

Introduction

This worksheet contains a bioaccumulation model to predict the concentration of PFOS in fish tissue, including the quantification of the proportion of exposure derived from surface sediment versus the water column.

The model makes the following primary assumptions:

1. Water and surface sediment are at steady state and that concentrations in water and sediment are independent of one another.
2. Fish diets are derived from epibenthic and/or benthic invertebrates that absorb PFOS directly from sediment or sediment porewater, and/or accumulate PFOS through ingestion of surface sediment.
3. Bioaccumulation constants derived from laboratory data (steady state) from water-only and food-only exposures to fish, and from data from laboratory exposures of benthic invertebrates to sediment are applicable to field organisms.
4. Fish are restricted to the area modeled in each of the three modeling scenarios and/or the accumulation kinetics for PFOS in fish are such that fish would reach steady state with respect to different exposures when moving to a new location exhibiting different concentrations of PFOS in sediment, water, and/or surface sediment invertebrates.
5. Water and surface sediment data obtained from the various studies reflect PFOS exposure conditions to fish at the time of fish sampling (2009).

Three modeling scenarios were investigated. Each scenario is represented by two tables: 1) raw data used to derive the average concentrations of PFOS in surface sediment (generally 0-10 cm in depth for most samples) and water, which are entered into the fish bioaccumulation model; and 2) the fish bioaccumulation model itself.

The following tables are included in this file:

- Table 1. Concentrations of PFOS in surface sediment and water samples obtained from Sections 1, 2, 3, and 4 upstream of 3M Cottage Grove.
- Table 2. Fish bioaccumulation model for Sections 1, 2, 3, and 4 upstream of 3M Cottage Grove.
- Table 3. Concentrations of PFOS in surface sediment and water samples obtained from Section 4 adjacent to 3M Cottage Grove shoreline, excluding East Cove and West Cove.
- Table 4. Fish bioaccumulation model for Section 4 adjacent to 3M Cottage Grove shoreline.
- Table 5. Concentrations of PFOS in surface sediment and water samples obtained from Section 4 downstream of 3M Cottage Grove.
- Table 6. Fish bioaccumulation model for Section 4 downstream of 3M Cottage Grove.
- Table 7. Tabular and figure summary of the results of the three modeling scenarios.
- Table 8. References cited.

Conclusions

1. Model-predicted concentrations of PFOS in fish compare well with observations from the MPCA (2010) study (Table 7).
2. The model suggests that the modeling scenario for the Mississippi River upstream of 3M Cottage Grove is not expected to result in concentrations of PFOS in fish above 200 ng/g, wet weight (ww) (Table 2), as supported by MPCA (2010) observations.
3. The model suggests that the modeling scenarios for the Mississippi River at and downstream of 3M Cottage Grove is expected to result in concentrations of PFOS in fish above 200 ng/g, wet weight (ww) (Tables 4 and 6), as supported by MPCA (2010) observations.
4. The model predicts that a majority of PFOS accumulated by fish is derived from ingesting sediment invertebrates (Tables 2, 4, 6 and 7); thus, the majority of PFOS in fish tissue is derived from sediment-associated PFOS.

Table 1. Concentrations of PFOS in surface sediment and water samples obtained from Sections 1, 2, 3, and 4 upstream of 3M Cottage Grove.

Sediment Sample	[Sediment PFOS] (ng/g, dw)	Reference	Note	Water Sample	[Water PFOS] (ng/L)	Reference	Note
XS-01a	0.837	Weston, 2007	Section 4 upstream of 3M Cottage Grove	Miss-up	5.14	MPCA, 2006	Section 4
XS-01b	1.34	Weston, 2007	Section 4 upstream of 3M Cottage Grove	1	2.56	MPCA, 2010	Value represents 1/2 DL; Section 1
XS-01c	0.289	Weston, 2007	Section 4 upstream of 3M Cottage Grove	2	2.53	MPCA, 2010	Value represents 1/2 DL; Section 1
XS-01d	0.343	Weston, 2007	Section 4 upstream of 3M Cottage Grove	3	2.53	MPCA, 2010	Value represents 1/2 DL; Section 1
XS-01e	0.472	Weston, 2007	Section 4 upstream of 3M Cottage Grove	4	2.53	MPCA, 2010	Value represents 1/2 DL; Section 2
Sediment upstream	1.57	MPCA, 2006	Section 4 upstream of 3M Cottage Grove	5	2.52	MPCA, 2010	Value represents 1/2 DL; Section 2
LS-821	0.125	Weston, 2007	Value represents 1/2 DL; Section 3	6	7.71	MPCA, 2010	Section 2
LS-824	0.524	Weston, 2007	Section 3	7	10.3	MPCA, 2010	Section 3
				8	8.51	MPCA, 2010	Section 3
				9	2.54	MPCA, 2010	Value represents 1/2 DL; Section 3
				10	2.5	MPCA, 2010	Value represents 1/2 of detection limit; Sample from Section 4 upstream of 3M Cottage Grove

