Environmental Toxicology and Chemistry, Vol. 9, pp. 1095–1106, 1990
Printed in the USA. Pergamon Press plc

0730-7268/90 $3.00 + .00

Hazard Assessment

EQUILIBRIUM PARTITIONING AND BIOACCUMULATION OF SEDIMENT-ASSOCIATED CONTAMINANTS BY INFAUNAL ORGANISMS

JAMES L. LAKE,* NORMAN I. RUBINSTEIN, HENRY LEE II, CAROL A. LAKE,†
JAMES HELTSHE‡ and SHARON PAVIGNANO§
United States Environmental Protection Agency, Environmental Research Laboratory, Narragansett, Rhode Island 02882, †Narragansett, Rhode Island 02882, ‡University of Rhode Island, Department of Statistics, Kingston, Rhode Island 02881, and §Science Applications International Corporation, Narragansett, Rhode Island 02882

(*Received* 4 *April* 1989; *Accepted* 29 *November* 1989)

Abstract—The utility and limits of applicability of a simple equilibrium partitioning model for predicting the maximum concentration of neutral organic compounds which can be accumulated by infaunal organisms exposed to a contaminated sediment were examined. Accumulation factors (AFs) for PCBs, the lipid normalized PCB concentration in organisms divided by the organic carbon normalized PCB concentration in sediments, were measured for PCBs in infaunal mollusks and polychaetes at field sites with a range of sediment Aroclor (A-1254) and total organic carbon (TOC) concentrations. The average AFs for A-1254 were found to be higher ($\bar{x} = 4.94$; range 3.76–7.27) at sites with lower contaminant concentrations (15.0–48.3 ng A-1254/g dry sediment) than at more contaminated sites (328–9,200 ng/g), where AFs were lower ($\bar{x} = 2.62$; range 1.14–5.04). AF data grouped on the basis of sediment A-1254 and TOC concentration differed statistically between, but not within each group. Significant differences in mean AFs were found between some species and between some PCB congeners. When all data were considered, the variability associated with AFs was lower than that found for bioaccumulation factors on a wet weight basis, indicating the utility of lipid and organic carbon normalization.

Keywords—Bioaccumulation Equilibrium partitioning PCBs

INTRODUCTION

The bioaccumulation of sediment-associated contaminants by infaunal organisms has been examined because residues accumulated by these organisms may be transferred up food chains and impact higher trophic level organisms and man. To assess bioaccumulation potential from contaminated sediments and dredged materials, present regulations require analyses of the concentrations of organic and inorganic contaminants in an infaunal polychaete, an infaunal mollusk and a crustacean following a 10-d laboratory exposure to the test sediment [1]. These tests are expensive to conduct and of a duration that is inadequate to assess bioaccumulation potential of sediment contaminants. For neutral organics, an alternative method using an equilibrium partitioning model for predicting the maximum bioaccumulation potential has been proposed [2–4]. This model considers the first level transfer of neutral organic compounds from sediment to infaunal organism to result from equilibrium partitioning, and uses the physical chemical concept of fugacity to express these distributions [5–7]. Fugacity f (Pa) is an expression of chemical potential or escaping tendency of a contaminant from a phase. Fugacity capacity Z (moles/m^3 Pa) describes the relative affinity a contaminant has for a phase. Using the terminology of MacKay [5] the relationship between fugacity and the concentration C (moles/m^3) of a contaminant, i, in a phase is given by:

$$C^i = f^i Z^i \quad (1)$$

For two phases (1 and 2) the distribution of contaminant is described by:

*To whom correspondence may be addressed.
Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

$$\frac{C_1^i}{C_2^i} = \frac{f_1^i Z_1^i}{f_2^i Z_2^i} \quad (2)$$

At equilibrium $f_1^i = f_2^i$ and the contaminant i will partition according to its relative affinity for each phase.

The controlling distributional phases for contaminant partitioning are lipids for organisms [8] and organic carbon for sediments [9]. To evaluate contaminant partitioning in infaunal organism-sediment systems we write:

$$AF = \frac{X_L^i}{X_{oc}^i} \quad (3)$$

where AF is the accumulation factor; X_L^i is the concentration of i in organism's lipids (ng i/g lipid) and X_{oc}^i is the concentration of i in the organic carbon of sediment (ng i/g organic carbon).

AFs for contaminants are useful because they can be used along with the measured contaminant concentration in the organic carbon to estimate the contaminant concentration in the lipid of exposed infaunal organisms. Assuming that all the contaminant is in the lipid, the concentration of contaminant in the whole organism can be obtained by multiplying the contaminant concentration in the lipid by the fraction of lipid in the organism. These calculations allow prediction of the maximum concentration of contaminant in an infaunal organism at equilibrium (with respect to contaminant) with a specific waste sediment or dredged material. The suitability of the test sediment for ocean disposal can be evaluated by comparing the maximum contaminant concentration in organisms with regulatory limits (e.g., FDA tolerance levels).

This simple construct of contaminant partitioning in infaunal organism-sediment systems assumes that no kinetic or structural barriers to the establishment of equilibrium are present. Other assumptions of this model are: there is no metabolism of accumulated compounds; oranisms are not impacted by exposure; and measured lipids and organic carbon are the sole distributional phases for the compounds and are compositionally uniform. In actual environmental exposures some contaminants may be excluded from bioaccumulation because of size, and some infaunal organisms can construct barriers (e.g., burrows) which limit contaminant exchange. In addition, infaunal organisms may metabolize accumulated compounds and may be impacted by contaminant exposure. Finally, the composition of distributional phases (lipids and organic carbon) vary within and between organisms and from site to site. Any of these realities may alter contaminant distribution, as perceived in the simple construct, and cause variability in model predictions.

Our objective was to determine if the AF model is a sufficiently accurate representation of contaminant partitioning to predict bioaccumulation of neutral organic compounds (e.g., PCBs) by infaunal organisms. Infaunal organisms and sediments were collected from 13 sampling sites, AFs were measured and evaluations were made of the general utility and limits of applicability of the AF model.

