APPENDIX I

Bioaccumulation Modeling Using C_{free}

BIOACCUMULATION MODELING USING C_{FREE}

INTRODUCTION

The laboratory bioaccumulation study exposed live organisms and SPMEs to subtidal plot ENR and ENR+AC material collected in Year 3. A main goal of this study was to compare PCB concentrations accumulated by the live organisms after exposure to ENR and ENR+AC sediment cores, providing a biological line of evidence to assess the potential difference in PCB bioavailability as a result of adding AC to ENR. SPME passive samplers were also added to the cores alongside organisms, enabling a comparison of the differences in porewater PCB concentrations (total C_{free} PCBs) after exposure to ENR and ENR+AC sediment cores. As noted in the main text, both SPME and tissue measurements confirmed there was no difference in PCB bioavailability between the subtidal ENR and ENR+AC subplots. This confirms observations in the *ex situ* SPME measurements made in Year 3. Additionally, it suggests that the SPME line of evidence corresponds to PCB bioavailability.

This appendix further evaluates the correlation between C_{free} PCB measurements made with SPMEs and concentrations in tissues. The goal of this evaluation was to determine if SPME passive sampler measurements of C_{free} are representative of bioavailability, as measured using concentrations of PCBs in tissues of clams and polychaetes exposed in the Year 3 laboratory bioaccumulation study.

C_{FREE} VERSUS CONCENTRATIONS IN TISSUE

PCB C_{free} from the bioaccumulation study was correlated with concentrations of PCBs in polychaetes and clams. To fully evaluate the data and allow the evaluation of more than just six sample points (i.e., total PCBs for the three ENR samples and the three ENR+AC samples), detected results from all individual PCB congeners were compared between SPME and tissue samples. Regressions were noted for the plots of PCB congener C_{free} versus concentrations in polychaetes and PCB congener C_{free} versus concentrations in clams (Figure 1), with r^2 values of 0.50 and 0.57, respectively.

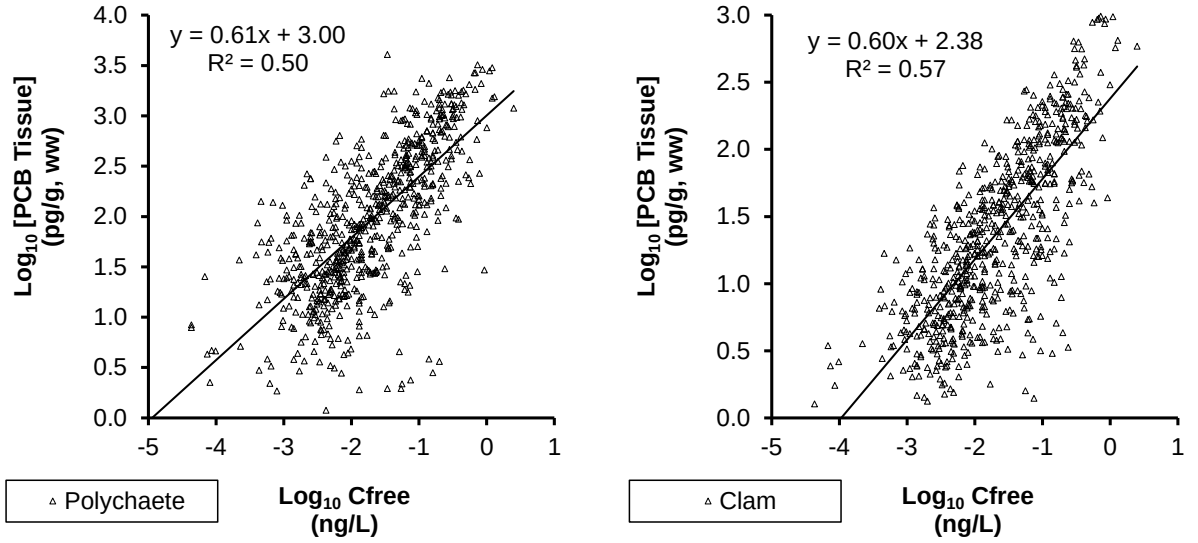

Figure 1. Log-Log comparison of concentrations of PCB congeners in polychaetes and clams compared to C_{free} PCBs in the subtidal ENR and subtidal ENR+AC cores from the laboratory bioaccumulation study.

Compared to measurements of PCBs in bulk sediment, C_{free} PCBs does a much better job of predicting the concentration of PCBs in tissue. Poor regression relationships were found for the plots of concentrations of PCBs in bulk sediment versus concentrations in polychaetes and clams (Figure 2), with r^2 values of 0.06 and 0.08, respectively. This is not surprising as the amount and type of carbon in the samples influences this relationship.

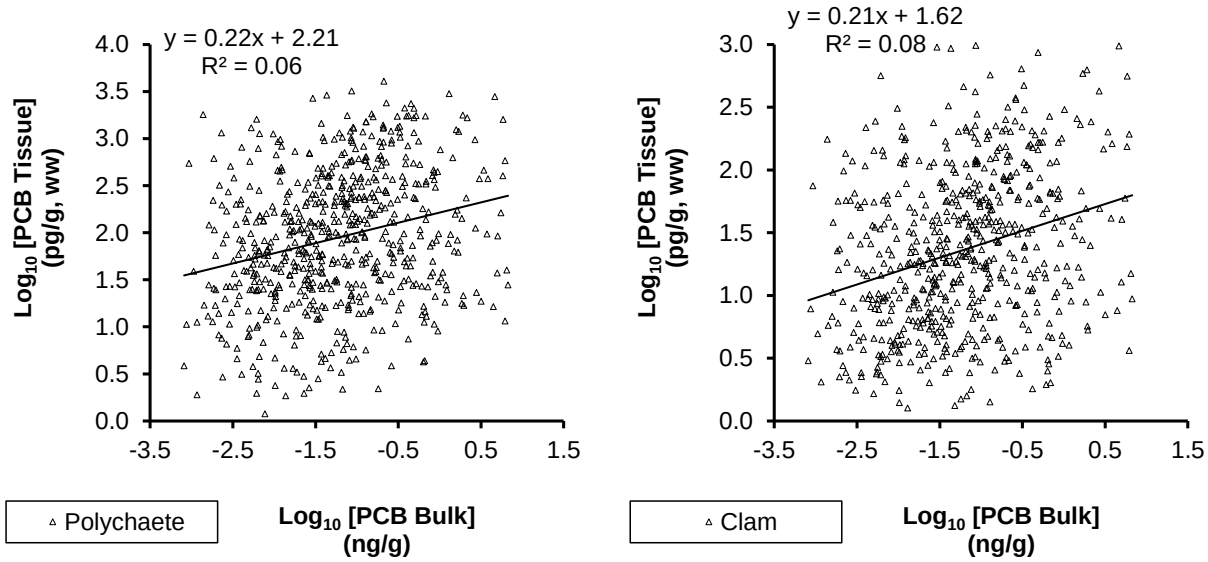

Figure 2. Log-Log comparison of concentrations of PCB congeners in polychaetes and clams compared to concentrations of PCBs in bulk sediment the subtidal ENR and subtidal ENR+AC cores from the laboratory bioaccumulation study.

