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Peter F. Landrum[1] *and Warren R. Faust*[1]

Effect of Variation in Sediment Composition on the Uptake Rate Coefficient for Selected PCB and PAH Congeners by the Amphipod, *Diporeia* sp.

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ABSTRACT: The exposure of benthic organisms to sediment-associated toxic organics is influenced by the sediment's organic carbon (OC) content because hydrophobic organic contaminants sorb to the organic and fine grain portions of sediments, and benthos ingest the OC associated with fine material. The effect of varying sediment composition, measured as the percent of combustible solids (CS), percent of OC, and percent of fine-grained material (FM) (the <63 μm fraction of the sediment), was examined by determining the accumulation of sediment-associated polychlorinated biphenyl and polycyclic aromatic hydrocarbon congeners by the Great Lakes amphipod, *Diporeia* sp. Prepared sediments (3 and 5% CS) and native sediment were dosed with pairs of contaminants: ^{3}H-pyrene and ^{14}C-2,5,2′,5′-tetrachlorobiphenyl, and ^{3}H-benzo(*a*)pyrene and ^{14}C-2,4,5,2′,4′,5′-hexachlorobiphenyl. Additionally, some of the dosed 5% CS sediment was recombined with the coarse material to recreate a 2% CS sediment where the fine material had been dosed preferentially. The accumulation of the radiolabeled compounds was followed for 27 days, and the partitioning between sediment particles and interstitial water was measured at the end of the experiment. When uptake rate coefficients (K_s) and the depuration rate constants (K_d) were estimated, the K_d values were found to be similar to those previously measured in *Diporeia*. The K_s values from the native and fine labeled sediments (both approximately 2% CS) were similar. K_s values declined with increasing CS, OC, and FM. Correlations indicated that the percent of OC best accounted for the variation resulting from changes in the sediment composition for each compound, both for K_s and for sediment-interstitial water partitioning. As in previous studies, the partition coefficient between sediment and interstitial water did not account for the changes in the bioavailability between different classes of compounds. Higher partitioning and higher uptake rate coefficients were found for the chlorinated hydrocarbons than for the polycyclic aromatic hydrocarbons, even when the hydrophobicity of the contaminants was accounted for. A linear solvation energy quantitative structure activity model was useful for describing the differences in the uptake rate coefficients by accounting for the differences in the molecular characteristics of the two compound classes.

KEY WORDS: sediments, polycyclic aromatic hydrocarbons, polychlorinated biphenyls, partition coefficients, bioaccumulation, *Diporeia* sp., linear solvation energy model, QSAR

Many important factors contribute to the bioavailability of organic contaminants sorbed to sediments. These factors can be divided into three classes: compound characteristics;

[1]Great Lakes Environmental Research Laboratory, NOAA, 2205 Commonwealth Blvd., Ann Arbor, MI 48105. This paper is GLERL Contribution No. 703.

sediment composition and characteristics; and biological characteristics, physiology and benthos behavior [*1*]. Several sediment characteristics influence contaminant bioavailability, including organic carbon content, particle size, clay types, cation exchange capacity, and pH. Organic carbon (OC) is a major factor because it can sorb or complex both metals and organic contaminants, and this sorption or complexation can reduce the bioavailability of contaminants [*2–8*]. Further, because benthic organisms preferentially ingest the organic fraction of the sediment, they are exposed to greater concentrations than would be suggested from contaminant concentrations measured in bulk (total) sediment [*9,10*]. The importance of the ingestion route to bioavailability for organic contaminants is greatest for those compounds with high octanol:water partition coefficients (K_{ow}) and becomes significant for compounds with a log K_{ow} of approximately 5 [*1,9*].

Because particulate OC affects both the sorption of contaminants to sediments and their bioavailability, we wished to examine the influence of organic matter and particle size on the uptake kinetics. In this study, the amphipod, *Diporeia* sp. was exposed to sediments containing differing levels of organic matter, and selected polycyclic aromatic hydrocarbon (PAH) and polychlorinated biphenyl (PCB) congeners. (Note: The organism *Diporeia* sp. was previously classified as *Pontoporeia hoyi* [*11*].)

Materials and Methods

Experimental Design

The accumulation of selected xenobiotics by *Diporeia* sp. from Lake Michigan sediment at 4°C was followed over a 27-day period. Radioactive tracers were added to three different sediments: native sediment, and two sediments modified to elevate the levels of fine-grained and combustible organic matter from the native material. In addition, tracers were added to a fine-grained enriched portion of native sediment, followed by reconstitution of the original sediment's organic matter composition.

Groups of 20 *Diporeia* were exposed to 40 g of sediment (wet weight) and 250 mL of lake water contained in a 400-mL beaker. The sediment was dosed with two radiotracers, ^{3}H-pyrene (PY) and ^{14}C-2,5,2′,5′-tetrachlorobiphenyl (TCBP). Three such beakers of animals were sampled at each time point (3, 6, 12, 20, and 27 days) for each of the four sediment types examined. A second uptake experiment was conducted similarly with ^{3}H-benzo(*a*)pyrene (BaP) and ^{14}C-2,4,5,2′,4′,5′-hexachlorobiphenyl (HCBP).

Sample Collection

Diporeia sp. were collected 2.5 miles southwest of Grand Haven, Michigan at a depth of 24 to 29 m with a PONAR grab sampler. The grab samples were mixed with lake water and the *Diporeia* were removed with a screen. The animals were placed in clean lake water and kept cold with ice during transportation to the laboratory. The *Diporeia* survived well in the laboratory in aquaria containing about 2 to 4 cm of sediment and 10 cm of lake water at 4°C.

Lake Michigan surface water was collected about 1 m below the surface and was stored at 4°C in 5-gallon carboys. Lake Michigan sediment was obtained by a PONAR grab approximately 5 miles off Grand Haven, Michigan at a depth of 45 m. The sediment was sieved through a 1-mm screen to remove debris and animals, and was kept at 4°C.