MATERIALS AND METHODS

Sampling locations, sediment A-1254 and TOC concentrations are shown (Table 1). Sediments and organisms were collected between September 1986 and March 1987 using a Smith-MacIntyre grab sampler (0.1 m^2). Sediment samples were taken by opening the doors of the grab and collecting approximately 100 g of the top 5-cm layer of sediment in a glass jar that had been cleaned by solvent rinsing and heating to 450°C. The remaining sediment sample was sieved using a 2-mm stainless steel sieve, and additional sediment grabs were taken at the station and sieved. Organisms (separated by species) were placed in separate glass jars. All samples were capped with aluminum foil and were kept on ice until arrival at the laboratory. In the laboratory, sediment adhering to organisms was removed by rinsing with small amounts of deionized water. Sediment and organisms were frozen until analysis.

The guts of organisms were not purged prior to analysis. A previous study examining the quantity of sediment present in field-collected *Nephtys incisa* without purging the gut showed the worms contained only 3.8% (SD, ±1.8%, $n = 7$) dry weight of sediment (J.L. Lake, unpublished data). If AF is approximately in the range of 1 to 10, then, at least for *Nephtys*, the organic contaminants associated with sediment in the gut are insignificant relative to amounts accumulated in the tissues of the organisms.

Sediment samples from each location and collection date were mixed thoroughly with a stainless steel spatula and a weighed aliquot was dried (90°C) to constant weight to determine sediment water content. A portion of the dried sediment was used for TOC analysis. Shell fragments were removed from sediment samples for TOC analysis. Sediment sample weights were determined on an electrobalance and TOC analyses were conducted with a Carlo Erba CHN analyzer (Model No. 1106).

Table 1. Locations and concentrations of A-1254 and TOC of sediment sampling sites[a]

Sample	Location	A-1254 (ng/g)	TOC percent
New Bedford 1	41°35.42'N 70°53.53'W	3070 (85)	4.15 (0.12)[b]
New Bedford 2	41°36.62'N 70°53.86'W	4510 (193)	4.67 (0.22)
New Bedford 3	41°37.82'N 70°54.45'W	9200 (384	4.84 (0.13)
New Bedford 4	41°38.06'N 70°54.79'W	6330 (378)	4.58 (0.090)
New Bedford 5	41°38.02'N 70°54.78'W	7760 (389)	5.24 (0.28)
New Bedford 6	41°38.01'N 70°54.77'W	7180 (567)	4.29 (0.11)
Long Island Sound SR	40°7.95'N 72°52.7'W	43.0 (2.64)	2.39 (0.16)
Long Island Sound 40	41°03.8'N 73°10.0'W	48.3 (2.08)	2.62 (0.066)
Long Island Sound 46	41°04.9'N 73°05.2'W	15.0 (1.41)[c]	0.673 (0.36)
Long Island Sound 55	41°06.2'N 73°00.2'W	40.3 (6.11)	2.45 (0.11)
Upper Narragansett Bay 1	71°22.0'W 41°43.5'N	328 (27.1)	3.57 (0.055)
Lower Narragansett Bay 2	71°22.5'W 41°34.5'N	39.0 (2.65)	1.97 (0.16)
Lower Narragansett Bay 3	71°22.5'W 41°34.6'N	27.0 (2.64)	2.02 (0.16)

[a]Aroclor 1254 and TOC concentrations are on a dry weight basis and are means of three analytical replicates. Standard deviations are in parentheses.
[b]Mean of five analytical replicates.
[c]Mean of two analytical replicates.

For each station the sediment sample was homogenized and three analytical replicates were taken from this pool and averaged to yield a mean sediment concentration. For Long Island Sound Station 46 only two sediment replicates were analyzed. For sediment PCB analysis each 1-g aliquot of the wet sediment was extracted with 5 ml acetone for 15 s using a Brinkman tissue homogenizer (Model PT/35). The sample was centrifuged to separate the phases and the acetone extract was saved. The extraction was repeated and the acetone extracts were combined with 5 ml deionized water plus 1 ml of hexane containing octachloronaphthalene. The sample extract was shaken for 30 s and centrifuged to separate the layers. The hexane extract was reacted with 1 ml concentrated H_2SO_4. The hexane layer was removed and reacted with reduced copper powder to remove elemental sulfur. This hexane extract was then analyzed for PCBs.

For each station all organisms of a species type were pooled and homogenized and three analytical replicates were averaged to obtain a mean organism concentration. Tissue samples were thawed and shells were removed from bivalves. The samples were homogenized using a Brinkman tissue homogenizer (Model PT/35). When sufficient tissue was available, a portion of the homogenized sample was removed and dried (90°C) for calculation of a wet to dry ratio. For each analytical replicate a 1-g aliquot of the tissue homogenate was extracted as described for sediments except that one half of the hexane extract was removed for lipid analysis prior to addition of H_2SO_4, and the extract was not reacted with copper powder.

Lipids were measured by placing 100-μl portions of the hexane tissue extract on a preweighed aluminum pan, allowing the sample to air dry and reweighing the pan. Repeated analysis for lipids in aliquots of homogenates of *Mytilus edulis* and *Petar* sp. using this lipid procedure gave coefficients of variation of 11.5% ($n = 16$) and 14.1% ($n = 18$).

The sediment and tissue extracts were analyzed for PCBs on a Hewlett-Packard 5890A gas chro-

matograph equipped with a splitless injection port, electron capture detector and a 30-m fused silica column coated with a 0.25-micron coating of phenyl-methyl silicone (DB-5) from J + W Scientific. The injection port was at 270°C, the detector at 300°C and the column was held at 160°C for 1 min and then programmed at 10°C per min to 290°C and held for 10 min. The output from the detector was collected on a Perkin-Elmer LIMS 3210 computer.

Peaks were identified by matching retention times of peaks of PCB congener standards with peaks in samples and by comparison of chromatograms with published analyses of Aroclor mixtures [10]. The peaks analyzed and their constituent congeners are shown (Table 2). The congener numbers used in this article refer to the dominant congener in these peaks. PCBs were also quantitated as Aroclor 1254 (A-1254) using the sums of the areas of seven peaks which were selected as representative of A-1254. The congeners comprising these seven peaks are shown (Table 2).

The analytical procedures used for the determination of organic contaminants have been tested with spiking experiments and have been successfully intercalibrated with other analytical procedures. Recoveries from spiked samples using these procedures ranged from 89.3% (SD, ±3.8%) for tetrachlorobiphenyl to 100.5% (SD, ±2.5%) for decachlorobiphenyl.

