BJC/OR-112

Biota Sediment Accumulation Factors for Invertebrates: Review and Recommendations for the Oak Ridge Reservation

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Biota Sediment Accumulation Factors for Invertebrates: Review and Recommendations for the Oak Ridge Reservation

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PREFACE

The purpose of this report is to acquire contaminant uptake data from published and unpublished literature, develop and present biota-sediment accumulation factors and regression equations for estimating chemical concentrations in benthic invertebrates for use on the Oak Ridge Reservation, and compare these to contaminant uptake data for emergent adult insects. This work was performed under Work break down Structure 1.4.12.2.3.04.05.03 (Activity Data Sheet 8304). The equations and biota-sediment accumulation factors presented in this report will facilitate the estimation of contaminant exposure experienced by wildlife consuming flying insects on the Oak Ridge Reservation. This report also provides a foundation for the process of developing body burden benchmarks for effects to benthic invertebrates and biota-sediment accumulation factors for fish. This report was originally issued as a draft under number ES/ER/TM-214.

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EXECUTIVE SUMMARY

Benthic invertebrates, fish, and flying insectivores are important assessment endpoints for the evaluation of ecological risks at aquatic sites on and near the Oak Ridge Reservation. One of the primary exposure pathways for these organisms is the consumption of contaminated food. Deposited sediments often act as a local sink for contaminants, which may increase the contaminant exposure for sediment-associated biota that indiscriminately ingest sediment particles while foraging. Benthic invertebrates are an important food source for fish and some terrestrial wildlife. Flying insectivores such as swifts, swallows, and bats, including the threatened and endangered grey bat, forage over water and consume adult insects that have aquatic larval stages (e.g., mayflies and midges). Therefore, larval infauna can be an important vector for the movement of chemicals out of sediment deposits and into the water column and terrestrial foodchains.

The simplest method for estimating contaminant loads in biota is the use of accumulation factors (AFS). AFs consist of ratios of the concentration of a given contaminant in biota to that in an abiotic medium. For the evaluation of sediments, this is commonly presented as the biota-sediment accumulation factor (BSAF). The concentration in biota may be estimated by multiplying the sediment concentration by the BSAF. This method is particularly useful for ecological risk assessments because ambient media concentrations are usually available; ambient media data are needed for the site characterization and human health assessments typically conducted in conjunction with ecological assessments. Concentrations in most biota are used only for the ecological risk assessment and are frequently not available, especially for screening level assessments. Separate BSAFs are required for each chemical because they are empirically derived, rather than based on general physico-chemical parameters. Bioavailability of contaminants for uptake can be influenced by sediment conditions including the pH and the amount of acid-volatile-sulfide that is available for complexing with divalent metals (e.g., Cd, Cu, Pb, Ni, and Zn).

The purpose of this report is to acquire contaminant uptake data from published and unpublished literature, develop and present BSAFs and regression equations for estimating chemical concentrations in benthic invertebrates for use on the Oak Ridge Reservation, and compare these to contaminant uptake data for emergent adult insects. The equations and BSAFs presented in this report will facilitate the estimation of contaminant exposure experienced by wildlife consuming flying insects on the Oak Ridge Reservation. This report also provides a foundation for the process of developing body burden benchmarks for effects to benthic invertebrates and BSAFs for fish.

1. INTRODUCTION

Benthic invertebrates, fish, and flying insectivores are important assessment endpoints for the evaluation of ecological risks at aquatic sites on and near the ORR. One of the primary exposure pathways for these organisms is the consumption of contaminated food. Deposited sediments often act as a local sink for contaminants, which may increase the contaminant exposure for sediment-associated biota that indiscriminately ingest sediment particles while foraging. Benthic invertebrates are an important food source for fish and some terrestrial wildlife. Flying insectivores such as swifts, swallows, and bats, including the Threatened and Endangered grey bat, forage over water and consume adult insects which have aquatic larval stages (e.g., mayflies and midges). Hence, larval infauna can be an important vector for the movement of chemicals out of sediment deposits and into the water column and terrestrial foodchains(Currie et al. 1997, Froese et al. 1998, and Larsson 1984)

Concentrations of bioavailable contaminants in sediment are needed to evaluate foodchain transfer and the potential toxicity of sediment contaminants. The bioavailable fraction can be measured directly by collecting and analyzing benthic invertebrates or it can be estimated. Contaminant concentrations in flying insects are needed to estimate the magnitude of contaminant exposure that flying insectivores may experience at a contaminated site. These concentrations also may be acquired either by direct measurement of contaminants in flying insects or by estimation. Direct measurement is the preferred approach because it contributes the least uncertainty to exposure estimates. That is, it provides information on the actual contaminant loading in on-site biota. However, direct measurement of contaminant concentrations in biota may not be feasible because of a lack time, personnel, or finances to support field sampling. When direct measurement of contaminants in biota is not possible, estimation is the only alternative.

Contaminant concentrations in biota may be estimated using a variety of methods, ranging from complex mechanistic process models to simple accumulation factors. While mechanistic process models for the estimation of contaminant concentrations in biota may give more accurate estimates, they require information which is not generally available for a risk assessment. An example of a mechanistic contaminant uptake model for fish is presented in Thomann et al. (1992).

The simplest method for estimation of contaminant loads in biota is the use of accumulation factors (AFs). AFs consist of ratios of the concentration of a given contaminant in biota to that in an abiotic medium. For the evaluation of sediments this is commonly presented as the biota-sediment accumulation factor (BSAF). The concentration in biota may be estimated by multiplying the sediment concentration by the BSAF. This method is particularly useful for ecological risk assessments because ambient media concentrations are usually available; ambient media data are needed for the site characterization and human health assessments typically conducted in conjunction with ecological assessments. Concentrations in most biota are used only for the ecological risk assessment and are frequently not available, especially for screening level assessments. Separate BSAFs are required for each chemical because they are empirically derived, rather than being based on generalizable physico-chemical parameters. Bioavailability of contaminants for uptake can be influenced by sediment conditions including the pH and the amount of acid-volatile-sulfide (AVS) that is available for complexing with divalent metals (i.e., Cd, Cu, Pb, Ni, and Zn).

The use of uptake factors, including BSAFs, depends on the assumption that the concentration of chemicals in organisms is a linear no threshold function of the concentration in sediment. This will not be the case if uptake or depuration of the chemical in question is well-regulated by the organism, either because it is an essential nutrient or because it is a toxicant for which the organism has inducible mechanisms for metabolism or excretion. Well regulated chemicals will have nearly constant concentrations regardless of sediment concentrations, at least within the effective concentration range for the regulating mechanism. Various complex patterns also are possible due to lack of induction at low concentrations, saturation kinetics at high concentrations, toxicity at high concentrations, or other processes. Despite these conditions that lead to violation of the assumptions, accumulation factors are commonly used in risk assessments.

The purpose of this report is to acquire contaminant uptake data from published and unpublished literature, develop and present BSAFs and regression equations for estimating chemical concentrations in benthic invertebrates for use on the ORR, and compare these to contaminant uptake data for emergent adult insects. Sediment to emergent adult BSAFs and regression equations also are included if sufficient data are available (i.e., PCBs). The equations and BSAFs presented in this report will facilitate the estimation of contaminant exposure experienced by wildlife consuming flying insects on the ORR. This report also provides a foundation for the process of developing body burden benchmarks for effects to benthic invertebrates and BSAFs for fish.

2. MATERIALS AND METHODS

2.1. LITERATURE REVIEW

To determine how contaminant uptake varies across locations, contaminant levels, and sediment conditions, we performed a literature search for studies reporting chemical concentrations in co-located sediment and invertebrate samples. Literature was reviewed for eight chemicals: arsenic, cadmium, chromium, copper, mercury, lead, nickel, zinc, and PCBs (Table 1). Sediment and invertebrate contaminant concentration data were extracted from each paper and used to calculate an accumulation factor.

Data were recorded for freshwater invertebrates, with particular emphasis on invertebrates that have terrestrial adult life stages (e.g., mayflies) or are generally consumed by fish (e.g., amphipods and tubificid worms). Data for marine and estuarine biota were not included in this evaluation. BSAFs and regression equations for metals were calculated on a dry weight basis. Biota concentrations reported in the literature only on a wet weight basis (e.g., mg Cu/kg fresh tissue) were included only if a wet-weight to dry-weight conversion factor also was presented. For PCBs, the BSAFs and regression equations were derived using sediment concentrations normalized to organic carbon content (e.g., ug PCB/g organic carbon) and organism concentrations normalized to lipid content (e.g., ug PCB/g lipid). Reported PCB concentrations were included only if organic carbon and lipid content values were presented. Biota concentrations presented only on a per organism basis (e.g., mg Cu/individual) were not included. Some studies were designed to elucidate mechanisms of uptake by using non-standard extraction methods. Only the results for methods typically used in environmental assessments

Table 1. Summary of Sources for Sediment and Invertebrate Concentration Data

Analytes	Study Locations	No. Sample Locations	Organisms	Depurated	Reference
			Benthic Organisms		
Cd, Cr, Cu, Ni, Pb, Zn	Wisconsin	3	Oligochaetes (*Lumbriculus variegatus)*	Yes	Ankley et at. 1944
Cd, Hg	Upper Miss. River	12	Mayfly (*Hexagenia spp.*)	No	Beauvais et al. 1995
Cu, Pb, Zn	Salmon River	2	Oligochaetes (*Limnodrilus hoffmeistri, Tubifex tubifex*)	Yes	Bindra & Hall 1977, cited in Chapman et al. 1979
As, Cd, Cu, Pb, Zn	Montana	9	Caddisfly, Mayfly, Stonefly, Hemiptera (Various species)	No	Cain et al. 1992
Cd, Cu, Pb	Montana	5	Caddisfly, Stonefly (Various species)	Yes	Cain et al. 1995
Cd	East River, Pequayman Lake, West Bearskin Lake	9	Oligochaetes (*Lumbriculus variegatus*)	Yes	Carlson et al. 1991
Cu, Hg, Ni, Pb, Zn	Canada	2	Oligochaetes (*Limnodrilus hoffmeistri, Tubifex tubifex*)	Yes	Chapman et al. 1979
As, Cd, Cu, Hg, Pb, Zn	S. Africa	1	Oligochaetes & Composite	No	Greichus et al. 1978
As, Cd, Cu, Zn	Quebec	1	Mayfly (*Hexagenia limbata*)	Yes	Hare et al. 1989
Cd, Cu, Zn	Quebec	3	Alderfly, Mayfly, Phantom midge, and Midge (*Sialis spp.*, *Hexagenia limbata*, *Chaorobus punctipennis*, *Chironomus sp.*, *Glyptotendipes sp.*, *Procladius spp.*)	Yes	Hare & Campbell 1992
Cd, Cu, Pb, Zn	Laboratory[a]	2	Midge (*Chironomus tentans*)	No	Harrahy & Clements 1997
As, Cd, Cu, Pb, Zn	Montana	7	Amphipod (*Hyallela azteca*)	No	Ingersoll et al. 1994

Table 1. (Continued)

Analytes	Study Locations	No. Sample Locations	Organisms	Depurated	Reference
Cd, Cr, Cu, Ni, Pb, Zn	Maryland	20	Dragonfly (Various species) & Composite[b]	No	Karouna-Renier 1995; MS Thesis
As, Cd, Cr, Cu, Ni, Pb, Zn	Lake Ontario	5	Oligochaetes	Yes	Krantzberg 1994
Pb	Illinois	3	Damselfly, Mayfly, Midge, Moth Flies, Oligochaetes (Anisoptera, Hexagenia limbata, Chirnomidae, Psychodidae, Tubificidae and Oligochaeta)	No	Leland & McNurney 1974
Cd, Cr, Cu, Ni, Pb, Zn	Illinois	1	Oligochaetes (*Limnodrilus hoffmeistri, Tubifex tubifex*)	No	Mathis & Cummings 1973
Cu, Pb, Zn	Oklahoma	1	Composite[b]	No	Namminga et al. 1974
As, Cd, Cu, Pb, Zn	Montana	6	Composite[b]	No	Poulton et al. 1995
Cr, Zn	North Carolina	8	Composite[b]	No	Shuman et al. 1977
Cd, Cu, Pb, Zn	Netherlands	1	Amphipod, Caddisfly, Dragonfly, Hemiptera, Isopod, Midge (Various species)	Yes	Timmermans et al. 1989
PCBs	Wisconsin	1	Oligochaetes (*Lumbriculus sp.* and *Lumbriculus variegatus*)	N/A[c]	Ankley et al. 1992
PCBs	Michigan	1	Mayfly (*Hexagenia limbata*)	N/A[c]	Drouillard et al. 1996
PCBs	Ontario	1	Mayfly (*Hexagenia limbata*)	N/A[c]	Gobas et al. 1989
PCBs	Lake Erie	1	Zebra mussel, Caddisfly, Amphipod, and Crayfish (*Dreissena polymorpha, Hydropsyche alterans, Gammarus fasciatus, and Orconectec propinquus*)	N/A[c]	Morrison et al. 1996

