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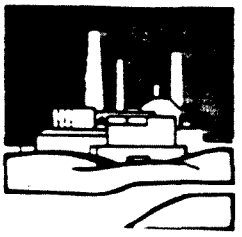
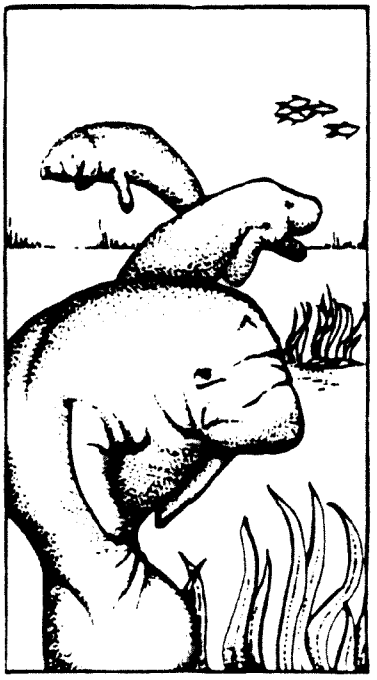
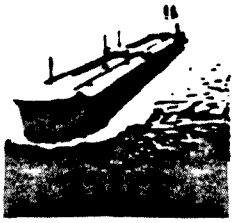
SEDIMENT QUALITY CRITERIA METHODOLOGY VALIDATION: UNCERTAINTY ANALYSIS OF SEDIMENT NORMALIZATION THEORY FOR NONPOLAR ORGANIC CONTAMINANTS







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SEDIMENT QUALITY CRITERIA METHODOLOGY VALIDATION: UNCERTAINTY ANALYSIS OF SEDIMENT NORMALIZATION THEORY FOR NONPOLAR ORGANIC CONTAMINANTS

Work Assignment 56, Task 3

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ABSTRACT

The U.S. Environmental Protection Agency (EPA), under the Criteria and Standards Division, is currently pursuing the development of numerical sediment quality criteria. Initial activities supporting this effort involved developing and evaluating sediment criteria methodologies. This study continues earlier work in which equilibrium partitioning (EP) theory was used to estimate permissible sediment contamination concentrations (PCCs) for nonpolar hydrophobic organic contaminants. The PCCs were computed from a simple predictive equation which expresses the PCC value as the product of the organic carbon-normalized sediment/water partition coefficient (K_{OC}) and the chronic water quality criterion (CWQC) for the compound in question. The applicable chronic water quality criterion is established by the EPA. For the development of sediment quality criteria, CWQC is applied to the interstitial water. Because benthic organisms are exposed to sediment contaminants for extended periods, chronic criteria are more appropriate than acute criteria for protecting benthic biota from impacts induced by chemical-specific exposure in their natural habitat.

In computing the PCCs, the following activities were performed: the pertinent partitioning literature was updated; empirically based regression equations which predict K_{OC} values from octanol/water partition coefficients (K_{OW}) were reexamined with refinement of the descriptive statistics; and the environmental variables influencing partitioning were evaluated.

The current study is an extension of the previous investigation. The main objective is quantification of the uncertainty associated with and the refinement of the initially predicted PCC values. This will allow the uncertainty inherent in any criterion value to be quantified, thereby permitting better-informed environmental and regulatory decisions. Two approaches were used to investigate uncertainties. The first approach employed parametric statistics assuming a log normal distribution on measured K_{OC} values. These K_{OC} values (distributions) were then subjected to a quantitative uncertainty analysis technique to define cumulative probability distribution functions (probability of exceedance curves). From these curves

one may determine the percentage of time (i.e., probability) that a given K_{oc} value will be equaled or exceeded for a specific chemical. PCC values are determined, based on EPA chronic water quality criteria, by multiplying the chemical-specific K_{oc} distribution function by the chronic criterion value for that chemical, converting the curve to a PCC distribution. The probability that any specific PCC value will be equaled or exceeded can then be determined, allowing selection of PCC values at various levels of protection. The second approach employed nonparametric statistics using Latin Hypercube sampling and computer-intensive (bootstrap) method of analysis. This second approach ultimately proved inconclusive due to the limited raw K_{oc}/K_{ow} data pairs from which the data distributions were generated.