Table 2. Congeners comprising peaks measured in this study

Peak	IUPAC numbers	Structures[a]
A	052	25-25
B[b]	95[c],66	236-25,24-34
C[b]	101[c],90	245-25, 235-24
D[b]	110[c],77	236-34,34-34
E	151[c],82	2356-25,234-23
F[b]	118[c],149	245-34,245-236
G	153	245-245
H[b]	138[c],158	245-234,2346-34
I[b]	128	234-234
J[b]	180	2345-245
K	195[c],208	23456-234,23456-2356
L	194	2345-2345
M	206	23456-2345
N	209	23456-23456

[a]Numbers refer to locations of chlorine substituents on biphenyl. Dash indicates separation of rings.
[b]Peak used for quantitation of Aroclor 1254.
[c]Dominant congener in peak.

Samples of commercial lunchmeat (as blanks) were taken through the wet sieving, sample collection, storage and analytical procedures. In addition, reagent blanks were carried through the analytical procedures with each set of samples. No contamination interfering with the analysis of PCBs was found in any of the blanks. To ensure satisfactory performance of the gas chromatograph, standards of A-1254 were run at intervals in each series of analyses.

The mean sediment concentration and the mean organism concentration were used along with the mean organic carbon and lipid concentrations to determine AF by Equation 3.

All concentrations used in this paper are on a dry weight basis except for those used in calculating bioaccumulation factors (BAFs), which were calculated as

$$\mathrm{BAF} = \frac{C^i\text{organism (wet weight)}}{C^i\text{sediment (wet weight)}} \qquad (4)$$

where i = contaminant and C = concentration. BAFs were calculated as wet weight concentrations because (for most organisms) insufficient tissue was available for determining wet to dry ratios.

Analysis of variance and Duncan's multiple range test were used to compare AFs and BAFs for each congener using a SAS statistical package. All tests were performed at the 5% level of significance.

RESULTS

A-1254 concentrations ranged from 3,070 to 9,200 ng/g in New Bedford Harbor, 27.0 to 328 ng/g in Narragansett Bay and 15.0 to 48.3 ng/g in Long Island Sound. Sediment TOC concentrations averaged 4.63% in New Bedford Harbor, 2.52% in Narragansett Bay and 2.03% in Long Island Sound (Table 1).

Organisms collected at each station and their feeding mode are listed in Table 3. The polychaete *Nephtys incisa*, the most ubiquitous species collected, was found at 12 of the 13 stations. The hard clam, *Mercenaria mercenaria*, and the bivalve, *Yoldia limatula*, were found at about half of the field sites.

Observations of the distribution of AFs for A-1254 against sediment A-1254 and TOC showed the data divided into two groups with two points between the groups (Fig. 1). A similar division of AFs by lipid concentration (wet weight basis) was not found. Although the middle points were from stations which were heavily contaminated [11] they were included with other contaminated sediments

Table 3. Organisms collected at field sampling sites[a]

	Location												
	New Bedford[b]						Long Island Sound[c]				Lower Narragansett Bay[c]		Upper Narragansett Bay[b]
Organisms	1	2	3	4	5	6	SR	40	46	55	2	3	1
Nephtys incisa[d]	3	1	1	1	1	1	3	3		3	3	3	
Mercenaria mercenaria[e]	3	3	3	3	1								3
Yoldia limatula[d]	1	1				1	2	3		3			2
Glycera sp.[f]	3	1	1				2						
Worm (Nemartine)[f]	3												
Astarte sp.[e]										3			

[a]Number in table refers to number of analytical replicates run on tissue.
[b]Samples at these locations were in the high group.
[c]Samples at these locations were in the low group.
[d]Deposit feeder.
[e]Filter feeder.
[f]Predator.

and AF data were divided into two groups, low sediments with A-1254 concentrations from 15.0 to 48.3 ng/g and TOC concentrations from 0.673 to 2.62% and high sediments with A-1254 concentrations from 328 to 9,200 ng/g and TOC concentrations from 3.57 to 5.24%. Analysis of AF data within these groups resulted in no significant relationships between AFs (for A-1254) and either sediment A-1254 or TOC concentration. This separation of AFs for data from all stations and spe-

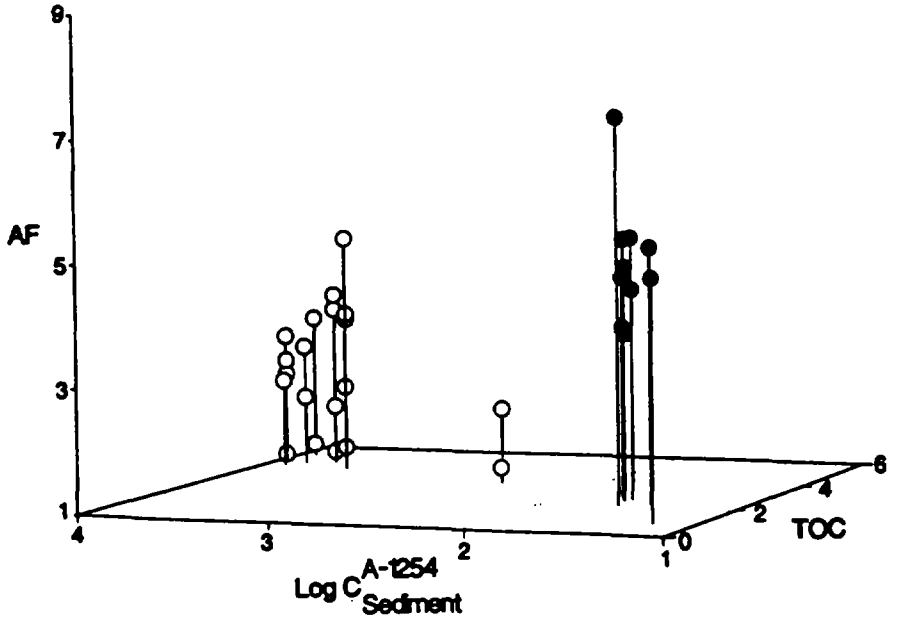

Fig. 1. Accumulation factor (AF) for Aroclor-1254 (A-1254) relative to sediment concentration of total organic carbon (TOC) (percent dry wt) and A-1254 (as $\log_{10}$) (dry wt). AFs are the lipid normalized tissue concentration of a congener or set of congeners for (A-1254) divided by the organic carbon normalized sediment concentration of that congener or set of congeners. Open balloons: high group sediments. Closed balloons: low group sediments. See text for details of sample sites, etc.

cies is tentative because the coverage of species at stations was not uniform, and only 13 sediments were sampled. Therefore, differences in AFs cannot be ascribed solely to differences in sediment A-1254 or TOC concentrations. This tentative separation was used to compare interspecies AFs and to examine differences in AFs between high and low sediment groups.