Extremely strong relations hips (e.g., as indicated by r^2 values of 0.95, 0.99, or other high values) are not necessarily expected between PCB C_{free} and concentrations in biota, as C_{free} measurements reflects PCB bioavailability in sediment porewater, external to the organism. Concentrations of PCBs in tissue reflect uptake of bioavailable PCBs, which is also governed by bioaccumulation processes and uptake and depuration rates that are independent of concentrations or availability conditions external to the organism. Examining congener fingerprints illustrates this point. The concentrations of individual detected PCB congeners for C_{free} and polychaetes in sample ENR+AC replicate C are shown in Figure 3 as an example[1]. In this figure, concentrations are shown for each of the congeners, plotted from PCB-1 (a monochlorinated biphenyl) on the left to PCB-209 (a decachlorinated biphenyl) on the right. C_{free} for the example sediment sample are enriched in the less-chlorinated PCB congeners (trichlorinated and tetrachlorinated biphenyls), which are consequently less hydrophobic (more water soluble). In contrast, PCBs in polychaetes exposed to this sediment are more enriched in the mid-range PCB congeners (tetrachlorinated, pentachlorinated, and hexachlorinated biphenyls) which are intermediate in hydrophobicity between the less chlorinated congeners and very hydrophobic congeners.

[1] PCB congener analytes identified in this figure (and other similar figures in this appendix) may represent more than one PCB congener (i.e., an analyte result representing multiple co-eluting PCBs). In these cases, multiple co-eluting PCB congeners are represented by their lowest-numbered PCB congener. Co-eluting congeners can be identified in data tables elsewhere in the Year 3 report.

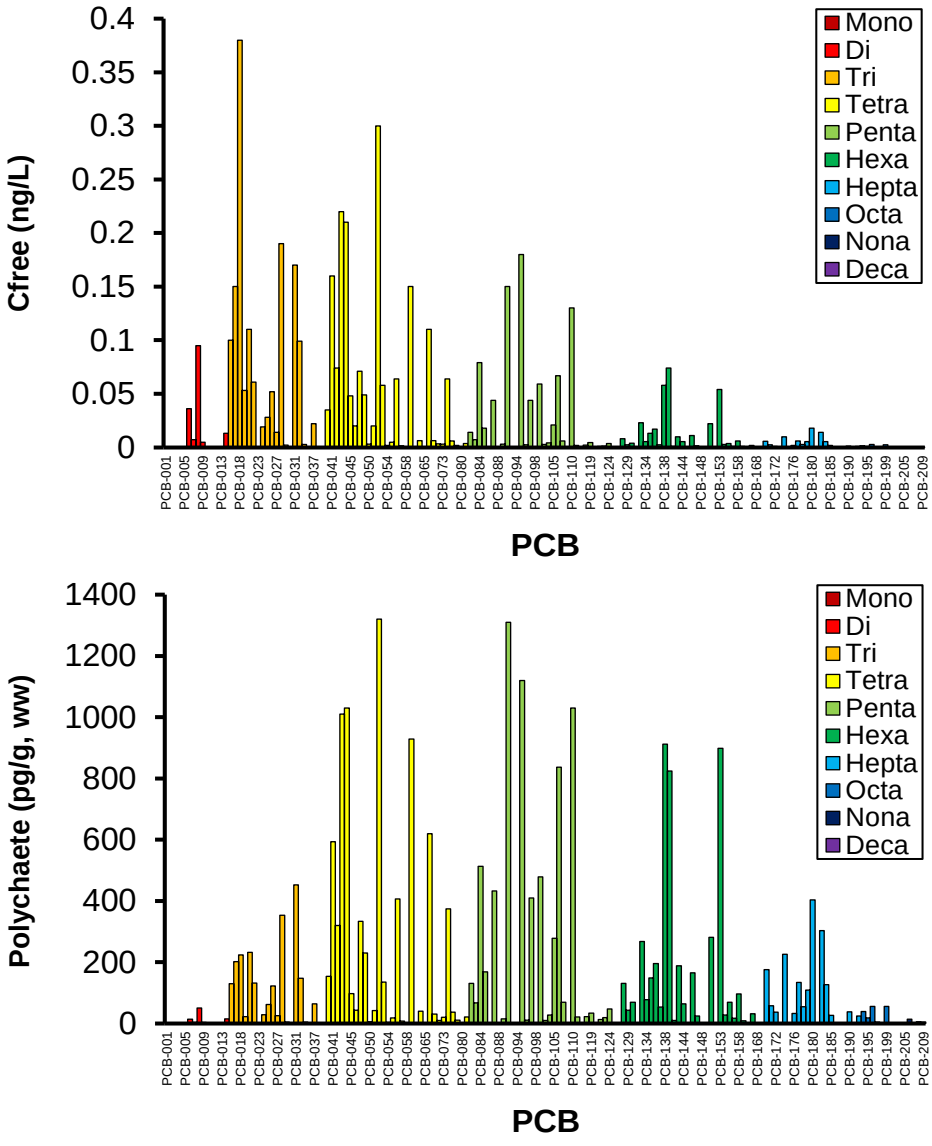

Figure 3. Polychaete and C_{free} PCB congener fingerprint for sample ENR+AC replicate C. Note: the X-axis does not depict every PCB congener label (only every 4th to 5th PCB congener) due to font size limitations.

BIOACCUMULATION MODELING USING C_{FREE} TO PREDICT CONCENTRATIONS IN TISSUE

As noted above, the bioaccumulation process is dependent on external availability (i.e., C_{free}) but also the inherent uptake factor. This uptake factor reflects chemical fugacity, which can be predicted if the hydrophobicity of a compound is known. An uptake factor such as the bioconcentration factor (BCF) can be used to predict equilibrium concentrations of a chemical in an aquatic organism using a measured or assumed concentration in water (or sediment porewater). BCF values for organic chemicals can be predicted using models if the chemicals hydrophobicity (as measured by the log of octanol-water partition coefficients [Log KNOW]) is known. Many

standard bioaccumulation models indicate that BCF values do not necessarily increase with hydrophobicity. BCF values may actually decrease with hydrophobicity for very hydrophobic compounds, as the molecule availability to tissue uptake decreases or the kinetics of the uptake process becomes so slow that equilibrium concentrations are not reached within the typical lifespan or exposure period of an aquatic organism. This relationship can be observed in the Arnot and Gobas Quantitative Structure Activity Relationship (QSAR) 2003 Model (Arnot and Gobas, 2003). This model can predict BCF values for chemicals if Log KOWs of the chemical are provided, as well as other parameters, such as the weight and lipid content of the organism. For this study, Log KOW values were obtained for the PCBs measured in C_{free} and tissues (Table 1). For congeners measured individually, values were obtained from Hawker and Connell (1988). For congeners that co-eluted during measurement, an average Log KOW was estimated (e.g., the Log KOW values for PCB-020 and PCB-021 were averaged since these congeners were measured as a PCB-020/PCB-021 combined analyte). Log KOWs used to generate BCFs are provided in Table 1.

To estimate BCFs for polychaetes, the Log KOWs presented in Table 1 were then input into the Arnot and Gobas (2003) "Arnot-Gobas BCF-BAF Model v1.2" assuming an organism weight of 0.3 g, ww and an organism lipid content of 0.6% (i.e., 0.006 g lipid/g organism). Both these organism-specific values were obtained from averages from polychaete data in the bioaccumulation study. The model-generated BCF values are shown in Table 1 and Figure 4. The model indicates that bioaccumulation is not always higher for the more hydrophobic PCBs. Model BCFs peak at a Log KOW of approximately 7.3 L/kg (Figure 4), predicting bioaccumulation is highest in the heptachlorinated biphenyls rather than the more hydrophobic octa-, nona-, or decachlorinated biphenyls.

