User's Manual

AFFF PFAS Terrestrial Ecological Risk Model Tool User's Manual

SERDP Project ER18-1614

MARCH 2021

Jason Conder Jennifer Arblaster Kristin Bridges **Geosyntec Consultants**

> *Distribution Statement A* This document has been cleared for public release



AFFF PFAS Terrestrial Ecological Risk Model Tool User's Manual Project: ER18-1614

TABLE OF CONTENTS

		Page
1.	OVERVIEW	1
1.	1.1 Purpose of the User's Manual and Model Tool	
	1.2 T&E Species Focus	
	1.3 Warning and Disclaimer	
	1.4 Model Uncertainties and Limitations	
	1.5 Remainder of the User's Manual	
2.	INTRODUCTION, TABLE OF CONTENTS, AND ACRONYMS &	2
2.	ABBREVIATIONS	
	(WORKSHEETS: INTRODUCTION, TOC, AND A&A)	1
3.	TABLE 1: EXPOSURE FACTORS FOR SELECTED RECEPTORS	
5.	(WORKSHEETS: EXPOSURE FACTORS AND EF LOOKUP)	5
4.	TABLE 2: BIOACCUMULATION PARAMETERS (WORKSHEET: BIO	
4.	ACCUMPARAMS)	
5.	TABLE 3: SITE-SPECIFIC DATA INPUT (WORKSHEET: DATA INPUT AND	0
5.	FWM)	
	1 vv ivi)	10
6.	TABLE 4: EXPOSURE SITE CONCENTRATION FOR ALL MEDIA	10
0.	(WORKSHEET: EPCS)	12
7.	TABLES 5 AND 6: TOXICITY REFERENCE VALUES FOR BIRDS AND	12
/.	MAMMALS (WORKSHEETS: TRVS BIRDS AND TRVS MAMMALS)	14
8.	TABLE 7: DIRECT CONTACT EXPOSURES (WORKSHEET: DIRECT	14
0.	CONTACT EXPOSURES)	16
9.	TABLES 8, 9, 10, 11, 12 AND 13: EXPOSURE ASSESSMENT AND HAZARD	10
9.	CHARACTERIZATION – BIRDS (WORKSHEETS: BIRD1, BIRD2, BIRD3)	
		17
10	AND MAMMALS (WORKSHEETS: MAMMAL1, MAMMAL2, MAMMAL3)	
10.	SUMMARY (WORKSHEET: HQSUM)	
	RENCES	
ALIA	ACHMENTS	23

LIST OF TABLES

TABLE 1 : EXPOSURE FACTORS FOR SELECTED RECEPTORS (WORKSHEETS: EXPOSURE FACTORS AND EF LOOKUP)	5
TABLE 2 : BIOACCUMULATION PARAMETERS (WORKSHEET: BIOACCUMPARAMS)	
· · · · · · · · · · · · · · · · · · ·	9
TABLE 3 : SITE-SPECIFIC DATA INPUT (WORKSHEET: DATA INPUT AND FWM)	
TABLE 4 : EXPOSURE SITE CONCENTRATION FOR ALL MEDIA (WORKSHEET: EPCS)	
TABLE 6 : TOXICITY REFERENCE VALUES FOR MAMMALS (WORKSHEET: TRVS MAMMALS)	
TABLE 7: DIRECT CONTACT EXPOSURES (WORKSHEET: DIRECT CONTACT EXPOSURES)	
TABLE 8: EXPOSURE ASSESSMENT AND HAZARD CHARACTERIZATION – TABLE 14: HAZARD QUOTIENT SUMMARY	17
	17

ACRONYMS AND ABBREVIATIONS

A&A	Acronyms and Abbreviations
AFFF	Aqueous Film Forming Foam
BCF	Bioconcentration factors sediment accumulation factors
BMF	Biomagnification factors
BSAF	Biota sediment accumulation factors
DoD	U.S. Department of Defense
EF	Exposure Factors
EPC	Exposure Point Concentrations
ERA	Ecological Risk Assessment
ESTCP	Environmental Security Technology Certification Program
HQ	Hazard Quotient
NOEC	No Observable Effect Concentration
PFAS	Per- and polyfluoroalkyl substances
PFOA	Perfluorooctanoic acid
PFOS	Perfluorooctanesulfonate
QSAR	Quantitative Structure Activity Relationship
SERDP	Strategic Environmental Research and Development Program
SSD	Species sensitivity distribution
T&E	Threatened and endangered
TDI	Total daily intake
TOC	Table of Contents
TRV	Toxicity reference value

		Form Approved
	DCUMENTATION PAGE	OMB No. 0704-0188
data needed, and completing and reviewing this collectio this burden to Department of Defense, Washington Head	s estimated to average 1 hour per response, including the time for reviewing instructior n of information. Send comments regarding this burden estimate or any other aspect or lquarters Services, Directorate for Information Operations and Reports (0704-0188), 12 or any other provision of law, no person shall be subject to any penalty for failing to cor YOUR FORM TO THE ABOVE ADDRESS	of this collection of information, including suggestions for reducing 215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-
1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
01-03-2021	SERDP User Manual	3/24/2020 - 5/31/2022
4. TITLE AND SUBTITLE		5a. CONTRACT NUMBER 20-P-0030
AFFF PFAS Terrestrial Eco	logical Risk Model Tool User's Manual	
		5b. GRANT NUMBER
		5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)		5d. PROJECT NUMBER
Jason Conder, Jennifer Ar	hlastor Kristin Bridges	ER18-1614
bason conder, benniter Al	Diaster, Kristin bildges	5e. TASK NUMBER
		5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME	E(S) AND ADDRESS(ES)	8. PERFORMING ORGANIZATION REPORT
Geosyntec Consultants		NUMBER
2100 Main St., Ste. 150,	7	ER18-1614
Huntington Beach, CA 9267	7	LIX10-1014
9. SPONSORING / MONITORING AGENC	CY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
Strategic Environmental R	esearch and Development Program	SERDP
4800 Mark Center Drive, S	uite 16F16	
Alexandria, VA 22350-36	505	11. SPONSOR/MONITOR'S REPORT
		NUMBER(S)
12. DISTRIBUTION / AVAILABILITY STA	TEMENT	ER18-1614
• Distribution A: Approved	for public release; distribution is u	nlimited.
13. SUPPLEMENTARY NOTES		
	is a user's manual for the customizabl	
-	eling tool ("Model Tool") for assessin	<u> </u>
	osure to perfluoroalkyl and polyfluoro	
	endangered (T&E) species in terrestri	al habitats potentially
	forming foam (AFFF)1. The Model Tool	
	M file) enables ecological risk assess	
	of PFAS in soil, surface water, and/o	
-	ecies of interest, and available toxic	5
	s consist of an evaluation of the pote	
	as well as model-predicted concentrati	
	model also features tables that provid	
	and risk characterization (i.e., hazar	d quotients) and other useful
information that can faci	litate ERA-based decision making.	
15. SUBJECT TERMS		
perfluoroalkyl, polyfluor	oalkyl, PFAS, aqueous film forming foam	m, AFFF, model tool,

ecological risk assessment

a. REPORT b. ABSTRACT c. THIS PAGE 33 19b. TELEPHONE NUMBER (inc	
UNCLASS Code)	clude area
UNCLASS UNCLASS UNCLASS 714-465-1226	

1. OVERVIEW

1.1 <u>Purpose of the User's Manual and Model Tool</u>

This document is a user's manual for the customizable Microsoft ExcelTM food web and wildlife exposure modeling tool ("Model Tool") for assessing the potential ecological risks associated with exposure to perfluoroalkyl and polyfluoroalkyl substances (PFAS) for common and threatened and endangered (T&E) species in terrestrial habitats potentially impacted by aqueous film forming foam (AFFF)¹. The Model Tool (a multi-worksheet ExcelTM file) enables ecological risk assessors to enter site-specific data (e.g., concentrations of PFAS in soil, surface water, and/or biota), exposure factors for site-relevant wildlife species of interest, and available toxicological information for common PFAS. Model outputs consist of an evaluation of the potential for direct effects to terrestrial communities, as well as model-predicted concentrations of PFAS in food webs and wildlife diet items. The model also features tables that provide ecological risk assessment (ERA) effects assessment and risk characterization (i.e., hazard quotients) and other useful information that can facilitate ERA-based decision making.

The Model Tool was based on a current state-of-the-practice overview of available methods, best practices, and key data gaps presented in the "Guidance for Assessing the Ecological Risks of PFAS to Threatened and Endangered Species at Aqueous Film Forming Foam Impacted Sites" document ("Guidance Document"; Conder et al., 2020), available on the ER18-1614 project page (<u>https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/ER18-1614</u>). This Model Tool was developed by Geosyntec Consultants with funding provided by the Strategic Environmental Research and Development Program (SERDP).

1.2 <u>T&E Species Focus</u>

This model tool was developed for use with T&E species, although it is also applicable for ecological risk assessments for common species. The quantitative ecological risk modeling tools, parameters, and receptors are specifically selected for assessing Federally listed T&E species present at AFFF release sites, particularly with regard to the characterization of effects, are much more conservative than approaches used for common species. For example, less conservative (higher) Toxicity Reference Values can be considered for use in the model to evaluate risks to common species. Please refer to the guidance regarding modifications that should be considered when focusing on common species.

¹ A second Model Tool is available for use in aquatic systems on the ER18-1614 project page and includes a separate User's Manual.

1.3 Warning and Disclaimer

Before proceeding further, it is recommended that the reader review the Guidance Document and confirm whether subsequent (improved) versions of the Model Tool and/or User's Manual are available at the URL provided in Section 1.1.

All cells and formulae in the Model Tool can be edited by the user (i.e., they're unprotected); therefore, updates to exposure factors, uptake models or toxicity reference values can be made by the user as data gaps are filled by additional research. However, it is recommended that the user save a backup (unedited) version of the original file before entering values or modifying parameters, equations, or algorithms in the model.

This Model Tool is intended to aid in quantitatively evaluating ecological risks from PFAS exposures, and to enable site managers to make defensible, risk-based management decisions using the best and most current scientific information and approaches available. This file outlines best practices, recommendations and suggestions that are based on the current state-of-the-science; it is not intended as regulation or a binding set of procedures. The user of this model takes full responsibility for the use and application of this model, including the input values, equations, assumptions and outputs. Therefore, it is recommended that all aspects of the model be evaluated by an experienced ecological risk assessor, prior to making site-specific or regulatory decisions.

1.4 Model Uncertainties and Limitations

Ecological risks assessments for PFAS, especially for PFAS beyond PFOS and PFOA, are in their infancy, and a high degree of uncertainty remains. Specifically, for the Model Tool, the uptake parameters included in the model are generally based on laboratory studies where model organisms are exposed to PFAS-spiked media. The use of model organisms may not reflect the same uptake rates as field species as PFAS-impacted sites. Additionally, the use of spiked media often results in uptake factors higher than those measured in the field studies due to higher bioavailability of contaminants in fresh versus aged media. As a result, the Model Tool is considered a conservative estimate of exposure but the uncertainty in over-predicting exposure is acknowledged. The Model Tool can be used to calculate site-specific risk-based thresholds however these should not be considered regulatory clean up goals or be used as such without risk management discussions with stakeholders. Where important site-specific remedial decisions making needs to be supported, modeled risks estimated should be confirmed in the field. For example, site-specific bioaccumulation studies with terrestrial or aquatic invertebrates or fish can be performed or samples of wildlife diet items can be collected and PFAS concentrations measured directly to better estimate exposures on a site-specific basis. The Model Tool is built with options for including site-specific tissue data to help refine preliminary risk estimates.