The resulting probability distribution based on the first approach yields the following PCC values for those compounds with CWQC (at the 95 percent protection level, in micrograms contaminant per gram of sediment normalized to organic carbon content (ug/goc)).

Fluoranthene	310
Chlordane	0.06
DDT	0.06
Dieldrin	0.002
Endrin	0.002
Heptachlor	0.006

In addition, PCC values based on acute-to-chronic toxicity ratio (ACR) estimations were developed for 13 other compounds for which no CWQC exist.

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1.0 INTRODUCTION

The U.S. Environmental Protection Agency (EPA), under the Criteria and Standards Division, is currently pursuing the development of numerical sediment quality criteria. Initial activities supporting this effort involved developing and evaluating sediment criteria methodologies. This study continues earlier work in which equilibrium partitioning (EP) theory was used to estimate permissible sediment contamination concentrations (PCCs) for nonpolar hydrophobic organic contaminants. The PCCs were computed from a simple predictive equation which expresses the PCC value as the product of the organic carbon-normalized sediment/water partition coefficient (K_{OC}) and the chronic water quality criterion (CWQC) for the compound in question. The applicable chronic water quality criterion is established by the EPA. For the development of sediment quality criteria, CWQC is applied to the interstitial water. This application is appropriate because the benthic organisms are subjected to a long-term exposure of sediment contaminants and therefore the chronic values are more appropriate for providing criteria that can protect benthic biota from any impacts induced by chemical-specific exposure in their natural habitat.

A brief background and rationale for the uncertainty analysis of the sediment normalization equilibrium partitioning theory, together with a summary of the uncertainty analysis approach, is presented in the following section.

1.1 BACKGROUND AND RATIONALE

Preliminary estimates of permissible sediment contamination concentrations (PCCs) based on equilibrium partitioning theory have been reported in earlier investigations (Kadeg et al. 1986; Pavlou 1984; Pavlou and Weston 1984) as part of an overall effort by the U.S. Environmental Protection Agency to evaluate and develop sediment criteria methodologies for the development of sediment quality criteria. These studies investigated PPC values based on both acute and chronic water quality criteria. The assumption of equilibrium and the exposure of benthic organisms to the sediment dictates that PCC values

based on CWQC are more appropriate than values based on acute criteria. Therefore, no further investigation of acute-based PCC values has been performed.

Work by Kadeg et al. (1985) confirmed that percent organic content of the sediments is the proper normalizing parameter for reporting equilibrium partition coefficients (K) for nonpolar organic contaminants. In addition, the study concluded that other parameters (salinity, temperature, dissolved organic carbon, sediment particle size, and suspended particulate matter) have a varying but limited influence on partitioning. There are insufficient data to quantify the effects of these factors. For the organic carbon-normalized sediment/water partition coefficient (K_{OC}) and the octanol/water partition coefficient (K_{OW}), evidence was also provided that the use of chemical class-specific K_{OC}/K_{OW} regression equations improved the estimation of partition coefficients for chemicals which did not have measured K_{OC} values. The recomputed PCC values were higher (less stringent) than those previously calculated by Pavlou (1984).

The results of this investigation pointed to the inherent limitations of using empirical regression equations to estimate PCCs and raised the question of how reliable these numbers are as "first-cut" sediment criteria for nonpolar hydrophobic chemicals without laboratory and field verification. To address the question of reliability and usefulness of these numbers, it was necessary to perform an uncertainty analysis on the mathematical expressions used to derive the PCCs. This was done by refining the values as appropriate and establishing a generic statistical methodology that could test the reliability of any criterion value determined by other methods.

This report discusses the methodology for the quantitative treatment of the data; the results of applying the methodology to the PCCs computed by the equilibrium partitioning approach; recommendations for laboratory and field studies to be performed to reduce the uncertainty inherent in the predictive equations; and appendices describing additional statistical investigations.