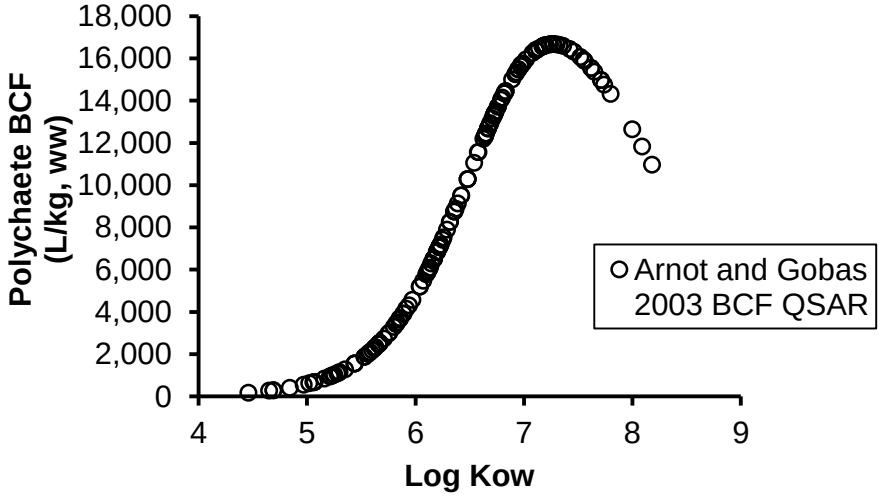

Figure 4. Polychaete BCF values predicted using the Arnot and Gobas (2003) BCF QSAR Model.

The model-generated polychaete BCFs can be used to predict concentrations in polychaetes using C_{free} PCBs for individual PCB congeners. For example, example calculations for C_{free} PCB-018 and PCB-153 measured in ENR+AC replicate C are shown in Figure 5 below.

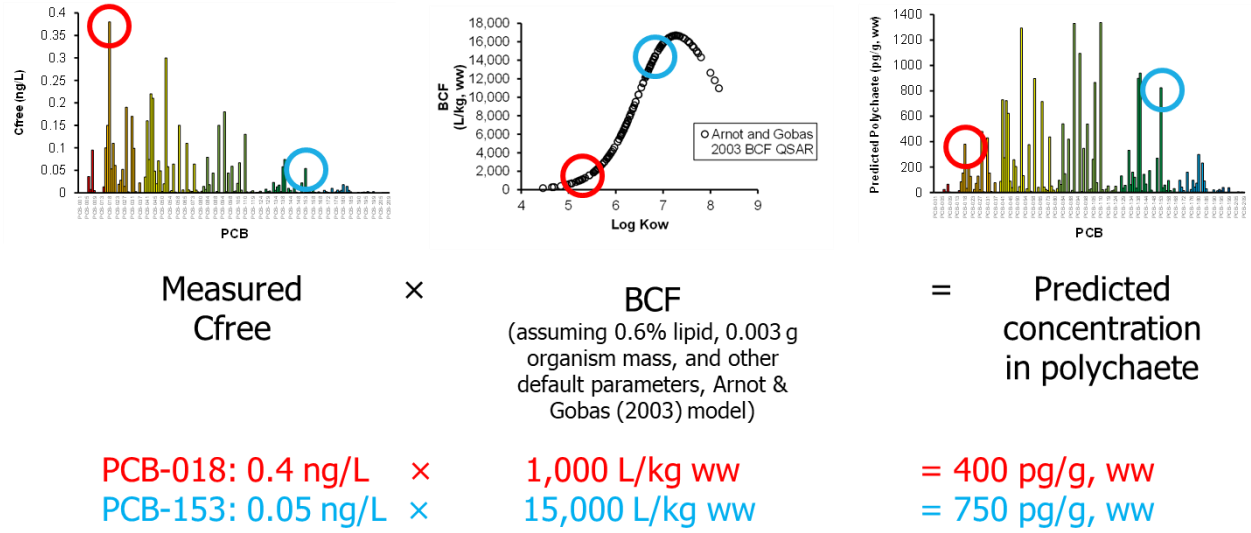

Figure 5. Example calculation of concentrations of PCB-018 and PCB-153 in polychaetes using the measured C_{free} in ENR+AC replicate C and model-generated BCFs (Table 1).

When all detected PCB congener C_{free} measurements in ENR+AC replicate C were used to predict the concentrations of PCB congeners in polychaetes using this approach, the match between the predicted and measured PCB fingerprint (Figure 6) indicates a good model performance. When all PCBs are summed, the concentration of total predicted PCBs (23 ng/g, ww) is also very comparable to that of the measured concentration (24 ng/g, ww), representing a factor or 1.1 difference between measured and predicted values.

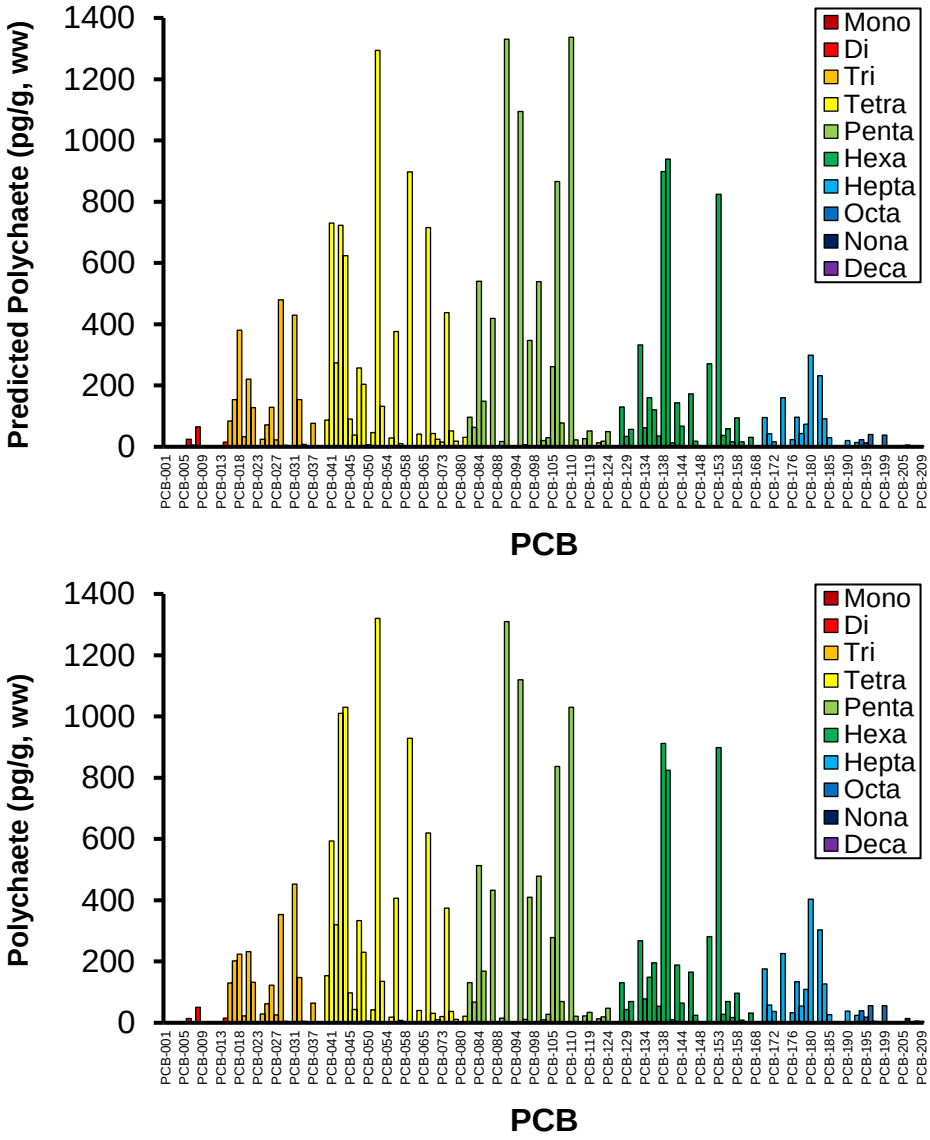

Figure 6. Predicted and measured polychaete PCB congener fingerprints for sample ENR+AC replicate C. Note: the X-axis does not depict every PCB congener label (only every 4th to 5th PCB congener) due to font size limitations.