1.5 <u>Remainder of the User's Manual</u>

The remainder of this User's Manual presents a step-by-step overview of the features and operations of the Model Tool and includes an explanation of the main worksheets contained within the ExcelTM file.

The references section also includes the citations for all references cited in this User's Manual and Model Tool.

The User's Manual also features two attachments:

- Attachment 1 provides supporting information used to fill data gaps in bioaccumulation uptake factors applied in the Model Tool.
- Attachment 2 provides a demonstration of the Model Tool using PFAS data from a hypothetical United States Navy site.

The Model Tool and Guidance Document can be cited as:

Conder, J.; Arblaster, J.; Larson, E.; Brown, J.; Higgins, C. (2020). Guidance for Assessing the Ecological Risks of PFAS to Threatened and Endangered Species at Aqueous Film Forming Foam-Impacted Sites. SERDP Project ER18-1614. September.

2. INTRODUCTION, TABLE OF CONTENTS, AND ACRONYMS & ABBREVIATIONS (WORKSHEETS: INTRODUCTION, TOC, AND A&A)

The first three worksheets in the Model Tool are un-numbered, and consist of the following:

- **Introduction:** The Introduction worksheet contains an overview of the file and critical information on the applicable version of the Model Tool.
- **Table of Contents (TOC):** The TOC worksheet contains a Table of Contents that provides a guide to the main model worksheets in the file. Users can input their Site name or model/file name in cell B2. This entry is carried forward in the remainder of the workbook.
- Acronyms and Abbreviations (A&A): The A&A worksheet contains a list of acronyms and abbreviations used in the Model Tool and User's Guide.

TABLE 1. EXPOSURE FACTORS FOR SELECTED RECEPTORS (WORKSHEETS: 3. EXPOSURE FACTORS AND EF LOOKUP)

> The first step in applying the Model Tool is to select vertebrate wildlife receptors (birds and mammals) that will be evaluated in the ecological risk model. Direct risks to terrestrial biota exposed to impacted soil are included by default and do not require species selection.

In the "Exposure Factors" worksheet (Table 1), the user can select three avian species and three mammalian species from different feeding guilds from a **drop-down menu** (see red box in the screenshot below). The user also defines the "Site Area" in acres (purple box), which will allow the model to generate a sitespecific "Area Use Factor" (AUF)². If impacted surface freshwater is present at your site, type an "X" in the green box to direct the model to evaluate the exposure of vertebrate terrestrial wildlife via drinking surface water. Salinity in freshwater considered suitable for wildlife use as drinking water should be less than 1 part per thousand. The green box should remain blank if surface water is not present at your site, as the inclusion of text in the green box will result in the addition of unnecessary columns pertaining to surface water throughout the workbook.

	10 actors for Selected Receptors	Type an "X" in the green box if surfac	rsite:		X	I.		
				Birds			Wildlife	
Parameter	Parameter Definition	Units	Avian Consumer (Herbivore)	Avian Consumer (Insectivore)	Avian Consumer (Omnivore)	Mammalian Consumer (Herbivore)	Mammalian Consumer (Insectivore)	Mammalian Consumer (Omnivore)
Parameter	Parameter Definition	Units	Willow Ptarmigan	Lapland Longspur	Florida Scrub-Jay (T&E)	Eastern Cottontail	Short-Tailed Shrew	Deer Mouse
			Lagopus lagopus	Calcarius lapponicus	Aphelocoma coerulescens	Sylvilagus floridanus	Blarina brevicauda	Peromyscus maniculatus
BW	Body Weight	kg	0.60	0.03	0.09	1.13	0.02	0.02
FIR _{dw}	Daily Food Ingestion Rate (dry matter) [1]	kg, dw/day	0.06	0.05	0.12	0.36	0.01	0.01
FIRww	Daily Food Ingestion Rate (wet matter) [2]	kg, ww/day	1.52	0.27	0.57	0.65	0.02	0.02
Pveg	Proportion of Diet - Vegetation	kg diet item, ww/kg diet, ww	0.93	0.00	0.20	1.00	0.05	0.65
Pinv	Proportion of Diet - Soil Invertebrates	kg diet item, ww/kg diet, ww	0.07	1.00	0.80	0.00	0.95	0.35
Pso	Proportion of Diet - Soil	kg sediment, dw/kg diet, dw	0.03	0.02	0.00	0.02	0.02	0.02
HR	Home Range	acres	9.00	4.30	22.00	1.98	0.96	0.13
AUF	Area Use Factor [3]	proportion	1.000	1.000	0.455	1.000	1.000	1.000
DWI	Daily Drinking Water Ingestion Rate	L/day	0.078	0.003	0.013	0.110	0.003	0.003

Notes and Abbreviations (see Acronyms & Abbreviations table for PFAS names)

Notes and Abbreview and Abbreview and Abbreview and Abbreview and Weight We were weight L. Iters kg - klogram [1] Dry weight FIR is applied to concentrations of PFAS in soil, generally reported on dry weight basis. The method FIR is applied to its and the source and weight abasis. The method FIR is applied to its and abar and the source and weight abas. The method FIR is applied to its weight abas [1] Ury weight FHK is applied to concentrations of PFAS in soil, generally reported on dry weight bass. [2] Wet weight FHK is applied to task and generally reported on fresh or vet weight bass. [3] AUF values for receptors were calculated by dividing home range by site area. At some sites for some receptors, it may be more accurate to express AUF with additional approaches that consider a minial foranging strategies at the site.

adoitional approaches that consider animal toraging strategies at the site. Details on Threatened & Endangered receptor selection are provided in Section 3.3 and Appendix A of Conder et al. 2019. References for all species-specific exposure factors are provided in the Exposure Factors Lookup Table

² It should be noted that the model will automatically calculate a "default" AUF for all receptors by dividing the user-specified Site Area by the receptor's Home Range. Although this approach generally provides a reasonably representative AUF value for many receptors, it may not be the most appropriate approach for all species. Therefore, after site-specific and receptor-specific considerations are made, the user may also opt to provide a modified equation or AUF value that considers additional species-specific factors and habitat preferences for some receptors.

The receptors available for user selection include examples of T&E species, as well as common species without any Federally protected status. This approach allows the user to more accurately represent various site-specific receptor traits, life histories, and/or statuses. Once the desired receptors have been selected by the user, the key exposure factor parameters inside the <u>blue box</u> in the image above will be pre-filled with values from the "EF Lookup" worksheet. Note that all the parameters in Table 1 can be supplanted or revised by the user. For example, if the user wants to use an alternate receptor species other than the Willow Ptarmigan (or other avian herbivores), one can simply revise the information in that column as desired. The information for that receptor will be used in the remainder of the worksheet as "Bird 1". The columns to the right refer to "Bird 2"and "Bird 3" respectively. The mammals to be modeled are "Mammal 1", "Mammal 2", and "Mammal 3", proceeding left to right.

The "EF Lookup" worksheet (an internal lookup worksheet at the end of the workbook) lists all parameter **values** that auto-populate cells inside the <u>blue box</u> in Table 1 following selection of avian and mammalian receptors from the <u>drop-down menus</u> on the "Exposure Factors" worksheet. The EF Lookup worksheet is also where users can find <u>references</u> for all exposure parameters, as well as any additional <u>notes</u> pertaining to a given parameter.

Note: The values in this table are initial suggestions only. Additional efforts should be considered to verify the use of these values with particular site-specific risk assessments, such as consultation of site conditions, and consultation with a biologist. Full citations are provided in the User Guidance

