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 if 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 Section 4 downstream of 3M Cottage Grove.
Table 7. Tabular and figure symmary 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**

Mean [PFOS Water] (ng/g, dw)	**4.5**

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	**Abbre-viation**	**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	**Abbre-viation**	**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	**Abbre-viation**	**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		W09f	25	Weston, 2007	Value represents 1/2 DL
IW19	3.53	Weston, 2007		W09f	25	Weston, 2007	Value represents 1/2 DL

IW19a	44.3	Weston, 2007		IW10	25	Weston, 2007	Value represents 1/2 DL
IW19b	6.86	Weston, 2007		IW11	113	Weston, 2007	
IW19c	1.81	Weston, 2007		IW12	25	Weston, 2007	Value represents 1/2 DL
IW19d	0.295	Weston, 2007		IW12	25	Weston, 2007	Value represents 1/2 DL
IW19e	0.535	Weston, 2007		IW13	53.9	Weston, 2007	
IW19f	1.42	Weston, 2007		IW13	59.4	Weston, 2007	
IW20	1.42	Weston, 2007		IW14	25	Weston, 2007	Value represents 1/2 DL
IW21	1.35	Weston, 2007		IW14a	111	Weston, 2007	
IW23	17.4	Weston, 2007		IW14a	130	Weston, 2007	
IW24	30.7	Weston, 2007		IW14b	63.1	Weston, 2007	
R3	8.28	Weston, 2008		IW14b	57.8	Weston, 2007	
SAB01	0.125	Weston, 2009		IW14c	25	Weston, 2007	Value represents 1/2 DL
SAB03	0.125	Weston, 2009		IW14d	25	Weston, 2007	Value represents 1/2 DL
SAB04	219	Weston, 2009		IW14d	25	Weston, 2007	Value represents 1/2 DL
SAB05	0.125	Weston, 2009		IW14e	25	Weston, 2007	Value represents 1/2 DL
SAB06	0.125	Weston, 2009		IW14e	25	Weston, 2007	Value represents 1/2 DL
SAB07	0.125	Weston, 2009		IW14f	25	Weston, 2007	Value represents 1/2 DL
SAB08	0.125	Weston, 2009		IW14f	25	Weston, 2007	Value represents 1/2 DL
				IW15	60.2	Weston, 2007	
				IW15	25	Weston, 2007	Value represents 1/2 DL
				IW16	155	Weston, 2007	
				IW17	116	Weston, 2007	
				IW17	122	Weston, 2007	
				IW18	115	Weston, 2007	
				IW18	110	Weston, 2007	
				IW19	105	Weston, 2007	
				IW19	96.6	Weston, 2007	
				IW19a	214	Weston, 2007	
				IW19a	206	Weston, 2007	
				IW19b	127	Weston, 2007	
				IW19b	88.9	Weston, 2007	
				IW19c	54.5	Weston, 2007	
				IW19d	25	Weston, 2007	Value represents 1/2 DL
				IW19d	25	Weston, 2007	Value represents 1/2 DL
				IW19e	25	Weston, 2007	Value represents 1/2 DL
				IW19e	25	Weston, 2007	Value represents 1/2 DL
				IW19f	25	Weston, 2007	Value represents 1/2 DL
				IW19f	25	Weston, 2007	Value represents 1/2 DL
				IW20	112	Weston, 2007	
				IW20	118	Weston, 2007	

				IW21	413	Weston, 2007	
				IW21	436	Weston, 2007	
				IW22	523	Weston, 2007	
				IW22	539	Weston, 2007	
				IW23	323	Weston, 2007	
				IW23	350	Weston, 2007	
				IW24	114	Weston, 2007	
				IW24	466	Weston, 2007	
				IW25	94.5	Weston, 2007	
				IW25	102	Weston, 2007	
				R2	25	Weston, 2008	
				R3	25	Weston, 2008	
				R4	25	Weston, 2008	
				11	90.07	MPCA, 2010	

Mean [PFOS Surface Sediment] (ng/g, dw)	**10**

Mean [PFOS Water] (ng/g, dw)	**88**

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	**Abbre-viation**	**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	**Abbre-viation**	**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	**Abbre-viation**	**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

Mean [PFOS Water] (ng/g, dw)	27

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

Model Input Variables				
Item	**Abbre-viation**	**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	**Abbre-viation**	**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	**Abbre-viation**	**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 symmary of the results of the three modeling scenarios.