Manipulation, Dosing, and Characterization of the Sediments

Sediments with increased levels of fine-grained material (FM), combustible solids (CS), and OC were generated from the native sediment by mixing the sediment with lake water, decanting the water with suspended lighter particles after several minutes of settling, and

allowing the suspended sediment to settle. Wet sediment (160 g) was dispersed in a 2-L graduated cylinder of lake water by shaking. After a 2-min settling period, the suspended material was decanted and collected to yield the sediment with approximately 5% CS, measured by loss on ignition. A similar procedure with 20 s settling time yielded the sediment with approximately 3% CS. This method was designed to create sediments with differing characteristics but without adding extraneous materials (Table 1).

The percent of CS and the dry-to-wet weight ratios for the sediment were determined by weighing a 1- to 2-g sample into a preweighed glass petri dish. The sediment's dry weight was determined after drying to constant weight at 60°C. After drying, the sediment was combusted at 500°C for 5 h and the CS weight was determined by taking the difference between the ash weight and the dry weight.

The OC content of the sediments was determined by treating 50 to 100 mg of dry sediment with 1 mL of 1 *N* HCl and shaking the sample on a shaker overnight to remove the carbonates. The sample was dried, and the organic carbon was determined on a Perkin-Elmer 2400 CHN Elemental Analyzer.

The percent of FM in the sediment was determined by wet sieving approximately one gram of sediment. After the addition of approximately 5 mL water, the sample was agitated until the sediment disaggregated. The material was then sieved wet through a 63-μm Nitex mesh screen, rinsed with distilled water, and each fraction washed into a 100-mL beaker. After drying to constant weight at 60°C, the two fractions were weighed and the proportion of the fine material was determined.

Wet sediment, corresponding to 700 g dry weight, was placed in a 4-L beaker with 2500 mL of lake water. The mixture was stirred vigorously at room temperature while a solution of PY in 262 μL of methanol and a solution of TCBP in 62 μL of methanol were slowly added dropwise. The mixture was stirred at room temperature for an additional 4 h and kept at 4°C thereafter. Sediments with CS values of 2, 3, and 5% were dosed as described. Additionally, one sediment was generated by adding the radiolabeled compounds to a smaller amount of fine sediment (with 5% CS) and stirring in the previously separated coarse material just before placing the sediments into individual beakers for exposing organisms. This procedure was intended to produce a 2% CS sediment in which the radiolabeled compounds resided preferentially on fine-grained material.

In a second experiment, BaP in 666 μL of methanol and HCBP in 100 μL of methanol were added to the four types of sediments as above. The small amount of methanol added as a carrier was not expected to affect the partitioning of the contaminants to the sediments [*12*].

Experimental Procedure

Two days after each dosed sediment was prepared, the overlying water was decanted to remove most of the methanol carrier. The sediment was stirred until visually homogeneous,

TABLE 1—*Characterization of sediments.*

Sediment Type (Nominal Percent Combustible)	Percent Combustible Solids (Actual)	Percent Organic Carbon	Percent Fine-Grained Material (<63 μm dia.)
2.0[a]	1.96 ± 0.16	0.46 ± 0.08	36.2 ± 0.5
2.0[b]	2.18 ± 0.18	0.40 ± 0.03	44.7 ± 0.9
3.0	3.18 ± 0.27	0.80 ± 0.02	77.2 ± 0.3
5.0	4.95 ± 0.44	1.03 ± 0.05	94.8 ± 0.9

[a]Original unmanipulated sediment.
[b]Fine-labeled sediment.

then 40 g of wet sediment was transferred to each of fifteen 400-mL beakers. The following samples were taken from each sediment at the beginning, middle, and end of the distribution to the beakers: 2 g for wet-to-dry weight determination and 5 g for desiccation with anhydrous sodium sulfate, extraction with ethyl acetate, and counting to determine radioisotope activity. Lake water (250 mL) was carefully added to each beaker to minimize disturbance of the sediment. On the following day (three days after the sediments were dosed), a 2-mL water sample was taken to determine the levels of radioisotopes in the aqueous phase and 20 test organisms (*Diporeia*) were added to each beaker.

Three beakers of animals exposed to each sediment type were sampled on days 3, 6, 12, 20, and 27 (a total of 15 beakers per sediment OC level per set of radiolabeled compounds) to obtain the following samples:

Overlying Water—A 2-mL water sample was counted to determine radioisotope activity in the aqueous phase.

Sediment—A sample was taken to determine the ratio of wet-to-dry weight, and the dry weight was determined as described above. A second sample was desiccated with anhydrous sodium sulfate and extracted with ethyl acetate to determine radioisotope activity in the sediment.

Test Organisms—The number of *Diporeia* found above the sediment was recorded to check for sediment-avoidance behavior. The number of organisms surviving was determined by removing the sediment and sieving the animals gently from the sediment. The wet weight and radioisotope content of several groups of three individuals was measured. The lipid content of two individuals was determined by the micromethod of Gardner et al. [*13*].

Interstitial Water—On day 27, the overlying water was removed by aspiration, the sediment was centrifuged, and the total, free, and bound concentration of the two radioisotopes in the interstitial water was determined as follows. Two milliters of interstitial water were counted for total activity. Then, the remaining water was filtered through glass fiber filters to remove particles (with a back-up filter to correct for sorption), and the radioisotope activities in a 2-mL sample of the filtrate were determined. The filtrate was passed through a Sep Pak® to absorb freely dissolved material. A 2-mL sample of the water passing through the Sep Pak® was collected, and the amount of dissolved organic matter bound compounds was measured as the amount of radioisotope activities in the sample [*14*].

The above sampling scheme results in measuring contaminant concentrations in 18 sediment samples and 15 organism samples for each type of sediment for each pair of radiolabeled compounds examined. The interstitial water was measured in triplicate for each sediment type with each pair of radiolabeled compounds examined.

Radioactivity Determination

All scintillation counting was done with an LKB 1217 RACKBETA liquid scintillation counter using RPI scintillation cocktail 3a70B. Quench corrections were made via the external standards ratio method after subtracting for background.