RECEPTOR TYPE	GUILD	Species	Parameter	Definition	Lookup Code	Value	Units	Reference	Notes
AVIAN	INSECTIVORE	American Robin	BW	Body Weight	American Robin_BW	0.077	kg	USEPA (1993)	
AVIAN	INSECTIVORE	American Robin	DWI	Daily Drinking Water Ingestion Rate	American Robin_DWI	0.0108	L/day	USEPA (1993)	
AVIAN	INSECTIVORE	American Robin	FIR _{dw}	Daily Food Ingestion Rate (dry	American Robin_FIRdw	0.012	kg, dw/day	Nagy (2001)	Calculated using DW allometric equation for Passerine birds from Nagy et al. 2001; see Nagy FIR variables tab for formulas
AVIAN	INSECTIVORE	American Robin	FIR _{ww}	matter) Daily Food Ingestion Rate (wet	American Robin_FIRww	0.034	kg, ww/day	Nagy (2001)	Calculated using WW allometric equation for Passerine birds from Nagy et al. 2001; see Nagy FIR variables tab for formulas
AVIAN	INSECTIVORE	American Robin	HR	matter) Home Range	American Robin_HR	2.0	Acres	USEPA (1993)	Foraging HR for fledglings (0.81 hectares) reported in USEPA (1993)
AVIAN	INSECTIVORE	American Robin	P _{inv}	Proportion of Diet - Invertebrates	American Robin_Pinv	0.900	kg diet item, ww/kg diet,	Assumed: USEPA (1993)	Forage for invertebrates and fruits in shrubs and low tree branches; proportion assumed based on dietary information provided in USEPA
AVIAN		American Robin	D	Proportion of Diet - Soil	American Robin_Pso	0.104	ww kg soil, dw/kg diet, dw	Assumed; Beyer et al. (1994)	(1993); assumed 90% invertebrates. Assumed based on soil consumption rates of American Woodcock
			r _{so}						
AVIAN		American Robin	P _{veg}	Proportion of Diet - Vegetation	American Robin_Pveg	0.100	kg diet item, ww/kg diet, ww		Forage for invertebrates and fruits in shrubs and low tree branches; proportion assumed based on dietary information provided in USEPA (1993); assumed 10% fruit/plants.
MAMMALIAN		Buena Vista Lake Shrew (T&E)	BW	Body Weight	Buena Vista Lake Shrew (T&E)_BW	0.005		NatureServe Explorer, 2020	https://explorer.natureserve.org
MAMMALIAN	INSECTIVORE	Buena Vista Lake Shrew (T&E)	DWI	Daily Drinking Water Ingestion Rate	Buena Vista Lake Shrew (T&E)_DWI	0.0011	L/day	USEPA (1993)	Based on the water ingestion rate of the Short-Tailed Shrew
MAMMALIAN	INSECTIVORE	Buena Vista Lake Shrew (T&E)	FIR _{dw}	Daily Food Ingestion Rate (dry matter)	Buena Vista Lake Shrew (T&E)_FIRdw	0.001	kg, dw/day	Nagy (2001)	Calculated using DW equation for rodentia from Nagy et al. 2001; see Nagy FIR variables tab for formulas
MAMMALIAN	INSECTIVORE	Buena Vista Lake Shrew (T&E)	FIR _{ww}	Daily Food Ingestion Rate (wet matter)	Buena Vista Lake Shrew (T&E)_FIRww	0.002	kg, ww/day	Nagy (2001)	Calculated using WW allometric equation for rodentia from Nagy et al. 2001; see Nagy FIR variables tab for formulas
MAMMALIAN	INSECTIVORE	Buena Vista Lake Shrew (T&E)	HR	Home Range	Buena Vista Lake Shrew (T&E)_HR	0.091	Acres	Assumed; NatureServe Explorer, 2020	Ornate Shrew (similar size) used as a surrogate; average home range in California (https://explorer.natureserve.org)
MAMMALIAN	INSECTIVORE	Buena Vista Lake Shrew (T&E)	P _{inv}	Proportion of Diet - Invertebrates	Buena Vista Lake Shrew (T&E)_Pinv	1.000	kg diet item, ww/kg diet, ww	Assumed; NatureServe Explorer, 2020	Assumed based on feeding guild and dietary information in NatureServe Explorer; consult additional literature for more information
MAMMALIAN	INSECTIVORE	Buena Vista Lake Shrew (T&E)	P _{so}	Proportion of Diet - Soil	Buena Vista Lake Shrew (T&E)_Pso	0.024		Assumed; USEPA (1993)	Based on reported values for Meadow Vole
MAMMALIAN	INSECTIVORE	Buena Vista Lake Shrew (T&E)	P _{veg}	Proportion of Diet - Vegetation	Buena Vista Lake Shrew (T&E)_Pveg	0	kg diet item, ww/kg diet,	Assumed; NatureServe Explorer,	Assumed based on feeding guild and dietary information in NatureServe Explorer; consult additional literature for more information
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	BW	Body Weight	Coastal California Gnatcatcher (T&E)_BW	0.006	kg	NatureServe Explorer, 2020	https://explorer.natureserve.org
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	DWI	Daily Drinking Water Ingestion Rate	Coastal California Gnatcatcher (T&E)_DWI	0.00084	L/day	USEPA (1993)	Based on the water ingestion rate of the American Robin
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	FIR _{dw}	Daily Food Ingestion Rate (dry matter)	Coastal California Gnatcatcher (T&E) FIRdw	0.0021	kg, dw/day	Nagy (2001)	Calculated using DW allometric equation for Passerine birds from Nagy et al. 2001; see Nagy FIR variables tab for formulas
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	FIR _{ww}	Daily Food Ingestion Rate (wet matter)	Coastal California Gnatcatcher (T&E) FIRww	0.0072	kg, ww/day	Nagy (2001)	Calculated using WW allometric equation for Passerine birds from Nagy et al. 2001; see Nagy FIR variables tab for formulas
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	HR	Home Range	Coastal California Gnatcatcher (T&E)_HR	4.0	Acres	NatureServe Explorer, 2020	https://explorer.natureserve.org; low end of typical range for California gnatcatcher
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	P _{inv}	Proportion of Diet - Invertebrates	Coastal California Gnatcatcher (T&E)_Pinv	1.000	kg diet item, ww/kg diet,	Assumed; NatureServe Explorer,	Assumed 100% invertebrate diet based on feeding guild and dietary information in NatureServe Explorer; consult additional literature for
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	P _{so}	Proportion of Diet - Soil	Coastal California Gnatcatcher (T&E)_Pso	0	kg soil, dw/kg diet, dw	2021 Assumed; NatureServe Explorer,	more information Assumed not to consume soil based on feeding strategies described in NatureServe Explorer profile
AVIAN	INSECTIVORE	Coastal California Gnatcatcher (T&E)	P _{veg}	Proportion of Diet - Vegetation	Coastal California Gnatcatcher (T&E)_Pveg	0	kg diet item, ww/kg diet,	2023 Assumed; NatureServe Explorer,	Assumed based on feeding guild and dietary information in NatureServe Explorer; consult additional literature for more information
MAMMALIAN	OMNIVORE	Deer Mouse	BW	Body Weight	Deer Mouse_BW	0.015	ww kg	2020 USEPA (1993)	Minimum mean body weight for adults reported for Deer Mice
MAMMALIAN	OMNIVORE	Deer Mouse	DWI	Daily Drinking Water Ingestion Rate	Deer Mouse_DWI	0.003	L/day	USEPA (1993)	
MAMMALIAN	OMNIVORE	Deer Mouse	FIR_{dw}	Daily Food Ingestion Rate (dry matter)	Deer Mouse_FIRdw	0.0027	kg, dw/day	Nagy (2001)	Calculated using DW equation for rodentia from Nagy et al. 2001; see Nagy FIR variables tab for formulas
MAMMALIAN	OMNIVORE	Deer Mouse	FIR _{ww}	Daily Food Ingestion Rate (wet matter)	Deer Mouse_FIRww	0.0061	kg, ww/day	Nagy (2001)	Calculated using WW allometric equation for rodentia from Nagy et al. 2001; see Nagy FIR variables tab for formulas
MAMMALIAN	OMNIVORE	Deer Mouse	HR	Home Range	Deer Mouse_HR	0.150	Acres	USEPA (1993)	Average of values reported for Deer Mice (male and female)
MAMMALIAN	OMNIVORE	Deer Mouse	P _{inv}	Proportion of Diet - Invertebrates	Deer Mouse_Pinv	0.350	kg diet item, ww/kg diet, ww	USEPA (1993)	Assumed 35% invertebrate diet based on dietary information in USEPA Wildlife EFH; Principally eat seeds, arthropods, some green vegetation, roots, fruits, and fungi as available; opportunistic omnivores with highly variable diets.
MAMMALIAN	OMNIVORE	Deer Mouse	P _{so}	Proportion of Diet - Soil	Deer Mouse_Pso	0.020	kg soil, dw/kg diet, dw	Assumed; USEPA (1993)	Based on reported values for White-Footed Mice
MAMMALIAN	OMNIVORE	Deer Mouse	P _{veg}	Proportion of Diet - Vegetation	 Deer Mouse_Pveg	0.650	kg diet item, ww/kg diet,		Principally eat seeds, arthropods, some green vegetation, roots, fruits, and fungi as available; opportunistic omnivores with highly
MAMMALIAN	HERBIVORE	Eastern Cottontail	BW	Body Weight	Eastern Cottontail BW	1.130	ww kg	USEPA (1993)	variable diets; assumed 65% vegetation. Minimum mean body weight reported.
MAMMALIAN		Eastern Cottontail	DWI	Daily Drinking Water Ingestion Rate	Eastern Cottontail_DWI	0.110	L/day	USEPA (1993)	
MAMMALIAN		Eastern Cottontail	FIR _{dw}	Daily Drinking Water Ingestion Rate	Eastern Cottontail_FIRdw	0.077		Nagy (2001)	Calculated using DW equation for rodentia from Nagy et al. 2001; see Nagy FIR variables tab for formulas
MAMMALIAN		Eastern Cottontail	FIR _{ww}	matter) Daily Food Ingestion Rate (wet	Eastern Cottontail FIRww	0.255	kg, ww/day	Nagy (2001)	Calculated using WW allometric equation for rodentia from Nagy et al. 2001; see Nagy FIR variables tab for formulas
			····ww	matter)		5.233	10, WW, duy		construction and the anometic equation for reaction many et al. 2001, see Magy in variables tab for formulas
MAMMALIAN		Eastern Cottontail	HR	Home Range	Eastern Cottontail_HR	7.4		USEPA (1993)	Based on the average reported home ranges for adult
MAMMALIAN	HERBIVORE	Eastern Cottontail	P _{inv}	Proportion of Diet - Invertebrates	Eastern Cottontail_Pinv	0	kg diet item, ww/kg diet, ww	USEPA (1993)	Assumed based on feeding guild and dietary information reported in USEPA (1993) - herbaceous plants, woody vines, shrubs, and trees.
MAMMALIAN	HERBIVORE	Eastern Cottontail	P _{so}	Proportion of Diet - Soil	Eastern Cottontail_Pso	0.063	kg soil, dw/kg diet, dw	USEPA (1993)	Based on soil ingestion rate of jackrabbit (Table 4-5).
			1						



4. TABLE 2. BIOACCUMULATION PARAMETERS (WORKSHEET: BIOACCUMPARAMS)

> The second step in applying the Model Tool is to consider the food web modeling parameters that will be used to predict concentrations of PFAS in the diet items of wildlife receptors (birds and mammals) that are being evaluated by the ecological risk model.

The Table 2 "BioaccumParams" worksheet contains experimentally determined bioaccumulation factors (BAF) and biota soil accumulation factors (BSAF) that have been published in the peer reviewed literature and recommended for use in modeling in the Guidance Document. Users should review the Guidance Document for details on the full selection of parameters evaluated, the selection process and criteria and full references to the supporting information. Additionally, the user is encouraged to consider alternate model parameters from additional resources (i.e., Gobas et al. (2020) and Zodrow et al. (2020), as discussed in the Guidance), or the use of site-specific uptake factors. For example, if site-specific BSAFs are developed as part of Remedial Investigations, these can be entered into the model in the BSAF table, however users should be cautious to enter uptake factors in the same units currently used in the model to avoid calculation errors.. The bioaccumulation parameters identified in Table 2 will be used to model site-specific concentrations in biota (on a nanogram per kilogram of body weight [ng/kg ww] basis) in subsequent steps.

Due to current gaps in knowledge, experimentally derived values are not available for all parameters in the "BioaccumParams" table for several PFAS. As an alternative, the user can opt to fill certain data gaps with Quantitative Structure Activity Relationship (QSAR)-modelled or read-across bioaccumulation parameters (i.e., BAFs, BSAFs) by typing "Yes" in the green shaded cell at the top of Table 2 (identified by the green highlighted cell in the image below). When the option to apply QSAR-modeled parameters is selected, a surrogate value derived using the technical approaches described in Attachment 1 is applied for plants and invertebrates.

data gaps type "Yes" in		d bioaccumulation param	eters to an	yes	shaded cell to replace dat
and gapstype res it		Plant	1	nvertebrates	gaps with QSAR-modeled
	Soil	to Terrestrial Plant BAF-TP (g.OC/g, ww)		rrestrial Invertebrate BSAF-TI g, OC/g, ww)	values
PFAS	Value	Source	Value	Source	
PFCAs	_				
PFBA	0.22	Blaine et al., 2013	0.0019	а	
PFPeA	1.3	Zhao et al., 2014	0.0034	Zhao et al., 2014	
PFHxA	0.81	Zhao et al., 2014	0.011	Zhao et al., 2014	
PFHpA	0.094	Zhao et al., 2014	0.012	Zhao et al., 2014	
PFOA	0.017	Zhao et al., 2014	0.047	Zhao et al., 2014	
PFNA	0.012	Zhao et al., 2014	0.091	Zhao et al., 2014	
PFDA	0.0084	Zhao et al., 2014	0.26	Zhao et al., 2014	
PFUnDA	0.0076	Zhao et al., 2014	0.39	Zhao et al., 2014	
PFDoDA	0.0067	Zhao et al., 2014	0.61	Zhao et al., 2014	
PFTrDA	0.0049	b	1.8	а	
PFTeDA	0.0039	b	3.8	а	
PFSAs					
PFBS	0.40	Zhao et al., 2014	0.092	Zhao et al., 2014	
PFHxS	0.087	Zhao et al., 2014	0.34	Zhao et al., 2014	
PFOS	0.046	Zhao et al., 2014	0.55	Zhao et al., 2014	
PFDS	0.0018	Blaine et al., 2013	0.017	Rich et al., 2015	
FASAs					
PFOSA	0.038	Bizkarguenaga et al., 2016	0.55	с	
EtFASAAs and MeFAS	AAs				
N-EtFOSAA	0.046	с	0.084	Zhou et al., 2016	
N-MeFOSAA	0.046	c	0.55	с	
Notes and Abbreviation	s (see Acrony	ns & Abbreviations table for	PFAS name	s):	
g - gram					
OC - Organic carbon					
ww - wet weight					
BAF - Bioaccumulation F					
BSAF - Biota Soil Accun				1	
Supporting information fo 2019	r recommended	bioaccumulation values are	provided in Ta	able 2c of Conder et al.	