Mean [PFOS Surface Sediment] (ng/g, dw)	0.69
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Mean [PFOS Water] (ng/g, dw)	4.5
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Abbreviations
DL: Detection Limit
dw: dry weight
g: gram
L: Liter

ng: nanogram
PFOS: perfluorooctane sulfonate
ww: wet weight

Note

Sediment samples reported at "NR" (Not Reported) and/or "NQ" (Not Quantifiable) by Weston were not included due to lack of numerical values.

Table 2. Fish bioaccumulation model for Sections 1, 2, 3, and 4 upstream of 3M Cottage Grove.

Model Input Variables				
Item	Abbreviation	Value	Units	Note
Measured [Water PFOS]	Wat	4.5	ng/L	Average of water samples in Sections 1-4, upstream of Cottage Grove.
Measured [Sediment PFOS]	Sed	0.69	ng/g, dw	Average of Section 3 and 4 surface sediment samples upstream of Cottage Grove.
Total organic carbon (OC) in sediment	TOC	0.01	g, OC/g, dw	Organic carbon not measured or data unavailable for sediment samples from Pool 2 investigations of PFOS in sediment. 0.01 (i.e., 1% TOC) represents a standard default modeling assumption for sediment.

Model Constants				
Item	Abbreviation	Value	Units	Note
Biota-Sediment Accumulation Factor (BSAF)	BSAF	1.22	g, OC/g, ww	Lab-derived steady state estimate with invertebrates and spiked sediment.
Bioaccumulation factor (BAF)	BAF	0.32	kg prey, ww/kg predator, ww	Lab-derived steady state estimate (fish carcass) for trout and PFOS-spiked food only exposure.
Bioconcentration Factor (BCF)	BCF	1,100	L/kg, ww	Lab-derived steady state estimate with trout (fish carcass) and PFOS-spiked water only exposure.

Model Predictions				
Item	Abbreviation	Value	Units	Note
[Sediment PFOS], OC-normalized	SedOC	69	ng/g, OC	Sed + TOC
Predicted [Sediment invertebrate PFOS]	Inv	84	ng/g, ww	SedOC × BSAF
[Fish PFOS] from Dietary (Sediment invertebrate) Source	Fsed	27	ng PFOS/g, ww	Inv × BAF
Predicted [Fish PFOS] from Direct Absorption from Water	Fwat	4.9	ng PFOS/g, ww	Wat × BCF ÷ 1,000 g, ww/kg, ww
Total [PFOS Fish]	F	32	ng PFOS/g, ww	Fsed + Fwat
Percentage of [Fish PFOS] from sediment	%Fsed	84	%	100% × Fsed / F
Percentage of [Fish PFOS] from water	%Fwat	16	%	100% × Fwat / F

Abbreviations

dw: dry weight
g: gram
kg: kilogram

L: Liter

ng: nanogram

OC: organic carbon

PFOS: perfluorooctane sulfonate

ww: wet weight

Reference
Table 1
Table 1

Reference
Higgins et al., 2007
Martin et al., 2003a
Martin et al., 2003b

Table 3. Concentrations of PFOS in surface sediment and water samples obtained from Section 4 adjacent to 3M Cottage Grove shoreline, excluding East Cove and West Cove.