Partition Coefficient Calculation

The partition coefficients were determined as the ratio of the contaminant concentration on the sediment particles divided by the "freely dissolved" contaminant concentration in the interstitial water. The freely dissolved concentration was determined in a manner similar to a previous study that examined the distribution of compounds between suspended particles, dissolved organic matter, and a freely dissolved fraction [*15*]. The freely dissolved concentration equals the sum of twice the amount of compound sorbed to the back-up filter,

which accounts for filter sorption when removing suspended particles from the interstitial water, divided by the total volume of the interstitial water filtered plus the difference between the concentration of the filtrate and the concentration of bound compound determined after passing the filtrate through a C-18 Sep Pak® [*14*]. The freely dissolved concentration is an operationally defined value and an estimate of "truly dissolved" compound.

Results

Sediment Characteristics

The variable OC levels in the sediments were generated through the removal of coarse material from the sediment. The range of OC concentrations was a factor of 2.5 between the lowest to highest OC content (Table 1). By increasing the OC content of the sediments, the percent of CS and FM were also comparably increased over the range of sediments by factors of 2.5 and 2.6, respectively (Table 1). The amount of FM and the CS content in the unmanipulated sediment are relatively consistent with previous collections [*16,17*]. Thus, the composition of bulk unmanipulated sediments resembled sediments previously collected from this station.

Partitioning

The extent of binding between the sediment interstitial water and sediment particles was determined at the end of the 27-day exposure (Table 2). The measured partition coefficient was the concentration of the compound on the solid phase divided by the freely dissolved concentration in the interstitial water. The amount of freely dissolved compound for the ^{14}C-labeled contaminants, the PCB congeners, was often very near background especially for the sediments containing the highest percent of OC. For these cases, the partition coefficients should be considered to be only minimal estimates of the actual partition coefficients. Where concentrations were below detection limits, the partition coefficients would have had to be larger than where partition coefficients could be measured. For both compound classes, several data points were lost because the interstitial water contained insufficient radioactivity to measure the freely dissolved contaminants. However, only in two cases were single values available as estimates; the remainder of the data were at least in duplicate and usually in triplicate. Since the lost data were usually for the PCB congeners, the differences in the partition coefficients between PCB and PAH congeners of similar K_{ow} may be greater than estimated by the measured data.

The partition coefficients were correlated with the OC content, percent of CS, and percent of FM in the sediments (Table 3). For the sediment with separately dosed, fine-enriched

TABLE 2—*Contaminant partition coefficients between sediment and interstitial water.*

Sediment (% CS)	PY	BaP	TCBP	HCBP
1.96	516 ± 67[a]	371 ± 40	1259 (144)[b]	873 (611)[b]
2.18	455[c]	443 ± 159	935[c]	634 (134)[b]
3.18	1130 ± 342	877 ± 191	4899 ± 1680	1195 ± 256
4.95	1112 ± 137	1446 ± 392	9158 (4473)[b]	8303 (4533)[b]

[a]The mean and standard deviations of the partition coefficients are presented, $n = 3$.
[b]The mean with the range in parentheses is presented, $n = 2$.
[c]Only single estimates are available because two of the three replicates were not measurable.

TABLE 3—*Linear regressions of the contaminant partition coefficients versus the sediment characteristics.*

Compound	Sediment Characteristic	Slope	Intercept	r^2	N	p
BaP	% FM	17.5 ± 3.4	−323 ± 228	0.702	12	0.000
PY	% FM	11.7 ± 3.3	85 ± 236	0.564	10	0.007
TCBP	% FM	130 ± 49	−4179 ± 3458	0.47	8	0.037
HCBP	% FM	99 ± 49	−3480 ± 3388	0.275	9	0.085
BaP	% CS	362 ± 63	−325 ± 207	0.744	12	0.000
PY	% CS	202 ± 79	217 ± 274	0.38	10	0.034
TCBP	% CS	2730 ± 950	−4157 ± 3214	0.51	8	0.028
HCBP	% CS	2538 ± 832	−5241 ± 2726	0.509	9	0.019
BaP	% OC	1628 ± 308	−310 ± 222	0.709	12	0.000
PY	% OC	1137 ± 336	46 ± 259	0.536	10	0.010
TCBP	% OC	12938 ± 4579	−4790 ± 3482	0.499	8	0.030
HCBP	% OC	9879 ± 4393	−4205 ± 3204	0.336	9	0.059

material that was recombined to give the 2% CS, the partition coefficients were consistent with the relative amount of organic matter for this sediment. Thus, partitioning of these organic contaminants probably is dominated by the properties of the fine sediment material, even when the sediments are dosed in bulk.

When comparing the various correlations between the partition coefficients and the sediment characteristics, the regressions with the various sediment characteristics were very similar (Table 3). Further, the percent of CS correlated significantly across all the sediments for all compounds while the regression for HCBP was not statistically significant when the percent of FM or OC was used as a regression variable (Table 3). Placing too much emphasis on the difference between the HCBP correlations for the different sediment variables is not appropriate because of the difficulties in measuring the freely dissolved concentrations for this compound. The differences may be due more to analytical variation than real differences in behavior. The fact that the regressions for the PCB congeners had greater relative slopes than those for the PAH congeners suggests that the partition coefficients for the PCB congeners depended more on the sediment characteristics than did those for the PAH congeners (Table 3).

The variation in the partition coefficients between the various sediments could not be explained better by multiple regression which uses more than one of the sediment characteristics. In all cases, multiple regressions resulted in lower r^2 values than the single-sediment characteristic regressions with the partition coefficient. Thus, the partitioning does not seem to be dominated by more than one phase. Further, because of the good correlations for the individual characteristics, the three characteristics are likely interrelated.