When the option to apply QSAR-modeled parameters is selected, a surrogate value is applied to precursor compounds (PFOSA, N-EtFOSAA, and N-MeFOSAA). Surrogate values used for precursor compounds were assumed to be equal to those of PFOS for each type of bioaccumulation parameter for several reasons. These include the potential for all three compounds to fully or partially transform to PFOS under certain environmental conditions, as well as laboratory evidence that tentatively suggests these compounds have similar bioaccumulative potentials to that of PFOS under controlled conditions (reviewed in Martin et al., 2010). It is important to note that there is no established scientific consensus regarding the selection of alternative PFAS as surrogates for predicting bioaccumulation of closely related and/or precursor compounds. Therefore, caution should be exercised when using modeled values as a basis for site-specific decision making and may be best applied as part of sensitivity analyses.

If the user does not type "yes" in the green shaded cell, the bioaccumulation parameters for which no experimentally derived values are available will remain blank and predictions for these PFAS will be unavailable for some of the biota. This may result in a potential underestimation of concentrations of PFAS in the food web diet items and subsequent calculations for estimating exposure and risks to wildlife, as noted in subsequent sections.

Please note: There is a hidden row (Row 1) at the top of the "BioaccumParams" worksheet that contains values supporting model formulae. This row should not be modified or deleted by the user, or a loss in model functionality may occur. Adding or deleting columns from this worksheet will also result in a loss of model functionality.

5. TABLE 3. SITE-SPECIFIC DATA INPUT (WORKSHEET: DATA INPUT & FWM)

> The third step in applying the Model Tool is to enter in available site-specific measurements to facilitate the calculation of PFAS in diet items for the wildlife receptors (birds and mammals) addressed in the ecological risk model.

The "Data Input & FWM" worksheet is where the user will enter the results of environmental sampling conducted at the site of interest, including physical parameters (total organic carbon), and concentrations of PFAS measured in abiotic media (e.g., soil and surface water) and biotic media (i.e., tissues), where available.

Concentrations of PFAS and TOC in soil are required model entry values in Table 3, while PFAS concentrations in surface water are optional:

- Under the header "Soil," the user should enter concentrations of PFAS into the "Site Specific Value" column of Table 3, using the units <u>nanograms per kilogram of dry weight (ng/kg dw)</u>. Laboratories often report concentrations of PFAS in soil as micrograms per kilogram (μg/kg), which would require conversion before entering data, specifically, multiplication of the μg/kg values by 1000. A "Basis" column, in which the origin of the site-specific soil PFAS concentrations can also be noted (e.g., maximum value [Max], 95% upper confidence limit [95 UCL]), is also included under the "Soil" heading as a bookkeeping measure for the user.
- If surface water is present at the site, a format similar to that of soil is used to enter <u>surface water</u> PFAS concentrations; however, the user should take care to enter water concentrations in <u>nanograms per liter (ng/L)</u>. If the user indicates that surface water is not present on the exposures factor tab, columns pertaining to <u>surface water</u> will not appear on the Data Input & FWM tab.
- Users must enter a site-specific value for the fraction organic carbon (kg OC/kg, soil, dw) in the green shaded cell at the top of Table 3 (identified by the green cell in the image below).
- If a User is including site-specific tissue data for use in the model, the data must be entered as nanograms per kilogram of wet weight (ng/kg ww).

Measured concentrations of PFAS in biota are not required for the model; however, in the event that measured data are available for a site, values can be entered into the "Site Specific Value" columns under the appropriate receptor type headings (i.e., terrestrial plant, soil invertebrate) in the model. Regardless of whether measured concentrations are entered into Table 3, the model will generate predicted PFAS concentrations for each receptor type, although if a measured value is available, the models will use the measured value instead of the model-predicted values in subsequent calculations.

Table 3: Site-specific Data Entry and Food Web Model Fraction Organic Carbon (kg OC/kg soil dw)											
ic Carbon (kg O	C/kg soil	dw)									
		Average carbon in the green s						shaded cell			
Soi	I	Terrestrial Plant		Soil Invertebrate		Surface Water					
Site- Specific Value ^[1]	Basis	Site- Specific Value ^[1]	Modele d Value	Site- Specific Value ^[1]	Modeled Value ^[3]	Site- Specific Value ^[1]	Basis				
(ng/kg dw)			(ng/kg ww	i)	(ng/kg ww)	(ng/L)		1			
1000	95 UCL		2.2		n/a	10	95 UCL	1			
1000	Max		12.5		0.21	10	Max				
1000	Max	100	8.1	100	0.71	10	Max	1			
1000	Max		0.94		0.75	10	Max	1			
40000000	95 UCL	100	6800	1000	120000	400000	95 UCL	1			
1000	95 UCL		0.12		5.7	10	95 UCL	1			
1000	Max		0.083		16	10	Max	1			
1000	95 UCL		0.076		24	10	95 UCL	1			
1000	Max		0.067		38	10	Max	1			
1000	Max		n/a		n/a	10	Max	1			
		10000		10000				1			
								1			
1000	95 UCL		4	1	5.8	10	95 UCL				
1000		100	0.87		21	10	Max	1			
					14000000	4000000		1			
								1			
1000	Max		0.38		n/a	10	Max				
MeFASAAs								1			
1000	95 UCL	1000	n/a	1000	0.84	10	95 UCL				
1000	Max		n/a		n/a	10	Max				
	Site- Specific Soi 0 1000	Soil Site- Specific Value ^[1] Basis (nq/kg dw) Basis 1000 95 UCL 1000 Max 1000 Max	Soil Terrestria Site- Specific Value ^[1] Basis Site- Specific Value ^[1] 1000 95 UCL 95 UCL 1000 Max 100 1000 Max 1000 1000 Max 1000 1000 Max 1000 1000 Max 1000 1000 Max 100 1000 Max 100 1000 Max 100 1000 Max 100 1000 Max 1000	Soil Terrestrial Plant Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Modele d Value (nq/kq dw) (nq/kq dw) (nq/kq ww) 1000 95 UCL 2.2 1000 Max 100 1000 95 UCL 2.2 1000 Max 0.94 40000000 95 UCL 0.12 1000 Max 0.083 1000 Max 0.067 1000 Max 0.067 1000 Max 1000 1000 Max 1000 1000 Max 1000 1000 Max 0.087 1000 Max 0.018 1000 Max 0.38 1000 Max 0.38 1000 Max 0.38	Soil Terrestrial Plant Soil Inv Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Modele d Value Site- Specific Value ^[1] Soil Inv (nq/kg dw) Basis Site- Specific Value ^[1] Modele d Value Site- Specific Value ^[1] Soil Inv 1000 95 UCL 2.2 Soil Soil Soil Inv 1000 Max 100 8.1 100 Soil Inv 1000 Max 0.083 1000 1000 1000 1000 Max 0.067 1000 1000 1000 1000 Max 100 0.87 1000 1000 1000 Max 100 0.38 1000 1000 1000 Max 0.38 Metototototototototototototototototototo	Soil Terrestrial Plant Soil Invertebrate Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Modele Site- Specific Value ^[1] Soil Invertebrate (nq/kq dw) (nq/kq ww) (nq/kq ww) (nq/kq ww) 1000 95 UCL 2.2 n/a 1000 Max 100 8.1 100 0.71 1000 Max 0.94 0.75 0.21 1000 Max 0.94 0.75 40000000 95 UCL 0.12 5.7 1000 Max 0.083 16 1000 Max 0.067 38 1000 Max n/a n/a 1000 Max 0.067 38 1000 Max 0.01 10000 1000 Max 0.01 10000 1000 Max 0.018 0.17 1000 Max 0.018 0.17 1000 Max 0.018 0.17 1000	Soil Terrestrial Plant Soil Invertebrate Surfactor (action in the carbon in the ca	Soil Terrestrial Plant Soil Invertebrate Surface Water Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Modele d Value Site- Specific Value ^[1] Modele d Value ^[1] Site- Specific Value ^[1] Modele d Value ^[1] Site- Specific Value ^[1]			

Notes and Abbreviations (see Acronyms & Abbreviations table for PFAS names):

ng - nanograms kg - kilograms

Toet Sito #1

L - liters

dw - dry weight

ww-wet weight

[1] Data must be added in provided units [2] Modeled value = Soil Concentration (OC normalized) x BAF-TP

[3] Modeled value = Soil Concentration (OC normalized) x BSAF-TI Uptake models are described in detail in Section 3.3 of Conder et al. 2019

If the user did not type "Yes" on the Table 2 (Bioaccumulation Parameters) worksheet, some predictions for PFAS in terrestrial plants and soil invertebrates will be listed as "n/a" and treated as zeros (i.e., no PFAS) in subsequent calculations. In these cases, concentrations of PFAS in diet items may be potentially underestimated, as indicated by the appearance of a "PU" note adjacent to the model-predicted values in subsequent tables. In cases where measured PFAS values in food web items (i.e., terrestrial plants or soil invertebrates) have been entered into the green cells, subsequent model calculations will preferentially use the measured value, and no PU note will be added.

6. TABLE 4. EXPOSURE POINT CONCENTRATIONS FOR ALL MEDIA (WORKSHEET: EPCS)

The fourth step in the Model Tool summarizes the available site-specific measurements and model predictions that will be used as Exposure Point Concentrations (EPCs) in the exposure modeling for wildlife receptors (birds and mammals) performed in the remainder of the ecological risk model.

The "EPCs" worksheet provides the user with a printer friendly summary of EPCs for PFAS in various environmental media at the site. While Table 4 does not require any user input, it serves as a lookup table that is referenced in a number of equations in subsequent steps of the model. Table 4 populates cells using values from the "Data Input & FWM" worksheet (Table 3). In the event that measured site-specific PFAS concentrations were provided by the user in previous steps, those values will be preferentially selected for inclusion in Table 4. Remaining cells will be populated with modeled values from Table 3.

Users should be aware that while the uptake factors in the Modeling Tool represent the current state-of-thescience, limited validation of the current Model Tools has been performed. This is due to the limited scope of the current project and the limited number of AFFF site investigations featuring sufficient data to conduct a robust assessment of model accuracy. Additional validation would improve confidence in the accuracy and conservatism of the model predictions. As with any modeling process within ecological risk assessment, users should consider and acknowledge uncertainty in modeled EPCs as part of evaluating risks, and carefully consider the need for model validation prior to final decision making.

Please note: There is a hidden row (Row 1) at the top of the "EPCs" worksheet that contains values supporting model formulae. This row should not be modified or deleted by the user, or a loss in model functionality may occur. Adding or deleting columns from this worksheet will also result in a loss of model functionality.

Table 4: Exposure Point Concentra						
Analyte	Soil EPC	Terrestrial F	Plant EPC	Terrestrial Inv	Surface Water EPC	
		Value	Basis [1]	Value	Basis ^[1]	
PFCAs	(ng/kg, dw)	(ng/kg, ww)		(ng/kg, ww)		(ng/L)
PFBA	1000.0	2.2	Modeled	n/a	n/a	10.0
PFPeA	1000.0	12.5	Modeled	0.2	Modeled	10.0
PFHxA	1000.0	5000.0	Measured	600000.0	Measured	10000.0
PFHpA	1000.0	0.9	Modeled	0.8	Modeled	10.0
PFOA	400000.0	100.0	Measured	5000000.0	Measured	400000.0
PFNA	40000.0	0.1	Modeled	5.7	Modeled	10.0
PFDA	1000.0	0.1	Modeled	16.0	Modeled	10.0
PFUnDA	1000.0	0.1	Modeled	24.0	Modeled	10.0
PFDoDA	1000.0	0.1	Modeled	38.0	Modeled	10.0
PFTrDA	1000.0	n/a	n/a	n/a	n/a	10.0
PFTeDA	1000.0	10000.0	Measured	10000.0	Measured	10.0
PFSAs						
PFBS	1000.0	4.0	Modeled	1.0	Measured	10.0
PFHxS	1000.0	100.0	Measured	21.0	Modeled	10.0
PFOS	100000.0	184000.0	Modeled	70000000.0	Measured	4000000.0
PFDS	1000.0	0.0	Modeled	0.2	Modeled	10.0
FASAs						
PFOSA	1000.0	0.4	Modeled	n/a	n/a	10.0
EtFASAAs and MeFASAAs	· · · · · · · · · · · · · · · · · · ·					
N-EtFOSAA	1000.0	1000.0	Measured	1000.0	Measured	10.0
N-MeFOSAA	1000.0	n/a	n/a	n/a	n/a	10.0

Test Site #1 Table 4: Exposure Point Concentrations for All Media

Notes and Abbreviations (see Acronyms & Abbreviations table for PFAS names):

dw - dry weight EPC - exposure point concentration kg - kilogram L - liters

ng - nanograms ww - wet weight

[1] Table selects for Site-specific empirical data over modeled values where available.

