SUPPORTING INFORMATION

Measurement and modeling of polychlorinated biphenyl bioaccumulation from sediment for the marine polychaete *Neanthes arenaceodentata* and response to sorbent amendment

Elisabeth M.L. Janssen, [†], Marie-Noële Croteau, [‡] , Samuel N. Luoma, [‡], Richard G. Luthy,[*,†]

[†]*Department of Civil and Environmental Engineering, Stanford University, Stanford, California USA 94305-4020*

[‡]*U.S. Geological Survey, Menlo Park, California USA 94025*

The supplementary section contains 3 tables and 12 figures and a total of 17 pages.

Integrated biodynamic model:

$$C_{org}(t) = \frac{IR \cdot AE_s \cdot C_s + k_w \cdot C_w}{(k_{e+g})} \cdot \left(1 - e^{-(k_{e+g}) \cdot t}\right) + C^0_{org} \cdot e^{-(k_{e+g}) \cdot t} \quad \text{(S1)}$$

for 0 < t < 70 with t=0 being equivalent to the age of 14days.

$$AE(t) = \left[(C_{org,t} - C^0_{org,t}) \cdot \frac{(k_{e+g})}{\left(1 - e^{-(k_{e+g}) \cdot t}\right)} - k_w \cdot C_w \right] \cdot \frac{1}{IR \cdot C_s} \quad \text{(S2)}$$

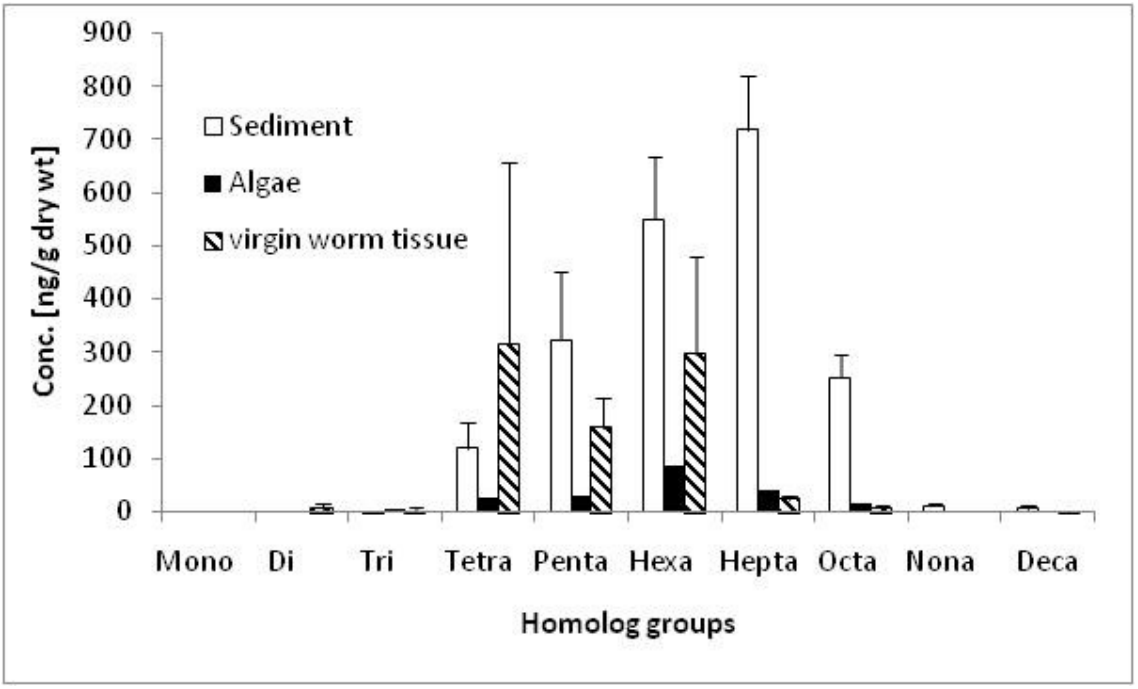

Figure S1. PCB homolog distribution in the virgin worm tissue, Hunters Point sediment, and algae obtained from worm bags from shipment. Error bars represent one standard deviation. (n=3-4).