Normalizing the partition coefficients for CS, OC content, or fraction of FM generally reduced the variability in the measured partition coefficients between the various sediments (Table 4). Considerable variability was still observed for the chlorinated biphenyls after normalization and was likely due to the analytical difficulties. This normalization did not result in a strong relationship between the partition coefficient and K_{ow}, regardless of whether all the compounds were considered together or when each class was considered independently (Fig. 1).

Bioavailability and Toxicity

Neither significant sediment avoidance nor mortality was observed for *Diporeia* in response to any of the treatments. The mean percent mortality after 20 days was 5.1 ± 4.9% (mean

TABLE 4—*Mean partition coefficients of contaminants normalized for sediment characteristics.*

Sediment Characteristic	BaP	PY	TCBP	HCBP
36.2 % FM	1024	1425	3478	2411
44.7 % FM	991	1018	2092	1418
77.2 % FM	1136	1464	6345	1547
94.8 % FM	1525	1173	9960	8758
1.96 % CS	23710	26327	64235	44541
2.18 % CS	20321	20871	42890	29083
3.18 % CS	27579	35535	154057	37579
4.95 % CS	29212	22465	185010	167737
0.46 % OC	80652	112174	273696	189783
0.40 % OC	110750	113750	233750	158500
0.80 % OC	109625	141250	612375	149375
1.03 % OC	140388	107961	889126	806117

± SD) for all treatments. Mortality could not be determined for the 27-day sample because some of the organisms were lost while transferring the sediment to the centrifuge tube to isolate the interstitial water. However, the number found dead on the sediment surface averaged less than one per beaker (0.25 dead per beaker). Further, the measured lipid content of *Diporeia* was not significantly different at the beginning (42.6 ± 9% on a dry weight basis) and the end of the experiments (42.9 ± 9 and 39.6 ± 6% for the PY/TCBP and BaP/HCBP experiments, respectively). Therefore, the organisms were considered to be in excellent health over the course of the study.

The accumulation of both the PAH and PCB congeners were reduced with increasing amount of OC in the sediments (Fig. 2). The sediment where the fine material had been

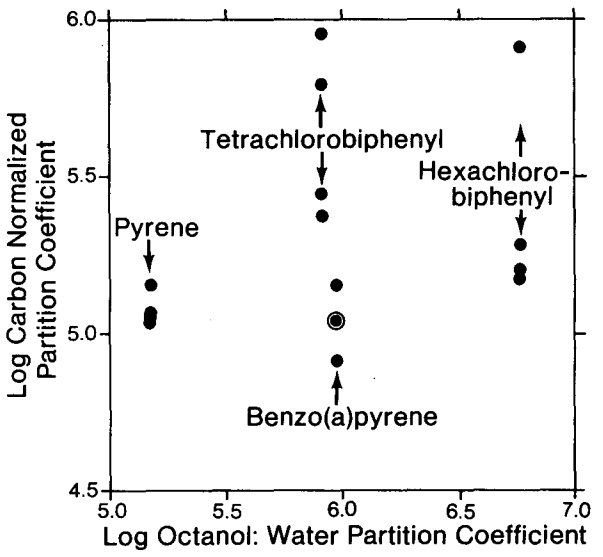

FIG. 1—*Scatter plot of the organic carbon normalized partition coefficient versus the log of the octanol:water partition coefficient* (K_{ow}) *for both the PAH and PCB congeners.*

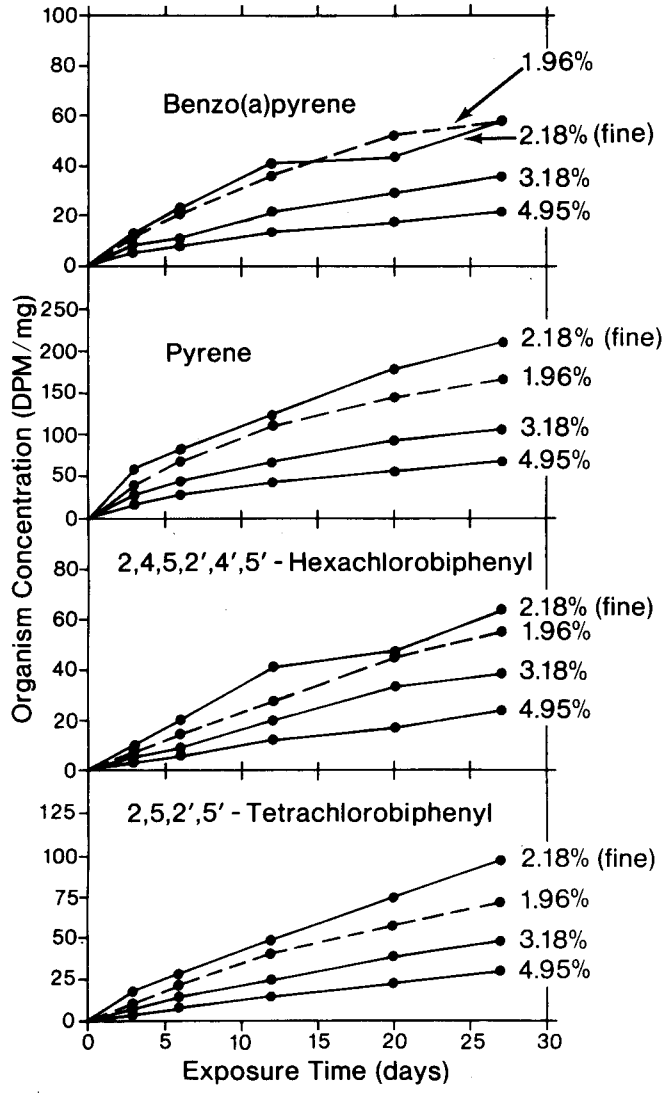

FIG. 2—*Accumulation curves for the accumulation of the PCB and PAH congeners from the various sediments. Percentages refer to the combustible solids content of the sediments.*

dosed preferentially had the lowest OC content and yielded the greatest amount of accumulation. The difference in accumulation between the 2% OC dosed in bulk and that with the fine material dosed preferentially was insignificant for BaP and HCBP.