7. TABLES 5 & 6. TOXICITY REFERENCE VALUES FOR BIRDS AND MAMMALS (WORKSHEETS: TRVS_BIRDS AND TRVS_MAMMALS)

> The fifth step in applying the Model Tool is to review and select PFAS toxicity benchmarks for comparison with wildlife (birds and mammals) exposure estimates.

Worksheets "TRVs_birds" and "TRVs_mammals" contain a range of <u>low and high toxicity reference</u> <u>values (TRVs)</u> reported in the literature for various PFAS. TRVs in Tables 5 and 6 will be used to generate hazard quotients for avian (Table 5) and mammalian (Table 6) receptors at AFFF impacted sites in subsequent steps of the model. The tables also provide the basis upon which each of the TRVs was established, as well as the source from which the value was retrieved (in their respective "Reference" columns). Additionally, the user is encouraged to consider alternate model parameters from additional resources (i.e., Gobas et al. (2020) and Zodrow et al. (2020), as discussed in the Guidance).

While a range of TRVs are available for mammalian receptors exposed to various PFAS, a significant number of data gaps still exist. This is particularly true for avian receptors, as evidenced by the lack of TRVs for most PFAS (Table 5). The lack of reliable TRVs for PFAS complicates the process of evaluating potential risks to ecological receptors. Users may opt to provide their own TRVs in the "<u>User Input TRV</u> <u>Value</u>" columns in Tables 5 and 6 values (an adjacent column for any notes/rationale that may accompany the user-selected TRV is also provided).

Tables 5 & 6 also provide the user with an option to apply "read across" surrogate TRVs (derived for other PFAS) to some or all of the PFAS that do not have available TRVs:

- For avian receptors (Table 5), the user can opt to apply the avian TRV for PFOS to the three precursor compounds (i.e., PFOSA, N-EtFOSAA, and N-MeFOSAA) by typing "Yes" in the green highlighted cell at the top of Table 5. Surrogate TRVs are not substituted for other PFAS with missing values, due to the paucity of reliable TRVs available for avian receptors.
- For mammalian receptors, typing "Yes" in the similarly placed green highlighted cell at the top of Table 6 will prompt the model to apply surrogate mammalian TRVs for <u>all missing values</u> (i.e., not just precursors) in Table 6. Mammalian surrogate TRVs were selected by examining TRVs from PFCAs or PFSAs (whichever is appropriate) with perfluorocarbon chain lengths of n + 1 and n 1 (where n = the number of carbons in the PFAS of interest) and selecting the more conservative (i.e., lower) of the two measured TRV values.

It is important to note that TRVs for individual PFAS may vary by orders of magnitude in relation to one another. Thus, while applying available TRVs for PFAS as surrogates for those missing values helps to provides some estimate of risk for PFAS for which a measured TRV is unavailable, this approach also introduces an additional source of uncertainty into the overall hazard evaluation. There is little scientific basis or precedent for the approaches used to derive the surrogate TRVs; therefore, the user should exercise appropriate professional caution and use professional judgement when selecting whether or not to apply surrogate values in the model. This approach is best used as a sensitivity analysis rather than primary risk estimate for decision making, and should include a thorough discussion of the inherent uncertainty involved when applied.

Test Site#1 Table 6: Toxicity Reference Values- Mamma OPTIONA L: To app		r PFOS to all data gaps type "Yes" in green cell:	Yes	Lear Manna	Type "yes" in the green shaded cell to ap the mammalian TRV for PFOS as a surrog					
Analyte	Analyte Low TRV		Reference	High TRV	Basis	Reference	User Input TRV Value	User Input TRV Value Notes or Rationale		
PFCAs										
PFBA	30	No effect on growth (bodyweight) in rats	van Otterdijk (2007b)	-	-	-				
PFPeA	30	Surrogate - PFHxA	-	200	Surrogate - PFHxA					
PFHxA	30	No effect on survival in rats	Klaunig et al. (2015)	200	14% control-adjusted decrease in survival in rats	Klaunig et al. (2015),				
PFHpA	1.3	Surrogate - PFOA	-	14	Surrogate - PFOA	-				
PFOA	1.3	No effect on growth (bodyweight) in rats	Butenhoff et al. (2012)	14	10% control-adjusted decrease in growth (body.weight) in rats	Buten hoff et al. (2012)				
PFNA	0.83	No effect on reproduction (# live pups) in mice	Wolfet al. (2010)	1.1	46% control-adjusted decrease in reproduction (# live pups) in mice	Wolfet al. (2010)				
PFDA	0.1	No effect on growth (fetal bodyweight per litter) in pregnant mice	Harris and Birnbaum (1989)	6.4	23% control-adjusted decrease in growth (fetal bodyweight per litter) in pregnant mice	Harris and Birnbaum (1989)				
PFUnDA	0.3	No effect on growth (body weight in adults and pups) in rats	Takahashi et al. (2014)	1	13-19% control-adjusted decrease in growth (body weight of pups) in rats	Takahashi et al. (2014)				
PFDoDA	0.5	No effect on growth (body weight in adults and pups) in rats	Kato et al. (2015)	2.5	20-40% control-adjusted decrease in growth (body weight in adults and pups) in rats	Kato et al. (2015)				
PFTrDA	0.5	Surrogate - PFDoDA	-	2.5	Surrogate - PFDoDA	-				
PFTeDA	3	No effect on growth (body weight in adults and pups) in rats	Hirata-Koizumi et al. (2015)	10	8-18% control-adjusted decrease in growth (body weight of pups) in rats	Hirata-Koizumi et al. (2015)				
PFSAs										
PFBS	300	No effect on growth (bodyweight) in rats	Lieder et al. (2009b)	1000	8% control-adjusted decrease in growth (body weight) in rats	Lieder et al. (2009b)				
PFHxS	0.3	No effect on reproduction (litter size) in mice	Chang et al. (2018)	1	14% control-adjusted decrease in reproduction (litter size) in mice	Chang et al. (2018)				
PFOS	0.1	No effect on growth (body weight gain) in rats	Luebkeretal. (2005)	0.4	14% control-adjusted decrease in growth (bodyweight gain) in mice	Luebker et al. (2005)				
PFDS	0.1	Surrogate - PFOS	-	0.4	Surrogate - PFOS					
FASAs				_						
PFOSA	0.1	Surrogate - PFOS	-	0.4	Surrogate - PFOS	-				
EtFASAAs and MeFASAAs										
N-EtFO SAA	0.1	Surrogate - PFOS	-		Surrogate - PFOS	-				
N-MeFO SAA	0.1	Surrogate - PFOS	-	0.4	Surrogate - PFOS	-				

Notes and Abbreviations (see Acronyms & Abbreviations table for PFAS nam ed): TRV - Toxicity Reference Value mg/kg-day-miligrams per kilogram body weight per day. Details and full references for all TRVs can be found in Section 3.4 and Appendix C of Conder et al. 2019.

8. TABLE 7. DIRECT CONTACT EXPOSURES (WORKSHEET: DIRECT CONTACT EXPOSURES)

> The sixth step in applying the Model Tool is to evaluate the potential for direct effects for terrestrial life, such as soil invertebrates and plants.

The "Direct Contact Exposures" worksheet provides a quantitative evaluation of the potential for direct effects of PFAS in soil to terrestrial biota, based on a comparison between the concentration of individual PFAS in impacted soil and toxicity reference values (TRVs) for terrestrial plants and soil invertebrates. At the time of model development, the only TRVs available for terrestrial plants and soil invertebrates are No Observable Effect Concentrations (NOECs) for PFOA and PFOS. Additional TRVs will be added to subsequent versions of the model as they become available; therefore, it is very important that users check the project website for the latest version of the model. Additionally, the user is encouraged to consider alternate terrestrial life risk-based concentrations from additional resources (i.e., Gobas et al. (2020) and Zodrow et al. (2020), as discussed in the Guidance).

Analyte	Soil EPC (ng/kg, dw)	Te	errestrial Invertet	orates	Terrestrial Plants			
		NOEC ^[1]	Study	HQ ^[2]	NOEC ^[1]	Study	HQ ^[2]	
PFCAs		(ng/kg ww)			(ng/kg ww)			
PFBA	1000.00							
PFPeA	1000.00							
PFHxA	1000.00							
PFHpA	1000.00							
PFOA	400000.00	1.00E+07	He et al., 2013	4.0E-02	8.40E+07	Zhou et al., 2016	4.8E-03	
PFNA	40000.00							
PFDA	1000.00							
PFUnDA	1000.00							
PFDoDA	1000.00							
PFTrDA	1000.00							
PFTeDA	1000.00							
PFSAs								
PFBS	1000.00							
PFHxS	1000.00							
PFOS	100000.00	8.00E+07	Xu et al., 2013	1.3E-03	3.90E+06	Brignole et al., 2003	2.6E-02	
PFDS	1000.00							
FASAs								
PFOSA	1000.00							
EtFASAAs and MeFASAAs		-			•			
N-EtFOSAA	1000.00							
N-MeFOSAA	1000.00							

Notes and Abbreviations (see Acronyms & Abbreviations table for PFAS names):

NOEC - No Observable Effect Concentration

EPC - Exposure Point Concentration

HQ - Hazard Quotient

[1] Additional details on soil NOEC derivation in Section 3.4.5 of Conder et al. 2019.

[2] Hazard Quotients are calculated as EPC/NOEC; HQ greater than 1 are shown in Bold

9. TABLES 8, 9, 10, 11, 12, AND 13. EXPOSURE ASSESSMENT AND HAZARD CHARACTERIZATION- BIRDS (WORKSHEETS: BIRD1, BIRD2, BIRD3) AND MAMMALS (WORKSHEETS: MAMMAL1, MAMMAL2, MAMMAL 3)

The seventh step in applying the Model Tool is to evaluate the potential for risks to avian and mammalian wildlife receptors.

Worksheets "Bird1" through "Bird3" and "Mam1" through "Mam3" provide estimates of the total daily PFAS intake (TDI) that user-specified avian and mammalian receptors are exposed to via consumption of various dietary items (i.e., soil, surface water, terrestrial vegetation, soil invertebrates).

TDIs are calculated using EPCs from Table 4 (on the "EPCs" worksheet), species-specific exposure parameters retrieved from Table 1 (on the "Exposure Factors" Worksheet), and the exposure model detailed on the worksheets³. In addition to providing numerical TDI estimates in Tables 8, 9, 10, 11, 12, and 13, the model also generates a stacked bar chart (located on worksheet "Figure1 – TDI") that provides the user with a visual representation of the relative contribution of individual PFAS to an organism's overall exposure.