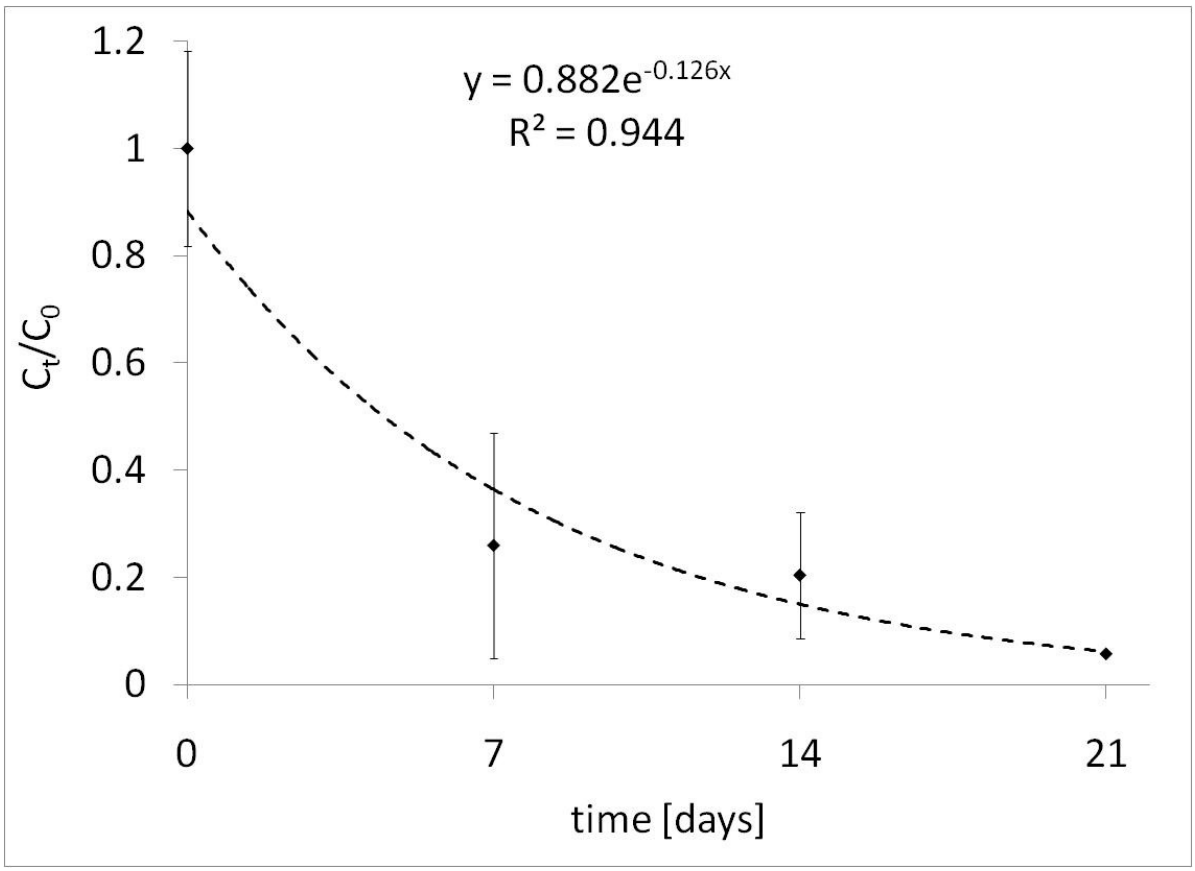

Figure S2. Determination of depuration rate by fitting the exponential function dc/dt=-kd*C(t), though the observed depuration data after 14 days exposure to untreated Hunters Point sediment.

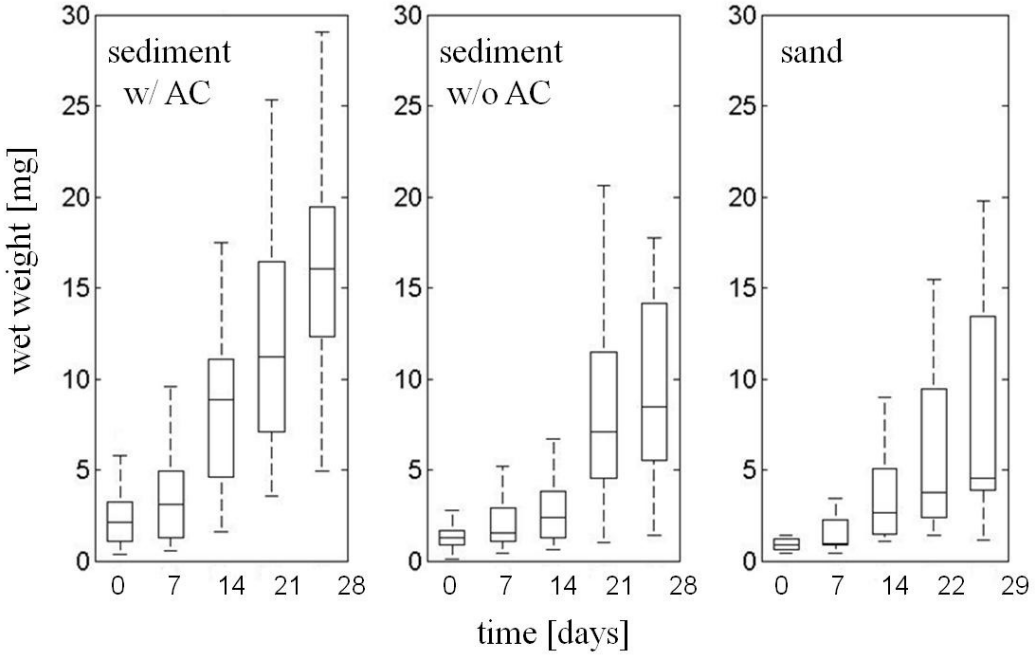

Figure S3. Growth of *N. arenaceodentata* (mg wet weight per individual) in untreated and AC-amended Hunters Point sediment and in silica sand; line = median, box = 25 and 75 percentile range, whisker = total range, and for each time point N = 27-36 (sediment), N = 10 (sand), N = 60-70 (juvenile, day 0).

