadie and Chevreuil 2011	3.8	2.9		2.1[c]		3.7				Orge River, France
Kwadijk et al. 2010	3.7 est.[b]	3.69	2.63			3.16		2.2 est.		21 rivers, lakes, and canals in the Netherlands
Vierke et al. 2014		3.8, 3.8	4.0, 3.9	3.0, 3.6	0.8, 2.7		1.2, 2.8	—, 2.7		40 and 80 cm depth riverbank sediment samples in Berlin
Munoz et al. 2015	3.7	3.6	3.0			3.4	2.9			133 rivers and lakes across France, f_{oc} < 0.4–22.9%
Jing et al. 2009									0.61 (K_p)	n/a
Theoretical log K_{ow} neutral form[d]	6.50	5.92	5.30	4.06	2.82	6.43	5.17	3.90	0.6	

[a] Computed using a log K_{oc} fragment constant for CF_2 of 0.5 using log K_{oc} for PFOA and PFOS as the basis for PFCAs and PFSAs, respectively.

[b] Estimated from graph.

[c] Value to be used for deriving sediment screening value.

[d] Wang et al. (2011); estimated using COSMOtherm model, assuming neutral form.

4.5 Prospects for Deriving Sediment Screening Values using the EqP Model

The growing body of empirically measured K_{oc} values in various freshwater and marine sediments exhibited in Table 4-1 suggests that it could be possible to derive sediment screening values using the EqP model. In addition, the empirically observed CF_2 fragment value of roughly 0.6, which comports well with the thermodynamically modeled value, provides a further basis for such derivation by demonstrating a quantitative structure-activity relationship for K_{oc} and chain length, especially for long-chain PFAS. However, although a sound theoretical and empirical basis exists for applying the EqP model, including observed linear or near-linear isotherms over useful concentration ranges, we conclude that sediment variabilities and model uncertainties are too great to derive sediment screening values at this time.

The above analysis does suggest, however, that ecological risk assessors would have a theoretical basis for deriving site-specific sediment screening values using measured K_{oc} values and/or porewater concentrations within an EqP framework. In making such measurements, analysts must be sure to filter out SPM from equilibrated water using submicron filters so as not to measure PFAS adsorbed to SPM as part of the dissolved fraction.

4.6 Method Uncertainties and Implications for Sediment ESV Derivation

Uncertainties in using the proposed EqP model and published K_{oc} values for the derivation of sediment ESVs lie in several areas, many of which are identified in the foregoing discussion. The implication of these uncertainties in deriving are explored further below.

- Applicability or protectiveness of WQBs, or aquatic screening values for sediment dwelling organisms. Jones et al. (1997) address this uncertainty directly, concluding that this assumption is valid for the purposes of deriving sediment criteria. They cite EPA (1993), which concluded that the sensitivities of benthic species are sufficiently similar to those of water column species to tentatively permit the use of WQBs for the derivation of sediment quality benchmarks. EPA (1993) applied WQBs derived for aquatic life to derive sediment benchmarks for numerous nonionic organic compounds through application of the EqP model and Koc estimates. Although EPA applied WQBs or criteria from chronic toxicity values for fish, daphnids and non-daphnid invertebrates, the current PFAS aquatic values were derived from species sensitivity distributions for as many genera as have published acute or chronic toxicity values. This approach includes the risk of underestimating impacts on benthic organisms more sensitive to PFAS than the most sensitive aquatic organisms, if any exist.

- Equilibrium pore-water concentrations as a basis for exposures to benthic organisms, including sediment feeders. Jones et al. (1997) addressed this uncertainty as well, as discussed above, concluding that use of the EqP method is preferable to direct measurements of pore water due to complicating factor of sorption on DOC (SPM). Regarding sediment feeders,

Jones et al. (1997) cites Maughan (1993): "if the organism is in equilibrium with the pore water, then the concentration in the pore water would reflect the sum of all exposure routes. Therefore, an organism that has accumulated contaminants, through feeding, at a higher concentration than the equilibrium with pore water would reestablish the equilibrium by losing contaminants to the pore water." This assumption includes a risk of underestimating impacts on sediment feeders.