AFs for A-1254 for data from all stations and species had a mean of 3.39 and a range factor of 6.38 (1.14–7.27), but sediment A-1254 concentrations and TOC concentrations differed by factors of 613 and 7.82. In high group sediments AFs for A-1254 had a mean of 2.62, a range factor of 4.42 (1.14–5.04) and sediment A-1254 and TOC concentrations ranged by factors of 28 and 1.47. In low group sediments the mean AF for A-1254 was 4.94, the range factor was 1.93 (3.76–7.27) and sediment A-1254 and TOC concentrations ranged by factors of 3.22 and 3.91.

Mean AFs (for A-1254 and for individual congeners) were compared between species with sufficient occurrence at stations in the high group. Mean AFs for *Nephtys incisa* (a deposit feeder), *Mercenaria mercenaria* (a filter feeder) and *Glycera* sp. (a predator) which were each found at the same three stations in New Bedford are compared (Table 4). For A-1254 and most congeners there is no significant difference between AFs for *N. incisa* and *Glycera* sp., but AFs for *M. mercenaria* are usually significantly lower. The data also show an increase in mean AFs for *Glycera* sp. relative to *N. incisa* with increasing number of chlorine atoms on the PCB molecule.

Mean AFs for A-1254 and congeners for the deposit feeders *Y. limatula* and *N. incisa* were compared at common low and high group stations (Table 5). No significant differences in mean AFs were found for eight of 11 congeners or for A-1254 in the low group. AFs were not different for eight of nine congeners and A-1254 between these species in the high group.

Comparisons of mean AFs for the individual PCB congeners showed that AFs for 8 of 12 congeners were not significantly different and values overall differed by less than a factor of 2.4. The highest mean AFs were found for PCBs containing five and six chlorine atoms (Table 6). The group with the lowest mean contained PCBs with eight and nine chlorine atoms.

The mean AFs and BAFs and the coefficients of variation for each congener for data from all stations and species are shown (Table 7). The coefficients of variation are greater for BAFs than AFs for all PCBs except congener No. 194. This demonstrates the increased precision, relative to that for BAF, afforded by lipid and organic carbon normalization in deriving AFs.

Table 4. Mean accumulation factors (AFs) by PCB congener or mixture for *Mercenaria mercenaria*, *Nephtys incisa* and *Glycera* sp. at common high group stations[a]

IUPAC No. or Aroclor mixture	Species	Mean AF (*n*)[b]
52	*N. incisa*	3.24 (2)[c]
	Glycera sp.	2.76 (3)[c]
	M. mercenaria	1.99 (3)[c]
101,90	*N. incisa*	3.60 (3)[c]
	Glycera sp.	2.71 (3)[cd]
	M. mercenaria	1.57 (3)[d]
151,82	*Glycera* sp.	3.26 (3)[c]
	N. incisa	3.26 (3)[c]
	M. mercenaria	0.79 (3)[d]
118,149	*N. incisa*	3.31 (3)[c]
	Glycera sp.	2.78 (3)[c]
	M. mercenaria	1.32 (3)[d]
153	*N. incisa*	4.14 (3)[c]
	Glycera sp.	3.92 (3)[c]
	M. mercenaria	1.49 (3)[d]
138,158	*N. incisa*	3.56 (3)[c]
	Glycera sp.	3.55 (3)[c]
	M. mercenaria	0.95 (3)[d]
128	*Glycera* sp.	3.64 (3)[c]
	N. incisa	3.12 (3)[c]
	M. mercenaria	0.79 (3)[d]
180	*Glycera* sp.	3.73 (3)[c]
	N. incisa	2.94 (3)[c]
	M. mercenaria	1.05 (3)[d]
195,208	*Glycera* sp.	1.61 (3)[c]
	N. incisa	1.06 (1)[c]
	M. mercenaria	0.84 (2)[c]
194	*Glycera* sp.	2.09 (3)[c]
	N. incisa	2.07 (3)[c]
	M. mercenaria	0.59 (3)[c]
206	*N. incisa*	2.19 (3)[c]
	Glycera sp.	1.60 (3)[c]
	M. mercenaria	1.03 (1)[c]
A-1254	*N. incisa*	3.22 (3)[c]
	Glycera sp.	2.79 (3)[c]
	M. mercenaria	1.27 (3)[c]

[a]New Bedford 1, 2 and 3.
[b]*n*, number of samples used for calculation of mean.
[c,d]Common Duncan groups for mean AFs within a PCB congener or mixture.

DISCUSSION

AFs show the equilibrium distribution of a contaminant between the lipid and organic carbon phases and, if the assumptions of the equilibrium partitioning model are valid, should be constant regardless of factors such as sediment contaminant

Table 5. Mean accumulation factors (AFs) by PCB congener or mixture for *Nephtys incisa* and *Yoldia limatula* at common stations grouped by sediment A-1254 and TOC concentrations

IUPAC No. or Aroclor mixture	Group[a]	Mean AF (n)[b] *N. incisa*	Mean AF (n)[b] *Y. limatula*
52	Low	4.52 (2)	2.48 (2)
	High[c]	3.16 (2)	4.89 (3)
101,90	Low	4.79 (3)	6.33 (3)
	High	3.55 (3)	4.38 (3)
151,82	Low	4.68 (3)	5.72 (3)
	High	3.28 (3)	4.10 (3)
118,149	Low[c]	4.48 (3)	5.73 (3)
	High	3.29 (3)	4.26 (3)
153	Low[c]	6.35 (3)	8.25 (3)
	High	4.15 (3)	5.10 (3)
138,158	Low[c]	5.14 (3)	5.60 (3)
	High	3.59 (3)	4.01 (3)
128	Low	3.66 (3)	4.80 (3)
	High	3.17 (3)	3.30 (3)
180	Low	4.27 (3)	3.77 (3)
	High	3.03 (3)	3.88 (3)
195,208	Low	4.49 (3)	3.58 (3)
	High	[d]	
194	Low	3.27 (3)	3.13 (3)
	High	2.12 (3)	1.35 (2)
206	Low	6.20 (3)	4.22 (3)
	High	[d]	
A-1254	Low	4.29 (3)	4.79 (3)
	High	3.22 (3)	4.07 (3)