When the congener-specific C_{free} measurements from all six bioaccumulation study samples are used to predict PCB concentrations in polychaetes, the approach reliably predicts concentrations in polychaetes that are comparable to measured values (Figure 7). Predicted congener-specific tissue concentrations were within a factor of 3 of measured concentrations in 83% of the 699 detected congener measurements.

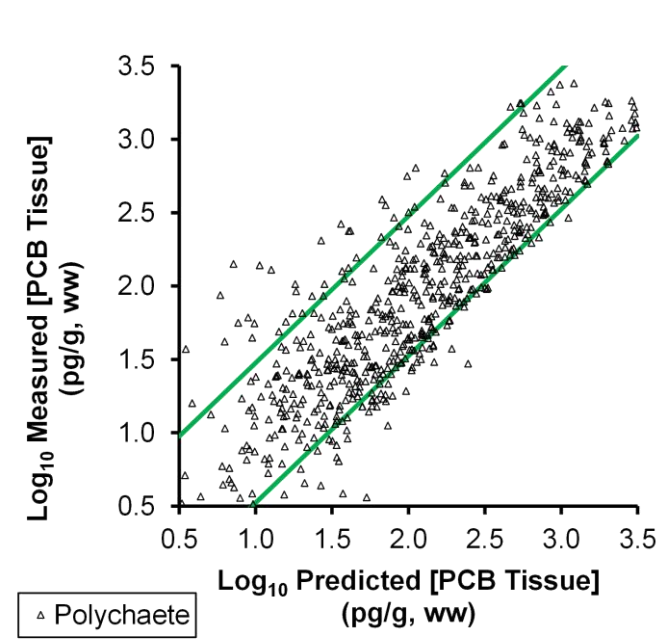

Figure 7. Predicted concentrations of PCB congeners in polychaetes versus measured concentrations for all six ENR and ENR+AC samples from the bioaccumulation study. Note: Symbols in between the green lines indicate predictions that are within a factor of 3 of measured values.

When this comparison is simplified to the total PCBs tissue concentration basis (see table below), all six predicted concentrations in polychaetes were within an approximate factor of 3 of measured values, as shown by the symbols within the green lines in Figure 8. In fact, six predicted concentrations in polychaetes were within a factor of 2 of measured values.

Sample		Concentration of Total PCBs in Polychaetes (ng/g, ww)	
		Predicted	Observed
ENR	A	19	40
ENR	B	115	61
ENR	C	34	31
ENR+AC	A	60	29
ENR+AC	B	35	17
ENR+AC	C	23	24

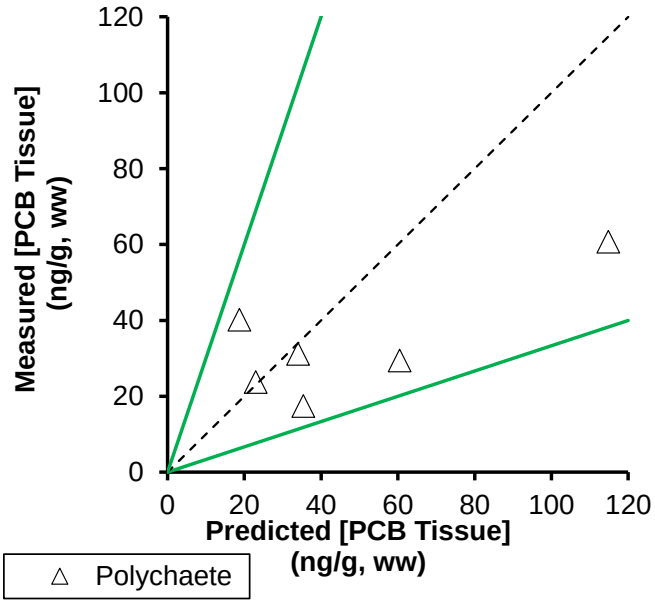

Figure 8. Predicted concentrations of total PCBs in polychaetes versus measured concentrations for all six ENR and ENR+AC samples from the bioaccumulation study. Note: Symbols in between the green lines indicate predictions that are within a factor of 3 of measured values, and the dashed black line is the 1:1 line.

This modeling approach was also conducted to explore the model's ability to predict PCBs concentrations in clam tissue using C_{free} PCBs. To estimate BCFs for clams, the Log KOWs presented in Table 1 were input into the Arnot and Gobas (2003) "Arnot-Gobas BCF-BAF Model v1.2" assuming an organism weight of 7 g, ww and an organism lipid content of 0.2% (i.e., 0.002 g lipid/g organism). Both these organism-specific values were obtained from averages from clams in the bioaccumulation study. The model-generated BCF values are shown in Table 1 and Figure 9. On average, clam BCF values are approximately 3 times less than polychaete BCFs. This is because the lipid content of the clams is approximately 3 times less than that of polychaetes, and lipids are the primary accumulation tissue for hydrophobic organic compounds like PCBs.

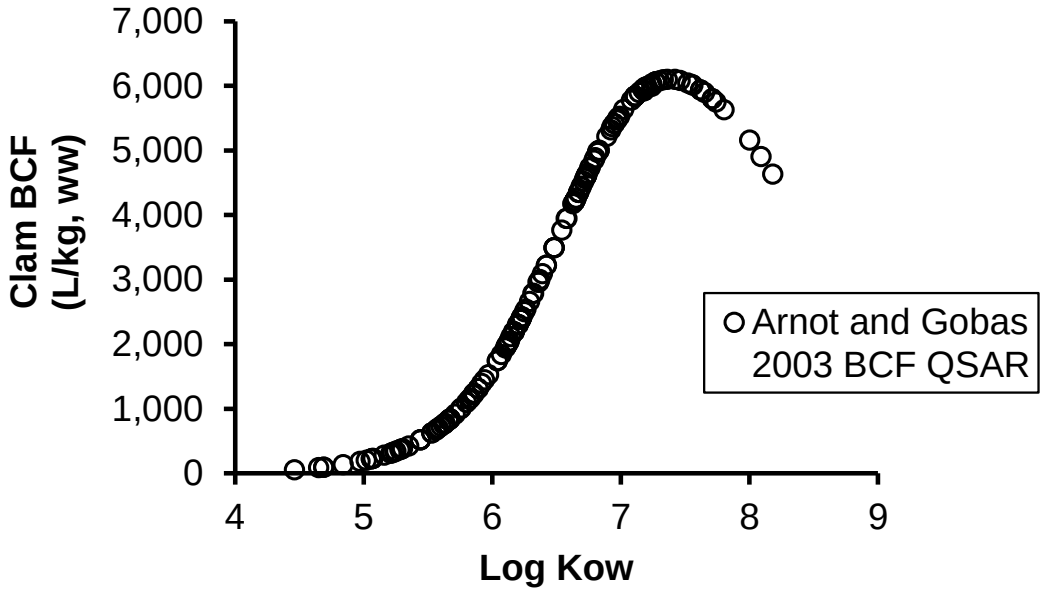

Figure 9. Clam BCF values predicted using the Arnot and Gobas (2003) BCF QSAR Model.