- Substitution of log K_{oc} for K_p in the EqP model; linearity of log K_{oc} over the relevant exposure concentration range. Substituting K_{oc} for K_p in the EqP model introduces uncertainties related to the adsorption behavior of PFAS on sediments as compared to the more ideal and linear absorption (partitioning) behavior assumed in the model. Several studies (as previously cited) examined the adsorption of PFAS on sediment and soils and identified linear or near-linear isotherms, which would mimic partitioning behavior. Thus, uncertainties in estimated porewater concentrations would be limited, but would result in underestimation of exposure concentrations due to reduced sorption at higher PFAS concentrations. Several studies have reported nonlinearity at concentrations of several parts per million, which is generally well above corresponding water quality criteria that serve as the basis for the sediment criteria using the EqP model. This uncertainty could be addressed by limiting the maximum solution concentration for which the EqP model could be applied. Consequences of this uncertainty would be underestimation of risk to benthic life at affected sites. Underestimates of such effects from nonlinear isotherms would be limited at low concentrations but would increase at higher concentrations.

- Representativeness of $K_{oc} \times f_{oc}$ as a model for K_d for sorption of PFAS on sediments. This uncertainty is related to the mechanisms of PFAS sorption on sediments and the primacy of sorption onto organic matter in sediments. Several studies have noted the role of sorption to mineral phases in sediments, particularly in low carbon sediments. EPA (1993) addresses this issue for nonionic chemicals by setting a minimum carbon content of 0.2%. This limit is adopted here for PFAS acids, which are anionic at environmental pH. This limit comports well with observations of PFAS sorption in low-carbon sediments reviewed in this study. Application of the K_{oc} model to low-carbon sediments could underestimate sorption and result in overestimates of exposures to benthic life, which would artificially reduce sediment screening values.

- Particle concentration effect. This uncertainty is discussed in some detail in Section 4.4, as drawn from EPA (1993). Briefly, sediment particle suspension experiments with nonionic organics have exhibited a decrease in the particle-water K_d values at increasing particle concentrations. This could imply that K_d and K_{oc} values derived from suspension experiments, which are most laboratory experiments, overestimate K_d and K_{oc} values for bedded sediments.

However, a cursory comparison of PFAS K_d and K_{oc} values measured in field studies with bedded sediments with those measured in laboratory spiked suspension studies suggest that this effect is not great in practice. Consequences of this effect would be overestimating sediment K_{oc} values resulting in artificially elevated sediment screening values.

- Applicability of sediment screening values derived from published K_{oc} values from diverse soil and sediment types of wide-ranging f_{oc} and including both freshwater and marine sediments. Applying mean K_{oc} values from a wide variety of soils and sediments, some with high f_{oc} values, to specific sites introduces the uncertainty in the representativeness of the mean K_{oc} values. Effects from including high-carbon soils and sediments would be small, because the studies which included them still found linear K_{oc} isotherms, while demonstrating the high f_{oc} range of the model. Including marine sediments in computing mean K_{oc} values might be expected to bias these values high, due to expected higher sediment adsorption of PFAS from marine water from the salting-out effect in saltwater. Including values for marine sediments could bias mean log K_{oc} toward higher values when applied to freshwater sediments, resulting in underestimates of exposure. Log K_{oc} values reported for marine sediments (Ahrens et al. 2010a, 2011) and salty river water (Li et al. 2011) in Table 4-1 are not obviously higher than those for freshwater sediments. Thus, any effect from including them in the computation of mean log K_{oc} would be small.

4.7 Recommendations and Data Gaps

Given all the uncertainties summarized above surrounding the derivation of sediment screening values from empirically measured K_{oc} values, it is premature to derive such values at this time from the compiled sorption studies via the EqP model. However, the foregoing analysis does suggest that such an approach could be valid if known uncertainties are reasonably quantified and appropriate uncertainty factors applied to the derivation. The above analysis may inform and provide a starting point for any such attempts, either for derivation of general sediment screening values or site-specific values employing local measurements of PFAS sorption. The following are some important data gaps that would need to be filled to reduce method uncertainty:

- Range of acceptable values for sediment sorption parameters for both OC and mineral components over which derived values would be valid.

- Understanding PFAS sorption mechanisms and behavior as a function of carbon chain length and assigning uncertainty ranges for specific PFAS. Note that longer chain PFAS, which have generally higher toxicities and thus lower screening values, have lower K_{oc} variabilities than do shorter chain PFAS.

- Range of PFAS water concentrations over which the EqP model is valid.

- Relative effects of other water quality parameters affecting PFAS sorption, including pH and divalent cations, such as Ca^{2+}.

- The effect of particle size and concentration in bedded sediments on K_{oc}, if any.

- The presence of active transport mechanisms in sensitive benthic species, which could invalidate PFAS uptake assumptions based solely on equilibrium partitioning.

- Confirmation of predicted effects levels with actual measurements of PFAS toxicity to benthic organisms via direct exposures in bulk sediment experiments.

4.8 References

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