[a]Low stations were Long Island Sound SR, 40 and 55 with sediment A-1254 concentrations from 40.3 to 48.3 ng/g (dry wt) and TOC concentrations from 2.39 to 2.62% (dry wt). High stations were New Bedford 1, 2 and 6 with sediment A-1254 concentrations from 3,070 to 7,180 ng/g (dry wt) and TOC concentrations 4.16 to 4.67% (dry wt).
[b]n, number of samples.
[c]A significant difference in mean AFs for *N. incisa* and *Y. limatula* was found for this congener and group. For unnoted groups no significant differences in mean AFs were found when separated by congeners and groups.
[d]Insufficient data.

concentration, organic carbon content or organism type and lipid content. We collected sediment that ranged from 15.0 to 9,200 ng A-1254/g sediment and 0.67 to 5.24% TOC and deposit, filter feeding and predatory infaunal organisms to cover a range in model parameters. Measured AFs between locations, species and congeners were used to determine limitations on the applicability of the model.

Plots of AFs for A-1254 for data from all stations and species showed two groups of points corresponding to differences in sediment A-1254 and TOC concentrations (Fig. 1). Division into low and

Table 6. Comparison of mean accumulation factors (AFs) of PCB congeners for data from all stations and species

IUPAC No.	Cl_n[a]	Mean AF (n)[b]
153	6	4.58 (29)[c]
138,158	6,6	3.92 (30)[cd]
101,90	5,5	3.86 (30)[cd]
118,149	5,6	3.56 (30)[cd]
151,82	6,5	3.44 (30)[d]
52	4	3.34 (25)[de]
128	6	3.12 (30)[de]
180	7	3.04 (30)[de]
206	9	2.92 (22)[def]
195,208	8,9	2.15 (22)[ef]
194	8	1.95 (28)[f]
209[g]	10	1.74 (6)

[a]Number of chlorine atoms on congener(s).
[b]n, number of samples used for calculation of mean.
[c,d,e,f]Common Duncan groups for mean AFs.
[g]Congener No. 209 was not used in analysis of comparisons of means because of the small sample size ($n = 6$).

Table 7. Mean accumulation factor (AF) and bioaccumulation factor (BAF)[a] for all stations and species by PCB congener or mixture

IUPAC No. or Aroclor mixture	Factor	Mean (n)[b]	C.V. (%)
52	AF	3.34 (25)	39.2
	BAF	1.18 (25)	64.1
101,90	AF	3.86 (30)	49.7
	BAF	1.87 (30)	103.7
151,82	AF	3.44 (30)	52.3
	BAF	1.64 (30)	86.1
118,149	AF	3.56 (30)	45.9
	BAF	1.68 (30)	87.7
153	AF	4.58 (29)	53.4
	BAF	2.23 (29)	95.1
138,158	AF	3.92 (30)	56.3
	BAF	1.90 (30)	89.7
128	AF	3.12 (30)	49.2
	BAF	1.54 (30)	97.6
180	AF	3.04 (30)	46.8
	BAF	1.38 (30)	76.3
195,208	AF	2.15 (22)	81.5
	BAF	1.23 (22)	121.2
194	AF	2.65 (29)	148.5
	BAF	1.28 (29)	146.2
206	AF	2.92 (22)	67.1
	BAF	1.52 (22)	88.0
209	AF	1.74 (6)	71.8
	BAF	0.809 (6)	89.9
A-1254	AF	1.60 (30)	83.8
	BAF	3.39 (30)	39.4

[a]BAF is on a wet weight basis.
[b]n, number of samples used for calculation of mean.

high groups on the basis of sediment A-1254 and TOC concentration resulted in AFs that did not significantly differ within each group. This suggests AFs may vary according to the degree of sediment contamination and TOC concentration. These differences in AFs from the high and low group sediments may have resulted from the greater affinity of organic contaminants for organic carbon of primarily anthropogenic origin (as found in high group sediments) than for natural organic carbon (as found in low group sediments) (S. Karickhoff, personal communication). In addition, the lowest concentration factors for oligochaete worms [$C_{worm}/C_{sediment}$] (dry weight basis) for a variety of chlorinated organics (including PCBs) in Lake Ontario sediments were associated with sediments with the highest organic content [12]. Similarly, higher AFs were found in sediments with low organic carbon content and lower AFs were found in sediments with higher organic carbon content for unsubstituted polycyclic aromatic hydrocarbons in the benthic organisms *Macoma balthica* and *Nereis succinea* [13]. Higher AFs also have been measured in sediments with lower sediment contaminant and organic carbon concentrations in laboratory studies [14,15].

In sediments of greater regulatory interest (high group) no functional relationship between AFs for A-1254 and sediment A-1254 or TOC concentrations were found, although the A-1254 concentration increased by a factor of 28 and TOC concentration increased by a factor of 1.5. The constancy in AFs with varying sediment contaminant concentration shows the utility of the AF approach for estimating the maximum PCB concentration in infaunal organisms exposed to sediments of regulatory concern.

Mean AFs for *N. incisa* (a deposit feeder), *Glycera* sp. (predatory species), and *M. mercenaria* (a filter feeder) which occurred at the same high group stations ranged from 0.79 to 4.14 (Table 4). For A-1254 and most congeners AF values did not differ between *N. Incisa* and *Glycera* sp., but AFs for *M. mercenaria* were significantly lower. This lack of difference between *N. incisa* and *Glycera* sp. suggests that biomagnification on a lipid normalized basis had not occurred for most congeners. Limited food chain transfer is suggested by the higher AFs for the more highly chlorinated PCB congeners in *Glycera* sp. relative to *N. incisa*. The selection of a higher molecular weight range of PCB congeners by predators also has been observed elsewhere [16]. The generally lower AFs for *M. mercenaria* may reflect accumulation of contaminants from suspended particulate matter and water in its feeding, the lack of a direct pathway of uptake from bedded sediment, or a difference in the fugacity capacity of its lipids.