Following the derivation of TDIs, the model will generate HQs by comparing TDIs with TRVs from Table 5 (on the "TRVs_birds" worksheet) or Table 6 (on the "TRVs_mammals" worksheet). Depending on the availability of TRVs, the model may generate up to three HQs for each PFAS, including a <u>Low-TRV HO</u>, <u>High-TRV HO</u>, and a <u>User-selected TRV-based HO</u>⁴.

If the user did not type "Yes" on the Table 2 (Bioaccumulation Parameters) worksheet, some predictions for PFAS in terrestrial plants and soil invertebrates will be listed as "n/a" and treated as zeros (i.e., no PFAS) in subsequent calculations. Consequently, the concentrations of PFAS in wildlife diet items (and thus, exposure and risk to wildlife) are potentially underestimated. TDI and HQ values that are potentially underestimated as a result of the user's choice not to apply QSAR modelled bioaccumulation parameters to data gaps on the "BioaccumParams" tab will be noted by a "PU" value in the rightmost "TDI and HQ note" column.

³ Model assumptions include a <u>relative bioavailability (RB)</u> of 1 for all PFAS (i.e., 100% dietary availability).

⁴ User-selected TRVs and HQs are hidden in the default model view.

Test Site #1 Table 8: Exposure Assessment and Hazard Characterization Receptor: Willow Ptarmigan

Analyte		S	oil	Surfac	e Water	Terrestrial Vegetation		Soil Invertebrates		TDI _{total} ^[1]	TDI _{total} ^[1]	Low TRV	High TRV	Low-TRV HQ ^[2]	High-TRV	User-selected	User-selected TRV-based	TDI and HQ
	RB	RB	EPC	TDI _{so}	EPC	TDI _{sw}	EPC	TDI _{veg}	EPC	TDI _{inv}	total	lotai		, ,	HQ 🖽	HQ ^[3]	TRV	HQ ^[3]
			RB	ng/kg dw	ng/kg-day	ng/L	ng/kg-day	ng/kg ww	ng/kg-day	ng/kg ww	ng/kg-day	ng/kg-day	mg/kg-day	mg/kg-day	mg/kg-day	unitless	unitless	mg/kg-day
PFCAs																		
PFBA	1	1.0E+03	4.4E-01	1.0E+01	1.3E+00	2.2E+04	3.9E+03	n/a		3.9E+03	3.9E-03	No TRV	No TRV			1.0E+00	3.9E-03	PU
PFPeA	1	1.0E+03	4.4E-01	1.0E+01	1.3E+00	1.3E+05	2.3E+04	3.4E+02	4.6E+00	2.3E+04	2.3E-02	No TRV	No TRV			2.0E+00	1.2E-02	
PFHxA	1	2.0E+03	8.8E-01	1.0E+01	1.3E+00	5.0E+00	9.0E-01	6.0E+01	8.1E-01	3.9E+00	3.9E-06	No TRV	No TRV			3.0E+00	1.3E-06	
PFHpA	1	2.0E+03	8.8E-01	3.0E+01	3.9E+00	1.9E+04	3.4E+03	2.4E+03	3.2E+01	3.4E+03	3.4E-03	No TRV	No TRV			4.0E+00	8.5E-04	
PFOA	1	3.0E+03	1.3E+00	1.0E+01	1.3E+00	1.0E+01	1.8E+00	1.0E+00	1.3E-02	4.4E+00	4.4E-06	1.0E+00	No TRV	4.4E-06				
PFNA	1	3.0E+03	1.3E+00	1.0E+01	1.3E+00	3.6E+03	6.4E+02	2.7E+04	3.7E+02	1.0E+03	1.0E-03	No TRV	No TRV					
PFDA	1	4.0E+03	1.8E+00	1.0E+01	1.3E+00	3.4E+03	6.0E+02	1.0E+05	1.4E+03	2.0E+03	2.0E-03	1.0E+00	No TRV	2.0E-03				
PFUnDA	1	4.0E+03	1.8E+00	1.0E+01	1.3E+00	3.0E+03	5.4E+02	1.6E+05	2.1E+03	2.6E+03	2.6E-03	No TRV	No TRV					
PFDoDA	1	5.0E+03	2.2E+00	1.0E+01	1.3E+00	3.4E+03	6.0E+02	3.1E+05	4.1E+03	4.7E+03	4.7E-03	No TRV	No TRV					
PFTrDA	1	5.0E+03	2.2E+00	1.0E+01	1.3E+00	n/a		n/a		3.5E+00	3.5E-06	No TRV	No TRV					PU
PFTeDA	1	6.0E+03	2.6E+00	1.0E+01	1.3E+00	n/a		2.5E+01	3.4E-01	4.3E+00	4.3E-06	No TRV	No TRV					PU
PFSAs																		
PFBS	1	1.0E+03	4.4E-01	1.0E+01	1.3E+00	4.0E+04	7.2E+03	5.0E+00	6.7E-02	7.2E+03	7.2E-03	8.8E+01	No TRV	8.1E-05				
PFHxS	1	2.5E+04	1.1E+01	1.0E+01	1.3E+00	2.2E+05	3.9E+04	8.5E+05	1.1E+04	5.0E+04	5.0E-02	No TRV	No TRV					
PFOS	1	1.0E+05	4.4E+01	5.0E+02	6.5E+01	4.6E+05	8.2E+04	5.5E+06	7.4E+04	1.6E+05	1.6E-01	7.7E-01	2.6E+00	2.0E-01	5.9E-02			
PFDS	1	1.0E+03	4.4E-01	1.0E+01	1.3E+00	1.8E+02	3.2E+01	1.7E+03	2.3E+01	5.7E+01	5.7E-05	No TRV	No TRV					
FASAs																		
PFOSA	1	1.0E+03	4.4E-01	1.0E+01	1.3E+00	3.3E+01	5.9E+00	n/a		7.6E+00	7.6E-06	No TRV	No TRV					PU
EtFASAAs and MeFASAAs																		
N-EtFOSAA	1	1.0E+03	4.4E-01	1.0E+01	1.3E+00	1.0E+01	1.8E+00	4.5E+01	6.1E-01	4.1E+00	4.1E-06	No TRV	No TRV					
N-MeFOSAA	1	1.0E+03	4.4E-01	1.0E+01	1.3E+00	n/a		n/a		1.7E+00	1.7E-06	No TRV	No TRV					PU

Notes:

[1] Media-specific Total Daily Dose (TDI) is calculated using the following general equation and receptor specific parameters:

TDI_{*i*,copc} = (EPC_{copc} x RB x FIR x P_{*i*}) + (DWI x EPC) x AUF x (1/BW), where:

Variable	Value	<u>Units</u>	Variable Description
TDI _i		mg/kg-day	Total Daily Intake for Dietary Item "i" for COPC
EPC _{copc}	see above	ng/kg, ng/L	Exposure Point Concentration for each media
RB		unitless	Relative Bioavailability (only for soil portion of diet; assumed to be 1 for all chemicals)
P_{veg}	0.93	proportion	Proportion of Diet Vegetation
P _{inv}	0.07	proportion	Proportion of Diet Terrestrial Invertebrates
P_{so}	0.01	proportion	Proportion of Diet Soil
FIR_{dw}	0.03	kg/day	Daily Food Ingestion (dry weight, used for soil)
FIRww	0.12	kg/day	Daily Food Ingestion (wet weight, used for tissue)
AUF	1.00	proportion	Area Use Factor
BW	0.60	kg	Body Weight
DWI	0.08	L/day	Daily Drinking Water Ingestion Rate

[2] HQ = TDI/TRV; HQ greater than 1 are shown in **Bold** [3] = In a scenarios where HQ values may be potentially underestimated, the "PU" designation will appear in either black or grey text. Black text indicates that the HQ is underestimated due to one or more missing EPCs related to Bird 1's diet items. Grey text indicates that the HQ cannot be calculated due to the lack of an available TRV

Abbreviations:

dw - dry weight TRV - Toxicity reference value PU - Potentially Underestimated ww - wet weight HQ - Hazard Quotient (unitless) ng - nanograms mg - milligram L - liters TDI - Total Daily Intake (mg/kg-day) kg - kilogram

10. SUMMARY (WORKSHEET: HQSUM)

The eighth step in applying the Model Tool is to review the summary of the potential for risks to avian and mammalian wildlife receptors.

The "HQSum" worksheet contains a table populated with all HQs (i.e., Low-HQ, High-HQ, User Selected TRV-based HQ) that were generated by the model for both avian and mammalian receptors. No inputs are required on this worksheet; rather, it serves as a printer-friendly summary table for the user.

Test Site #1 Table 14: Hazard Quotient Summary

	Hazard Quotients (HQ) - Recommended TRVs													
Analyte			American			ξE)		Cottontail		led Shrew				
	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ		
PFCAs														
PFBA							1.7E-04		1.6E-05		2.1E-04			
PFPeA														
PFHxA							3.5E-07	5.3E-08	1.1E-06	1.7E-07	4.6E-07	6.9E-08		
PFHpA														
PFOA	4.4E-06		3.8E-05		1.5E-06		1.2E-05	1.1E-06	1.2E-05	1.1E-06	1.1E-05	1.0E-06		
PFNA							1.0E-03	7.5E-04	1.3E-02	9.6E-03	3.7E-03	2.8E-03		
PFDA	2.0E-03		3.3E-02		1.2E-02		2.6E-03	7.8E-04	1.3E-01	4.0E-02	2.9E-02	8.6E-03		
PFUnDA							2.4E-03	7.1E-04	2.0E-01	6.0E-02	4.1E-02	1.2E-02		
PFD₀DA							1.6E-03	3.1E-04	2.3E-01	4.7E-02	4.7E-02	9.3E-03		
PFTrDA														
PFTeDA							8.9E-06	2.7E-06	1.3E-05	3.8E-06	7.3E-06	2.2E-06		
PFSAs														
PFBS	8.1E-05		1.6E-05		3.4E-05		3.0E-05	9.0E-06	3.0E-06	8.9E-07	3.9E-05	1.2E-05		
PFHxS							1.6E-01	4.9E-02	1.1E+00	3.3E-01	4.2E-01	1.3E-01		
PFOS	2.0E-01	5.9E-02	2.3E+00	6.7E-01	8.5E-01	2.5E-01	1.0E+00	2.6E-01	2.1E+01	5.3E+00	5.4E+00	1.3E+00		
PFDS														
FASAs														
PFOSA														
EtFASAAs and MeFASAAs														
N-EtFOSAA														
N-MeFOSAA														

Notes:

HQ greater than 1 are shown in **Bold** See Acronyms & Abbreviations table for PFAS names.