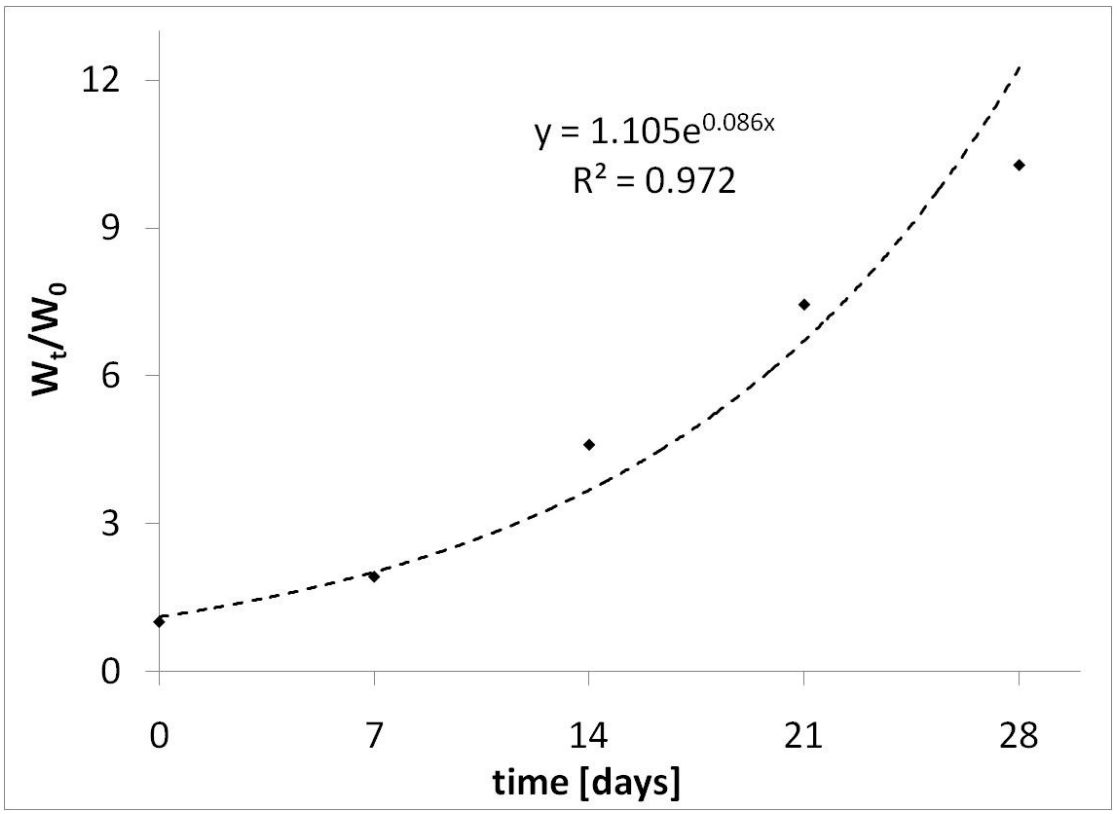

Figure S4. Observed exponential growth from *N. arenaceodentata* in sediment for average values of all measurements in treated and untreated sediment (N=50-66 for each time point).

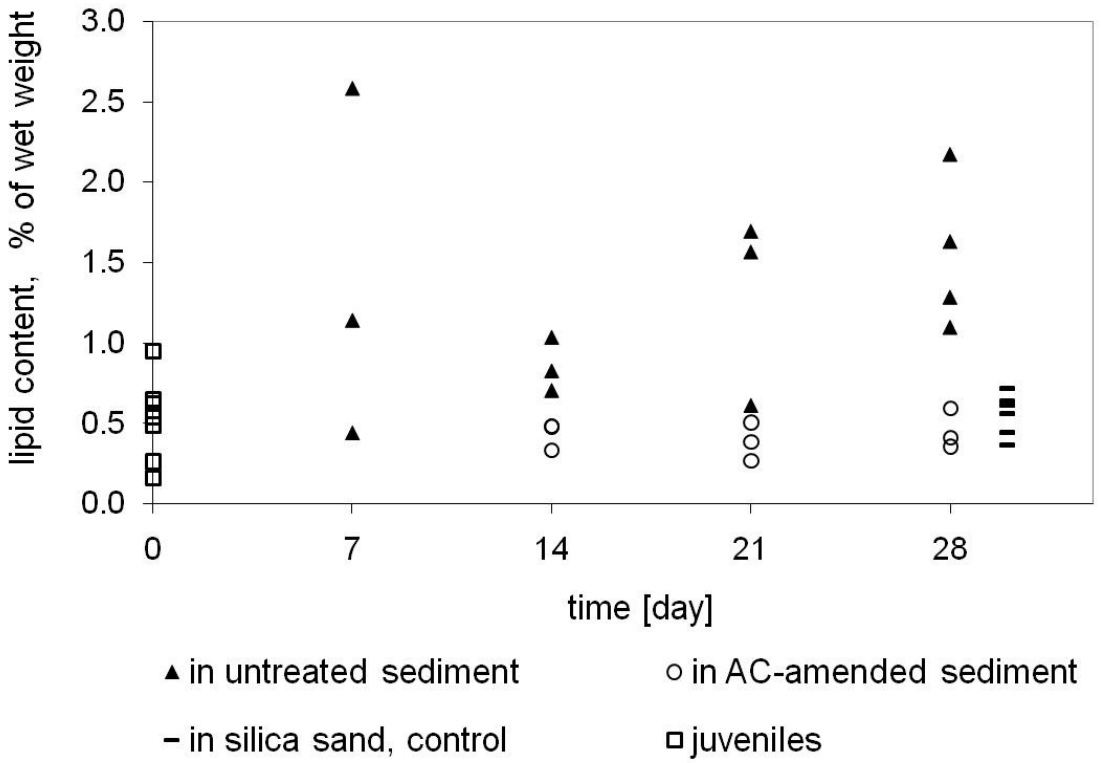

Figure S5: Temporal distribution of lipid content in percent of the organism's wet weight for juvenile *N. arenaceodentata* and after exposure to untreated and AC-amended Hunters Point sediment and silica sand.