Table 1. (Continued)

Analytes	Study Locations	No. Sample Locations	Organisms	Depurated	Reference
PCBs	Lake Ontario	6	Oligochaetes (*Limnodrilus hoffmeistri and Tubifex tubifex*)	N/A[c]	Oliver 1987
PCBs	Netherlands	1	Mollusc and Crustaceans (*Dreisena polymorpha* and various species)	N/A[c]	van der Oost et al. 1988
			Emergent Adults		
Cd	Ontario	1	Dragonfly and Mayfly (*Odonata spp. And Hexagenia spp.*)	N/A[d]	Currie et al. 1997
As, Pb, Hg, Zn	Tennessee	3	Mayfly (*Hexegenia rigida*)	N/A[d]	Department of Energy 1996
Cd, Cu, Zn	Michigan	2	Midge (Chironomidae spp.)	N/A[d]	Young and Harvey 1988
PCBs	Michigan	1	Emergent Insects (Various species)	N/A[d]	Froese et al. 1998
PCBs	Laboratory[a]	9	Midge (*Chironomus plumosus*)	N/A[d]	Larsson 1984

[a] Results from a spiked-sediment bioassay.
[b] Composite of various benthic invertebrates analyzed together
[c] Not Applicable for analyses of PCBs, which are normalized to the organism lipid content.
[d] Not applicable to analyses of emergent adults.

(e.g., hot acid extraction of sediment metals) were used from such studies. Unfortunately, many potentially useful studies had to be eliminated for the aforementioned reasons.

Metal concentrations in biota were recorded as "depurated" for organisms that were allowed to purge their gut contents in clean water or sediment or were dissected to remove their gut contents. Biota concentrations that included gut contents were recorded as "Non-Depurated." Gut contents are presumed to be a negligible source of error for lipid-normalized organic chemical concentrations and were not explicitly accounted for in this evaluation.

Other relevant sediment and biota characteristics also were recorded. Sediment characteristics included percent sand, silt, and clay; percent organic carbon content; AVS and simultaneously extracted metal (SEM) concentrations; and interstitial water concentrations. Biota characteristics included the scientific and common name; life stages analyzed (larvae, pupae, or adult); feeding behavior (water column filter feeders, sediment ingesters, etc.); organism habits and habitats (e.g., burrowing in sediment depositional areas); and concurrently measured adverse effects (e.g., survival or density). These sediment and biota characteristics were recorded for future use and were not explicitly incorporated into the current evaluation.

2.2. MODEL DEVELOPMENT

2.2.1 Metals

BSAFs were calculated for each analyte, site, and species combination reported in a given study. Replicate sediment and biota measurements for a site and species combination were averaged together. Most of the available studies reported uptake from a limited number of locations or represented only a small range of sediment concentrations. However, a broad range of sediment concentrations are needed to best evaluate the relationship between concentrations of contaminants in sediment and those in benthic invertebrates. To that end, biota and sediment concentrations and the resulting BSAFs for each analyte were placed in one of two groups: those for which depurated organisms were analyzed ("Depurated") and those for which undepurated organisms were analyzed ("Non-Depurated"). BSAFs and accumulation models were subsequently developed for each group independently and for the entire data set ("All").

Summary statistics were calculated for BSAFs for each chemical and data set combination. The Shapiro-Wilk test (PROC UNIVARIATE; SAS Inst. Inc. 1988a) was applied to the untransformed and log-transformed BSAFs for each analyte to determine if the distribution of the BSAFs was normal or log-normal, respectively. Distributions were fit only for data sets with four or more BSAFs. A uniform distribution (i.e., all values are equally likely) was assumed if there were fewer than four BSAFs.

Regression analyses of the sediment and biota data also were performed for each chemical and data set combination. Because data concerning the number of individuals included in composites or means were not available for all observations, no weighting of observations was applied. Data were evaluated graphically and considered to be best fit by a power model. This is consistent with evaluations reported elsewhere (Sample et al. 1997). The power model of the form

$$y = a(x)^b \tag{1}$$

was linearized for the regression analyses by log-transforming the sediment and biota concentrations. The transformed model is:

$$\log(y) = a' + b \log(x). \qquad (2)$$

where:

y = chemical concentration in the organism (mg/kg dry wt.)
x = chemical concentration in sediment (mg/kg dry wt.)
a' = log-transformed y intercept
b = slope

2.2.2 PCBs

BSAFs were calculated for each site and species combination reported in a given study. Replicate measurements for a site and species combination were averaged together. Most of the available studies were designed to evaluate the uptake of non-ionic organic chemicals relative to chemical-specific characteristics (e.g., the organic carbon-partitioning coefficient). Such studies generally presented concentrations of individual congeners. The reported coongener concentrations were summed to obtain a total PCB concentration, because congener-specific data are not typically available for screening ecological risk assessments.

Summary statistics were generated for the PCB BSAFs. As with the BSAFs for metals, the Shapiro-Wilk test (PROC UNIVARIATE; SAS Inst. Inc. 1988a) was applied to the untransformed and log-transformed BSAFs to determine if the distribution of the BSAFs was normal or log-normal, respectively.

Regression analyses of the sediment and biota data also were performed for PCBs using the linearized power model (Eq. 2). Where "y" is the PCB concentration in the organism (ug/g lipid) and "x" is the PCB concentration in sediment (ug/g organic carbon)

2.3 VALIDATION

BSAFs and regression models developed from the benthos data were applied to the sediment concentration data in the validation dataset, and estimated contaminant concentrations in emergent adult insects were generated. "Most likely" estimates were generated using the median BSAF and the regression model. Conservative estimates for use in screening assessments were generated using the 90th percentile BSAF and the upper 95% prediction limit (95% UPL) for the regression models. The 95% UPL was calculated according to Dowdy and Wearden (1983) [Note: methods and parameters for calculating the 95% UPL are presented in Appendix A].

The appropriateness and accuracy of the estimation methods was evaluated for each analyte, data set, and estimation method. Differences between estimated and measured concentrations in emergent adults were evaluated using Wilcoxon signed-rank tests (PROC UNIVARIATE; SAS Inst. Inc. 1988a). Differences were considered significant if $p(H_0=0) \leq 0.05$. Relative accuracy and quality of different estimation methods were evaluated by calculating the proportional deviation of the estimate from the measured value:

$$PD = (Mi - Ei) / Mi$$

where

PD= proportional deviation
Mi = measured concentration in emergent adult insects at sediment concentration (i)
Ei = estimated concentration in emergent adult insects at sediment concentration (i)

Negative values for PD indicate overestimation while positive PD values indicate underestimation. The percentage of estimated values that exceeded their corresponding measured value was also tabulated for each chemical and estimation method. Relative quality of the "Most Likely" estimation methods was evaluated by the following criteria:

1) median PD closest to 0 (indicates estimates center around measured values);
2) PD with narrowest range (indicates relative accuracy of method);
3) percentage overestimation closest to 50% (indicates estimates center around measured values);
4) difference between estimated and measured values not significantly different as determined by Wilcoxon signed-rank tests.

Relative quality of conservative estimation methods was evaluated by

1) smallest, negative median PD value (indicates method overestimates while minimizing the degree of overestimation);
2) PD with narrowest range (to minimize the degree of overestimation);

In addition to the use of PD values, the concentrations in emergent adult insects relative to that of benthic organisms was evaluated graphically. Validation data (concentrations in adults and sediment) were included in the scatter plots of the model data (concentrations in benthos and sediment) to allow comparison of the ranges of sediment concentrations, the trends in biota concentrations relative to sediment concentrations, and the trends in observed adult concentrations relative to those predicted by the regression model. BSAFs for emergent adults and benthos also were plotted to allow comparison of the trends of predictions based on accumulation factors.

There was sufficient PCB validation data (ten observations) to develop a linear regression equation for the log-transformed sediment and emergent adult concentrations. This model was compared to regressions developed from the benthos data using the F-test procedure for comparing regression lines outlined in Draper and Smith (1981). Differences were considered significant if $p \leq 0.05$.

3. RESULTS

3.1 MODELING RESULTS

Summary statistics for the BSAFs for each chemical and data set combination are presented in Table 2. Data sets for which the median BSAFs were less than 1 included the "All"

Table 2. Summary statistics for literature-derived sediment-invertebrate accumulation factors

Analyte	Data Set[a]	N	Mean	Standard Deviation	Minimum	Median	90th Percentile	Maximum	Mean of Log-Trans-formed Values	Standard Deviation of Log-Trans-formed Values	Distribution
As	All	55	0.329	0.597	0.018	0.143	0.690	4.330	-0.764	0.476	Lognormal
As	Non-Dep.	49	0.240	0.236	0.018	0.127	0.675	0.889	-0.828	0.442	Lognormal
As	Dep.	6	1.058	1.611	0.278	0.373	4.330	4.330	-0.245	0.457	Lognormal[b]
Cd	All	120	2.822	5.227	0.001	0.600	7.990	41.550	-0.099	0.749	Lognormal[b]
Cd	Non-Dep.	88	3.438	5.938	0.049	0.614	9.240	41.550	0.005	0.710	Lognormal[b]
Cd	Dep.	32	1.126	1.362	0.001	0.459	3.073	4.878	-0.387	0.789	Lognormal[b]
Cr	All	34	0.179	0.227	0.015	0.100	0.468	1.101	-0.941	0.390	Lognormal
Cr	Non-Dep.	26	0.206	0.252	0.015	0.108	0.588	1.101	-0.883	0.396	Lognormal
Cr	Dep.	8	0.090	0.055	0.018	0.083	0.186	0.186	-1.133	0.322	Normal b
Cu	All	112	2.424	3.755	0.032	1.556	5.250	23.870	0.005	0.633	Lognormal[b]
Cu	Non-Dep.	74	2.140	2.621	0.032	1.647	3.872	16.630	0.050	0.565	Lognormal[b]
Cu	Dep.	38	2.976	5.318	0.047	0.661	7.957	23.870	-0.084	0.750	Lognormal
Hg	All	15	1.422	0.940	0.286	1.136	2.868	3.981	0.074	0.275	Lognormal
Hg	Non-Dep.	13	1.204	0.653	0.286	1.081	1.735	2.868	0.022	0.245	Lognormal[c]
Hg	Dep.	2	2.837	1.619	1.692	2.837	3.981	3.981	0.414	0.263	Lognormalv
Ni	All	26	0.857	1.230	0.055	0.486	2.320	5.746	-0.375	0.534	Lognormal

Table 2. (continued)