Using the same approach as shown for polychaetes in Figure 5, the concentrations in clams were predicted using C_{free} PCBs for individual PCB congeners from each of the six bioaccumulation study samples (Figure 10). Predicted concentrations were within a factor of 3 of measured concentrations for 72% of the 675 detected congener measurements. When this comparison is simplified to the total concentration of PCBs basis, three of the six predicted concentrations in clams were within an approximate factor of 2 of measured values (all were within a factor of 4).

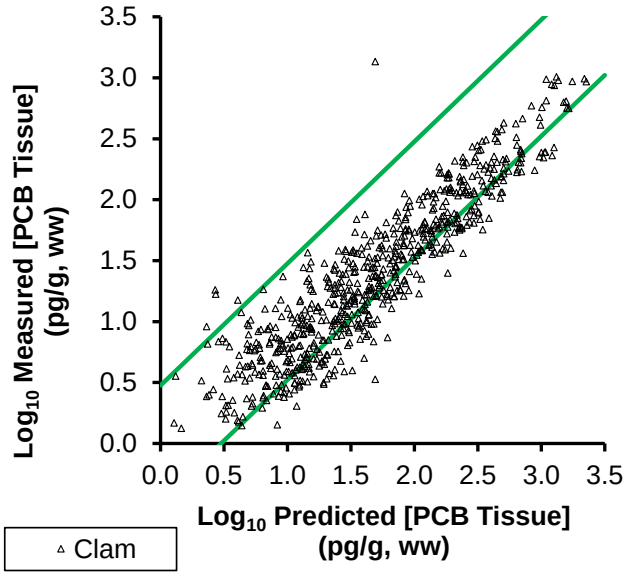

Figure 10. Predicted concentrations of PCB congeners in clams versus measured concentrations for all six ENR and ENR+AC samples from the bioaccumulation study. Note: Symbols in between the green lines indicate predictions that are within a factor of 3 of measured values.

The observed model fit for clams (Figure 10) is not as precise as that observed for polychaetes (Figure 7). Many of the predicted concentrations in clams fall below the lower green line in Figure 10, suggesting that the model tends to predict concentrations that are more than 3 times higher than the measured concentrations. On average, for the concentration of total PCBs, predictions were approximately 2 times higher than measurements.

The tendency of the model to overestimate concentrations in the clam tissue is not completely unexpected given the likely exposure source for the clam. Clams used in the bioaccumulation study (*Mya arenaria*) are filter feeders that siphon water from the surface water overlying the sediment. Some experiments have concluded that the majority of clam chemical exposures in sediment bioassays (and under field conditions) is to the overlying water, not the sediment in which they reside (USACE, 2017). The BCF modeling approach used to generate the predictions shown in Figure 10 assumes that the clams are exposed only to C_{free} PCBs in the top 10 centimeters (cm) of the ENR and ENR+AC layers in which the SPMEs were placed. Thus, the model is likely to overestimate exposure to the clams, considering total C_{free} PCBs in the laboratory-supplied water continuously refreshing the overlying water in the test chambers was 0.003 ng/L, approximately 2,000 to 3,000 times lower than total C_{free} PCB in the ENR and ENR+AC layers.

To account for the likelihood that a significant portion of the clam exposure was to comparatively PCB-free overlying water, it was assumed that 50% of the clam exposure originated in the top 10 cm of the ENR and ENR+AC layers (represented by the SPME measurement of C_{free} PCBs)

and that 50% originated in the overlying water (which was assumed to be negligible). With regards to the bioaccumulation model approach, this equated to multiplying the predicted concentrations in clam tissue by an exposure adjustment factor of 0.5 to reduce the predictions by 50%. Results of the adjusted model (Figure 11) indicate a much better fit than shown in Figure 7. Predicted concentrations with the adjusted model were within a factor of 3 of measured concentrations for 92% of the 675 detected congener measurements.

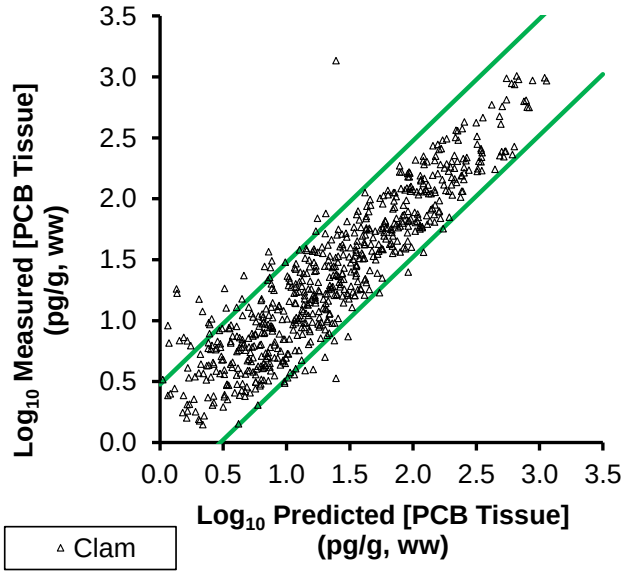

Figure 11. Predicted concentrations of PCB congeners in clams versus measured concentrations for all six ENR and ENR+AC samples from the bioaccumulation study using the 0.5-adjustment factor applied to the model predictions shown in Figure 10. Note: Symbols in between the green lines indicate predictions that are within a factor of 3 of measured values.

When this comparison is simplified to the total concentration of PCBs basis (see table below), all six predicted concentrations in clams were within an approximate factor of 3 of measured values, as shown by the symbols within the green lines in Figure 12. In fact, six predicted concentrations in polychaetes were within a factor of 2 of measured values.

Sample		Concentration of Total PCBs in Clams (ng/g, ww)	
		Predicted	Observed
ENR	A	3.2	3.9
ENR	B	19.5	22.6
ENR	C	5.8	3.9
ENR+AC	A	10.3	5.1
ENR+AC	B	6.1	4.9
ENR+AC	C	3.9	6.7

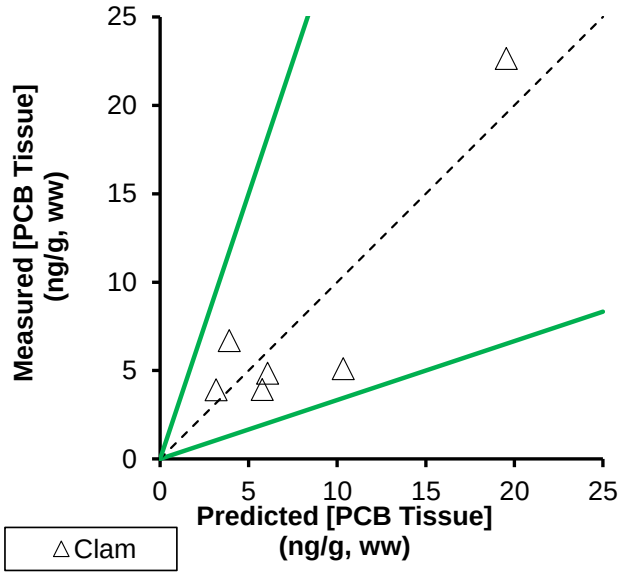

Figure 12. Predicted concentrations of total PCBs in clams versus measured concentrations for all six ENR and ENR+AC samples from the bioaccumulation study (using the 0.5-adjustment factor). Note: Symbols in between the green lines indicate predictions that are within a factor of 3 of measured values, and the dashed black line is the 1:1 line.

As with polychaetes, when all detected PCB congener C_{free} measurements in ENR+AC replicate C were used to predict the concentrations of PCB congeners in clams using this approach, the match between the predicted and measured PCB fingerprint (Figure 13) indicates a good model performance. When all PCBs are summed, the concentration of total predicted PCBs (3.9 ng/g, ww) is also comparable to that of the measured concentration (6.7 ng/g, ww), representing a factor or 1.7 difference between measured and predicted values.