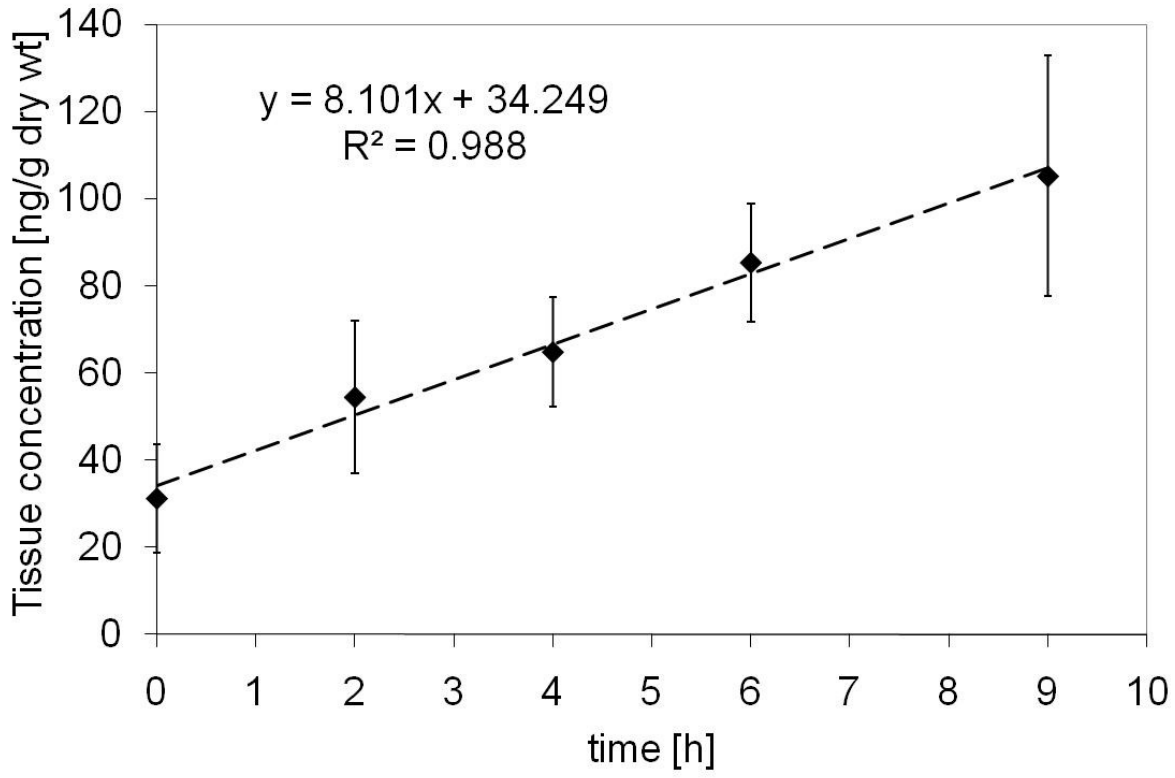

Figure S6. PCB concentration in worm tissue during aqueous exposure at 370 ng/L aqueous PCB concentrations for 2 to 9 hours.

Uptake from water:

$$C_{org}(t) = \frac{k_w \cdot C_w}{(k_{e+g})} \cdot \left(1 - e^{-(k_{e+g}) \cdot t}\right) \quad \text{(S3)}$$

Table S1: Relative contribution of PCB uptake from the aqueous phase.

	Total uptake day 28	Uptake from water, day 28	Maximum uptake from water	Uptake from water, day 70*
Determined by	sediment bioassay measured	equation S3 calculated	equation 2 calculated	equation S3 calculated
Sediment	6534 ng/g 100%	140 ng/g 2.1%	444 ng/g 6.8%	147ng/g 2.2%
AC-amendment	327 ng/g 100%	0.77 ng/g 0.2%	0.8 ng/g 0.2%	0.79 ng/g 0.2%

*Nearing end of *N. arenaceodentata's* life-cycle.

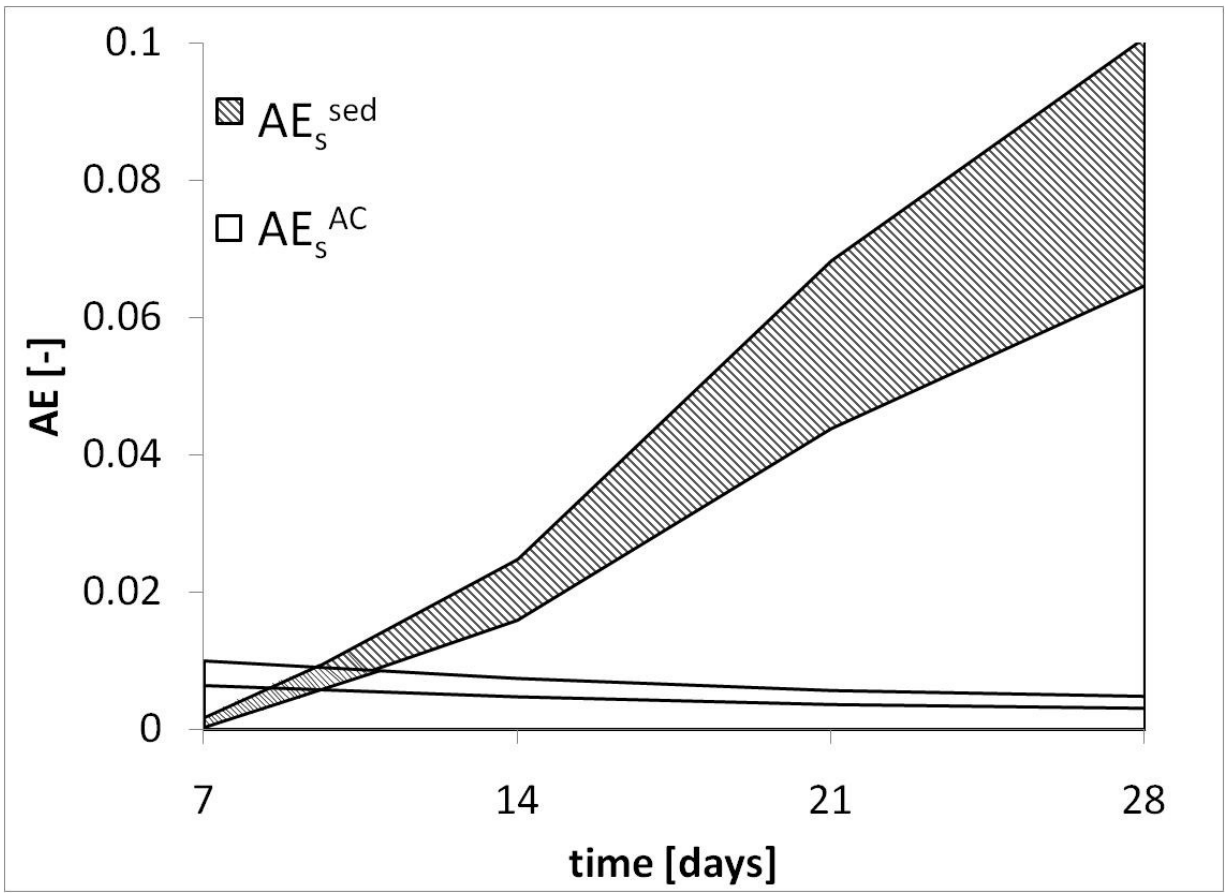

Figure S7. Assimilation efficiencies for sediment (AE_s^{sed}) and AC amendment (AE_s^{AC}) calculated for *N. arenaceodentata* considering the range of measured ingestion rates from 6.7 to 10.6 g/g dw per day.