Sediment Sample	[Sediment PFOS] (ng/g, dw)	Reference	Note	Water Sample	[Water PFOS] (ng/L)	Reference	Note
IW01	0.458	Weston, 2007		IW01	25	MPCA, 2006	Value represents 1/2 DL. The DL (50 ng/L) for water analysis in Weston (2007) is 10X higher than other studies examined in this modeling effort.
IW02	0.321	Weston, 2007		IW01	25	Weston, 2007	Value represents 1/2 DL
IW03	0.363	Weston, 2007		IW02	25	Weston, 2007	Value represents 1/2 DL
IW04	0.23	Weston, 2007		IW02	25	Weston, 2007	Value represents 1/2 DL
IW05	0.32	Weston, 2007		IW03	25	Weston, 2007	Value represents 1/2 DL
IW06	0.469	Weston, 2007		IW03	25	Weston, 2007	Value represents 1/2 DL
IW07	0.502	Weston, 2007		IW04	25	Weston, 2007	Value represents 1/2 DL
IW08	0.753	Weston, 2007		IW04	25	Weston, 2007	Value represents 1/2 DL
IW09	0.589	Weston, 2007		IW05	25	Weston, 2007	Value represents 1/2 DL
IW09a	27	Weston, 2007		IW05	25	Weston, 2007	Value represents 1/2 DL
IW09b	1.6	Weston, 2007		IW06	25	Weston, 2007	Value represents 1/2 DL
IW09c	0.802	Weston, 2007		IW06	25	Weston, 2007	Value represents 1/2 DL
IW09d	0.358	Weston, 2007		IW07	25	Weston, 2007	Value represents 1/2 DL
IW09e	0.279	Weston, 2007		IW07	25	Weston, 2007	Value represents 1/2 DL
IW09f	0.737	Weston, 2007		IW08	25	Weston, 2007	Value represents 1/2 DL
IW10	1.37	Weston, 2007		IW08	25	Weston, 2007	Value represents 1/2 DL
IW11	4.84	Weston, 2007		IW09	162	Weston, 2007	
IW12	4.12	Weston, 2007		IW09	183	Weston, 2007	
IW13	3.62	Weston, 2007		IW09a	25	Weston, 2007	Value represents 1/2 DL
IW14	4.2	Weston, 2007		IW09a	25	Weston, 2007	Value represents 1/2 DL
IW14a	74.5	Weston, 2007		IW09b	25	Weston, 2007	Value represents 1/2 DL
IW14c	10.4	Weston, 2007		IW09b	25	Weston, 2007	Value represents 1/2 DL
IW14d	0.125	Weston, 2007	Value represents 1/2 DL	IW09c	25	Weston, 2007	Value represents 1/2 DL
IW14e	0.125	Weston, 2007	Value represents 1/2 DL	IW09c	25	Weston, 2007	Value represents 1/2 DL
IW14f	0.513	Weston, 2007		IW09d	25	Weston, 2007	Value represents 1/2 DL
IW15	1.31	Weston, 2007		IW09d	25	Weston, 2007	Value represents 1/2 DL
IW16	0.654	Weston, 2007		IW09e	25	Weston, 2007	Value represents 1/2 DL
IW17	1.47	Weston, 2007		IW09e	25	Weston, 2007	Value represents 1/2 DL
IW18	3.17	Weston, 2007		IW09f	25	Weston, 2007	Value represents 1/2 DL
IW19	3.53	Weston, 2007		IW09f	25	Weston, 2007	Value represents 1/2 DL