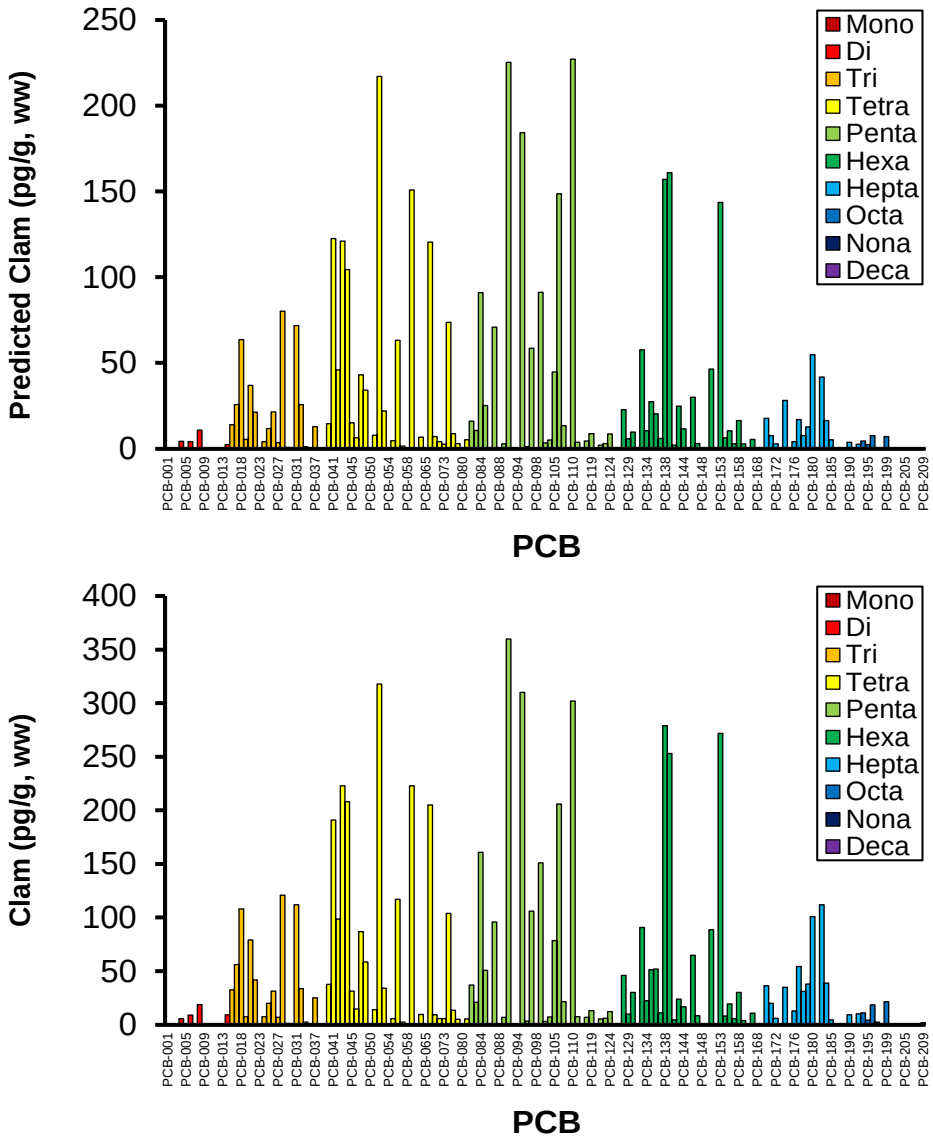

Figure 13. Predicted and measured clam PCB congener fingerprints for sample ENR+AC replicate C. Note: the X-axis does not depict every PCB congener label (only every 4th to 5th PCB congener) due to font size limitations.

BIOACCUMULATION MODELING USING C_{FREE} TO EVALUATE DIFFERENCES BETWEEN ENR AND ENR+AC

This modeling exercise is also helpful in evaluating the differences in ENR and ENR+AC performance in reducing the concentrations of PCBs likely to accumulate in organisms. In general, evaluating ENR versus ENR+AC on the basis of predicted concentrations in tissues yields the same general conclusions as comparing total C_{free} PCBs between ENR and ENR+AC. For example, C_{free} PCB data from the baseline and Year 3 monitoring events at the intertidal plots can

be used to predict concentrations in polychaetes as if they had been measured in a bioaccumulation study:

- For the intertidal ENR+AC subplot, the geomean predicted concentration of total PCBs in polychaetes in the Baseline and Year 3 events were 120 and 5 ng/g, ww, respectively, indicating a 96% reduction in bioavailability from Baseline to Year 3. This 96% reduction in predicted concentrations in polychaetes is similar to the 97% reduction in measured total C_{free} PCBs from Baseline to Year 3.

- For the intertidal ENR subplot, the geomean predicted concentration of total PCBs in polychaetes in the Baseline and Year 3 events were 140 and 11 ng/g, ww, respectively, indicating a 92% reduction in bioavailability from Baseline to Year 3. This 92% reduction was similar to the 95% reduction in total C_{free} PCBs from Baseline Year 3.

As with all environmental modeling, uncertainty is associated with the predictions of the bioaccumulation models with regards to their ability to accurately predict concentrations of PCBs in biota tissues. For example, the model is sensitive to the lipid content of the organism, which is used to derive the BCF values shown in Table 1. For this exercise, the lipid contents were based on measurements in the bioaccumulation test organisms at the beginning of the test. Changes in the lipid content over the duration of the 28-day bioaccumulation test could affect BCF values and model results. Additionally, the assumption that clams were only 50% exposed to the sediment porewater C_{free} (measured by the passive samplers) carries uncertainty. Despite these uncertainties, the model performance was sufficient to confirm a strong quantitative correlation between passive sampling C_{free} measurements and tissue concentrations. Additionally, model uncertainty is low enough to assume that tissues data would have likely yielded the same pilot study conclusions reached for bioaccumulation by comparing total C_{free} PCBs between ENR and ENR+AC. Overall these results show passive samplers provided a good surrogate for evaluating PCB bioavailability and update by benthic organisms to evaluate effectives of ENR+AC compared to ENR alone at this site.

CONCLUSIONS

Results of this evaluation show that passive sampler C_{free} PCB concentrations can be used to accurately indicate PCB bioavailability to worms and clams. This “translation” approach can be used to relate passive sampler C_{free} measurements to concentrations expected in organisms. In general, the above examples indicate that concentrations in biota (if they had been measured in the baseline and post-amendment monitoring events) would indicate the same general pattern of conclusions as using measured C_{free} values with regards to the ability of ENR and ENR+AC to reduce PCB bioavailability. Overall, these results show passive samplers provided a good

surrogate for evaluating PCB bioavailability and uptake by benthic organisms to evaluate effectives of ENR+AC compared to ENR alone.

REFERENCES

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Hawker, D.W., and Connell, D.W., 1988. Octanol-Water Partition Coefficients of Polychlorinated Biphenyl Congeners. Environ. Sci. Technol. 22:382-387.

United States Army Corps of Engineers (USACE), 2017. The Biology of Bioavailability: The Role of Functional Ecology in Exposure Processes, SERDP ER-1750. ERDC/EL TR-17-2. https://www.serdp-estcp.org/content/download/42120/401460/file/ER-1750%20Final%20Report.pdf.