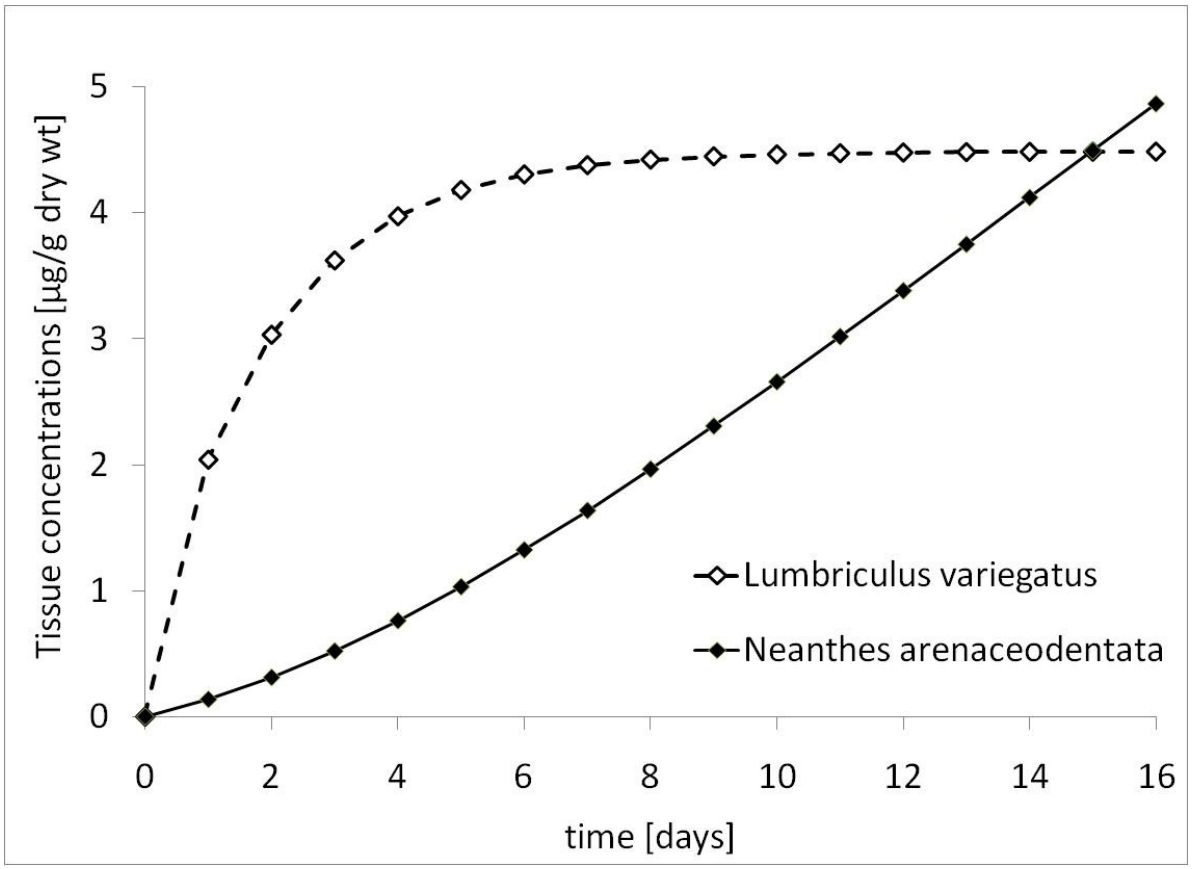

Figure S8. Solid line: PCB uptake behavior for polychaete with time-dependent AE predicted with biodynamic model input parameters presented in Table S1; Dashed Line: PCB uptake behavior for oligochaete with constant AE predicted with biodynamic input parameters published by Sun et al. ***[Sun, X.; Ghosh, U., PCB bioavailability control in Lumbriculus variegatus through different modes of activated carbon addition to sediments. Environ. Sci. & Tech. 2007, 41, 4774-4780.]***

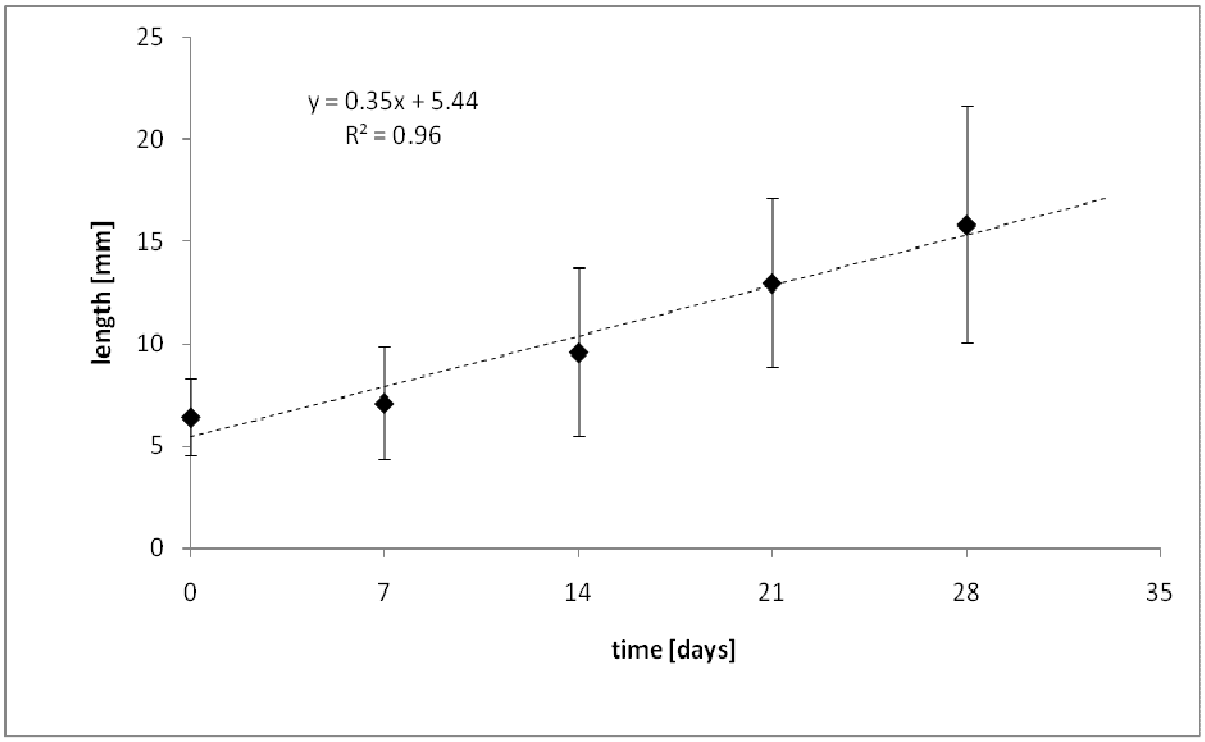

Figure S9: Average growth rate of *N. arenaceodentata* in Hunters Point sediment with linear regression.