The uptake rate coefficient (K_s) and depuration rate constant (K_d) were determined by fitting the time-dependent organism concentration data to a two-compartment donor-dependent model [*16*]. The resulting K_s values for BaP and HCBP from the unmanipulated sediments were approximately two times larger (Table 5) than previously reported values where the sediment characteristics were similar as previously discussed [*16*]. The K_s for PY

TABLE 5—*Uptake rate coefficients and depuration rate constants.*

Compound	Sediment (% CS)	K_s (g sed. g^{-1} h^{-1})	K_d (h^{-1})	BAF (K_s/K_d)	AF[a]
BaP	1.96	0.0046 ± 0.0003	0.0022 ± 0.0003	2.1	0.085
BaP	2.18	0.0046 ± 0.0008	0.0031 ± 0.0009	1.5	0.053
BaP	3.18	0.0022 ± 0.0002	0.0018 ± 0.0003	1.2	0.087
BaP	4.95	0.0015 ± 0.0002	0.0025 ± 0.0006	0.6	0.056
HCBP	1.96	0.0121 ± 0.0008	0.0007 ± 0.0003	17.3	0.71
HCBP	2.18	0.0146 ± 0.0024	0.0018 ± 0.0008	8.1	0.29
HCBP	3.18	0.0064 ± 0.0008	0.0006 ± 0.0005	10.7	0.76
HCBP	4.95	0.0036 ± 0.0003	0.0005 ± 0.0003	7.2	0.66
PY	1.96	0.0139 ± 0.0002	0.0028 ± 0.0001	5.0	0.20
PY	2.18	0.0147 ± 0.0016	0.0025 ± 0.0006	5.9	0.21
PY	3.18	0.0076 ± 0.0005	0.0026 ± 0.0003	2.9	0.21
PY	4.95	0.0048 ± 0.0004	0.0025 ± 0.0004	1.9	0.18
TCBP	1.96	0.0197 ± 0.0007	0.0013 ± 0.0002	15.2	0.62
TCBP	2.18	0.0212 ± 0.0017	0.0009 ± 0.0003	23.6	0.84
TCBP	3.18	0.0108 ± 0.0004	0.0011 ± 0.0002	10.8	0.77
TCBP	4.95	0.0060 ± 0.0004	0.0006 ± 0.0002	10.0	0.91

[a]BAF normalized to both the lipid content in the organism and the organic carbon content in the sediment.

from the unmanipulated sediment was similar but somewhat lower than previously measured values [*16*]. The K_s for TCBP was essentially identical to previous values [*17*]. In all cases, the K_s values declined as the OC content and fraction of FM increased for the different sediments (Table 5).

As with previous studies [*16,17*], the availability of contaminants for accumulation from sediments, reflected by the K_s values, was not proportional to the partition coefficient determined between sediment interstitial water and particles. Both the partition coefficients and the K_s values were larger for the chlorinated biphenyls than for the polycyclic aromatic hydrocarbons. This was the case for all levels of organic carbon (Tables 2 and 5).

When the K_s values were correlated to the individual sediment characteristics, percent of FM, CS, and OC content, the percent of OC provided the best variable for describing the variability between sediments based on the generally smaller p values for the regressions across all the compounds (Table 6). When OC was used in the regressions, the PY and TCBP yielded more highly significant regressions than BaP and HCBP.

If the K_s values are normalized for the fraction of OC and plotted against the respective log K_{ow} for the compounds, the two classes of compounds each show a decline in K_s with increasing log K_{ow}. However, the K_s values for the chlorinated hydrocarbons are larger than the corresponding values for the polycyclic aromatic hydrocarbons (Fig. 3). The decline in K_s between PY and BaP relative to K_{ow} is similar to previous findings [*16*]. Further, the higher K_s values for the chlorinated biphenyls compared to PAH congeners are also similar to previous results [*16,17*].

Bioaccumulation factors (BAF), concentration in the organisms (wet weight) divided by the concentration in the sediment (dry weight), can be calculated from the kinetics constants by dividing the uptake rate coefficient by the depuration rate constant (K_s/K_d) (Table 5). In all cases, the BAF tended to decline with increasing amounts of OC. This reflects the decline in the K_s values with increasing OC. Because the contaminant in the organism will concentrate in the lipid pools of the animals and the sorption to the sediment is dominated by the OC content, the BAF was normalized for both factors. To normalize for the amount

TABLE 6—*Correlations between the uptake rate coefficients and sediment characteristics.*

Compound	Sediment Characteristic	Slope	Intercept	r^2	N	p
BaP	% FM	-5.8 ± 0.7^a	0.007 ± 0.001	0.957	4	0.014
HCBP	% FM	-1.7 ± 0.4^b	0.020 ± 0.003	0.842	4	0.054
PY	% FM	-1.7 ± 0.2^b	0.021 ± 0.002	0.943	4	0.019
TCBP	% FM	-2.6 ± 0.4^b	0.031 ± 0.003	0.934	4	0.022
BaP	% CS	-1.1 ± 0.3^c	0.007 ± 0.001	0.775	4	0.078
HCBP	% CS	-3.4 ± 1.1^c	0.020 ± 0.004	0.748	4	0.088
PY	% CS	-3.3 ± 0.8^c	0.020 ± 0.003	0.826	4	0.060
TCBP	% CS	-5.1 ± 1.2^c	0.030 ± 0.004	0.85	4	0.051
BaP	% OC	-5.4 ± 0.6^c	0.007 ± 0.0005	0.958	4	0.014
HCBP	% OC	-1.7 ± 0.2^d	0.021 ± 0.001	0.966	4	0.011
PY	% OC	-1.6 ± 0.1^d	0.021 ± 0.001	0.989	4	0.004
TCBP	% OC	-2.5 ± 0.1^d	0.031 ± 0.001	0.997	4	0.001

[a]Slope × 10^5.
[b]Slope × 10^4.
[c]Slope × 10^3.
[d]Slope × 10^2.