TABLES

Table 1
Log KOW and BCF Values
Used in Predicting Concentrations of PCBs in Polychaetes and Clams using C_{free}

PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-001	Mono	4.46	4.46		173	58
PCB-002	Mono	4.69	4.69		291	98
PCB-003	Mono	4.69	4.69		291	98
PCB-004	Di	4.65	4.65		266	89
PCB-005	Di	4.97	4.97		549	184
PCB-006	Di	5.06	5.06		671	225
PCB-007	Di	5.07	5.07		687	230
PCB-008	Di	5.07	5.07		687	230
PCB-009	Di	5.06	5.06		671	225
PCB-010	Di	4.84	4.84		409	137
PCB-011	Di	5.28	5.28		1,094	366
PCB-012	Di	5.22	5.22		959	321
PCB-013	Di	5.29	5.29		1,119	374
PCB-014	Di	5.28		SPME PRC (not modeled)		
PCB-015	Di	5.30	5.30		1,143	382
PCB-016	Tri	5.16	5.16		839	281
PCB-017	Tri	5.25	5.25		1,024	343
PCB-018	Tri	5.24	5.24		1,002	335
PCB-019	Tri	5.02	5.02		614	205
PCB-020	Tri	5.57	5.56	Average of PCB-020, PCB-021	2,004	670
PCB-021	Tri	5.51		Co-eluting PCB (modeled with other PCB, noted above/below)		
PCB-022	Tri	5.58	5.58		2,091	699
PCB-023	Tri	5.57	5.57		2,047	685
PCB-024	Tri	5.35	5.35		1,276	427
PCB-025	Tri	5.67	5.67		2,523	844

Table 1
Log KOW and BCF Values
Used in Predicting Concentrations of PCBs in Polychaetes and Clams using C_{free}

PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-026	Tri	5.66	5.66		2,471	827
PCB-027	Tri	5.44	5.44		1,551	519
PCB-028	Tri	5.67	5.67		2,523	844
PCB-029	Tri	5.60	5.60		2,181	730
PCB-030	Tri	5.44	5.44		1,551	519
PCB-031	Tri	5.67	5.67		2,523	844
PCB-032	Tri	5.44	5.44		1,551	519
PCB-033	Tri	5.60		Co-eluting PCB (modeled with other PCB, noted above/below)		
PCB-034	Tri	5.66	5.66		2,471	827
PCB-035	Tri	5.82	5.82		3,419	1,145
PCB-036	Tri	5.88		SPME PRC (not modeled)		
PCB-037	Tri	5.83	5.83		3,487	1,168
PCB-038	Tri	5.76	5.76		3,032	1,015
PCB-039	Tri	5.89	5.89		3,921	1,314
PCB-040	Tetra	5.66	5.66		2,471	827
PCB-041	Tetra	5.69	5.97	Average of PCB-041, PCB-064, PCB-071, PCB-072	4,565	1,532
PCB-042	Tetra	5.76	5.86	Average of PCB-042, PCB-059	3,699	1,240
PCB-043	Tetra	5.75	5.80	Average of PCB-043, PCB-049	3,285	1,101
PCB-044	Tetra	5.75	5.75		2,972	995
PCB-045	Tetra	5.53	5.53		1,881	629
PCB-046	Tetra	5.53	5.53		1,881	629
PCB-047	Tetra	5.85	5.85		3,627	1,216
PCB-048	Tetra	5.78	5.92		4,153	1,393

Table 1
Log KOW and BCF Values
Used in Predicting Concentrations of PCBs in Polychaetes and Clams using C_{free}

PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-049	Tetra	5.85		C043		
PCB-050	Tetra	5.63	5.63		2,322	777
PCB-051	Tetra	5.63	5.63		2,322	777
PCB-052	Tetra	5.84	5.94	Average of PCB-052, PCB-069	4,314	1,447
PCB-053	Tetra	5.62	5.62		2,274	761
PCB-054	Tetra	5.21	5.21		938	314
PCB-055	Tetra	6.11	6.11		5,877	1,977
PCB-056	Tetra	6.11	6.11	Average of PCB-056, PCB-060	5,877	1,977
PCB-057	Tetra	6.17	6.17		6,510	2,192
PCB-058	Tetra	6.17	6.17		6,510	2,192
PCB-059	Tetra	5.95		C042		
PCB-060	Tetra	6.11		C056		
PCB-061	Tetra	6.04	6.12	Average of PCB-061, PCB-070	5,980	2,012
PCB-062	Tetra	5.89	5.89		3,921	1,314
PCB-063	Tetra	6.17	6.17		6,510	2,192
PCB-064	Tetra	5.95		C041		
PCB-065	Tetra	5.86	5.86		3,699	1,240
PCB-066	Tetra	6.20	6.17	Average of PCB-066, PCB-076	6,510	2,192
PCB-067	Tetra	6.20	6.20		6,842	2,305
PCB-068	Tetra	6.26	6.26		7,532	2,541
PCB-069	Tetra	6.04		C052		
PCB-070	Tetra	6.20		C061		
PCB-071	Tetra	5.98		C041		
PCB-072	Tetra	6.26		C041		

Table 1
Log KOW and BCF Values
Used in Predicting Concentrations of PCBs in Polychaetes and Clams using C_{free}

PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-073	Tetra	6.04	6.04		5,191	1,744
PCB-074	Tetra	6.20	6.20		6,842	2,305
PCB-075	Tetra	6.05		C048		
PCB-076	Tetra	6.13		C066		
PCB-077	Tetra	6.36	6.36		8,750	2,961
PCB-078	Tetra	6.35		PRC		
PCB-079	Tetra	6.42	6.42		9,511	3,225
PCB-080	Tetra	6.48	6.48		10,283	3,495
PCB-081	Tetra	6.36	6.36		8,750	2,961
PCB-082	Penta	6.20	6.20		6,842	2,305
PCB-083	Penta	6.26	6.36	Average of PCB-083, PCB-112	8,750	2,961
PCB-084	Penta	6.04	6.20	Average of PCB-084, PCB-092	6,842	2,305
PCB-085	Penta	6.30	6.32	Average of PCB-085, PCB-116	8,254	2,790
PCB-086	Penta	6.23	6.23		7,182	2,422
PCB-087	Penta	6.29	6.42	Average of PCB-087, PCB-117, PCB-125	9,511	3,225
PCB-088	Penta	6.07	6.10	Average of PCB-088, PCB-091	5,776	1,942
PCB-089	Penta	6.07	6.07		5,478	1,841
PCB-090	Penta	6.36	6.37	Average of PCB-090, PCB-101	8,876	3,004
PCB-091	Penta	6.13		C088		
PCB-092	Penta	6.35		C084		
PCB-093	Penta	6.04	6.04		5,191	1,744
PCB-094	Penta	6.13	6.13		6,084	2,047

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Log KOW and BCF Values
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PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-095	Penta	6.13	6.13		6,084	2,047
PCB-096	Penta	5.71	5.71		2,739	917
PCB-097	Penta	6.29	6.29		7,889	2,664
PCB-098	Penta	6.13	6.15	Average of PCB-098, PCB-102	6,295	2,119
PCB-099	Penta	6.39	6.39		9,128	3,092
PCB-100	Penta	6.23	6.23		7,182	2,422
PCB-101	Penta	6.38		C090		
PCB-102	Penta	6.16		C098		
PCB-103	Penta	6.22	6.22		7,068	2,383
PCB-104	Penta	5.81		SPME PRC (not modeled)		
PCB-105	Penta	6.65	6.65		12,443	4,262
PCB-106	Penta	6.64	6.69	Average of PCB-106, PCB-118	12,924	4,436
PCB-107	Penta	6.71	6.71	Average of PCB-107, PCB-108	13,159	4,522
PCB-108	Penta	6.71		C107		
PCB-109	Penta	6.48	6.48		10,283	3,495
PCB-110	Penta	6.48	6.48		10,283	3,495
PCB-111	Penta	6.76	6.63	Average of PCB-111, PCB-115	12,197	4,173
PCB-112	Penta	6.45		C083		
PCB-113	Penta	6.54	6.54		11,057	3,767
PCB-114	Penta	6.65	6.65		12,443	4,262
PCB-115	Penta	6.49		C111		
PCB-116	Penta	6.33		C085		
PCB-117	Penta	6.46		C087		
PCB-118	Penta	6.74		C106		