Analyte	Data Set[a]	N	Mean	Standard Deviation	Minimum	Median	90th Percentile	Maximum	Mean of Log-Trans-formed Values	Standard Deviation of Log-Trans-formed Values	Distribution
Ni	Non-Dep.	16	1.313	1.395	0.397	0.818	3.150	5.746	-0.024	0.329	Lognormal
Ni	Dep.	10	0.129	0.059	0.055	0.134	0.214	0.237	-0.935	0.214	Normal[c]
Pb	All	114	0.276	0.787	0.004	0.071	0.607	7.080	-1.069	0.575	Lognormal[b]
Pb	Non-Dep.	83	0.331	0.915	0.004	0.066	0.946	7.080	-1.063	0.624	Lognormal[b]
Pb	Dep.	31	0.129	0.132	0.009	0.080	0.326	0.503	-1.084	0.423	Lognormal
Zn	All	112	3.092	3.335	0.026	1.936	7.527	14.512	0.160	0.622	Lognormal[b]
Zn	Non-Dep.	84	3.473	3.577	0.026	2.330	8.465	14.512	0.229	0.610	Lognormal[b]
Zn	Dep.	28	1.952	2.141	0.079	0.840	4.759	8.479	-0.047	0.622	Lognormal
PCBs	Model (infauna)	16	9.016	12.796	0.739	4.670	21.886	51.313	0.652	0.530	Lognormal
PCBs	Validation (adult)	10	37.193	19.118	11.176	36.215	64.122	67.132	1.508	0.261	Normall[c]

[a] All = depurated and non-depurated invertebrates combined, Dep. = invertebrates depurated prior to analysis, Non-Dep. = invertebrates not depurated prior to analysis, Model = benthic invertebrates analyzed for PCBs, Validation = emergent adult insect analyzed for PCBs.
[b] $p<0.05$ for both normal and lognormal distributions
[c] $p>0.05$ for both normal and lognormal distributions

and “Non-Depurated” data for As, Cd, Cr, Ni, and Pb and the “Depurated” data for Cu and Zn. This indicates that the invertebrates analyzed in most of the evaluated studies did not accumulate these analytes to levels greater than those measured in the associated sediments. The maximum BSAFs for Cr, Ni, and Pb in depurated organisms also were less than 1. However, at least one reported BSAF was greater than 1 for all chemicals. The maximum BSAF for all metals was 23.9 for Cu in depurated organisms. The maximum BSAF for PCBs were 51.3 for benthos and 67.1 for emergent adults. The minimum BSAF for all analytes was 0.001 for Cd in depurated organisms.

For three metals (As, Hg, and Pb) the median BSAF for depurated organisms was greater than the median BSAF for non-depurated organisms. This is consistent with expected results for Hg, which should accumulate in the tissue to concentrations higher than those found in sediment. For As and Pb, it is more likely because of sampling error (measured sediment concentrations not representative of organism exposures) or differences in the taxa included in the two data sets. The median BSAF for all organisms was between the median BSAFs for each of the individual data sets for all metals. The 90th percentile BSAF for three metals (As, Cu, and Hg) in depurated organisms was greater than that for the non-depurated organisms.

The distributions of BSAFs for most analytes and data set combinations (22 of 26) were better described by a lognormal distribution than by a normal distribution. The three BSAF distributions that were better described by a normal distribution were also not significantly different ($p < 0.05$) from a lognormal distribution. Only one distribution better described by a lognormal distribution was also not significantly different ($p < 0.05$) from a normal distribution. Each of these four data sets was relatively small(8 to 13 observations). Ten of BSAF distributions better described by a lognormal distribution were significantly different ($p < 0.05$) from both a normal and lognormal distribution. This determination appeared to be independent of sample size. There also was no obvious relationship between the type of distribution and the range of sediment concentrations (Table 3).

Results of the regression analyses are presented in Table 3. Figures 1-5 present the log-log scatter plots of sediment and biota concentrations, the fitted line, and the 95% prediction interval. The regression lines presented in each figure are based on all of the available data (depurated and non-depurated) for all metals except Ni, for which the equations for depurated and non-depurated organisms are presented separately.

The metal concentrations in all invertebrates (depurated and non-depurated) were significantly positively correlated with the sediment concentrations for all but two analytes (Hg and Ni). That is, higher biota concentrations were observed at higher sediment concentrations. For those models with significantly positive slopes ($p < 0.05$), the amount of variation in biota metal concentrations explained by the sediment metal concentrations (R^2) ranged from 60% for As to 20% for Cr. Sediment PCB concentrations explained 65% of the variation in biota PCB concentrations. The slope for Hg was not significantly different from zero ($p > 0.05$), but the available sediment data covered a very small range of concentrations (0.038 mg/kg to 0.28 mg/kg). The ranges of sediment concentrations for most other analytes covered two or three orders of magnitude.

Table 3. Summary results for regression analyses of log-transformed sediment and invertebrate metal concentrations reported in the literature[a]

Analyte	Data Set[b]	N	Range of X (mg/kg dry wt.)	Est. (a′)	s.e. (a′)	Est. (b)	s.e. (b)	Slope > Zero[c]	R^2
As	All	55	1.15 - 764	-0.292	0.174	0.754	0.0851	Y ($p<0.001$)	0.60
As	Non-Dep.	49	4 - 764	-0.572	0.200	0.873	0.0943	Y ($p<0.001$)	0.65
As	Dep.	6	1.15 - 79	0.566	0.150	0.289	0.118	Y ($p<0.05$)	0.60
Cd	All	120	0.179 - 3000	0.0395	0.0685	0.692	0.0623	Y ($p<0.001$)	0.51
Cd	Non-Dep.	88	0.2 - 3000	0.191	0.0739	0.668	0.0608	Y ($p<0.001$)	0.58
Cd	Dep.	32	0.179 - 63.1	-0.314	0.132	0.513	0.192	Y ($p<0.01$)	0.19
Cr	All	34	10.4 - 1648	0.2092	0.237	0.365	0.128	Y ($p<0.01$)	0.20
Cr	Non-Dep.	26	10.4 - 1648	0.246	0.280	0.341	0.160	Y ($p<0.05$)	0.16
Cr	Dep.	8	54.15 - 279	0.0445	0.817	0.448	0.380	N ($p=0.14$)	0.19
Cu	All	112	2.765 - 7820	1.089	0.0623	0.278	0.0369	Y ($p<0.001$)	0.34
Cu	Non-Dep.	74	3.44 - 7820	1.037	0.0680	0.359	0.0394	Y ($p<0.001$)	0.54
Cu	Dep.	38	2.765 - 729	1.23	0.094	0.079	0.0583	N ($p=0.09$)	0.05
Hg	All	15	0.038 - 0.28	-0.67	0.279	0.327	0.246	N ($p=0.10$)	0.12
Ni	All	26	6.38 - 93	1.48	0.213	-0.425	0.159	N[d] ($p<0.01$)	0.23

Table 3. (continued)

Analyte	Data Set[b]	N	Range of X (mg/kg dry wt.)	Est. (a′)	s.e. (a′)	Est. (b)	s.e. (b)	Slope > Zero[c]	R^2
Ni	Non-Dep.	16	6.38 - 27	1.59	0.275	-0.463	0.247	N[d] ($p<0.05$)	0.20
Ni	Dep.	10	21.9 - 93	-0.440	0.491	0.695	0.300	Y ($p<0.05$)	0.40
Pb	All	114	6.89 - 679	-0.776	0.160	0.801	0.102	Y ($p<0.001$)	0.35
Pb	Non-Dep.	83	6.89 - 679	-0.864	0.205	0.859	0.137	Y ($p<0.001$)	0.33
Pb	Dep.	31	10.555 - 375	-0.515	0.223	0.653	0.129	Y ($p<0.01$)	0.47
Zn	All	112	12.02 - 10100	1.80	0.0720	0.208	0.0328	Y ($p<0.001$)	0.27
Zn	Non-Dep.	84	12.02 - 10100	1.77	0.0828	0.242	0.0384	Y ($p<0.001$)	0.33
Zn	Dep.	28	29.84 - 3210	1.89	0.1274	0.126	0.0549	Y ($p<0.05$)	0.17
PCBs	Model (benthos)	16	0.398 - 41.5[e]	0.59	0.177	1.110	0.2174	Y ($p<0.001$)	0.65
PCBs	Validation (adults)	10	0.126 - 326[e]	1.60	0.148	0.939	0.0841	Y ($p<0.001$)	0.94

[a] Equation is $\log(y) = a' + b[\log(x)]$, where y = concentration in biota and x = concentration in sediment, a′ = estimated intercept in log units, and b = estimated slope in log units.

[b] All = depurated and non-depurated invertebrates combined, Dep. = invertebrates depurated prior to analysis, Non-Dep. = invertebrates not depurated prior to analysis, Model = benthic invertebrates analyzed for PCBs, Validation = emergent adult insect analyzed for PCBs.

[c] Significantly different from zero based on the one-tailed t-test with (n-2) degrees of freedom.
[d] Slope is significantly different from zero, but is negatively correlated with sediment concentrations.
[e] Sediment concentrations are ug PCB/g organic carbon

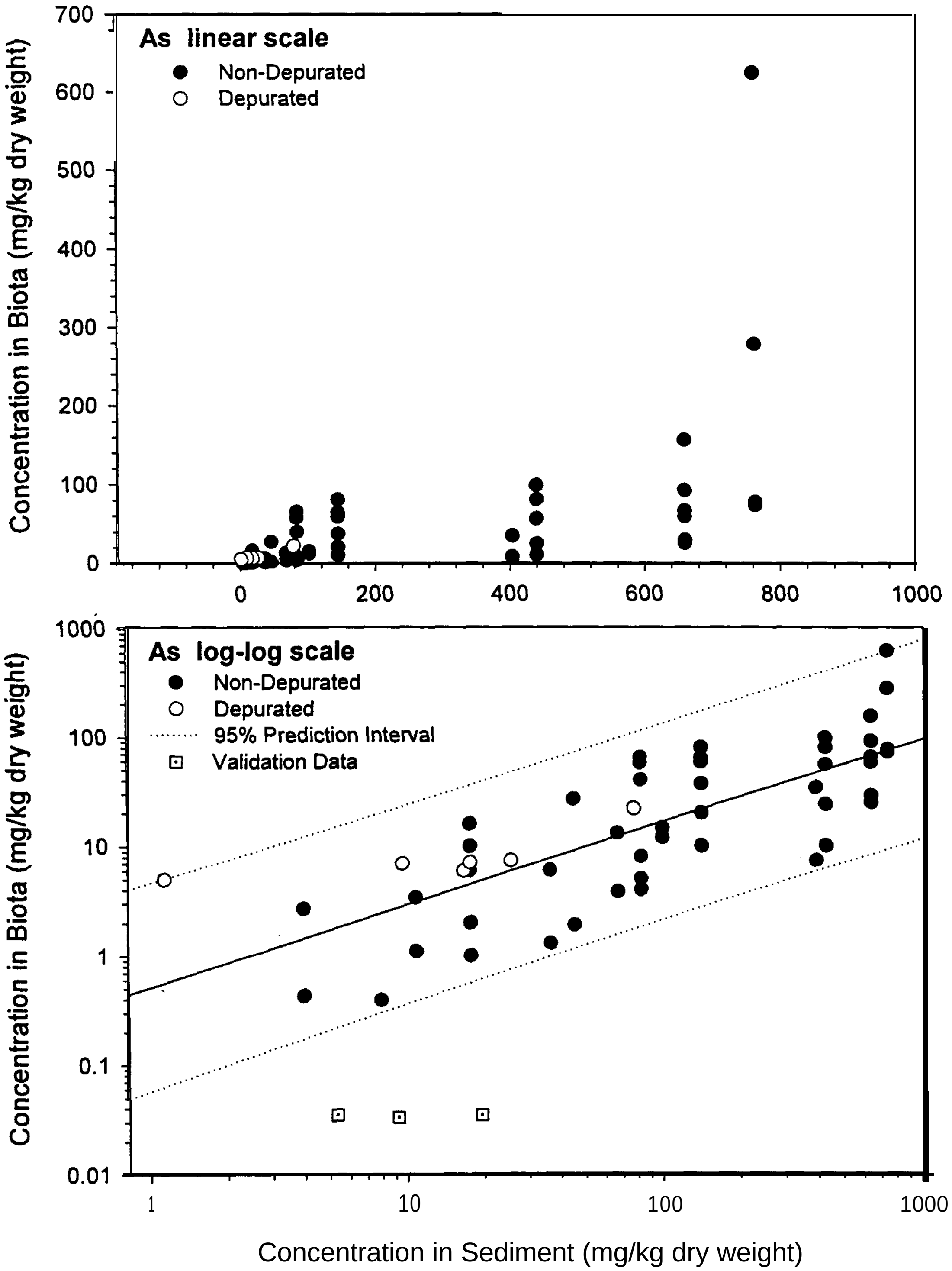


Figure 1. Linear and Log-log scatterplots of arsenic concentrations in sediment, benthic invertebrates, and emergent adult insects, The regression lines are based on all of the available data for benthics (depurated and non-depurated).