IV19a	44.3	Weston, 2007	IV10	25	Weston, 2007	Value represents 1/2 DL
IV19b	6.86	Weston, 2007	IV11	113	Weston, 2007	
IV19c	1.81	Weston, 2007	IV12	25	Weston, 2007	Value represents 1/2 DL
IV19d	0.295	Weston, 2007	IV12	25	Weston, 2007	Value represents 1/2 DL
IV19e	0.535	Weston, 2007	IV13	53.9	Weston, 2007	
IV19f	1.42	Weston, 2007	IV13	59.4	Weston, 2007	
IV20	1.42	Weston, 2007	IV14	25	Weston, 2007	Value represents 1/2 DL
IV21	1.35	Weston, 2007	IV14a	111	Weston, 2007	
IV23	17.4	Weston, 2007	IV14a	130	Weston, 2007	
IV24	30.7	Weston, 2007	IV14b	63.1	Weston, 2007	
R3	8.28	Weston, 2008	IV14b	57.8	Weston, 2007	
SAB01	0.125	Weston, 2009	IV14c	25	Weston, 2007	Value represents 1/2 DL
SAB03	0.125	Weston, 2009	IV14d	25	Weston, 2007	Value represents 1/2 DL
SAB04	219	Weston, 2009	IV14d	25	Weston, 2007	Value represents 1/2 DL
SAB05	0.125	Weston, 2009	IV14e	25	Weston, 2007	Value represents 1/2 DL
SAB06	0.125	Weston, 2009	IV14e	25	Weston, 2007	Value represents 1/2 DL
SAB07	0.125	Weston, 2009	IV14f	25	Weston, 2007	Value represents 1/2 DL
SAB08	0.125	Weston, 2009	IV14f	25	Weston, 2007	Value represents 1/2 DL
			IV15	60.2	Weston, 2007	
			IV15	25	Weston, 2007	Value represents 1/2 DL
			IV16	155	Weston, 2007	
			IV17	116	Weston, 2007	
			IV17	122	Weston, 2007	
			IV18	115	Weston, 2007	
			IV18	110	Weston, 2007	
			IV19	105	Weston, 2007	
			IV19	96.6	Weston, 2007	
			IV19a	214	Weston, 2007	
			IV19a	206	Weston, 2007	
			IV19b	127	Weston, 2007	
			IV19b	88.9	Weston, 2007	
			IV19c	54.5	Weston, 2007	
			IV19d	25	Weston, 2007	Value represents 1/2 DL
			IV19d	25	Weston, 2007	Value represents 1/2 DL
			IV19e	25	Weston, 2007	Value represents 1/2 DL
			IV19e	25	Weston, 2007	Value represents 1/2 DL
			IV19f	25	Weston, 2007	Value represents 1/2 DL
			IV19f	25	Weston, 2007	Value represents 1/2 DL
			IV20	112	Weston, 2007	Value represents 1/2 DL
			IV20	118	Weston, 2007	

				IW/21	413 Weston, 2007	
				IW/21	436 Weston, 2007	
				IW/22	523 Weston, 2007	
				IW/22	539 Weston, 2007	
				IW/23	323 Weston, 2007	
				IW/23	350 Weston, 2007	
				IW/24	114 Weston, 2007	
				IW/24	466 Weston, 2007	
				IW/25	94.5 Weston, 2007	
				IW/25	102 Weston, 2007	
				R2	25 Weston, 2008	
				R3	25 Weston, 2008	
				R4	25 Weston, 2008	
				11	90.07 MPCA, 2010	11

Mean [PFOS Surface Sediment] (ng/g, dw)	10
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Mean [PFOS Water] (ng/g, dw)	88
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Abbreviations

DL: Detection Limit

dw: dry weight

g: gram

L: Liter

ng: nanogram

PFOS: perfluorooctane sulfonate

ww: wet weight

Note

Sediment samples reported at "NR" (Not Reported) and/or "NQ" (Not Quantifiable) by Weston were not included due to lack of numerical values.

Table 4. Fish bioaccumulation model for Section 4 adjacent to 3M Cottage Grove shoreline.

Model Input Variables				
Item	Abbreviation	Value	Units	Note
Measured [Water PFOS]	Wat	88	ng/L	Average of water samples in Section 4 adjacent to 3M Cottage Grove shoreline.
Measured [Sediment PFOS]	Sed	10	ng/g, dw	Average of surface sediment samples in Section 4 adjacent to 3M Cottage Grove shoreline
Total organic carbon (OC) in sediment	TOC	0.01	g, OC/g, dw	Organic carbon not measured or data unavailable for sediment samples from Pool 2 investigations of PFOS in sediment. 0.01 (i.e., 1% TOC) represents a standard default modeling assumption for sediment.