Our AF results for *N. incisa* and *Y. limatula* from the field agree with some laboratory results, but disagree with others. The present study found no significant differences in mean AFs for A-1254 and 8 of nine congeners between *Y. limatula* and *N. incisa* at three common stations in the high group, and no significant differences in mean AFs for A-1254 and eight of eleven congeners between these organisms at the three common low group stations (Table 5). A lack of difference would be expected because of the common deposit feeding mode.

To compare AFs between studies, data regarding congener No. 153 are used (Table 8), because it is highly bioaccumulated and resistant to metabolism. Further it was the only congener used in one of two laboratory studies [14].

Rubinstein et al. [15] found no significant differences in mean AFs between *Y. limatula* and *N. incisa* for congener No. 153 in a 60-d laboratory exposure (Table 8). In contrast, McElroy and Means [14] found significantly different AFs for congener No. 153 between *Y. limatula* and *N. incisa* from 30-d laboratory exposures to spiked sediments from Narragansett Bay. In the present study mean AFs for PCB No. 153, except for *Y. limatula* in the high group, were significantly lower (by about a factor of 2) than those of Rubinstein et al. [15]. Mean AFs for congener No. 153 of McElroy and Means [14] are a factor of 5 to 18 below ours and were lower than the lower 95% confidence bound constructed from the means of the present study (Table 8). The disparate results found between the laboratory and field studies may have resulted from: (a) lack of attainment of equilibrium with respect to contaminant in the laboratory and field studies, (b) differences in methodologies for measuring PCBs and lipids between the studies, or (c) differences in dosing—the 30-d laboratory study used spiked sediments, but the other studies used environmentally contaminated sediments.

For the congeners examined in this study, the average AF for all stations and species ranged from 1.74 for congener No. 209 to 4.58 for congener No.153. The means of the AFs for the PCBs separated into four overlapping groups (Table 6). The PCBs in the group with the highest AFs were those congeners containing five and six chlorine atoms with structures which make them resistant to metabolism and which are known to accumulate in

Table 8. Interstudy comparison of accumulation factors (AFs) for PCB Congener 153 in *N. incisa*

Study (reference no.)	Exposure			AF		
	Group[a]	Site	Duration (d)	Mean	C.V. (%)	n^b
Rubinstein et al. 1987 [15]	Low	Lab	60	16.6[c]	40	3
Present Study	Low	Field		7.05[d]	20	3
McElroy and Means 1988 [14]	Low	Lab	30	0.42[e]		4
Rubinstein et al. 1987 [15]	High	Lab	60	7.12[f]	34	6
Present Study	High	Field		3.75[g]	25	6
McElroy and Means 1988 [14]	High	Lab	30	0.21[e]		4

[a]Low group defined as sediment A-1254 concentrations from 15 to 48.3 ng/g (dry wt) and TOC from 0.673 to 2.39% (dry wt). High group defined as sediment A-1254 concentrations from 328 to 9,200 ng/g (dry wt) and TOC from 3.57 to 5.24% (dry wt).
[b]Number of samples used in calculation of mean.
[c,d]Denote significant difference in mean AF in low group.
[f,g]Denote significant difference in mean AF in high group.
[e]Variance term could not be computed from data.

tissues of infaunal organisms [17,18]. The congeners in the groups with the lower AFs were those with greater numbers of chlorine atoms which may cause structural barriers to bioaccumulation [19]. These findings indicate that all congeners do not partition similarly and that differences in AFs for congeners may result from differences in physical-chemical properties of the congener. This suggests that, depending on the accuracy required from model predictions, a range of applicability of the model may have to be specified based on the properties of the congeners.

For the All Station and Species Data Set the coefficients of variation were lower for AFs, for all congeners except No. 194, than for bioaccumulation factors based on a wet organism weight and wet sediment weight (Table 7). Therefore, normalization for the lipid content of organisms and the organic carbon of sediments improves predictability of tissue concentrations from sediment concentrations.

Mean AFs for A-1254 for the deposit feeders *N. incisa* and *Y. limatula* from a laboratory study were generally significantly higher than those reported in this work and in other field studies (Table 9). With the exception of AFs for *Y. limatula* in the high group, the results of the laboratory exposures are approximately a factor of 2 higher than the AFs reported here. These results may reflect dif-

Table 9. Interstudy comparison of accumulation factors (AFs) for A-1254 in *N. incisa* and *Y. limatula*

Study (reference no.)	Exposure				AF		
	Group[a]	Site	Duration (d)	Organism	Mean	C.V. (%)	n^b
Rubinstein et al. 1987 [15]	Low	Lab	60	*N. incisa*	10.9[c]	29	3
Present Study	Low	Field		*N. incisa*	5.07[d]	26	5
Lake et al. 1987 [4]	Low	Field		*N. incisa*	4.55[d]	60	9
Lake et al. 1987 [4]	Low	Field		*N. incisa*	4.01[d]	5.6	2
Rubinstein et al. 1987 [15]	High	Lab	60	*N. incisa*	6.67[c]	45	6
Present Study	High	Field		*N. incisa*	3.12[d]	17	6
Rubinstein et al. 1987 [15]	Low	Lab	60	*Y. limatula*	13.1[c]	2.7	2
Present Study	Low	Field		*Y. limatula*	4.79[d]	18	3
Lake et al. 1987 [4]	Low	Field		*Y. limatula*	3.39[d]	2.5	3
Rubinstein et al. 1987 [15]	High	Lab	60	*Y. limatula*	4.92[c]	29	3
Present Study	High	Field		*Y. limatula*	3.61[d]	32	4

[a]Low group defined as sediments with A-1254 concentrations from 15 to 48.3 ng/g (dry wt) and TOC from 0.673 to 2.39% (dry wt). High group defined as sediments with A-1254 concentrations from 328 to 9,200 ng/g (dry wt) and TOC from 0.673 to 2.39% (dry wt).
[b]Number of samples used in calculation of mean.
[c,d]Represent Duncan groupings within each combination of group and organism.

ferences in exposure (i.e., impact of laboratory exposure on organisms), lack of attainment of equilibrium or methodological differences for quantifying PCBs and lipids between the laboratory study [15] and the field studies.