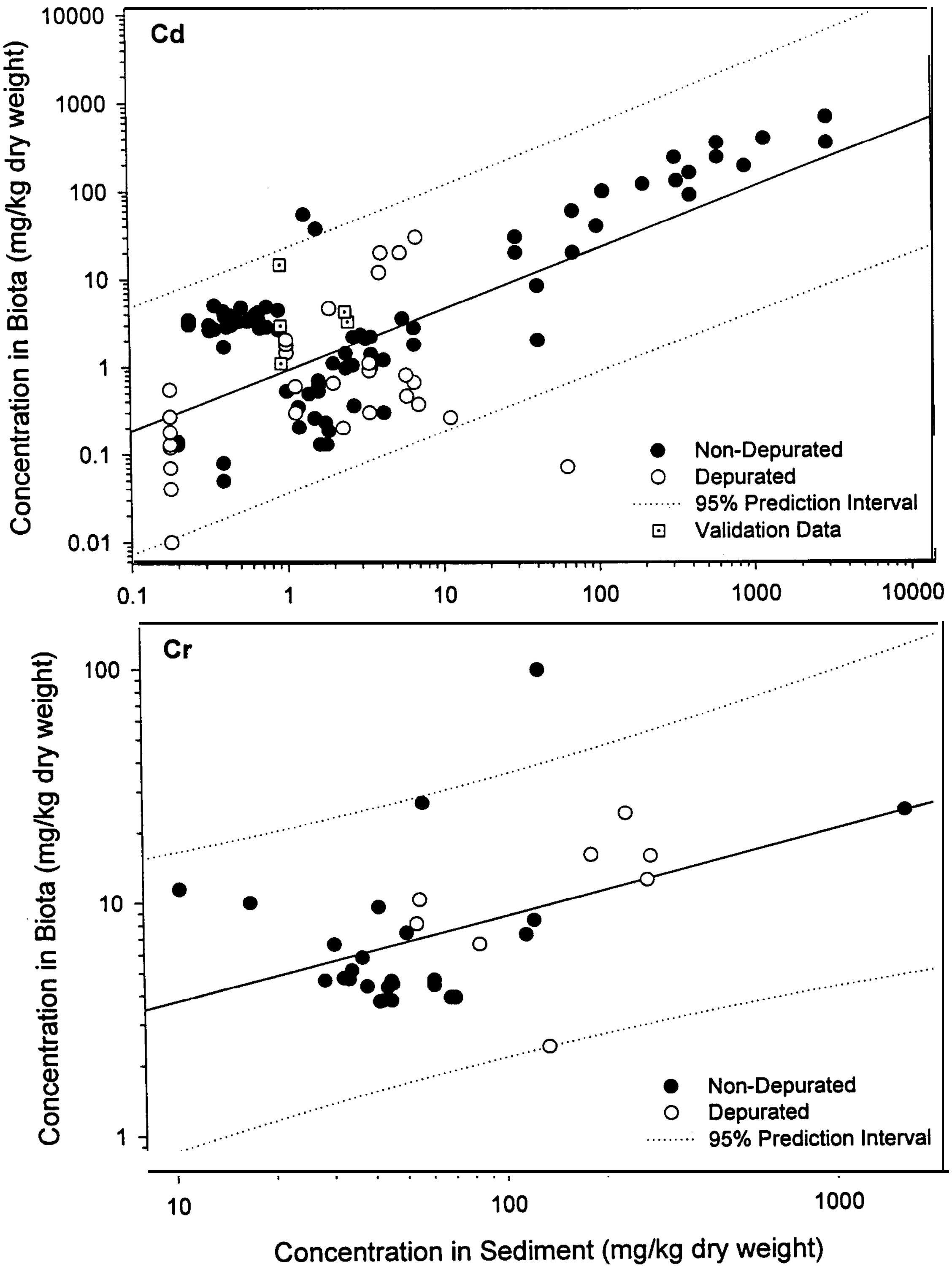


Figure 2. Log-log scatterplots of cadmium and chromium concentrations in sediment, benthic invertebrates, and emergent adult insects. The regression lines are based on all of the available data for benthics (depurated and non-depurated).

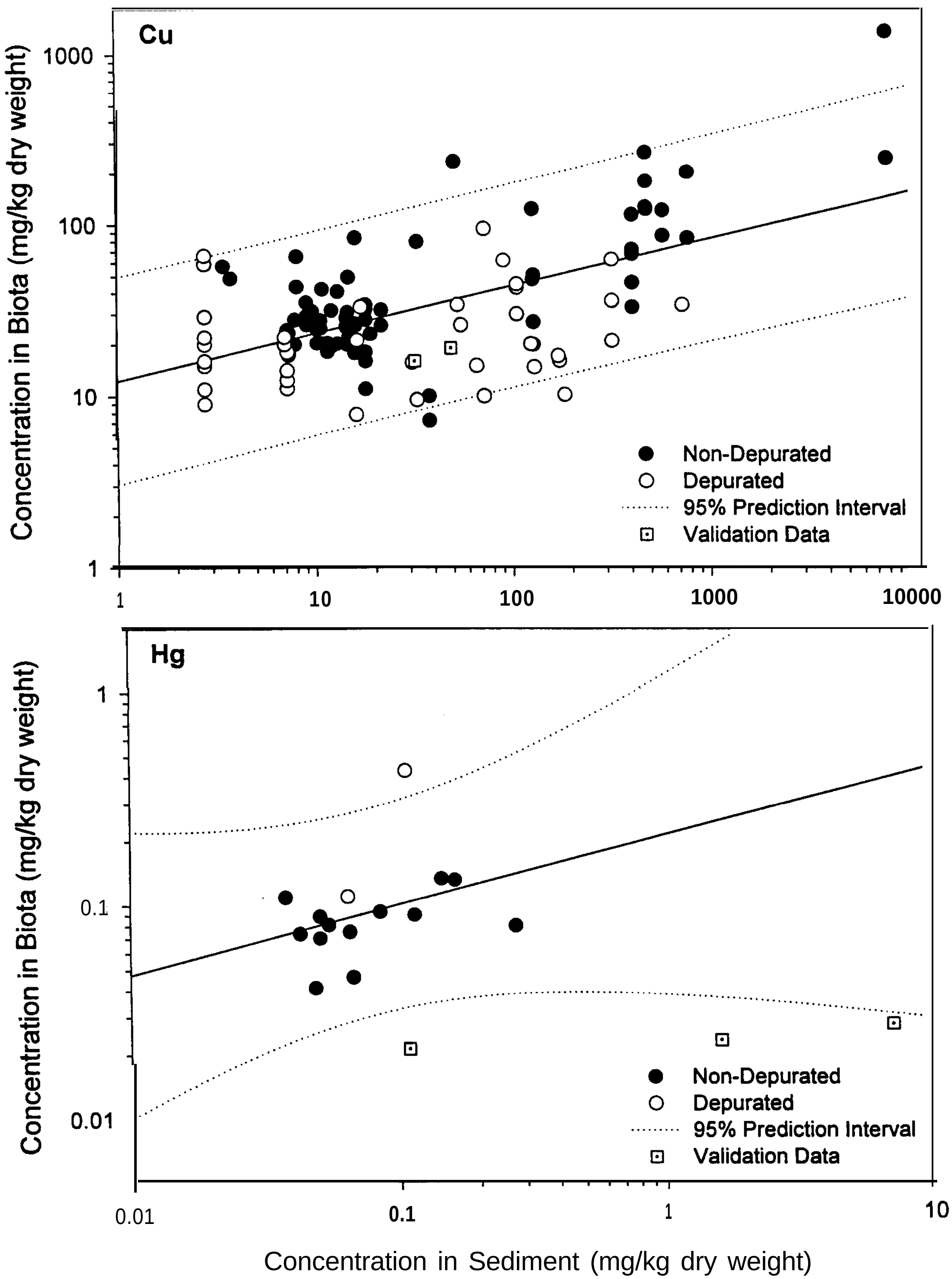


Figure 3. Log-log scatterplots of copper and mercury concentrations in sediment, benthic invertebrates, and emergent adult insects. The regression lines are based on all of the available data for benthics (depurated and non-depurated).

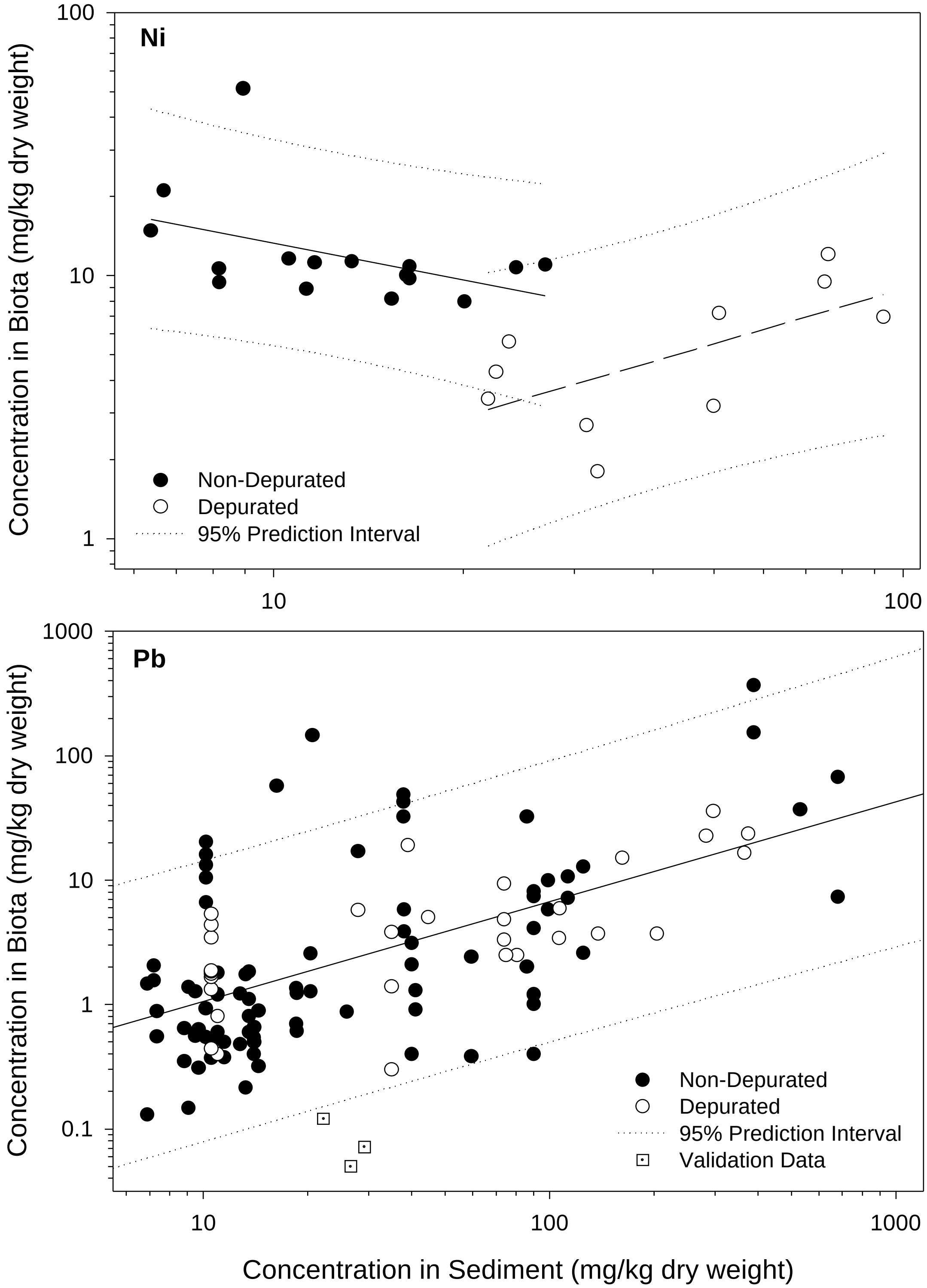


Figure 4. Log-log scatterplots of nickel and lead concentrations in sediment, benthic invertebrates, and emergent adult insects. The regression lines for lead are based on all of the available data for benthics (depurated and non-depurated).