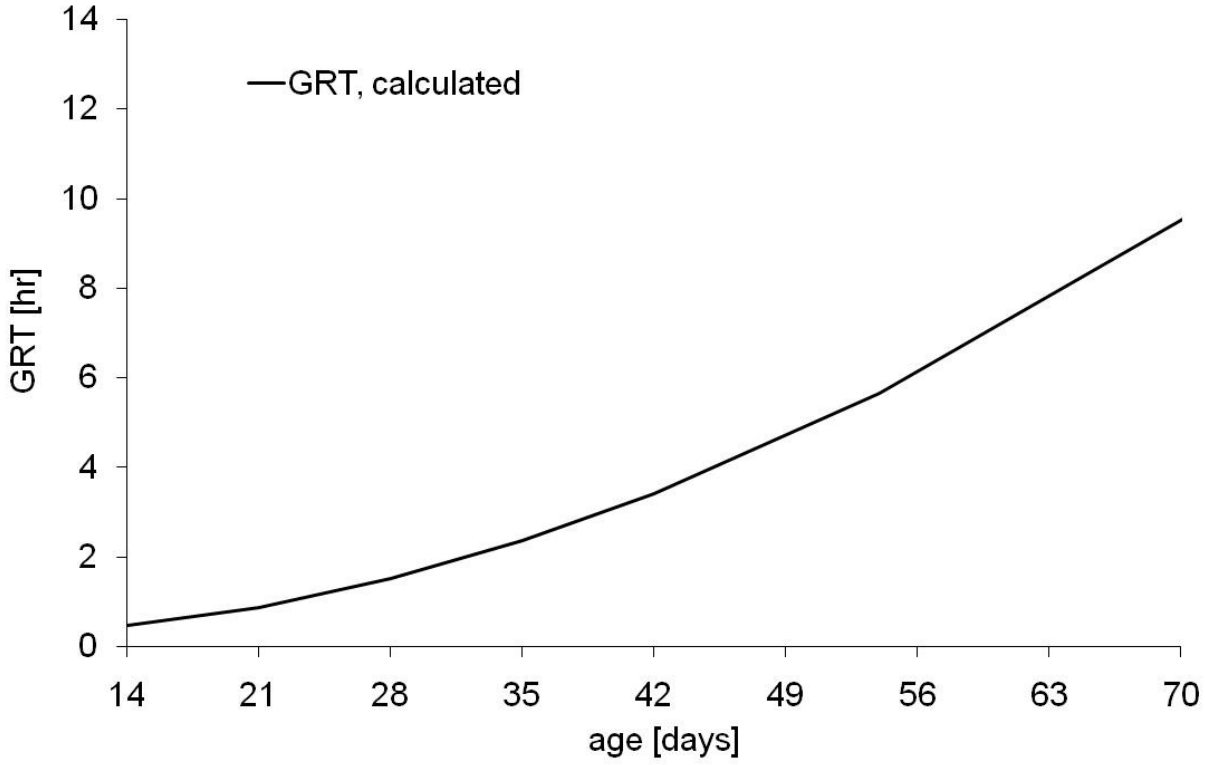

Figure S10: Calculated gut residence time (GRT) for *N. arenaceodentata* from the relationship of ingestion rate and gut volume with polynomial regression.