Model Scenario	Predicted [Fish PFOS] Sediment Source	Water Source	Total	% from Sediment	Observed [Fish Minimum Average	Maximum Average	Note	Observed cc Midpoint
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

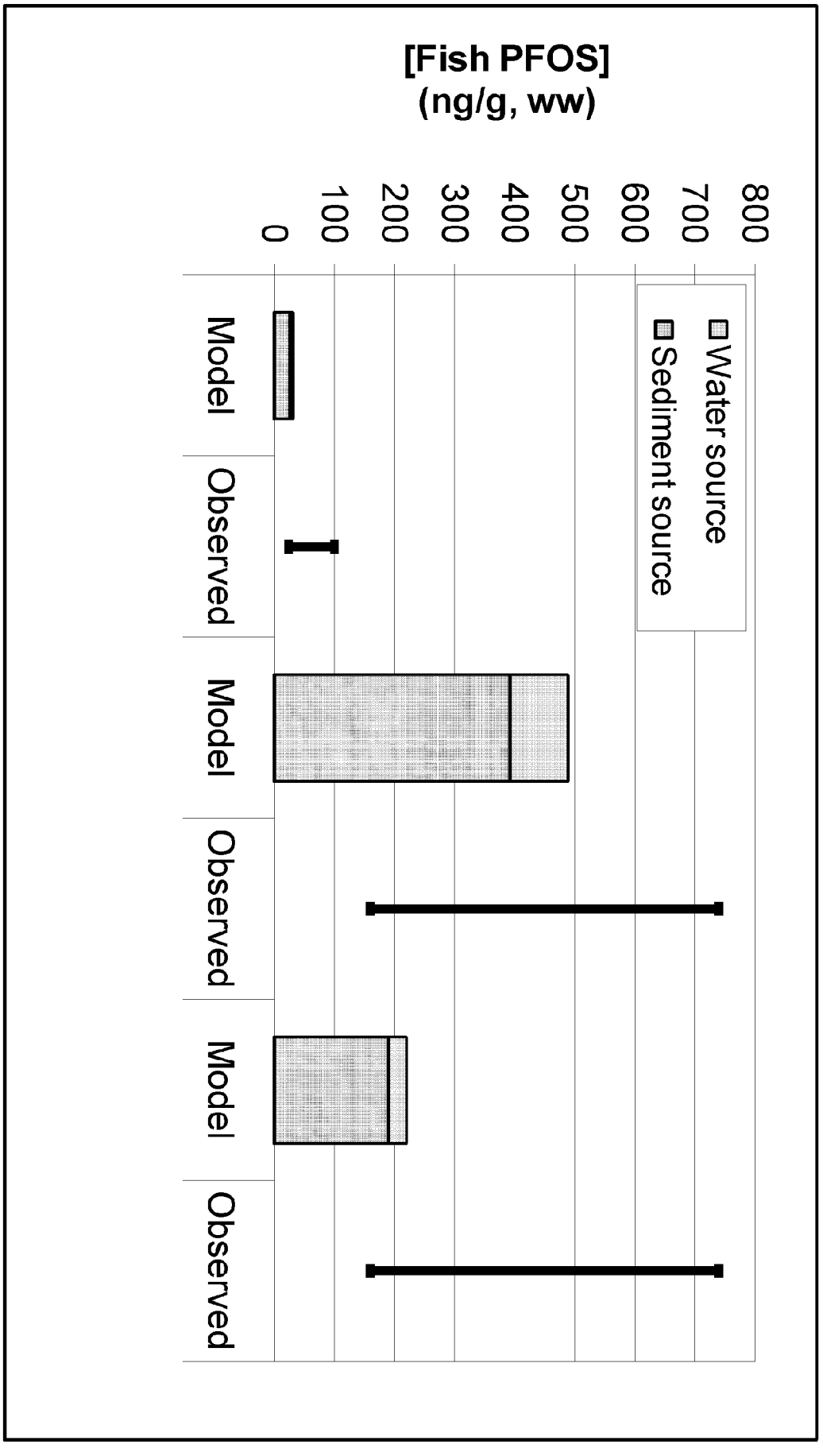
Pool 2 Section 4: 3M Cottage Grove (Shoreline)

Pool 2 Section 4: Downstream of 3M Cottage Grove

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

)ncentrations (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



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