Model Constants				
Item	Abbreviation	Value	Units	Note
Biota-Sediment Accumulation Factor (BSAF)	BSAF	1.22	g, OC/g, ww	Lab-derived steady state estimate with invertebrates and spiked sediment.
Bioaccumulation factor (BAF)	BAF	0.32	kg prey, ww/kg predator, ww	Lab-derived steady state estimate (fish carcass) for trout and PFOS-spiked food only exposure.
Bioconcentration Factor (BCF)	BCF	1,100	L/kg, ww	Lab-derived steady state estimate with trout (fish carcass) and PFOS-spiked water only exposure.

Model Predictions				
Item	Abbreviation	Value	Units	Note
[Sediment PFOS], OC-normalized	SedOC	1,006	ng/g, OC	Sed ÷ TOC
Predicted [Sediment invertebrate PFOS]	Inv	1,227	ng/g, ww	SedOC × BSAF
[Fish PFOS] from Dietary (Sediment invertebrate) Source	Fsed	393	ng PFOS/g, ww	Inv × BAF
Predicted [Fish PFOS] from Direct Absorption from Water	Fwat	97.0	ng PFOS/g, ww	Wat × BCF ÷ 1,000 g, ww/kg, ww
Total [PFOS Fish]	F	490	ng PFOS/g, ww	Fsed + Fwat
Percentage of [Fish PFOS] from sediment	%Fsed	80	%	100% × Fsed / F
Percentage of [Fish PFOS] from water	%Fwat	20	%	100% × Fwat / F

Abbreviations

dw: dry weight
g: gram
kg: kilogram

L: Liter

ng: nanogram

OC: organic carbon

PFOS: perfluorooctane sulfonate

ww: wet weight

Reference
Table 3
Table 3

Reference
Higgins et al., 2007
Martin et al., 2003a
Martin et al., 2003b

Table 5. Concentrations of PFOS in surface sediment and water samples obtained from Section 4 downstream of 3M Cottage Grove.

Sediment Sample	[Sediment PFOS] (ng/g, dw)	Reference	Note	Water Sample	[Water PFOS] (ng/L)	Reference	Note
XS-02a	2.31	Weston, 2007		Miss-down #1	14.5	MPCA, 2006	
XS-02a	2.66	Weston, 2007		Miss-down #2	6	MPCA, 2006	
XS-02b	0.603	Weston, 2007		Miss-down #3	2.555	MPCA, 2006	Value represents 1/2 DL
XS-02c	0.798	Weston, 2007		12	15	MPCA, 2010	
XS-02d	0.702	Weston, 2007		R5	98	Weston, 2008	
XS-02e	1.24	Weston, 2007					
Sed-Miss-down #1	27.9	MPCA, 2006					
Sed-Miss-down #2	8.26	MPCA, 2006					
Sed-Miss-down #3	1.71	MPCA, 2006					
R5	6.13	Weston, 2008					
R6	1.35	Weston, 2008					

Mean [PFOS Surface Sediment] (ng/g, dw)	4.9
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Mean [PFOS Water] (ng/g, dw)	27
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Abbreviations

DL: Detection Limit
dw: dry weight
g: gram
L: Liter
ng: nanogram
PFOS: perfluorooctane sulfonate

www: wet weight

Note

Sediment samples reported at "NR" (Not Reported) and/or "NQ" (Not Quantifiable) by Weston were not included due to lack of numerical values.

Table 6. Fish bioaccumulation model for Section 4 Section 4 downstream of 3M Cottage Grove.

Model Input Variables				
Item	Abbreviation	Value	Units	Note
Measured [Water PFOS]	Wat	27	ng/L	Average of water samples in Section 4 adjacent to 3M Cottage Grove shoreline.
Measured [Sediment PFOS]	Sed	5	ng/g, dw	Average of surface sediment samples in Section 4 adjacent to 3M Cottage Grove shoreline
Total organic carbon (OC) in sediment	TOC	0.01	g, OC/g, dw	Organic carbon not measured or data unavailable for sediment samples from Pool 2 investigations of PFOS in sediment. 0.01 (i.e., 1% TOC) represents a standard default modeling assumption for sediment.