Our results agree with results of a laboratory exposure study by Rubinstein et al. [15] in the following ways: (a) the highest AFs were found in exposures with sediments containing the lowest concentrations of A-1254 and TOC, (b) significant differences in AFs were found for some congeners, (c) AFs for congener No. 153 were highest, lower AFs were found for some congeners containing seven or more chlorine atoms and (d) normalization for lipids (organisms) and organic carbon (sediments) reduced the variability in bioaccumulation data.

The mean AF for A-1254 for high group sediments ($\bar{x} = 2.62$) was higher than the AFs of 1.92 [2] or 1.72 [3], which were calculated from the differences in regression lines relating K_{oc}, for sediment, and BCFs (lipid), for fish, to K_{ow}. Our AF values were similar to a mean AF of 2.98 which was measured in fish (eight species) and crayfish (one species) exposed in a combined disposal facility to Lake Michigan sediments with PCB and TOC concentrations similar to the high group sediments [20].

Cumulative frequency distribution plots of AFs for congeners using data from all stations and species show that about 95% of the AFs are at or below 6.5 (Fig. 2A); for *N. incisa* and *Y. limatula* in high group sediments about 95% of the AFs are at or below 4.5 (Fig. 2B). These plots can be used to select a level of protection for infaunal organisms. For example, use of an AF of 4.5 in the model will result in predictions of tissue concentration (lipid weight basis) being exceeded 5% of the time for *N. incisa* and *Y. limatula* in high group sediments. A higher level of protection (less probability of a predicted tissue concentration being exceeded) can be obtained by increasing the AF used in the predictive model.

The concept of equilibrium partitioning of contaminants has been applied in other bioaccumulation studies. Equilibrium with respect to PCBs was found between water and zooplankton [21]. These authors also found equilibrium for PCBs in fish and in water, but they suggested equilibrium for PCBs may not be established in organisms which lacked appropriate exchange surfaces (gills). No difference in PCB concentrations in the lipids of crayfish and fish were found after long-term exposure to constant levels of PCBs in a combined disposal facility in Lake Michigan [20]. These findings suggest that the simple equilibrium partitioning

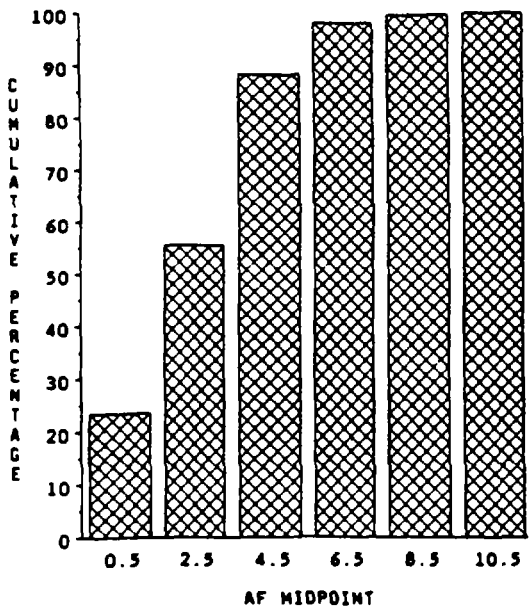

Fig. 2. (A) Cumulative frequency distribution plot of accumulation factor (AF) for 12 PCB congeners from six infaunal species and stations in New Bedford Harbor,

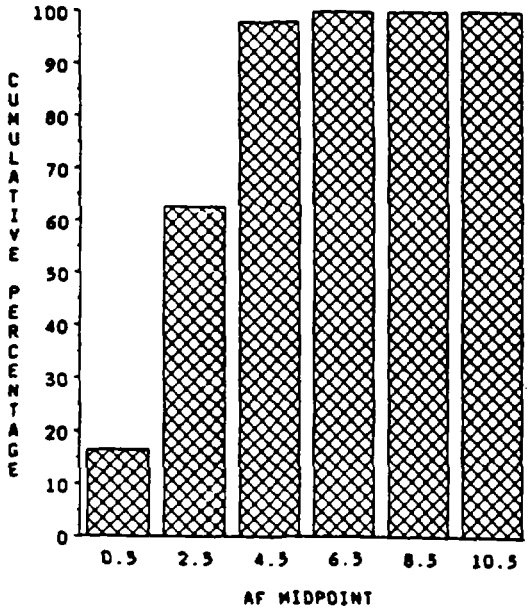

Fig. 2. (B) Cumulative frequency distribution plot of accumulation factor (AF) for 12 PCB congeners for *N. incisa* and *Y. limatula* at high group stations (sediments

approach may be applicable to contaminant bioaccumulation in aquatic organisms including fish.

Other field studies, however, have found that simple closed system equilibrium partitioning models are not appropriate for predicting accumulations by higher trophic level organisms. One study found differences in AFs between species and between congeners and evidence for the biomagnification of higher chlorinated congeners in some predators [22]. Kinetic and thermodynamic approaches have been compared for evaluating the bioaccumulation and biomagnification (the increase in contaminant concentration with increase in trophic level) of PCBs in aquatic systems [23]. Using field data, they found the fugacity of PCBs in water was lower than in fish lipid, and a direct relationship between the fugacity in fish lipid and its trophic level. These findings suggest that disequilibrium with respect to PCBs existed, biomagnification had occurred and the simple equilibrium partitioning approach was not applicable for PCBs in these fish. If biomagnification of PCBs and other contaminants occurs, as the results of the latter studies suggest, then simple closed system equilibrium partitioning models are not appropriate for predicting accumulations by higher trophic level organisms. For these applications, kinetic models or nonequilibrium fugacity models are appropriate, but these models require considerable input data (contaminant concentrations in prey, consumption rates of prey, assimilation efficiencies, depuration rates for contaminants and growth rates) to predict contaminant concentrations in higher trophic level organisms.

The findings of this study indicate the simple equilibrium partitioning model has use as a first level screening tool for estimating the maximum PCB concentration with infaunal organisms exposed to sediments of regulatory concern. However, to increase the precision of model predictions, limitations for the model's applicability may need to be specified based on the concentration of contaminants in sediments, organism type and physical-chemical properties of the contaminant.

Acknowledgement—The authors thank David Hansen, Richard Pruell and Walter Galloway for their comments on a draft of this manuscript.