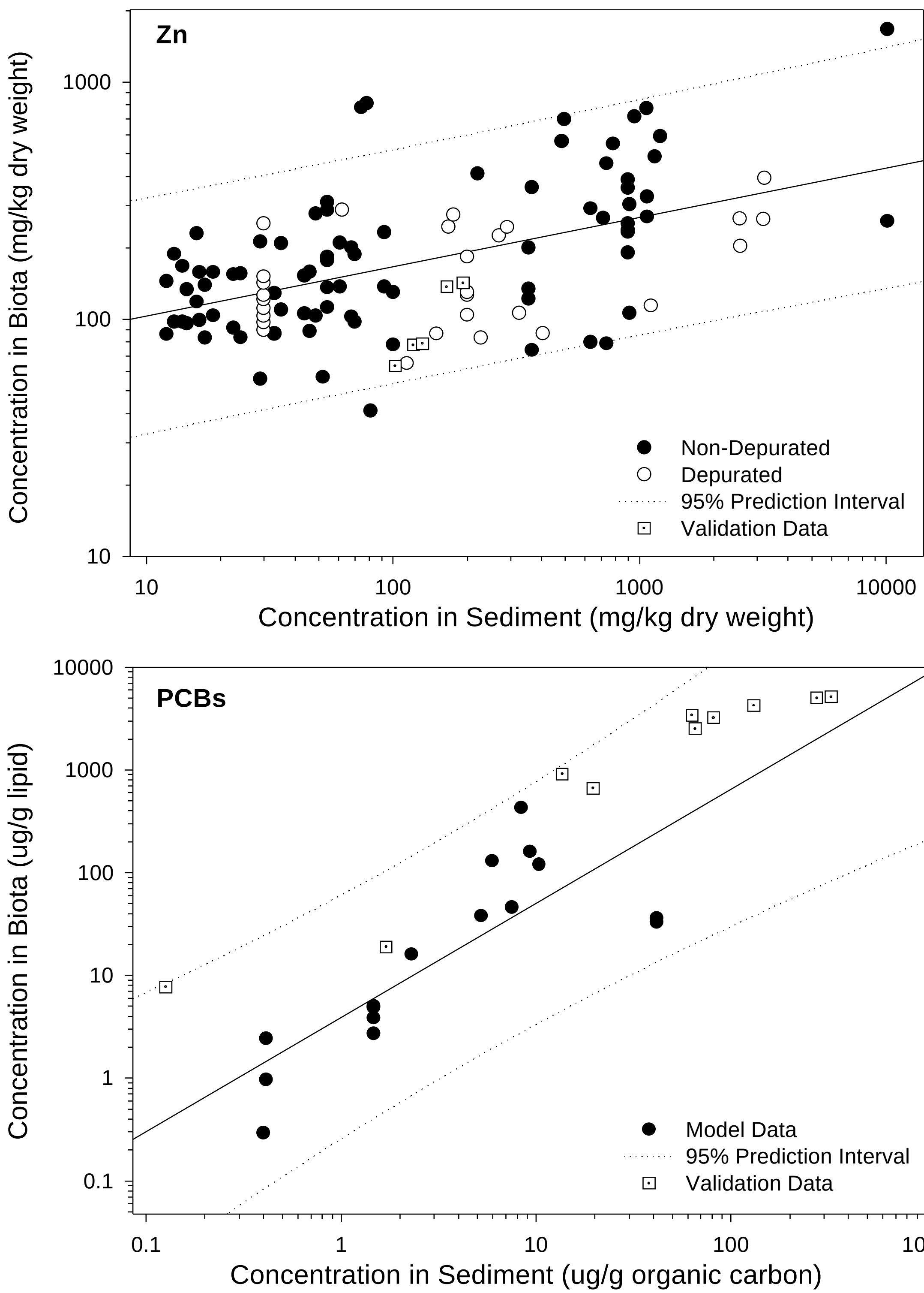
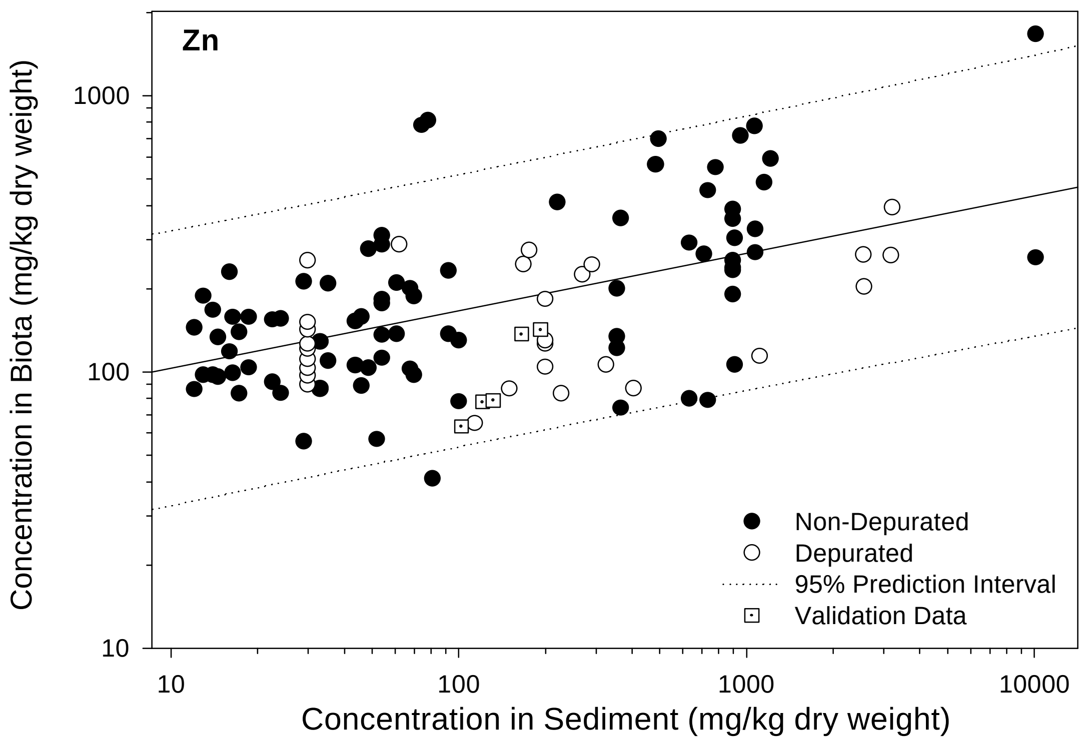


Figure 5. Log-log scatterplots of zinc and PCB concentrations in sediment, benthic invertebrates, and emergent adult insects. The regression lines for zinc are based on all of the available data for benthics (depurated and non-depurated). The regression lines for PCBs are based on the data for benthics.



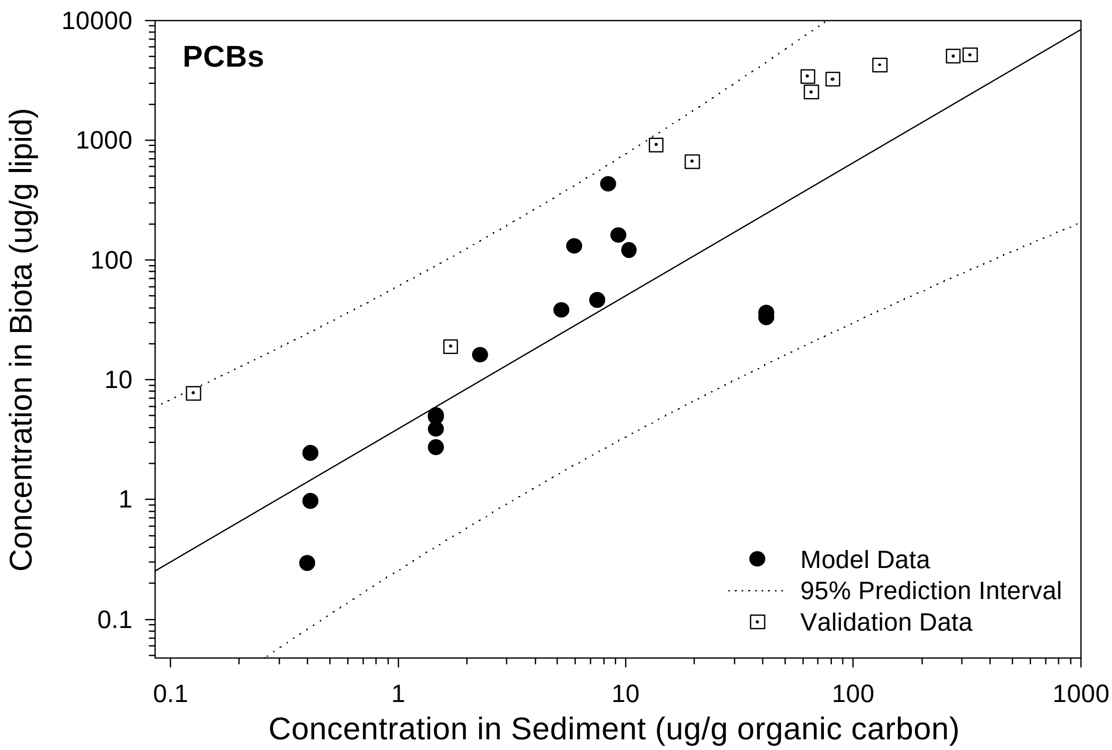


Figure 5. Log-log scatterplots of zinc and PCB concentrations in sediment, benthic invertebrates, and emergent adult insects. The regression lines for zinc are based on all of the available data for benthics (depurated and non-depurated). The regression lines for PCBs are based on the data for benthics.

The range of sediment concentrations also may have affected the observed relationship between sediment and organism concentrations for Ni. Concentrations of Ni in all invertebrates (depurated and non-depurated combined) were significantly negatively correlated with the sediment concentrations. Although the slope was significantly different from zero ($p < 0.05$), the depurated and non-depurated data sets appear to represent very different relationships (Figure 4). The regression model for non-depurated organisms is consistent with that of the combined data sets. Ni concentrations in depurated organisms are significantly positively correlated with sediment concentrations ($\alpha \leq 0.05$) and the model explains a higher proportion of the variation in organism concentrations than does either of the other two models (Table 3). However, comparison of these data sets is complicated by the narrow range of sediment concentrations for each data set and the limited overlap of these ranges.

3.2 VALIDATION RESULTS

Data for model validation were available for all analytes except Cr and Ni. However, the number of observations was very small (two to five) for all metals and they were associated with a relatively small range of sediment concentrations for all metals except Hg (Figures 1-5). Slightly more validation data (ten observations) were available for PCBs (Figure 5). The sediment concentrations cover three orders of magnitude, but nine of those exposures were from one study using spiked-sediment concentrations.

Concentrations estimated using the “Most Likely” estimation methods (i.e., the median BSAF and the log-log regression model) were not significantly different ($p < 0.05$) from the concentrations observed in emergent adults for each metal and data set combination (Table 4). The median BSAF overestimated 100% of the concentrations for all metals except Cd, for which it underestimated 100% of the concentrations. The regression models also overestimated 100% of the concentrations for all metals except Cd. The model based on non-depurated organisms underestimated four of the five observed concentrations (Table 4). Figures 1-5 depict the emergent adult data relative to the model data and the regression model based on “All” data. Arsenic and Pb concentrations in adults are clearly overestimated by the regression model, whereas Cd, Cu, and Zn concentrations fall within the 95% Prediction Intervals. Figures 6-8 depict the BSAFs for emergent adults relative to the BSAFs for benthos. These also indicate consistent overestimation of concentrations in adults for As and Pb. For Cd, Cu, and Zn, the ratios of concentrations in emergent adults and associated sediment are within the range of benthos-sediment ratios for each data set (i.e., depurated, non-depurated, and all organisms). Mercury appears to be slightly overestimated by the BSAFs for depurated benthos, but not by the BSAFs for non-depurated organisms (Figure 7). Based on the selection criteria outlined above, the best estimates of adult concentrations are provided by the regression models for Cd and Cu and by the median BSAFs for Hg and Zn. All estimates for As and Pb are likely to be conservative, though the BSAFs appear to be somewhat better than the regression models.