of lipid in the organisms, the organism weight had to be corrected to a dry weight basis using the dry-to-wet weight ratio (0.27) [*18*] and then adjusted for the lipid content. The average lipid fraction (0.417) was used for all calculations. The sediment concentration could simply be corrected for the fraction OC since the weight was already expressed on a dry weight basis. These normalized values are accumulation factors (AF) and have a suggested theoretical value of approximately two [*19,20*]. These AF are the inverse of preference

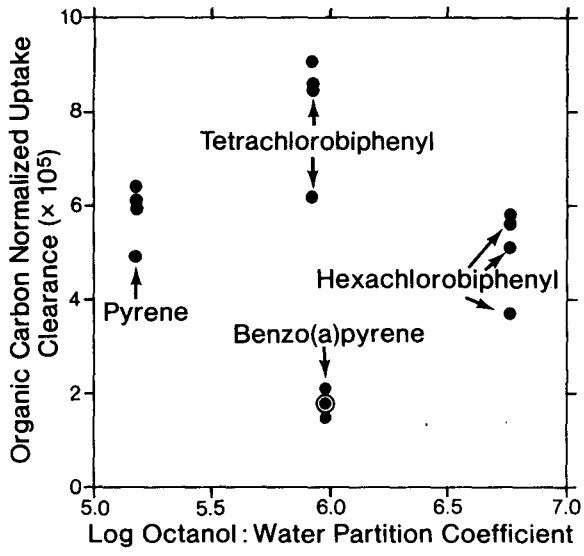

FIG. 3—*Scatter plot of the uptake rate coefficient normalized for percent OC versus the log octanol:water partition coefficient* (K_{ow}) *for both the PCB and PAH congeners.*

factors [*8,21*]. The AF values were relatively consistent across the various sediments but were considerably different between the two classes of contaminants with the PCB congeners exhibiting the larger values (Table 5).

Discussion

Partitioning

Measuring the partition coefficients between the sediment particles and the interstitial water is difficult even with radiotracers. The levels of radioactivity employed for this work were 8 000 to 10 000 DPM g^{-1} dry sediment for the ^{14}C-labeled compounds and 30 000 to 50 000 DPM g^{-1} dry sediment for the ^{3}H-labeled compounds. At these levels, the amount of radioactivity found in the freely dissolved fraction of the interstitial water was often low and in some cases not measurable, particularly for the ^{14}C-labeled compounds and in the cases where the amount of organic matter was greatest. The ^{3}H-labeled compounds, BaP and PY, were usually not as difficult to measure because they had generally greater levels of activity in the sediment and lower partition coefficients compared to the chlorinated biphenyls. The partition coefficients measured for the unmanipulated sediments were similar to previously determined values for BaP and TCBP [*17*] and for PY [*34*] in sediments collected from the same station. The similarity of results among various studies with sediments collected from the same station over a variety of studies suggests consistency in the method. Despite measurement difficulties, the partition coefficients provide insights into the factors that may govern partitioning of hydrophobic organic contaminants to sediments and those factors that influence their bioavailability.

While partitioning of organic contaminants to suspended sediments has routinely been attributed to the organic carbon content of the sediments [*22,23*], the partitioning between interstitial water and the sediment particles has not been well studied. As in the case of suspended sediments, the amount of organic matter best describes the variability in the measured partition coefficients for sediments with different OC contents. Although the change in the OC content occurred with a corresponding change in the percent of FM, the percent of FM was not quite as useful for describing the variability in the contaminant partitioning between the sediments. The percent of CS yielded almost as good a description of the variance in the partition coefficients between the various sediment types as did the OC content. However, the percent of CS is not expected to be as consistently useful across a wide range of sediment compositions because of differences in the relative amount of trapped water among sediment types.

The observed difference for the measured organic carbon content of the unmanipulated sediment between this collection (0.46%) and previous collections (1.0%) seems too large to be accounted for by sampling variability [*24*]. Therefore, part of the variability is likely due to the differences in the techniques used to measure the OC. This finding suggests that consistent approaches are needed for characterizing sediments, especially when making comparisons between laboratories. The method for determining the organic matter content should be well specified, and data for the percent of CS should be included for comparison, as this is a method that most laboratories will be able to perform.

Even after normalizing the partition coefficients for the OC content of the sediment, there was not a strong relationship between K_{ow} and the partition coefficient across all the compounds. Further, even within a compound class the normalized partition coefficient is not directly proportional to K_{ow}. This absence of direct proportionality between the partition coefficients and hydrophobicity contrasts markedly with partition coefficients measured for suspended solids after normalization for the organic carbon content. Partition coefficients measured for suspended solids exhibit a regular increase with increasing K_{ow} [*25*]. The

partitioning of organic contaminants between sediment and interstitial water has been measured for three PAH congeners, phenanthrene, pyrene and benzo(*a*)pyrene, spanning a range of log K_{ow} from 4.2 to 5.98. The partition coefficients were greatest for pyrene (420, [*34*]), while the partition coefficients for phenanthrene (317, [*34*]) and BaP (378 ± 18, [*17*]) were lower. A similar finding of a larger interstitial water-sediment partition coefficient compared to those for phenanthrene and benzo(*a*)pyrene has also been observed for field-collected sediments (B. J. Eadie, personal communication, Great Lakes Environmental Research Laboratory, Ann Arbor, Mich.). The differences in the physical environment may contribute to the difference in the partitioning behavior between water and sediments or suspended particles. Additionally, the partition coefficients may not represent equilibrium values because the time required to reach equilibrium for contaminants partitioning to particles may be long—on the order of years [*26,27*]. This finding will require additional effort to determine the mechanisms that cause the apparent absence of correlation between the normalized partition coefficient and K_{ow}.