Model Constants				
Item	Abbreviation	Value	Units	Note
Biota-Sediment Accumulation Factor (BSAF)	BSAF	1.22	g, OC/g, ww	Lab-derived steady state estimate with invertebrates and spiked sediment.
Bioaccumulation factor (BAF)	BAF	0.32	kg prey, ww/kg predator, ww	Lab-derived steady state estimate (fish carcass) for trout and PFOS-spiked food only exposure.
Bioconcentration Factor (BCF)	BCF	1,100	L/kg, ww	Lab-derived steady state estimate with trout (fish carcass) and PFOS-spiked water only exposure.

Model Predictions				
Item	Abbreviation	Value	Units	Note
[Sediment PFOS], OC-normalized	SedOC	488	ng/g, OC	Sed + TOC
Predicted [Sediment invertebrate PFOS]	Inv	595	ng/g, ww	SedOC × BSAF
[Fish PFOS] from Dietary (Sediment invertebrate) Source	Fsed	190	ng PFOS/g, ww	Inv × BAF
Predicted [Fish PFOS] from Direct Absorption from Water	Fwat	29.9	ng PFOS/g, ww	Wat × BCF ÷ 1,000 g, ww/kg, ww
Total [PFOS Fish]	F	220	ng PFOS/g, ww	Fsed + Fwat
Percentage of [Fish PFOS] from sediment	%Fsed	86	%	100% × Fsed / F
Percentage of [Fish PFOS] from water	%Fwat	14	%	100% × Fwat / F

Abbreviations

dw: dry weight
g: gram
kg: kilogram

L: Liter

ng: nanogram

OC: organic carbon

PFOS: perfluorooctane sulfonate

ww: wet weight

Reference
Table 5
Table 5

Reference
Higgins et al., 2007
Martin et al., 2003a
Martin et al., 2003b

Table 7. Tabular and figure summary of the results of the three modeling scenarios.

Model Scenario	Predicted [Fish PFOS]				Observed [Fish]		Note	Observed cc Midpoint
	Sediment Source	Water Source	Total	% from Sediment	Minimum Average	Maximum Average		
Pool 2 Upstream of 3M Cottage Grove	27	4.9	32	84	24	100	Fish from Sections 1-3	62
Pool 2 Section 4: 3M Cottage Grove (Shoreline)	393	97	490	80	160	740	Fish from Section 4	450
Pool 2 Section 4: Downstream of 3M Cottage Grove	190	30	220	86	160	740	Fish from Section 4	450

For Graphing
Pool 2
Upstream of
3M Cottage
Grove

Pool 2
Section 4: 3M
Cottage Grove
(Shoreline)

Pool 2
Section 4:
Downstream
of 3M Cottage
Grove

Abbreviations

g: gram
ng: nanogram
PFOS: perfluorooctane sulfonate
ww: wet weight

Concentrations (for
Low (-) High (+)