PCB concentrations estimated using the “Most Likely” estimation methods were significantly different ($P < 0.01$) from the observed concentrations (Table 4). Concentrations of PCBs observed in emergent adults were within the 95% Prediction Interval for the regression model (Figure 5) and the range of BSAFs for adults were within the range for benthos (Figure 9). However, the data for emergent adults was consistently underestimated by both methods, which is consistent with the PD results presented in Table 4. Based on these evaluations, neither estimation method appears to be appropriate.

Table 4. Quality of "Most Likely" estimation methods as determined by the proportional deviation (PD) of the estimated values from measured values[a]

			Log-Log Model				Median BSAF			
Analyte	Data set[b]	N	Median	Minimum	Maximum	Over	Median	Minimum	Maximum	Over
As	All	3	-81.53	-138.87	-50.76	100%	-39.09	-80.75	-20.96	100%
As	Non-Dep.	3	-55.52	-103.74	-32.20	100%	-34.65	-71.69	-18.53	100%
As	Dep.	3	-210.87	-252.29	-170.47	100%	-103.49	-212.05	-56.24	100%
Cd	All	5	0.53	0.06	0.93	0%	0.67	0.49	0.96	0%
Cd	Non-Dep.	5	0.35	-0.34	0.90	20%	0.66	0.48	0.96	0%
Cd	Dep.	5	0.82	0.58	0.97	0%	0.74	0.61	0.97	0%
Cu	All	2	-0.96	-1.01	-0.90	100%	-2.56	-3.01	-2.11	100%
Cu	Non-Dep.	2	-1.34	-1.36	-1.32	100%	-2.77	-3.25	-2.29	100%
Cu	Dep.	2	-0.30	-0.39	-0.21	100%	-0.51	-0.71	-0.32	100%
Hg	All	3					-79.48	-294.17	-4.90	100%
Hg	Non-Dep.	3					-75.59	-279.89	-4.61	100%
Hg	Dep.	3					-199.92	-735.87	-13.72	100%
Pb	All	3	-33.89	-45.59	-15.67	100%	-28.07	-37.11	-12.15	100%
Pb	Non-Dep.	3	-33.62	-44.97	-15.27	100%	-25.98	-34.37	-11.20	100%
Pb	Dep.	3	-37.56	-51.18	-18.18	100%	-31.54	-41.66	-13.72	100%
Zn	All	5	-1.22	-1.63	-0.34	100%	-2.00	-2.23	-1.33	100%
Zn	Non-Dep.	5	-1.40	-1.82	-0.47	100%	-2.62	-2.89	-1.81	100%
Zn	Dep.	5	-0.84	-1.22	-0.07	100%	-0.30	-0.40	-0.01	100%
PCBs	Model	10	0.84	0.53	0.95	0%	0.87	0.58	0.93	0%

[a] PD = (measured-estimated)/measured. Negative PD values indicate overestimates; positive PD values indicate underestimates.
[b] All = depurated and non-depurated invertebrates combined, Dep. = invertebrates depurated prior to analysis, Non-Dep. = invertebrates not depurated prior to analysis, Model = benthic invertebrates analyzed for PCBs.

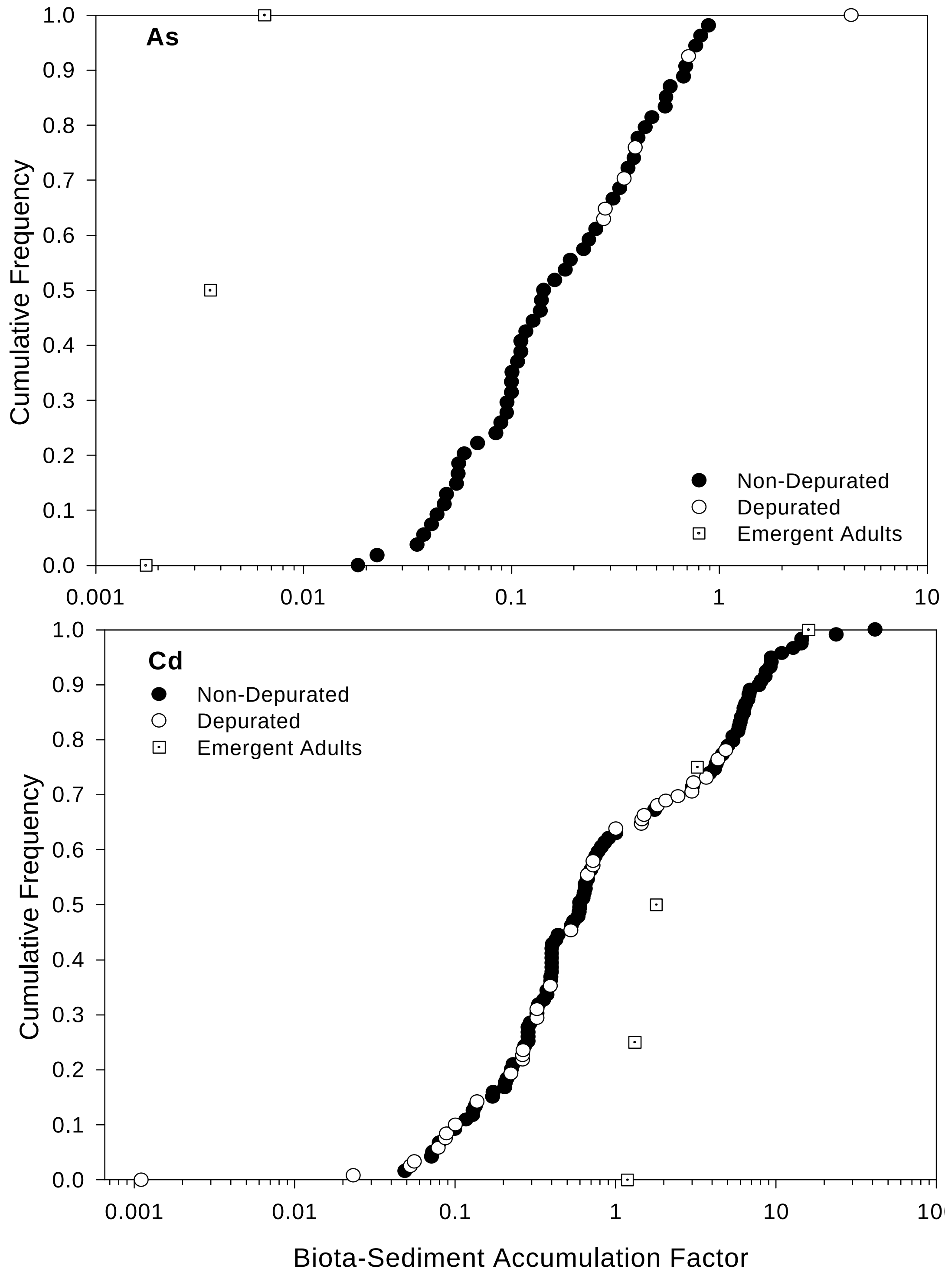


Figure 6. Cumulative distributions of arsenic and cadmium BSAFs for benthic invertebrates (depurated and non-depurated) and emergent adult insects.

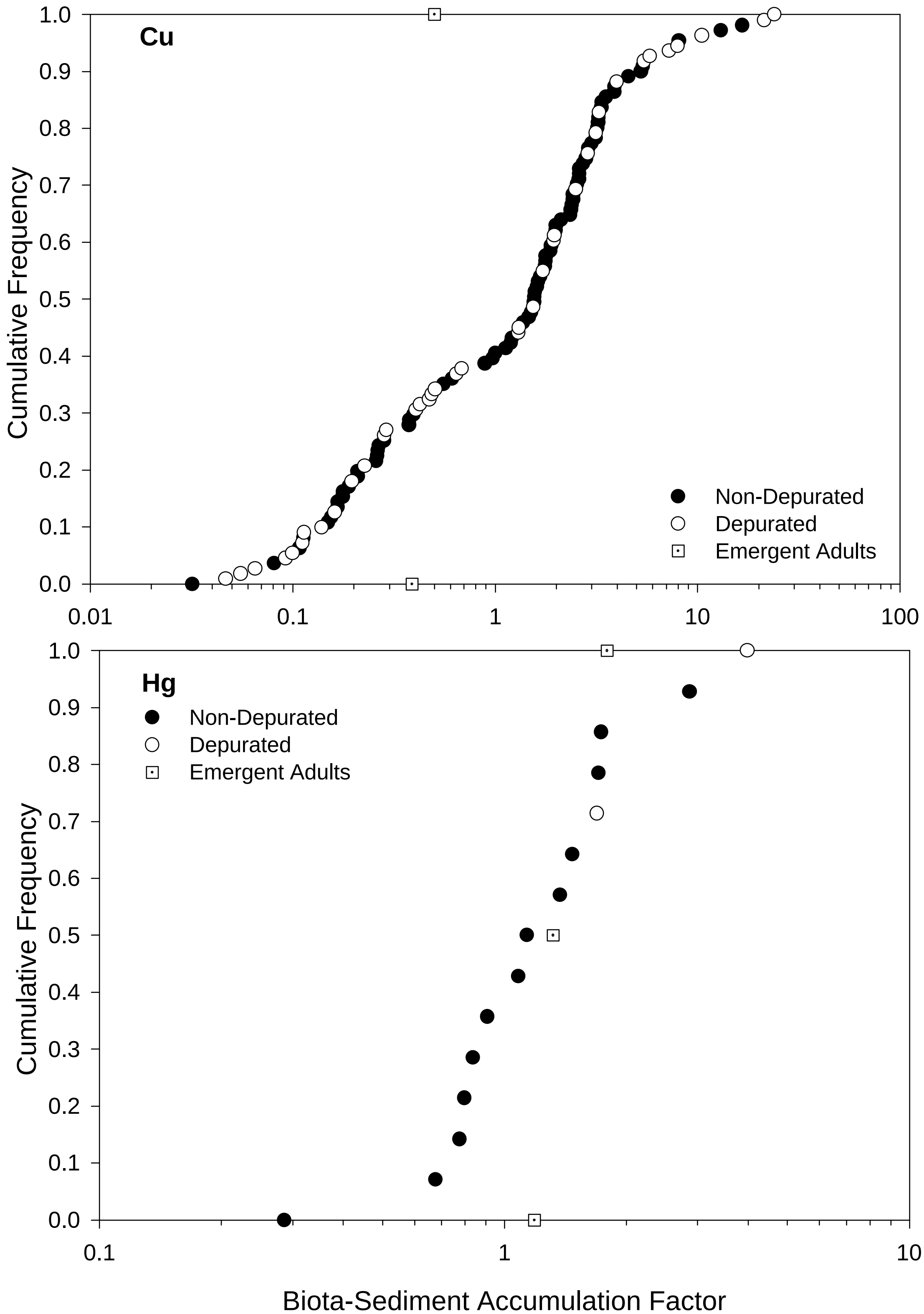


Figure 7. Cumulative distributions of copper and mercury BSAFs for benthic invertebrates (depurated and non-depurated) and emergent adult insects.