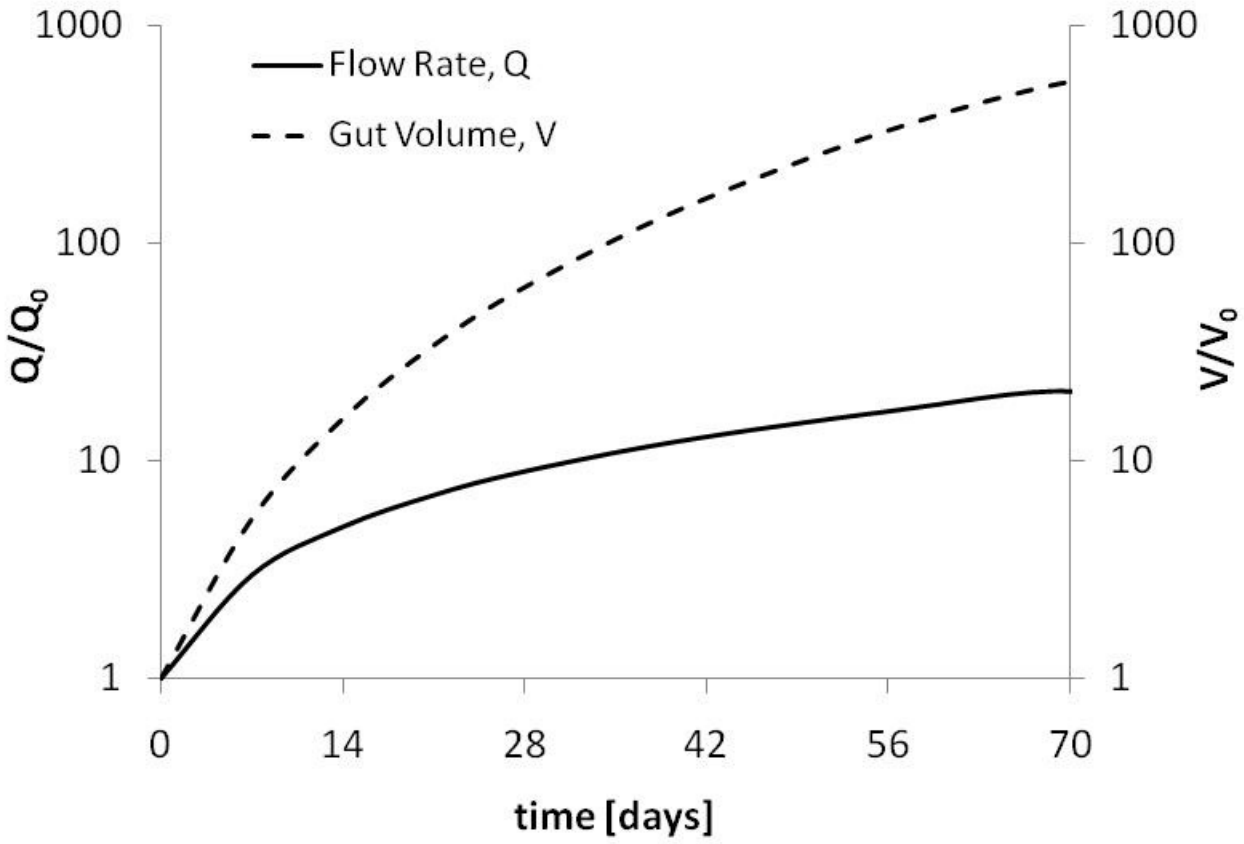

Figure S11. Calculated mass flow, Q, of ingested matter in growing polychaete and observed increase in body volume, V, for *N. arenaceodentata*.

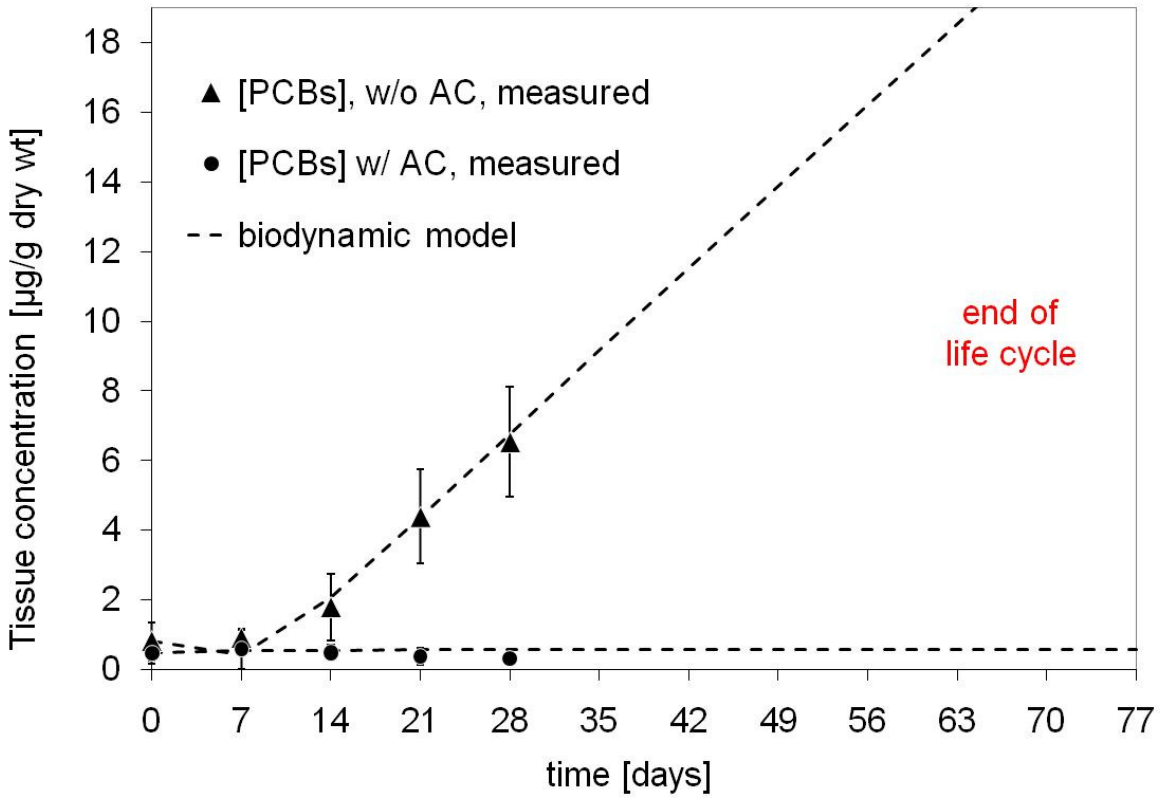

Figure S12. Measured data and modeled range of PCB tissue concentrations for organisms in sediment w/ and w/o AC-amendment.

Food ingestion rate calculations.

Labeling flagellates. For the pulse-case feeding study, the marine flagellate *Isochrysis* (University of Toronto Culture Collection) was exposed for 24 h to isotopically enriched ^{65}Cu and ^{106}Cd. Specifically, *Isochrysis* was grown for several generations in a f/2 medium (*23*). The flagellates were harvested onto a 1.2 µm polycarbonate filter, rinsed with AMW, and re-suspended into a 20-mL acid-washed glass scintillation vial filled with AMW spiked with commercially purchased standards (Trace Sciences International), isotopically enriched with ^{65}Cu (99.4%) and ^{106}Cd (96.5%). After exposure, labeled flagellates were harvested onto 1.2 µm polycarbonate filter and rinsed with AMW. Five small sections of the filters holding the labeled flagellates were sampled, dried for 24 h at 50 °C, and analyzed as described in the paper. The remaining filters were offered as food in the feeding study.