Abbreviations:

HQ - Hazard Quotient (unitless) TRV - Toxicity reference value

11. REFERENCES

- Bizkarguenaga, E., Zabaleta, I., Mijangos, L., Iparraguirre, A., Fernández, L. A., Prieto, A., & Zuloaga, O. (2016). Uptake of perfluorooctanoic acid, perfluorooctane sulfonate and perfluorooctane sulfonamide by carrot and lettuce from compost amended soil. Science of The Total Environment, 571, 444–451. https://doi.org/10.1016/j.scitotenv.2016.07.010
- Brignole, A. J., Porch, J. R., Krueger, H. O., & Van Hoven, R. L. (2003). PFOS: A Toxicity Test to Determine the Effects of the Test Substance on Seedling Emergence of Seven Species of Plants (No. Project No. 454-110; p. 135). St. Paul, MN: Wildlife International, Ltd. (sponsored by 3M).
- Blaine, A. C., Rich, C. D., Hundal, L. S., Lau, C., Mills, M. A., Harris, K. M., & Higgins, C. P. (2013). Uptake of Perfluoroalkyl Acids into Edible Crops via Land Applied Biosolids: Field and Greenhouse Studies. Environ. Sci. Technol., 47(24), 14062–14069. <u>https://doi.org/10.1021/es403094q</u>
- Butenhoff, J. L., Kennedy, G. L., Chang, S.-C., & Olsen, G. W. (2012). Chronic dietary toxicity and carcinogenicity study with ammonium perfluorooctanoate in Sprague–Dawley rats. Toxicology, 298(1–3), 1–13. <u>https://doi.org/10.1016/j.tox.2012.04.001</u>
- Chang, S., Butenhoff, J. L., Parker, G. A., Coder, P. S., Zitzow, J. D., Krisko, R. M., ... Seed, J. G. (2018). Reproductive and developmental toxicity of potassium perfluorohexanesulfonate in CD-1 mice. Reproductive Toxicology, 78, 150–168. https://doi.org/10.1016/j.reprotox.2018.04.007
- Conder J, Arblaster J, Larson E, Brown J, Higgins C. (2020). Guidance for Assessing the Ecological Risks of PFAS to Threatened and Endangered Species act Aqueous Film Forming Foam-Impacted Sites. SERDP Project ER18-1614. <u>https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/ER18-1614</u>.
- Cornell Lab of Ornithology, 2020. All About Birds. Bird Guide Search. Available at: <u>https://www.allaboutbirds.org/guide</u>
- Gallagher, S. P., Van Hoven, R. L., Beavers, J. B., & Jaber, M. (2005). Final Report T-7485: A Reproduction Study with the Northern Bobwhite (Project No. 454-116; p. 444). St. Paul, MN: Wildlife International, LTD (3M Corporation sponsor).
- Gobas, F. A. P. C., Kelly, B., Kim, J. (2020). A Framework for Assessing Bioaccumulation and Exposure Risks of Per- and Polyfluoroalkyl Substances in Threatened and Endangered Species on Aqueous Film Forming Foam (AFFF)-Impacted Sites. SERDP Contract Report ER18-1502. <u>https://www.serdpestcp.org/Program-Areas/Environmental-Restoration/ER18-1502</u>
- Harris, M. W., & Birnbaum, L. S. (1989). Developmental Toxicity of Perfluorodecanoic Acid in C57BL/6N Mice. Fundamental and Applied Toxicology, 12, 442–448.
- He, W., Megharaj, M., & Naidu, R. (2016). Toxicity of perfluorooctanoic acid towards earthworm and enzymatic activities in soil. Environ Monit Assess., 188(7). <u>https://doi.org/10.1007/s10661-016-5416y</u>
- Hirata-Koizumi, M., Fujii, S., Hina, K., Matsumoto, M., Takahashi, M., Ono, A., & Hirose, A. (2015). Repeated dose and reproductive/developmental toxicity of long-chain perfluoroalkyl carboxylic acids in rats: perfluorohexadecanoic acid and perfluorotetradecanoic acid. Fundamental Toxicological Sciences, 2(4), 177–190. <u>https://doi.org/10.2131/fts.2.177</u>

- Kato, H., Fujii, S., Takahashi, M., Matsumoto, M., Hirata-Koizumi, M., Ono, A., & Hirose, A. (2015). Repeated dose and reproductive/developmental toxicity of perfluorododecanoic acid in rats. Environmental Toxicology, 30(11), 1244–1263. <u>https://doi.org/10.1002/tox.21996</u>
- Klaunig, J. E., Shinohara, M., Iwai, H., Chengelis, C. P., Kirkpatrick, J. B., Wang, Z., & Bruner, R. H. (2015). Evaluation of the Chronic Toxicity and Carcinogenicity of Perfluorohexanoic Acid (PFHxA) in Sprague-Dawley Rats. Toxicologic Pathology, 43(2), 209–220. https://doi.org/10.1177/0192623314530532
- Lieder, P. H., York, R. G., Hakes, D. C., Chang, S.-C., & Butenhoff, J. L. (2009). A two-generation oral gavage reproduction study with potassium perfluorobutanesulfonate (K+PFBS) in Sprague Dawley rats. Toxicology, 259(1–2), 33–45. <u>https://doi.org/10.1016/j.tox.2009.01.027</u>
- Luebker, D. J., York, R. G., Hansen, K. J., Moore, J. A., & Butenhoff, J. L. (2005). Neonatal mortality from in utero exposure to perfluorooctanesulfonate (PFOS) in Sprague–Dawley rats: dose–response, and biochemical and pharamacokinetic parameters. Toxicology, 215(1-2), 149-169.
- Martin J.W., Asher B.J., Beesoon S., Benskin J.P., Ross M.S. (2010). PFOS or PreFOS? Are perfluorooctane sulfonate precursors (PreFOS) important determinants of human and environmental perfluorooctane sulfonate (PFOS) exposure? J Environ Monit 12:1979-2004. https://doi.org/10.1039/c0em00295j
- Nagy K. 2001. Food requirements of wild animals: predictive equations for free-living mammals, reptiles, and birds. Nutrition Abstracts and Reviews:21R-31R.
- NatureServe (2020). NatureServe Explorer: An Online Encyclopedia of Life. Available from: http://explorer.natureserve.org/
- Newsted, J. L., Jones, P. D., Coady, K., & Giesy, J. P. (2005). Avian toxicity reference values for perfluorooctane sulfonate. Environmental science & technology, 39(23), 9357-9362.
- Newsted, J. L., Coady, K. K., Beach, S. A., Butenhoff, J. L., Gallagher, S., & Giesy, J. P. (2007). Effects of perfluorooctane sulfonate on mallard and northern bobwhite quail exposed chronically via the diet. Environmental Toxicology and Pharmacology, 23(1), 1-9.
- Rich, C. D., Blaine, A. C., Hundal, L., & Higgins, C. P. (2015). Bioaccumulation of Perfluoroalkyl Acids by Earthworms (*Eisenia fetida*) Exposed to Contaminated Soils. Environ. Sci. Technol., 49(2), 881– 888. <u>https://doi.org/10.1021/es504152d</u>
- Sample, B.E., Aplin, M.S., Efroymson, R.A., Suter G.W. II, Welsh, C.J.E. (1997). Methods and tools for estimation of the exposure of terrestrial wildlife to contaminants.
- Takahashi, M., Ishida, S., Hirata-Koizumi, M., Ono, A., & Hirose, A. (2014). Repeated dose and reproductive/developmental toxicity of perfluoroundecanoic acid in rats. J. Toxicol. Sci., 39(1), 97– 108. <u>https://doi.org/10.2131/jts.39.97</u>
- Tyron, P.R., MacLean, S.F. (1980). Use of space by Lapland longspurs breeding in Arctic Alaska. The Auk 97, 509-520.U.S. EPA. (1993). Wildlife exposure factors handbook [EPA Report]. (EPA/600/R-93/187). Washington, DC: Office of Research and Development.

- van Otterdijk, F. M. (2007). Repeated Dose 90-Day Oral Toxicity Study with MTDID 8391 by Daily Gavage in the Rat Followed by a 3-week Recovery Period (3M Study No. 06-398; NOTOX Project 484492; p. 346). The Netherlands: NOTOX B.V. (sponsored by 3M Medical Department).
- Virginia DGIF, 2020. Wildlife Information: Pungo white-footed mouse (*Peromyscus leucopus easti*). Available at: <u>https://www.dgif.virginia.gov/wildlife/information/pungo-white-footed-mouse/#:~:text=This%20is%20a%20medium%20sized,subspecies%20is%20distinguished%20from%20P.</u>
- Wolf, C. J., Zehr, R. D., Schmid, J. E., Lau, C., & Abbott, B. D. (2010). Developmental Effects of Perfluorononanoic Acid in the Mouse Are Dependent on Peroxisome Proliferator-Activated Receptor-Alpha. PPAR Research, 2010, 1–11. <u>https://doi.org/10.1155/2010/282896</u>
- Xu, D., Li, C., Wen, Y., & Liu, W. (2013). Antioxidant defense system responses and DNA damage of earthworms exposed to Perfluorooctane sulfonate (PFOS). Environmental Pollution, 174, 121–127. <u>https://doi.org/10.1016/j.envpol.2012.10.030</u>
- Yeung, L. W., Loi, E. I., Wong, V. Y., Guruge, K. S., Yamanaka, N., Tanimura, N., ... & Lam, P. K. (2009). Biochemical responses and accumulation properties of long-chain perfluorinated compounds (PFOS/PFDA/PFOA) in juvenile chickens (*Gallus gallus*). Archives of environmental contamination and toxicology, 57(2), 377-386.
- Zhao, H., Chen, C., Zhang, X., Chen, J., & Quan, X. (2011). Phytotoxicity of PFOS and PFOA to *Brassica chinensis* in different Chinese soils. Ecotoxicology and Environmental Safety, 74(5), 1343–1347. <u>https://doi.org/10.1016/j.ecoenv.2011.03.007</u>
- Zhao, S., Fang, S., Zhu, L., Liu, L., Liu, Z., & Zhang, Y. (2014). Mutual impacts of wheat (*Triticum aestivum* L.) and earthworms (*Eisenia fetida*) on the bioavailability of perfluoroalkyl substances (PFASs) in soil. Environmental Pollution, 184, 495–501. https://doi.org/10.1016/j.envpol.2013.09.032
- Zhao, S., Ma, X., Fang, S., & Zhu, L. (2016). Behaviors of N-ethyl perfluorooctane sulfonamide ethanol (N-EtFOSE) in a soil-earthworm system: Transformation and bioaccumulation. Science of The Total Environment, 554–555, 186–191. <u>https://doi.org/10.1016/j.scitotenv.2016.02.180</u>
- Zhou, L., Xia, M., Wang, L., & Mao, H. (2016). Toxic effect of perfluorooctanoic acid (PFOA) on germination and seedling growth of wheat (*Triticum aestivum L*.). Chemosphere, 159, 420–425. <u>https://doi.org/10.1016/j.chemosphere.2016.06.045</u>
- Zodrow, J., Frenchmeyer, M., Dally, K., Osborn, E., Anderson, P., Divine, C. (2020). Per- and Polyfluoroalkyl Substances Ecological Risk-Based Screening Levels. SERDP Contract Report ER18-1653. https://www.serdp-estcp.org/Program-Areas/Environmental-Restoration/ER18-1653

ATTACHMENT 1: SUPPORTING INFORMATION REGARDING THE DERIVATION SURROGATE BIOACCUMULATION PARAMETERS

This attachment describes the derivation of the surrogate bioaccumulation parameters that are available to be selected in cases for which bioaccumulation parameters are not available (as detailed in the Guidance Document).

Terrestrial Plant Bioaccumulation Factors

The BAF values for PFTrDA and PFTeDA in terrestrial plants were extrapolated using the model shown in the figure below, which was derived from available empirical information from other PFCAs of 7, 8, 9, 10, and 11 perfluorocarbons (BAFs are reviewed in Conder et al. (2020)).



Terrestrial Invertebrate Biota-Soil Accumulation Factors

The BSAF-TI values for PFBA, PFTrDA and PFTeDA in terrestrial invertebrates were extrapolated using the model shown in the figure below, which was derived from available empirical information from other PFCAs (BSAF-TIs are reviewed in Conder et al. (2020)).



Precursor PFAS

Where empirical values were unavailable, BAF and BSAF values for precursor compounds (PFOSA, N-EtFOSAA, and N-MeFOSAA) were assumed to be equal to their respective values for PFOS. This assumption was made due to a combination of factors, including the potential for all three compounds to fully or partially transform to PFOS under certain environmental conditions, as well as laboratory evidence that tentatively suggests these compounds have similar bioaccumulative potentials to that of PFOS under controlled conditions (reviewed in Martin et al., 2010).