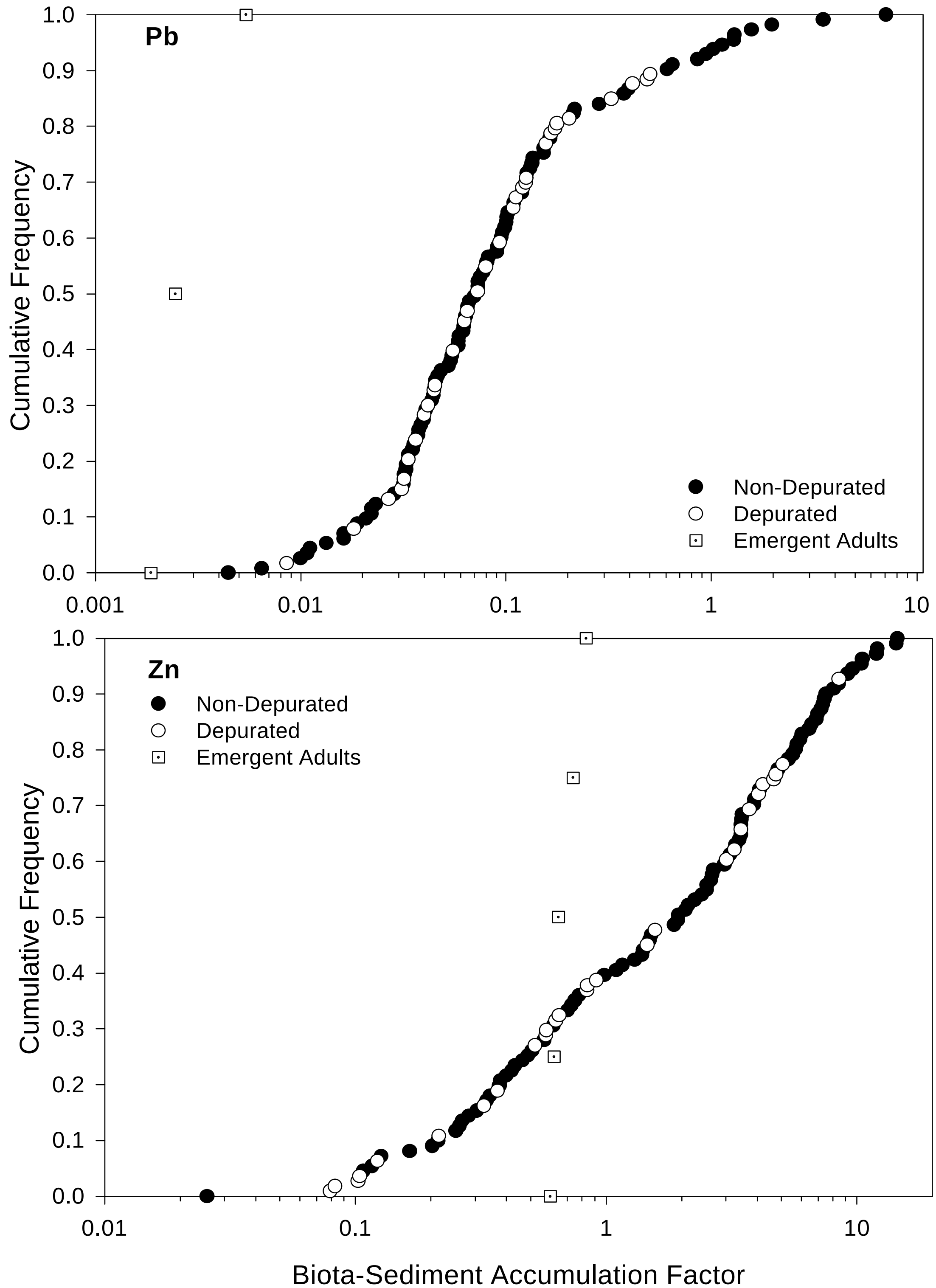


Figure 8. Cumulative distributions of lead and zinc BSAFs for benthic invertebrates (depurated and non-depurated) and emergent adult insects.

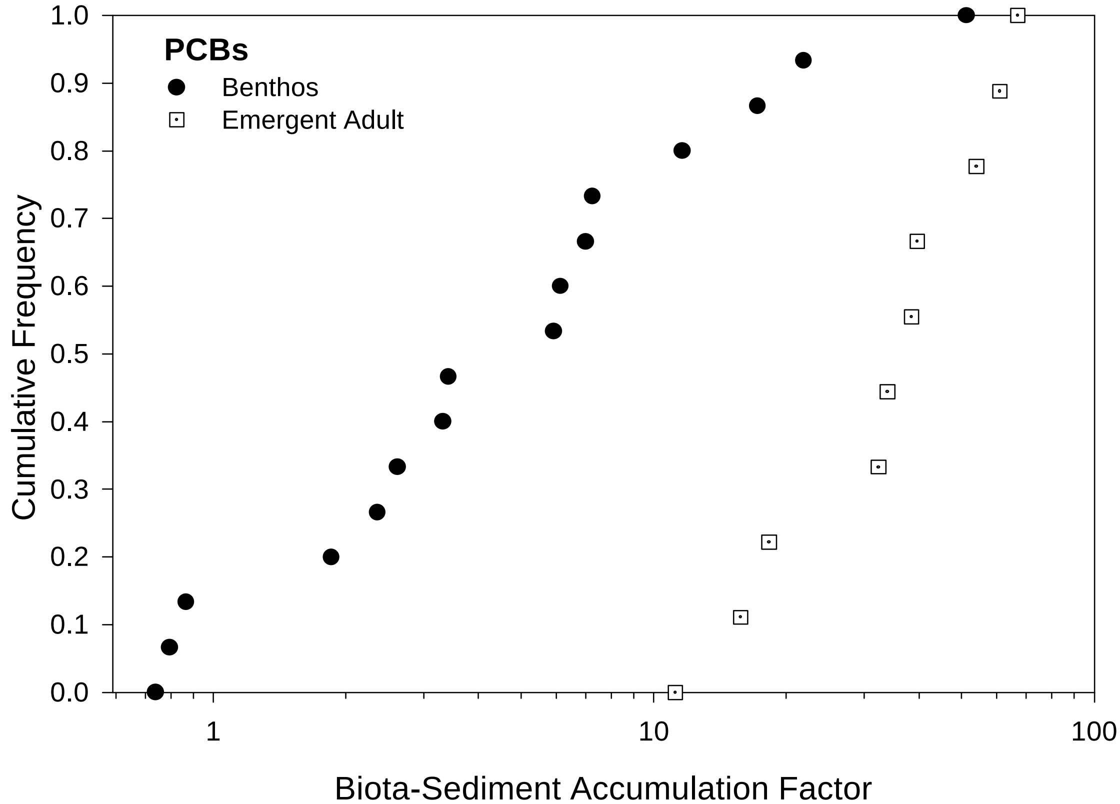


Figure 9. Cumulative distributions of PCB BSAFs for benthic invertebrates (depurated and non-depurated) and emergent adult insects.

Concentrations estimated using the conservative estimation methods (i.e., the 90th percentile BSAF and the upper 95% prediction limit of the regression model) were not significantly different ($p < 0.05$) from the concentrations observed in emergent adults for each metal and data set combination (Table 5). The BSAFs and 95%UPLs overestimated 100% of the concentrations for all metals except Cd. The BSAFs underestimated one or two of the five observed concentrations and the 95% UPLs (depurated and all organisms) underestimated two of the five observed concentrations (Table 5). Based on the aforementioned selection criteria and the an evaluation of Figures 1-8, both estimation methods appear to be adequately conservative for all metals except Hg, for which a model could not be fit. The degree of overestimation is minimized with the 90th percentile BSAFs for Cd (depurated organisms) and the 95% UPLs for Cu (all organisms) and Zn (depurated). For As and Pb, the “Most Likely” estimation methods are expected to be sufficiently conservative for screening, while minimizing the degree of overestimation.

PCB concentrations estimated from the 95% UPL were significantly different ($P < 0.05$) from the observed concentrations, whereas those estimated from the 90th Percentile BSAF were not (Table 5). However, the data for emergent adults was consistently underestimated by both (Table 5). Based on the results in Table 5 and an evaluation of Figures 5 and 9, neither estimation method appears to be appropriately conservative.

Table 5. Quality of conservative estimation methods as determined by the proportional deviation (PD) of the estimated values from measured values[a]

			Log-Log Model UPL				BSAF 90th Percentile			
Analyte	Data set[b]	N	Median	Minimum	Maximum	Over	Median	Minimum	Maximum	Over
As	All	3	-465.98	-792.14	-291.20	100%	-192.40	-393.33	-104.95	100%
As	Non-Dep.	3	-310.24	-577.24	-181.39	100%	-188.06	-384.50	-102.57	100%
As	Dep.	3	-495.83	-593.20	-397.75	100%	-1211.91	-2472.13	-663.45	100%
Cd	All	5	-5.43	-11.85	0.04	80%	-3.46	-5.74	0.50	80%
Cd	Non-Dep.	5	-5.91	-13.10	-0.05	100%	-4.16	-6.79	0.42	80%
Cd	Dep.	5	-1.35	-5.31	0.53	80%	-0.71	-1.59	0.81	60%
Cu	All	2	-5.20	-5.36	-5.03	100%	-11.02	-12.54	-9.50	100%
Cu	Non-Dep.	2	-5.48	-5.54	-5.42	100%	-7.86	-8.99	-6.74	100%
Cu	Dep.	2	-2.76	-3.02	-2.50	100%	-17.22	-19.52	-14.91	100%
Hg	All	3					-202.15	-744.06	-13.88	100%
Hg	Non-Dep.	3					-121.90	-449.74	-8.00	100%
Hg	Dep.	3					-280.98	-1033.18	-19.66	100%
Pb	All	3	-306.71	-409.83	-145.95	100%	-246.40	-323.34	-110.91	100%
Pb	Non-Dep.	3	-381.53	-507.03	-178.83	100%	-384.42	-504.30	-173.35	100%
Pb	Dep.	3	-177.32	-240.30	-87.65	100%	-131.80	-173.10	-59.07	100%
Zn	All	5	-4.77	-5.84	-2.48	100%	-10.68	-11.56	-8.07	100%
Zn	Non-Dep.	5	-5.43	-6.57	-2.94	100%	-12.13	-13.13	-9.20	100%
Zn	Dep.	5	-2.99	-3.80	-1.32	100%	-6.38	-6.94	-4.73	100%
PCBs	Model	10	0.25	-2.15	0.77	22%	0.39	-0.96	0.67	30%

[a] PD = (measured-estimated)/measured. Negative PD values indicate overestimates; positive PD values indicate underestimates.
[b] All = depurated and non-depurated invertebrates combined, Dep. = invertebrates depurated prior to analysis, Non-Dep. = invertebrates not depurated prior to analysis, Model = benthic invertebrates analyzed for PCBs.

A regression model also was developed from the PCB concentrations in emergent adults and sediments. Results of the regression analyses are presented in Table 3. Figure 10 presents the log-log scatter plots of sediment and biota concentrations, the fitted line, and the 95% prediction interval. The PCB concentrations in adult insects were significantly positively correlated ($p < 0.001$) with the sediment concentrations and the sediment concentrations explained 94% of the variation in biota concentrations.