REFERENCES

1. **U.S. Environmental Protection Agency/U.S. Army Corps of Engineers—Technical Committee on Criteria for Dredging and Fill Material.** 1977. Ecological evaluation of proposed discharge of dredged material into ocean water. Implementation Manual for Section 103 of Public Law 92-532 (Marine Protection, Research and Sanctuaries Act of 1972). Environmental Effects Laboratory, U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.
2. **McFarland, V.A.** 1984. Activity-based evaluation of potential bioaccumulation from sediments. *Proceedings*, Dredging and Dredged Material Disposal '84, American Society of Civil Engineers, Clearwater Beach, FL, November 14–16, pp. 461–467.
3. **McFarland, V.A. and J.U. Clarke.** 1986. Testing bioavailability of polychlorinated biphenyls from sediments using a two-level approach. *Proceedings*, U.S. Army Engineers Committee on Water Quality Sixth Seminar, New Orleans, LA, February 25–27, pp. 220–229.
4. **Lake, J.L., N. Rubinstein and S. Pavignano.** 1987. Predicting bioaccumulation: Development of a simple partitioning model for use as a screening tool for regulating ocean disposal of wastes. In K.L. Dickson, A.W. Maki and W.A. Brungs, eds., *Fate and Effects of Sediment-Bound Chemicals in Aquatic Systems*. Pergamon Press, Elmsford, NY, pp. 151–166.
5. **Mackay, D.** 1979. Finding fugacity feasible. *Environ. Sci. Technol.* 13:1218–1223.
6. **Mackay, D. and S. Paterson.** 1981. Calculating fugacity. *Environ. Sci. Technol.* 15:1006–1014.
7. **Mackay, D. and S. Paterson.** 1982. Fugacity revisited. *Environ. Sci. Technol.* 16:654A–660A.
8. **Schneider, R.** 1982. Polychlorinated biphenyls (PCBs) in cod tissues from the western Baltic: Significance of equilibrium partitioning and lipid composition in the bioaccumulation of lipophilic pollutants in gill-breathing animals. *Meeresforsch.* 29:69–79.
9. **Karickhoff, S.** 1981. Semi-empirical estimation of sorption of hydrophobic pollutants in natural sediments and soils. *Chemosphere*, 8:833–846.
10. **Schulz, D.E., G. Petrick and J.C. Duinker.** 1989. Complete characterization of polychlorinated biphenyl congeners in commercial Aroclor and clopher mixtures by multidimensional gas chromatography-electron capture detection. *Environ. Sci. Technol.* 23:852–859.
11. **Lake, J.L., C. Norwood, C. Dimock and R. Bowen.** 1979. Origins of polycyclic aromatic hydrocarbons in estuarine sediments. *Geochim. Cosmochim. Acta* 43:1847–1854.
12. **Oliver, B.G.** 1987. Bio-uptake of chlorinated hydrocarbons from laboratory spiked and field sediments by oligochaete worms. *Environ. Sci. Technol.* 21: 785–790.
13. **Foster, G.D. and D.A. Wright.** 1988. Unsubstituted polynuclear aromatic hydrocarbons in sediment, clams and clam worms from Chesapeake Bay. *Mar. Pollut. Bull.* 19:459–465.
14. **McElroy, A.E. and J.C. Means.** 1988. Factors affecting the bioavailability of hexachlorobiphenyls to benthic organisms. In W.J. Adams and G.A. Landis, eds., *Aquatic Toxicology and Hazard Assessment, 10th Volume*. STP 971. Philadelphia, PA, pp. 149–158.
15. **Rubinstein, N.I., J.L. Lake, R.J. Pruell, H. Lee II, B. Taplin, J. Heltshe, R. Bowen and S. Pavignano.** 1987. Predicting bioaccumulation of sediment associated organic contaminants: Development of a regulatory tool for dredged material evaluation. Technical Report D-87. U.S. Environmental Protection Agency, Narragansett, RI for U.S. Army Corps of Engineers, Vicksburg, MS.

16. **Oliver, B.G. and A.J. Niimi.** 1988. Trophodynamic analysis of polychlorinated biphenyl congeners and other chlorinated hydrocarbons in the Lake Ontario ecosystem. *Environ. Sci. Technol.* 22:388–397.
17. **Boon, J.P. and J.C. Duinker.** 1986. Monitoring of cyclic organochlorines in the marine environment. *Environ. Monit. Assess.* 7:189–208.
18. **Duinker, J.C., M.T.J. Hillebrand and J.P. Boon.** 1983. Organochlorines in benthic invertebrates and sediments from the Dutch Wadden Sea; Identification of individual PCB components. *Neth. J. Sea Res.* 17:19–38.
19. **Tulp, M.T.M. and O. Hutzinger.** 1978. Some thoughts on aqueous solubilities and partition coefficients of PCB and mathematical correlation between bioaccumulation and physio-chemical properties. *Chemosphere* 7:849–860.
20. **Clark, J.U., V.A. McFarland and J. Dorkin.** 1988. Evaluating bioavailability of neutral organic chemicals in sediments—A combined disposal facility case study. In W.G. Wiley, ed., *Proceedings*, Seminar on Water Quality '88, Charleston, SC, February 23–25, pp. 751–768.
21. **Clayton, J.R., S.P. Pavlou and N.F. Breitner.** 1977. Polychlorinated biphenyls in coastal marine zooplankton: Bioaccumulation by equilibrium partitioning. *Environ. Sci. Technol.* 11:676–682.
22. **Van der Oost, R., H. Heida and O. Opperhuizen.** 1988. Polychlorinated biphenyl congeners in sediments, plankton, molluscs, crustaceans and eel in a freshwater lake: Implications of using reference chemical and indicator organisms in bioaccumulation studies. *Arch Environ. Contam. Toxicol.* 17: 721–729.
23. **Connolly, J.P. and C.J. Pedersen.** 1988. A thermodynamic-based evaluation of organic chemical accumulation in aquatic organisms. *Environ. Sci. Technol.* 22:99–103.
24. **Lake, J.L., W. Galloway, G. Hoffman, W. Nelson and K.J. Scott.** 1987. Comparison of field and laboratory bioaccumulation of organic and inorganic contaminants from Black Rock Harbor dredged material. Technical Report D-87-6. U.S. Environmental Protection Agency, Narragansett, RI, for the U.S. Army Engineer Waterways Experiment Station, Vicksburg, MS.