Table 1
Log KOW and BCF Values
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PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-119	Penta	6.58	6.58		11,569	3,948
PCB-120	Penta	6.79	6.79		14,044	4,851
PCB-121	Penta	6.64		SPME PRC (not modeled)		
PCB-122	Penta	6.64	6.64		12,320	4,217
PCB-123	Penta	6.74	6.74		13,501	4,648
PCB-124	Penta	6.73	6.73		13,388	4,607
PCB-125	Penta	6.51		C087		
PCB-126	Penta	6.89	6.89		15,005	5,220
PCB-127	Penta	6.95	6.95		15,487	5,414
PCB-128	Hexa	6.74	6.99	Average of PCB-128, PCB-162	15,766	5,530
PCB-129	Hexa	6.73	6.73		13,388	4,607
PCB-130	Hexa	6.80	6.80		14,148	4,890
PCB-131	Hexa	6.58	6.72	Average of PCB-131, PCB-133	13,274	4,565
PCB-132	Hexa	6.58	6.83	Average of PCB-132, PCB-161	14,450	5,005
PCB-133	Hexa	6.86		C131		
PCB-134	Hexa	6.55	6.58	Average of PCB-134, PCB-143	11,569	3,948
PCB-135	Hexa	6.64	6.64		12,320	4,217
PCB-136	Hexa	6.22	6.22		7,068	2,383
PCB-137	Hexa	6.83	6.83		14,450	5,005
PCB-138	Hexa	6.83	6.95	Average of PCB-138, PCB-163, PCB-164	15,487	5,414
PCB-139	Hexa	6.67	6.67	Average of PCB-139, PCB-149	12,685	4,350

Table 1
Log KOW and BCF Values
Used in Predicting Concentrations of PCBs in Polychaetes and Clams using C_{free}

PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-140	Hexa	6.67	6.67		12,685	4,350
PCB-141	Hexa	6.82	6.82		14,351	4,967
PCB-142	Hexa	6.51		SPME PRC (not modeled)		
PCB-143	Hexa	6.60		C134		
PCB-144	Hexa	6.67	6.67		12,685	4,350
PCB-145	Hexa	6.25	6.25		7,414	2,501
PCB-146	Hexa	6.89	6.97	Average of PCB-146, PCB-165	15,631	5,474
PCB-147	Hexa	6.64	6.64		12,320	4,217
PCB-148	Hexa	6.73	6.73		13,388	4,607
PCB-149	Hexa	6.67		C139		
PCB-150	Hexa	6.32	6.32		8,254	2,790
PCB-151	Hexa	6.64	6.64		12,320	4,217
PCB-152	Hexa	6.22	6.22		7,068	2,383
PCB-153	Hexa	6.92	6.92		15,256	5,320
PCB-154	Hexa	6.76	6.76		13,723	4,730
PCB-155	Hexa	6.41		SPME PRC (not modeled)		
PCB-156	Hexa	7.18	7.18		16,581	5,926
PCB-157	Hexa	7.18	7.18		16,581	5,926
PCB-158	Hexa	7.02	6.98	Average of PCB-158, PCB-160	15,700	5,502
PCB-159	Hexa	7.24	7.24		16,663	5,995
PCB-160	Hexa	6.93		C158		
PCB-161	Hexa	7.08		C132		
PCB-162	Hexa	7.24		C128		
PCB-163	Hexa	6.99		C138		
PCB-164	Hexa	7.02		C138		
PCB-165	Hexa	7.05		C146		

Table 1
Log KOW and BCF Values
Used in Predicting Concentrations of PCBs in Polychaetes and Clams using C_{free}

PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-166	Hexa	6.93	6.93		15,335	5,373
PCB-167	Hexa	7.27	7.27		16,674	6,061
PCB-168	Hexa	7.11	7.11		16,380	5,842
PCB-169	Hexa	7.17	7.17		16,559	5,947
PCB-170	Hepta	7.42	7.42		16,448	6,100
PCB-171	Hepta	7.27	7.27		16,674	6,061
PCB-172	Hepta	7.11	7.11		16,380	5,842
PCB-173	Hepta	7.33	7.33		16,638	6,095
PCB-174	Hepta	7.02	7.02		15,951	5,636
PCB-175	Hepta	7.11	7.11		16,380	5,842
PCB-176	Hepta	6.76	6.76		13,723	4,744
PCB-177	Hepta	7.08	7.08		16,258	5,780
PCB-178	Hepta	7.14	7.14		16,480	5,898
PCB-179	Hepta	6.73	6.73		13,388	4,619
PCB-180	Hepta	7.36	7.36		16,592	6,102
PCB-181	Hepta	7.11	7.11		16,380	5,842
PCB-182	Hepta	7.20	7.19	Average of PCB-182, PCB-187	16,601	5,975
PCB-183	Hepta	7.20	7.20		16,618	5,989
PCB-184	Hepta	6.85		SPME PRC (not modeled)		
PCB-185	Hepta	7.11	7.11		16,380	5,842
PCB-186	Hepta	6.69	6.69		12,924	4,448
PCB-187	Hepta	7.17		C182		
PCB-188	Hepta	6.82	6.82		14,351	4,983
PCB-189	Hepta	7.71	7.71		14,971	5,803
PCB-190	Hepta	7.46	7.46		16,317	6,085
PCB-191	Hepta	7.55	7.55		15,927	6,020
PCB-192	Hepta	7.52		SPME PRC (not modeled)		

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PCB	Homolog Group	Log KOW (L/kg) Hawker and Connell (1988)	Log KOW (L/kg) Used for BCF Model	Note	Model-generated Polychaete BCF (L/kg, ww)	Model-generated Clam BCF (L/kg, ww)
PCB-193	Hepta	7.52	7.52		16,071	6,047
PCB-194	Octa	7.80	7.80		14,317	5,634
PCB-195	Octa	7.56	7.56		15,877	6,010
PCB-196	Octa	7.65	7.65	Average of PCB-196, PCB-203	15,364	5,898
PCB-197	Octa	7.30	7.30		16,665	6,081
PCB-198	Octa	7.62	7.62		15,546	5,939
PCB-199	Octa	7.62	7.62		15,546	5,939
PCB-200	Octa	7.20	7.20		16,618	5,989
PCB-201	Octa	7.27	7.27		16,674	6,061
PCB-202	Octa	7.24	7.24		16,663	6,034
PCB-203	Octa	7.65		C196		
PCB-204	Octa	7.30		SPME PRC (not modeled)		
PCB-205	Octa	8.00	8.00		12,648	5,160
PCB-206	Nona	8.09	8.09		11,823	4,908
PCB-207	Nona	7.74	7.74		14,761	5,750
PCB-208	Nona	7.71	7.71		14,971	5,803
PCB-209	Deca	8.18	8.18		10,966	4,636

Abbreviations:

BCF = bioconcentration factor
L/kg = liter(s) per kilogram
L/kg, ww = liter(s) per kilogram, wet weight
Log KOW = log of octanol-water partition coefficients
PCB = polychlorinated biphenyl
PRC = performance recovery compound
SPME = solid-phase micro extraction