ATTACHMENT 2: MODEL TOOL DEMONSTRATION FOR NAVY SITE 1

To demonstrate the use of the Model Tool, data for PFAS in surface water and soil were obtained for a representative DoD Site (referred to herein as Navy Site 1). This demonstration is a hypothetical example of how the model can be used using real-world data, and does not represent a complete ERA for Navy Site 1. The use of this data is included only as demonstration of the Model Tool and the risk-focused conclusions from the model output are for illustrative purposes only.

First, the representative species for the terrestrial portion of the site were selected from the drop-down menu of Table 1: Exposure Factors for Selected Receptors. Terrestrial receptors were selected from the drop-down menus (note, the receptors selected would not likely to co-occur at the same site given their respective geographical distributions – this is a hypothetical exercise). Since Navy Site 1 includes a freshwater body, drinking water use by the terrestrial wildlife was selected by making an "X" in the green selection cell. A terrestrial exposure area was estimated by evaluating the size of the habitat assumed to be represented by the available PFAS soil samples. This value (7 acres) was entered into the green Site Area cell.



Second, On the Bioaccumulation Parameters tab (Table 2: Bioaccumulation Parameters), the option to include surrogates/QSARs for data gaps was checked "Yes" by making an "X" in the green selection cell to allow the evaluation of as many PFAS as possible.

Third, 95 Upper Confidence Limits on the Mean (95UCL) were calculated for the concentrations of PFAS in surface water using measurements of samples collected at the site. Units were converted from μ g/kg to ng/kg for concentrations in soils. Due to a low sample count, maximum values were used as EPCs for soils. These values were input manually into Table 3: Site-specific Data Entry and Food Web Model. To the right of the values, "Max" or '95UCL" was entered to specify the basis for the values. No site-specific tissue data have been collected, so only abiotic data were entered (green cells under the "Site-specific Value" for plants and invertebrates were left blank). PFAS that were all non-detect in soil and water at the site were not included. As organic carbon data for soil was not available, the default of 1% was assumed.

ic Carbon (kg (OC/kg soi	ldw)		0.01				
				Average				
So	il	Terrestr	ial Plant	Soil Inve	ertebrate	Surface Water		
Site- Specific Value ^[1]	Basis	Site- Specific Value ^[1]	Modeled Value ^[2]	Site- Specific Value ^[1]	Modeled Value ^[3]	Site- Specific Value ^[1]	Basis	
(na/ka dw)			(ng/kg ww)		(na/ka ww)	(ng/L)		
(lightg uti)						7	95UCL	
			0		0	13	95UCL	
			0		0	120	95UCL	
			0		0	13	95UCL	
2,810	MAX		4,777		13,207	140	95UCL	
			0		0	2	95UCL	
			0		0	0.67	95UCL	
			0		0	0.57	95UCL	
			0		0			
			n/a		n/a			
			n/a		n/a			
187	MAX		7,480		1,720	15	95UCL	
			0		0	460	95UCL	
44,070	MAX		202,722		2,423,850	157	95UCL	
			0		0			
			0		n/a	2	95UCL	
MeFASAAs								
			n/a		0			
	Carbon (kg)	ic Carbon (kg OC/kg soi Soil Site- Specific Value ^[1] Basis (ng/kg dw) 2 2 2 3 3 3 3 4 3 3 3 3 3 3 3 3 3 3 3 3	ic Carbon (kg OC/kg soil dw) Soil Terrestr Site- Specific Value ^[1] Basis Site- Specific Value ^[1] (ng/kg dw)	Soil Terrestrial Plant Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Modeled Modeled Value ^[2] (ng/kg dw) (ng/kg ww) (ng/kg ww) (ng/kg ww) (ng/kg dw) 0 0 (ng/kg dw) 0 0 (ng/kg dw) 0 0 2,810 MAX 4,777 0 0 0 10 0 0 10 0 0 11 1 0 12 1 0 137 MAX 7,480 187 MAX 202,722 0 0 0 44,070 MAX 0 0 0 0	Soil Terrestrial Plant Soil Inverse Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Site- Specific Value ^[1] Site- Specific Value ^[1] (ng/kg dw) (ng/kg ww) (ng/kg ww) (ng/kg ww) 2,810 MAX 4,777 0 0 0 2,810 MAX 4,777 0 0 0 187 MAX 7,480 187 MAX 202,722 0 0 0 0 0 0 0 0 0	Soil Terrestrial Plant Soil Invertebrate Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Modeled Value ^[2] Site- Specific Value ^[1] Modeled Value ^[2] Modeled Value ^[1] (ng/kg dw) (ng/kg ww) (ng/kg ww) (ng/kg ww) (ng/kg dw) 0 n/a 2,810 MAX 4,777 13,207 0 0 0 0 2,810 MAX 4,777 13,207 0 0 0 0 0 1 0 0 0 0 1 0 0 0 0 1 1 0 0 0 1 1 1,720 0 0 1 1 0 0 0 1 0 0 0 0 1 0 0 0 0 1 0 0 0 0 1 0 0 0	Soil Terrestrial Plant Soil Invertebrate Surface Site- Specific Value ^[1] Basis Site- Specific Value ^[1] Modeled Value ^[2] Site- Specific Value ^[1] Modeled Value ^[1] Site- Specific Value ^[1] Site- Specific Value ^[1] Modeled Value ^[1] Site- Specific Value ^[1]	

Fourth, to illustrate the ability to customize TRVs in the model, an alternate avian TRV for PFOS was entered into the green "User Input TRV Value" cell for PFAS in Table 5: Toxicity Reference Values-Birds. This value was 0.077 mg/kg-day. Surrogate TRVs were not included for analysis by leaving the green selection box blank.

Did not include surrogate TRVs here

Navy Site 1

Table 5: Toxicity Reference Values- Bird	ds							
	OPTIONAL: To apply Sur	rogate TRVs to precursors only (F	ASAs and FASAAs)	type "Yes" in green cell: Birds (mg/kg-day)				
Analyte	Low TRV	Basis	Reference	High TRV	Basis	Reference	User Input TRV Value	User Input TRV Value Notes or Rationale
PFCAs								
PFBA	No TRV		-	No TRV				
PFPeA	No TRV			No TRV				
PFHxA	No TRV			No TRV				
PFHpA	No TRV	-		No TRV				
PFOA	1	No effect on growth (body weight) of 1-day old chickens; exposed to PFOA/PFDA/PFOS mixture	Yeung et al. 2009	No TRV				
PFNA	No TRV			No TRV				
PFDA	1	No effect on growth (body weight) of 1-day old chickens; exposed to PFOA/PFDA/PFOS mixture	Yeung et al. 2009	No TRV				
PFUnDA	No TRV			No TRV				
PFD₀DA	No TRV			No TRV				
PFTrDA	No TRV			No TRV				
PFTeDA	No TRV			No TRV				
PFSAs								
PFBS	88	No effect on growth (body weight) of northern bobwhite quail	Gallagher et al. (2005)	No TRV	No High-TRV available			
PFHxS	No TRV			No TRV				
PFOS	0.77	No true 'no effect' values were available. 17% control-adjusted decrease in reproduction (14-day old survivors/eggs set) for northern bobwhite quail	Newsted et al. (2005, 2007)	2.64	16% control-adjusted decrease in survival of northern bobwhite quail	Newsted et al. (2005, 2007)	0.077	
PFDS	No TRV			No TRV				
FASAs								
PFOSA	No TRV		-	No TRV		-		
EtFASAAs and MeFASAA	s							
N-EtFOSAA	No TRV		-	No TRV		-		
N-MeFOSAA	No TRV	-		No TRV	-	-		

Manually added Alternate TRV here

Following the last step, hazard quotients automatically update in Table 7 through 13 (Receptor-specific Total Daily Intake and HQ) and the Table 14: Wildlife Hazard Quotient Summary.

As shown below in the hazard quotient summary, five hazard quotient values (ranging from 2.3 to 9.3) exceeded 1 and were auto-bolded. This result indicated that the site-specific exposures for Short-Tailed Shrew, Deer Mouse, American Woodcock, and Lapland Longspur to PFOS were predicted to exceed the user-selected PFOS TRVs. For mammals (Short-Tailed Shrew and Deer Mouse), predicted exposures exceeded the PFOS TRVs (by a factor of 2.3 to 9.4). For birds (American Woodcock and Lapland Longspur), predicted exposures exceeded the user-selected PFOS TRV of 0.077 mg/kg-day (by a factor of 6.8 to 9.3).

		Hazard Quotients (HQ) - Recommended TRVs													Hazard Quotients (HQ) - User Selected TRVs (if applicable)						
Analyte	America Willow Ptarmigan Woodco					ngspur Eastern Cottontail		Short-Tailed Shrew		Deer Mouse						Short-					
	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Low-TRV HQ	High-TRV HQ	Willow Ptarmigan	American Woodcock	Lapland Longspur	Eastern Cottontail	Tailed Shrew	Deer Mouse			
PFCAs																					
PFBA	-		-			-	2.1E-08		5.0E-08	-	4.2E-08		-	-		-		-			
PFPeA	-		-				-			-	-	-	-	-		-					
PFHxA	-		-	-		-	3.7E-07	5.5E-08	8.9E-07	1.3E-07	7.6E-07	1.1E-07	-	-	-	-		-			
PFHpA	-	1	1			-	1		-		-	-			1	-					
PFOA	8.2E-04	1	4.1E-03		3.9E-03	1	8.0E-04	7.5E-05	4.0E-03	3.7E-04	2.4E-03	2.3E-04	-	-	1	-					
PFNA	-		1			-	2.2E-07	1.7E-07	5.4E-07	4.1E-07	4.6E-07	3.5E-07	-	-	-		-				
PFDA	6.8E-08		6.1E-08		4.8E-08	-	2.1E-07	6.2E-08	5.0E-07	1.5E-07	4.3E-07	1.3E-07	-		-		-				
PFUnDA	-		1			-	1.7E-07	5.2E-08	4.2E-07	1.3E-07	3.6E-07	1.1E-07		-	-	-					
PFDoDA	-		1			-	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00		-	-	-					
PFTrDA			1			-	1	-			-			-	-	-					
PFTeDA	-		-			-	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	0.0E+00	-	-	-	-		-			
PFSAs							-														
PFBS	1.2E-05	-	8.5E-06	-	2.8E-05		5.3E-06	1.6E-06	2.8E-06	8.3E-07	7.4E-06	2.2E-06	-	-		-		-			
PFHxS		-	1				1.4E-04	4.2E-05	3.4E-04	1.0E-04	2.9E-04	8.7E-05		-	-	-	-				
PFOS	7.0E-02	2.0E-02	9.3E-01	2.7E-01	6.8E-01	2.0E-01	4.4E-01	1.1E-01	9.4E+00	2.3E+00	4.0E+00	1.0E+00	7.0E-01	9.3E+00	6.8E+00	1					
PFDS	-		1				1				-			-		-					
FASAs			-																		
PFOSA		-					-							-							
EtFASAAs ar	nd MeFAS	AAs																			
N-EtFOSAA		1	1				1	-			-	-		-	1	-					
N-MeFOSAA		-	-	-	-		1		-	-		-	-	-		-		-			

Notes: HQ greater than 1 are shown in **Bold** See Acronyms & Abbreviations table for PFAS names.

Abbreviations: HQ - Hazard Quotient (unitless) TRV - Toxicity reference value