38 38

290 290

290 290

Model 27 5

Observed 0 62 38
Model 393 97

Observed 0 450 290
Model 190 30

Observed 0 450 290

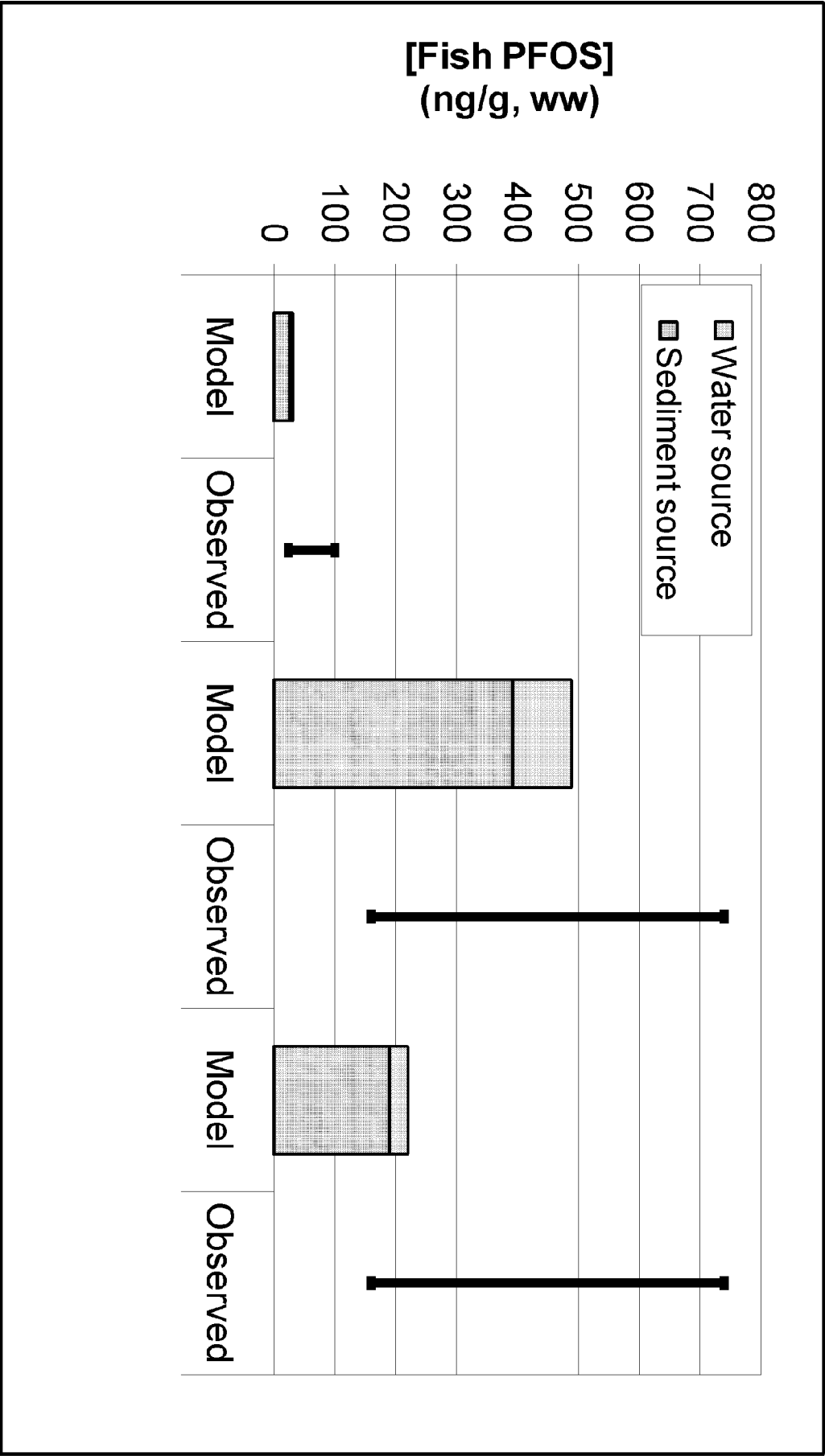


Table 8. References cited.

- Higgins, C.P., McLeod, P.B., MacManus-Spencer, L.A., Luthy, R.G. 2007. Bioaccumulation of perfluorochemicals in sediments by the aquatic oligochaete *Lumbriculus variegatus*. Environ. Sci. Technol. 41:4600-4606.
- Martin, J.W., Mabury, S.A., Solomon, K.R., Muir, D.C.G. 2003a. Dietary accumulation of perfluorinated acids in juvenile rainbow trout (*Oncorhynchus mykiss*). Environ. Toxicol. Chem. 22:189-195
- Martin, J.W., Mabury, S.A., Solomon, K.R., Muir, D.C.G. 2003b. Bioconcentration and tissue distribution of perfluorinated acids in rainbow trout (*Oncorhynchus mykiss*). Environ. Toxicol. Chem. 22:196-204.
- MPCA. 2006. INVESTIGATION OF PERFLUOROCHEMICAL (PFC) CONTAMINATION IN MINNESOTA PHASE ONE, Report to Senate Environment Committee.
- MPCA. 2010. Mississippi River Pool 2 Intensive Study of Perfluorochemicals in Fish and Water: 2009. 8 March.
- Weston. 2007. REMEDIAL INVESTIGATION REPORT, PHASE 2, FLUOROCHEMICAL (FC) DATA ASSESSMENT REPORT FOR THE COTTAGE GROVE, MN SITE. June.
- Weston. 2008. Feasibility Study, Cottage Grove Site, Cottage Grove, MN. March.
- Weston. 2009. Feasibility Study Report Addendum No. 2, (Pre-Design Data Report and Alternative Refinement), Cottage Grove Site, Cottage Grove, MN. January.