Mass-balance calculation using as the total amount of tracer (i.e., 65Cu and 106Cd) retained in the polychaetes after depuration, $I_{organism}$ in ng, the amount of tracer egested in the feces during depuration, I_{feces} in ng, the tracer concentration in the food, $[I]_{food}$ in ng g^{-1}, the worm's dry weight, $wt_{organism}$ in g, and the exposure duration, *t* in days.

$$IR = \frac{I_{organism} + I_{feces}}{[I]_{food} \cdot wt_{organism} \cdot t} \tag{S4}$$

Isotope tracing technique to establish the relative abundance of each tracer (e.g., ^{65}Cu and ^{106}Cd) from signal intensities of each isotope in the calibration standards, i.e.

$$p^i = \left(\frac{\text{Intensity } {}^{i}E}{\sum_{j}^{jj} \text{Intensity } {}^{j}E} \right)_{\text{Standard}} \tag{S5}$$

where p^i is the relative abundance of the natural isotope ${}^{i}E$ (an element *E* of atomic weight *i*), *j* and *jj* are the lightest and heaviest isotopes of the metal *E*, respectively. Concentrations of tracer in the experimental organisms ($[{}^{i}E]_{\hat{e}}$) are calculated as the product of p^i and the total metal concentrations inferred by the ICP-MS software from tracer intensity ($[T^{i}E]$), i.e.,

$$[^{i}E]_{\hat{e}} = p^{i} \cdot [T^{i}E] \quad \text{(S6)}$$

The original load of tracer ($[^{i}E]_{\hat{e}}^{0}$) that occurred in each sample in the absence of a spike is calculated as the product of p^{i} and the total metal concentrations inferred from the intensity of the most abundant isotope ($[T^{k}E]$), i.e.,

$$[^{i}E]_{\hat{e}}^{0} = p^{i} \cdot [T^{k}E] \quad \text{(S7)}$$

The net tracer uptake ($\Delta[^{i}E]_{\hat{e}}$) is derived from the total experimental metal concentration ($[^{i}E]_{\hat{e}}$, equation 3) minus the pre-existing concentration of tracer ($[^{i}E]_{\hat{e}}^{0}$, equation 4), which gives after algebra simplifications:

$$\Delta[^{i}E]_{\hat{e}} = p^{i} \cdot (\cdot [T^{i}E] - [T^{k}E]) \quad \text{(S8)}$$

The background concentration of tracer in the organism's tissue is calculated in the absence of a spike as the product of p^{i} and the total metal concentrations inferred from the intensity of the most abundant isotope. The net tracer uptake is derived from the difference of total experimental metal concentration and background concentration of tracer.

Conversion from flagellate IR to sediment IR. The food IR was measured in laboratory-controlled feeding experiments using the flagellate algae Isocrysis labeled with stable metal tracers. We assume that these algae represent 100% organic matter (OM). Hence, the algae IR also represents the organic matter IR. OM is represented by $C_5H_7O_2N$ with 53.09% organic carbon (OC) by molecular weight. The algae IR was measured as 0.14 ± 0.08 gram OM per gram body weight per day. This translates into ingestion of 0.074 ± 0.042 gram OC per gram body weight per day. The OC content of the sediment was measured as 0.7 to 1.1% at Hunters Point. In order to consume 0.074 ± 0.042 g OC/g d, the sediment ingestion rate has to be 6.8 to 10.6 g/g d or an average of 8.7 g/g d.

Table S2. Parameters in biodynamic model for *N. arenaceodentata*.

Parameter	*Symbol*	*Unit*	*Average value* ± standard deviation
Ingestion rate, average	IR	$\frac{g_{\text{sediment, dry wt}}}{g_{\text{organism, dry wt}} \cdot day}$	8.7 ± 1.9
Lipid content	f_{lipid}	$\frac{g_{\text{lipid}}}{g_{\text{organism, dry wt}}}$	1.2 ± 0.7
- Untreated sediment			0.4 ± 0.1
- AC-amended sediment			
Aqueous uptake rate constant (linear)	k_w	$\frac{L}{g_{\text{organism, dry wt}} \cdot day}$ 1	0.5 ± 0.1
Elimination rate constant (exponential)	k_e	$\frac{g_{\text{PCBs lost}}}{g_{\text{PCBs, total}} \cdot day}$	0.04 ± 0.02
Growth rate constant (exponential)	k_g	$\frac{g_{\text{organism, dry wt gained}}}{g_{\text{organism, dry wt, total}} \cdot day}$	0.086 ± 0.008
Assimilation efficiency			
- untreated sediment (linear)	AE(t)	$\frac{g_{\text{PCBs assimilated}}}{g_{\text{PCBs ingested}} \cdot \text{day}}$	0.004 t - 0.03 (see regression in Figure 3)
- AC-amended sediment	AE	$\frac{g_{\text{PCBs assimilated}}}{g_{\text{PCBs ingested}}}$	0.006 (see Figure 3)
Sediment concentration Hunters Point (Plot B)	C_{sed}	$\frac{ng_{\text{PCBs}}}{g_{\text{sediment, dry wt}}}$	1200 ± 300
Aqueous concentration	C_{aq}	$\frac{ng_{\text{PCBs}}}{L_{water}}$	
- untreated sediment			37 ± 11
- AC-amended sediment			0.2 ± 0.1

Sensitivity Analysis. To test the sensitivity of the biodynamic model to variability in input parameters, estimated 28-d polychaete bioaccumulation in untreated Hunters Point sedimentwas calculated for a 10% increase of each parameter while the other parameters were held constant. Table S3 shows the average values determined for the biodynamic model when increased by 10% and the relative change compared to the predicted uptake using average input parameters for 28-day exposure. The uptake after 28 days exposure could be predicted using average input parameters as 6534 ng/g and 327 ng/g for sediment and AC-amendment, respectively.

Table S3: Model sensitivity to biodynamic parameters used to describe PCB accumulation in *Neanthes arenaceodentata* (for units please see Table S2).

Parameter	**Average values + 10%**	**% change**
Ingestion rate (IR)	9.6	+10%
Assimilation efficiency from (AE_s^{sed})	0.090	+10%
Concentrations in sediment (C_{sed})	1320	+10%
Rate constant of growth (k_g)	0.095	-6%
Rate constant of loss (k_e)	0.055	-4%
Aqueous uptake rate constant (k_w)	0.55	+0.21%
Concentrations in the pore water (C_w)	40.7	+0.21%
Organic carbon of sediment (f_{oc})	0.99	+10%