Bioavailability

The main purpose of this work was to investigate the role that organic matter and fine material in sediments play in altering organic contaminant bioavailability. Altering the organic matter content of sediment, either by the method employed here or by adding organic-rich material, results in changes in the particle size distributions as well as in the OC content. These changes in particle size may be as important as the differences in the organic matter concentration when assessing bioavailability. Our purpose in manipulating the sediments was to alter the OC concentration without altering the composition of the OC, since changes in OC composition can affect partitioning behavior [*28,29*] and bioavailability [*29*]. As in the case of partitioning between sediment and interstitial water, the OC content yields the best regressions with K_s for explaining the variability between the sediment types for each compound. Thus, bioavailability apparently depends on the amount of OC in the sediment, all other factors being equal.

Preferentially dosing the fine fraction of the sediments did not seem to have any specific influence on K_s when the amount of OC or FM was taken into account. Even when sediments were dosed in bulk, the sorption appeared to occur to the FM or OC fraction of the sediments. Thus, the amount of FM and OC are important for determining the relative bioavailability of organic contaminants even when the bulk concentrations are similar.

As in previous work [*17*], the measured partition coefficients are insufficient to describe the extent of bioavailability or to describe the changes in bioavailability in terms of changes in compound characteristics. This is likely due, in part, to the role of ingestion in the bioaccumulation of the organic contaminants [*1,16*]. Even when the variability between sediment types is normalized by the percent of OC in the sediments, K_s values of the PCB and PAH congeners still vary significantly. These differences are not explained either by the measured partition coefficients or by the respective K_{ow} for the various compounds because compounds such as the PCB congeners with similar and, in some cases, greater measured partition coefficients compared to the PAH congeners are biologically more available from sediments than are PAH congeners (Fig. 3). An understanding of the factors influencing the desorption of the various contaminants from particles and the compounds' assimilation efficiencies is required to account for this difference between compound classes.

For both PY and TCBP, the correlations between OC and K_s are highly significant, while the regressions for HCBP and BaP are somewhat less significant. The slight difference between the pairs of compounds may exist because accumulation of HCBP and BaP by *Diporeia* is less dependent on desorption and uptake from interstitial water than the ac-

cumulation of PY and TCBP, based on a previous modeling effort [*1*]. Desorption and uptake of PY and TCBP from interstitial water accounted for approximately 75 to 80% of the total accumulated contaminant in *Diporeia*, while desorption and uptake of BaP and HCBP was estimated to contribute 50% or less of the contaminant accumulation. Thus, if the partitioning to sediments is governed largely by the OC content, and if the uptake of PY and TCBP occur predominantly from desorption and uptake from interstitial water, then these factors may explain why PY and TCBP exhibit slightly better correlations with OC than do BaP and HCBP.

The differences in the bioaccumulation potential of the two classes of compounds from sediment was also exhibited by the differences in the calculated AF values. While theoretical calculations have suggested that the AF value should be approximately two [*19,20*], even the PCB congeners were not calculated to reach this value at steady state, based on the kinetics. Deviations from the theoretical value could result from differences in the basis for the theoretical calculation, which was taken from relationships found for bioconcentration in fish and partitioning to solids both related to K_{ow}. Biotransformation of compounds could also account for changes in the AF value. Thus, while PCB congeners are widely recognized as metabolically stable, the PAH congeners are metabolized by many organisms.

However, for *Diporeia*, even the PAH congeners are metabolically stable [*18*]. Thus, the deviations from theoretical expectations cannot be explained by biotransformation for these compounds in *Diporeia*. Further, differences from the theoretical calculation likely reflect differences between fish and benthos and kinetic limitations in the accumulation of contaminants by benthos. The accumulation of contaminants from sediments has been successfully modeled as a kinetically limited system that cannot be accurately described by thermodynamic relationships [*1*]. The differences in the AF values between the two classes of compounds are another clear example of significant kinetic limitations for the accumulation of contaminants from sediments. These differences are a result primarily of reduced availability of the PAH congeners compared to the PCB congeners as reflected by the markedly lower K_s values. Even the PCB congener accumulation is likely kinetically limited since the expected value falls below the theoretical value. Such kinetic limitations are supported by the absence of correlations in the accumulation of contaminants from sediments either with the measured partition coefficients between sediment and interstitial water or K_{ow}.

Structure Activity Relationships

Understanding and predicting the accumulation of contaminants is the goal of toxicokinetic studies such as this. As shown in Fig. 3 and in previous studies [*16,17*], K_{ow} does not sufficiently explain the variability in K_s values normalized for the percent of OC in the sediment when comparisons are made between the PAH and PCB congeners. The data in Fig. 3 suggest that no single variable can describe the variability between the normalized K_s values for the two compound classes. Thus, any model selected must account for more than a single property of the compounds to satisfactorily describe K_s.

Because single variables such as K_{ow} will not describe the data, an alternative model such as the linear solvation energy model [*30*] may improve both our understanding and predictions of K_s across classes of compounds. The model uses compound characteristics that account for both the steric characteristics of molecules, specifically the molecular volume expressed as the intrinsic molecular volume divided by 100 (VI/100), and the electronic characteristics such as dipolarity (π^*) and hydrogen-bonding characteristics α and β. The molecular characteristics used for modeling the structure activity were obtained from the literature [*31*] (Table 7). All the α values were zero for our compounds, so no discrimination would be obtained from this characteristic. Regressions were performed with VI/100 com-

bined with π^* or β or both. With K_s normalized to the fraction OC in the sediment, the best regression was obtained using VI/100 and π^*: normalized $K_s = 0.00022 \pm 0.00003 - 0.00021 \pm 0.00003$ (VI/100) $+ 0.00010 \pm 0.00001\ \pi^*$, with $r^2 = 0.84$, $n = 16$, $p < 0.001$. The regression using VI/100 and β was only slightly less significant with $r^2 = 0.828$. The multiple regression with all three variables VI/100, π^*, and β gave the best r^2 value (0.874) but the F-ratio was less than that obtained from the regression with only VI/100 and π^*. From these regression results, it seems clear that the steric properties of the compounds and the dipolarity of the molecules best describes the molecular factors that influence the K_s values normalized to OC.