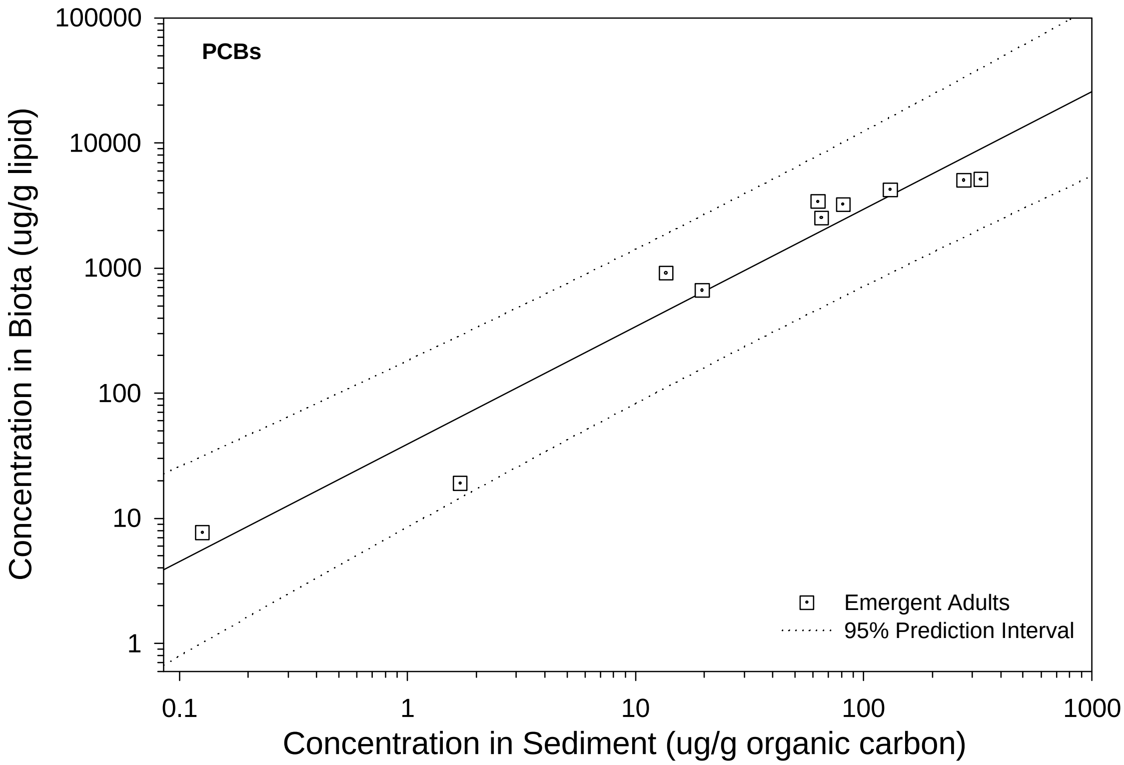


Figure 10. Log-log scatterplot of PCB concentrations in sediment and emergent adult insects. The regression lines are based on the available data for emergent adults.

4. DISCUSSION

This report presents a preliminary, exploratory analysis of the sediment-invertebrate accumulation data available in the literature. While it provides better accumulation factors than are currently available, it suggests the need to incorporate more explanatory factors into the estimation of chemical accumulation. It also suggests that aquatic stages may not be predictive of emergent stages for PCBs and some metals. However, the conservative estimation methods presented herein (i.e., 90th percentile BSAFs and 95% UPLs) appear to be appropriately conservative for screening sediment contaminant concentrations for the potential risks to flying insectivores. These data might also be used in uncertainty analyses to indicate the benefits of measuring site-specific contaminant concentrations in flying insects when such data are not available.

A preliminary evaluation of the regression models suggests that few of the relationships shown in this report fit the assumptions required for use of accumulation factors. Conventionally, an accumulation factor assumes a linear no threshold relationship between the biota concentration and the sediment concentration (i.e., biota concentrations are directly proportional to sediment concentrations across all sediment concentrations). The BSAF is represented in a linear model by the biota concentration (y) divided by the sediment concentration (x). This corresponds to the slope (b) of the linear regression equation (i.e., b = y/x and y = bx). Therefore, the BSAF will describe the relationship between x and y only if the y-intercept (a) of the linear model is zero (i.e., y = 0 + bx). However, in the power model ($y = a(x)^b$) the BSAF is represented by the y-intercept (a), rather than the slope (b). Therefore, the slope (b) must be 1 (i.e., $x^1 = x$) for the accumulation factor to accurately describe the relationship between the sediment concentration (x) and the biota concentration (y). When the slope is 1 the biota concentration is equal to the BSAF times the sediment concentration (i.e., y=ax). However, nearly all of the estimated slopes (b) presented in Table 3 are less than 1 by at least two times the standard error of (b).

It is not clear whether the apparent non-linearity indicates that the assumptions are violated (i.e., uptake or depuration is well-regulated by the organism) or that the true relationship is obscured by the influences of confounding factors (e.g., variations in pH). For biologically well-regulated chemicals (e.g., Cu and Zn), the use of an uptake factor will tend to overestimate exposures at high concentrations and underestimate exposure at low concentrations. This is not unacceptable in practice because it tends to result in conservative (i.e., protective) risk estimates at contaminated sites but not at uncontaminated sites. However, it is undesirable to use models and assumptions that are not supported by the available evidence. Therefore, the effects of confounding factors should be further evaluated in future revisions of this document to help clarify the influence of these factors on the equilibrium concentrations of the chemicals in invertebrates.

Some of these factors include the lack of depuration of biota and the speciation of analytes. Including the gut contents in the analysis of biota tends to obscure the true accumulation factor. Specifically, the BSAF is forced towards 1 as the amount of sediment in the gut increases. Chemicals with true BSAFs less than 1 will be over estimated because the concentration in the sediment is greater than the tissue concentration. True BSAFs greater than 1 will be underestimated because the sediment has lower chemical concentrations than the tissue. However, excluding all data for non-depurated organisms may increase the uncertainty in the analyses, because it would greatly reduce the number of measurements and range of sediment concentrations. This may be of less concern for some chemicals (e.g., Cu, Pb, and Zn) and of more concern for others (As and Cr). Also, total analyte concentrations in sediment and gut contents may not accurately represent the bioavailable fractions, because some analyte species may be more readily available than others. All of the available studies determined total analyte concentrations in sediment and biota and provided no information on the relative proportions of different analyte species or forms.

Comparison of the data for benthic invertebrates and adult insects suggests that the models and BSAFs in this report can be used to provide conservative estimates of metal concentrations in emergent insects. However, the data available for model validation is very limited. The number of observations was small and they generally constituted a small range of sediment concentrations. Further research is needed to provide sufficient data for a thorough evaluation of these models.

PCB concentrations in emergent adults were consistently underestimated by the concentrations in benthos. This may be due to differences in the types of lipids found in immature and adult life stages (Larsson 1984). Ideally, sufficient adult insect data would be available to allow for model development *and* validation. In the absence of such data, conservative estimates (i.e., the 95%UPL or the 90th percentile BSAF) from models and BSAFs based on the emergent adult data should be adequate for screening purpose.

5. RECOMMENDATIONS

These BSAFs and regression models are intended for use in ERAs performed on the Oak Ridge Reservation. To facilitate the most appropriate and consistent use of these values, the following recommendations should be followed.

1) The available BSAFs and regressions model are appropriate for use in screening ecological risk assessments to determine the need for further evaluation or site-specific data. The uncertainties in the estimation of emergent insect concentrations indicate that these data should not be used as the sole basis for a definitive characterization of risks to flying insectivores.

2) The 90th percentile BSAFs and the 95% UPLs are adequately conservative for all metals and can be used as a preliminary screening tool. The degree of overestimation can be minimized by using the 90th percentile BSAFs for Cd (depurated organisms), the 95% UPL for Cu (all organisms) and Zn (depurated), and the median BSAFs for As (non-depurated) and Pb (non-depurated). These values can be used as a secondary screening level as needed, provided that the limitations of the available validation data are explicitly included in the assessment.

3) Models and BSAFs for PCBs based on benthic invertebrate data should not be used to estimate PCB concentrations in emergent adult insects. Rather, the models derived using the PCB data for adult insects should be used.

4) Contaminants for which the models could not be validated (PCBs in adults and Cr and Ni in benthics) can be estimated using the 90th percentile BSAF and the 95% UPL for statistically significant regression equations (e.g., Ni in depurated benthos). The regression models should be used to the extent practicable. Most of these data do not appear to satisfy the assumptions for use as accumulation factors (i.e., linear no-threshold uptake). Although the regressions models developed herein also fail to address some confounding factors, they are likely to describe the sediment-invertebrate relationships better than the BSAFs.

3) If the uptake data are to be used in Monte Carlo simulation, selection of values to use is dependent on the distribution that best fits the data. If the distribution of the BSAF is fit better by the lognormal than the normal distribution, then the lognormal mean and standard deviation should be used. If the distribution of the BSAF is fit better by the normal than the lognormal distribution, then the normal mean and standard deviation should be used. If the distribution of the BSAF is uniform, the minimum and maximum observed BSAFs should be used.

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APPENDIX A

PROCEDURE FOR CALCULATION OF PREDICTION LIMITS FOR ESTIMATES GENERATED BY THE REGRESSION MODELS

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Prediction limits for estimates generated by the regression models presented in Table 3 may be calculated using the following equation (Dowdy and Wearden 1983):

$$Prediction\ Limit = \hat{y} \pm t_{\alpha=0.05,\ df=n-2} * RMSE * \sqrt{1 + \frac{1}{n} + \frac{(x^* - \bar{x})^2}{Sxx}}$$

$\hat{y}$	= log-transformed concentration of analyte in emergent adults estimated using regression models from Table 3.
$t_{\alpha=0.05,\ df=n-2}$	= t-statistic for 95% one-tailed limits or 90% two-tailed intervals with n-2 degrees of freedom. (Presented in Table A-1).
n	= Sample size for regression model. (Presented in Table A-1).
RMSE	= Root mean square error for regression model. (Presented in Table A-1).
x^*	= log-transformed sediment concentration for which emergent adult concentrations are being estimated. (Site specific).
$\bar{x}$	= Mean log-transformed sediment concentration from regression model. (Presented in Table A-1).
Sxx	= Variance of sediment concentrations from regression model. $Sxx = (\sum x^2 - (\sum x)^2)/n$. (Presented in Table A-1).

The procedure for calculating an upper 95% prediction limit for an estimate ($\hat{y}_{UPL}$) is as follows:

1) Use regression model from Table 3 and estimate the log-transformed concentration of analyte in emergent adults ($\hat{y}$) from the log-transformed sediment concentration of the analyte of concern (x^*).

2) Obtain values for t, n, RMSE, $\bar{x}$, and Sxx from Table A-1.

3) Apply the values from step 2 along with x^* to the equation outlined above and add the product to $\hat{y}$ to generate the upper 95% prediction limit for $\hat{y}$ ($\hat{y}_{UPL}$).

4) $\hat{y}_{UPL}$ as calculated by the above equation is log-transformed and must be back-transformed.

A lower 95% prediction limit ($\hat{y}_{LPL}$) can be calculated by subtracting the product from step 3 from $\hat{y}$, then back transforming the result. The 90% prediction interval (PI) is calculated if both the UPL and LPL are calculated. In application, 95% of all estimates are expected to fall below or above the UPL and LPL, respectively, and 90% of all estimates are expected to fall between the UPL and LPL.

Table A-1. Values for estimating upper and lower prediction limits for estimates generated by regression models.

Analyte	Data Set	n	$\bar{x}$	$\sum x$	$\sum x^2$	Root Mean Square Error (RMSE)	Sxx	t statistic (α = 0.05, df = n-2)
As	All	55	1.916	105.364	229.370	0.447	-197.68	1.674
As	Non-Dep.	49	2.011	98.515	219.692	0.438	-193.58	1.678
As	Dep.	6	1.142	6.849	9.677	0.161	-6.21	2.132
Cd	All	120	0.451	54.100	145.153	0.684	-23.18	1.658
Cd	Non-Dep.	88	0.560	49.280	130.086	0.615	-26.12	1.663
Cd	Dep.	32	0.151	4.820	15.067	0.728	-0.255	1.697
Cr	All	34	1.812	61.611	117.076	0.298	-108.20	1.694
Cr	No	26	1.714	44.565	80.137	0.309	-73.30	1.711
Cu	All	112	1.501	168.165	318.839	0.301	-249.65	1.659
Cu	Non-Dep.	74	1.541	114.028	220.270	0.263	-172.73	1.666
Ni	Yes	10	1.621	16.210	26.780	0.213	-23.60	1.860
Pb	All	117	1.462	171.011	281.205	0.568	-247.55	1.658
Pb	Non-Dep.	86	1.398	120.232	189.139	0.624	-165.89	1.663
Pb	Dep.	31	1.638	50.779	92.066	0.385	-80.21	1.699
Zn	All	112	2.077	232.627	540.751	0.249	-478.34	1.659
Zn	Non-Dep.	84	2.029	170.424	390.170	0.256	-341.12	1.664
Zn	Dep.	28	2.222	62.203	150.581	0.193	-132.81	1.706
PCBs	Model (benthos)	16	0.523	8.367	10.635	0.516	-3.71	1.761
PCBs	Validation (adults)	10	1.435	14.352	30.752	0.268	-17.52	1.860

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