To examine whether this model would work with all the sediment uptake data that had been collected for *Diporeia*, including data from previous studies [*16,17*], the K_s values, normalized to the percent of CS, were fit by multiple linear regression as above. The data were normalized to percent of CS because the OC content, measured by the same technique, was not available for all the data. The best fit to the data was obtained by using molecular volume and β as the independent variables, and resulted in the following equation: normalized $K_s = 0.0018 \pm 0.0001 - 0.0011 \pm 0.0001$ (VI/100) $- 0.00085 \pm 0.00014\ \beta$, with $r^2 = 0.82$, $n = 34$, $p < 0.001$ (Fig. 4). The use of π^* in place of β resulted in a multiple linear regression that had only a slightly smaller r^2 value (0.81), but a much smaller F-ratio. A multiple regression with VI/100, π^*, and β resulted in a less significant regression than either of the regressions containing only two variables.

Whether modeling only the data from this study or all the available data, this structure activity model suggests that the normalized K_s values for sediment-associated contaminants

TABLE 7—*Normalized uptake rate coefficients and molecular characteristics for structure activity modeling.*

Compound Log K_{OW}	K_s^* (OC) (g OC g^{-1} h^{-1})	K_s^* (CS) (g CS g^{-1} h^{-1})	Molecular Characteristics[a] VI/100	π^*	β
Benzo(*a*)pyrene					
5.98[b]	0.000021	0.00009	1.418[b]	1.0[b]	0.3[b]
	0.000018	0.0001	1.418	1.0	0.3
	0.000018	0.00007	1.418	1.0	0.3
	0.000015	0.00008	1.418	1.0	0.3
Hexachlorobiphenyl					
6.77[c]	0.000056	0.00024	1.46[b]	1.5[b]	0.0[b]
	0.000058	0.00032	1.46	1.5	0.0
	0.000051	0.00020	1.46	1.5	0.0
	0.000037	0.00050	1.46	1.5	0.0
Pyrene					
5.18[b]	0.000064	0.00027	1.156[b]	0.9[b]	0.25[b]
	0.000059	0.00032	1.156	0.9	0.25
	0.000061	0.00024	1.156	0.9	0.25
	0.000049	0.00024	1.156	0.9	0.25
Tetrachlorobiphenyl					
5.92[c]	0.000091	0.00039	1.28[b]	1.3[d]	0.06[d]
	0.000085	0.00046	1.28	1.3	0.06
	0.000086	0.00034	1.28	1.3	0.06
	0.000062	0.00030	1.28	1.3	0.06

[a]VI = intrinsic molecular volume, π^* = dipolarity, β = hydrogen bonding characteristics.
[b][*31*].
[c][*33*].
[d]Solvatochromic parameters calculated from Kamlet et al. [*31*].

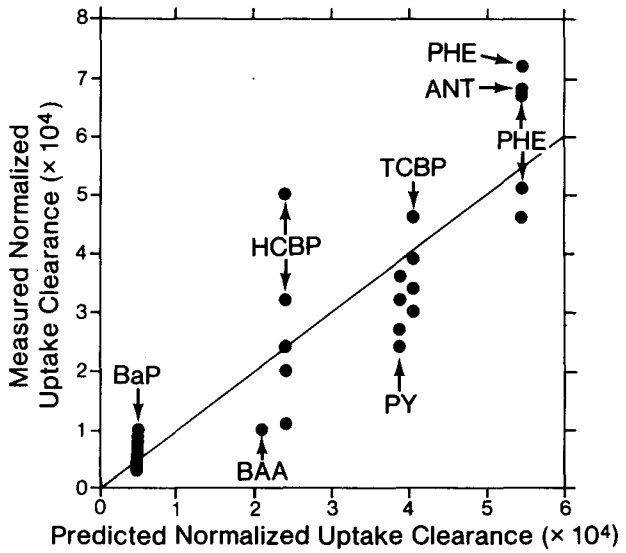

FIG. 4—*Scatter plot of the measured uptake rate coefficient normalized to percent combustible solids for data from this study and literature values* [16,17] *versus the predicted uptake rate coefficient. PY = pyrene, BaP = benzo(a)pyrene, TCBP = tetrachlorobiphenyl, HCBP = hexachlorobiphenyl, ANT = anthracene, PHE = phenanthrene, BAA = benz(a)anthracene.*

depend on both steric and electronic characteristics of the molecules. The steric term is strongly related to the partitioning characteristics of molecules, and in many cases molecular size has shown excellent correlations with log K_{ow} for single compound classes [*32*]. While the π^* term was most appropriate for the data restricted to this study, which represented a smaller data set, the β term was better when the larger data set representing all studies was used in the model. In spite of the somewhat better regression with β and the larger data set, it is difficult to decide conclusively which of the electronic terms is more appropriate for describing the variability not explained by the steric term because there are only small differences between the regressions using π^* and β. The major impact of this model is its ability to describe most of the variability in the data for two classes of compounds by using only molecular characteristics. When data are available for more compound classes, the resolution of which electronic term, π^* or β, is more appropriate may be easier to make. The fact that both steric and electronic terms are required to model the accumulation of nonpolar organic contaminants from sediments, and the failure of characteristics such as log K_{ow} to describe the accumulation from sediments, suggest that approaches such as the equilibrium partitioning approach, which are based on simple partitioning relationships related to log K_{ow}, are not likely to be adequate to describe bioaccumulation from sediments.

Overall, the K_s values for sediment-associated nonpolar contaminants seem to depend more on the amount of organic material in the sediment than on the amount of fine-grained matter for these sediments. Since the variation in organic matter did not incorporate differences in organic composition, based on the fact that the original sediment was manipulated to differing organic matter contents, further examination is needed to determine whether the relationship with percent of OC will remain the best descriptor for normalization over a range of sediment types. The utility of a linear solvation energy model to describe the variation in the normalized K_s values for two classes of compounds is promising, and further testing of this model may lead to useful predictive relationships.

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