1.2 SUMMARY OF UNCERTAINTY ANALYSIS APPROACH

To quantify the uncertainty in the calculated PCCs for sediment, the sources of uncertainty must first be identified. PCC values of chemicals for which measured K_{oc} values exist are calculated from

$$PCC = \hat{K}_{oc} \times CWQC \quad (1.1)$$

where $\hat{K}_{oc}$ = true K_{oc} + bias + error
CWQC = EPA-specified chronic water quality criterion.

Because K_{oc} values are measured and therefore subject to error, any observation is composed of the true (actual) K_{oc} value plus-or-minus measurement error. Because the available K_{oc} data reflect observations from numerous laboratories and, commonly, multiple observations from any single laboratory, the error within any reported K_{oc} value is composed of the potential bias of the laboratory reporting the value and the within-laboratory variability (errors) of these measurements.

For chemicals for which no measured K_{oc} values exist but for which measured K_{ow} values are found, the PCC value can be expressed as

$$PCC = \hat{K}_{oc} \times CWQC \quad (1.2)$$

where
$$\hat{K}_{oc} = B_0 + B_1 \hat{K}_{ow} + \text{error} \quad (1.3)$$
$\hat{K}_{ow}$ = true K_{ow} + bias + error.

For any chemical without a measured K_{oc}, the value can be estimated from the linear regression model for that compound's chemical class. The model describes the empirical relationship between measured K_{oc} and K_{ow} values as observed from chemicals with both K_{ow} and K_{oc} data in chemically similar (in terms of structure and behavior) classes. B_0 and B_1 are the model constants determined for each of the chemical classes. The estimated K_{oc} carries error due to the imperfect prediction of K_{oc} from K_{ow} values for that chemical class plus the measurement error of K_{ow} which in turn contains both bias and precision errors (as K_{oc} measurements, above).

Two observations on Equations (1.1) and (1.2) are pertinent to the methods applied in the current analysis. First, comparison of the equations indicates that errors/uncertainty accrued to PCC values for chemicals requiring prediction of K_{oc} will be greater than the errors accrued to PCC values for chemicals whose K_{oc} values have been measured. This observation is true unless the measurement error on K_{ow} is much smaller than measurement error on K_{oc} and/or K_{ow} functions as a perfect predictor of K_{oc}. Hence, the assumption that Equation (1.1) will yield a smaller error/uncertainty is intuitively reasonable because confidence in a measured value is generally greater than in a predicted value. Second, in both equations, the estimated PCC value is found by multiplying the observed K_{oc} or predicted K_{oc} by the CWQC for that compound. It is recognized that CWQCs, which are developed from toxicological data with some known or unknown variance, carry error themselves. This study focuses on the variances of K_{ow} and K_{oc} as they affect predicted PCC values. Therefore, it has initially been assumed that the error associated with CWQC values is zero. The actual nonzero error associated with CWQC values may require further evaluation in the future.

Figure 1.1 schematically describes the analytical sequence followed in the current study. The first phase of the study involved extensive exploratory analyses and resulted in distributions of K_{ow} and K_{oc} for each chemical with any reported measurements. The representativeness of these distributions was examined within the context of the extremely limited raw data and the comparative data indicated by the dashed feed-back line from the paired K_{oc}-K_{ow} box to the raw K_{oc}-K_{ow} data box.

Following the exploratory analyses, two approaches were used. The first approach applied straightforward parametric statistics to the measured K_{oc} distributions for those compounds for which measured K_{oc} values exist. Previous work (Kadeg et al. 1986) has verified the log normal distribution of these data and appropriateness of using this approach. A decision-modelling system employing Latin Hypercube sampling was then applied to the K_{oc} distribution Equation (1.1) to define cumulative probability distribution function (CDF) curves for the corresponding PCC values. The 0.01 and 0.05 probability fractiles, corresponding to the 99 and 95 percentile protection levels, were then calculated, yielding PCC values for these levels of protection. This procedure is discussed in Chapter 2.

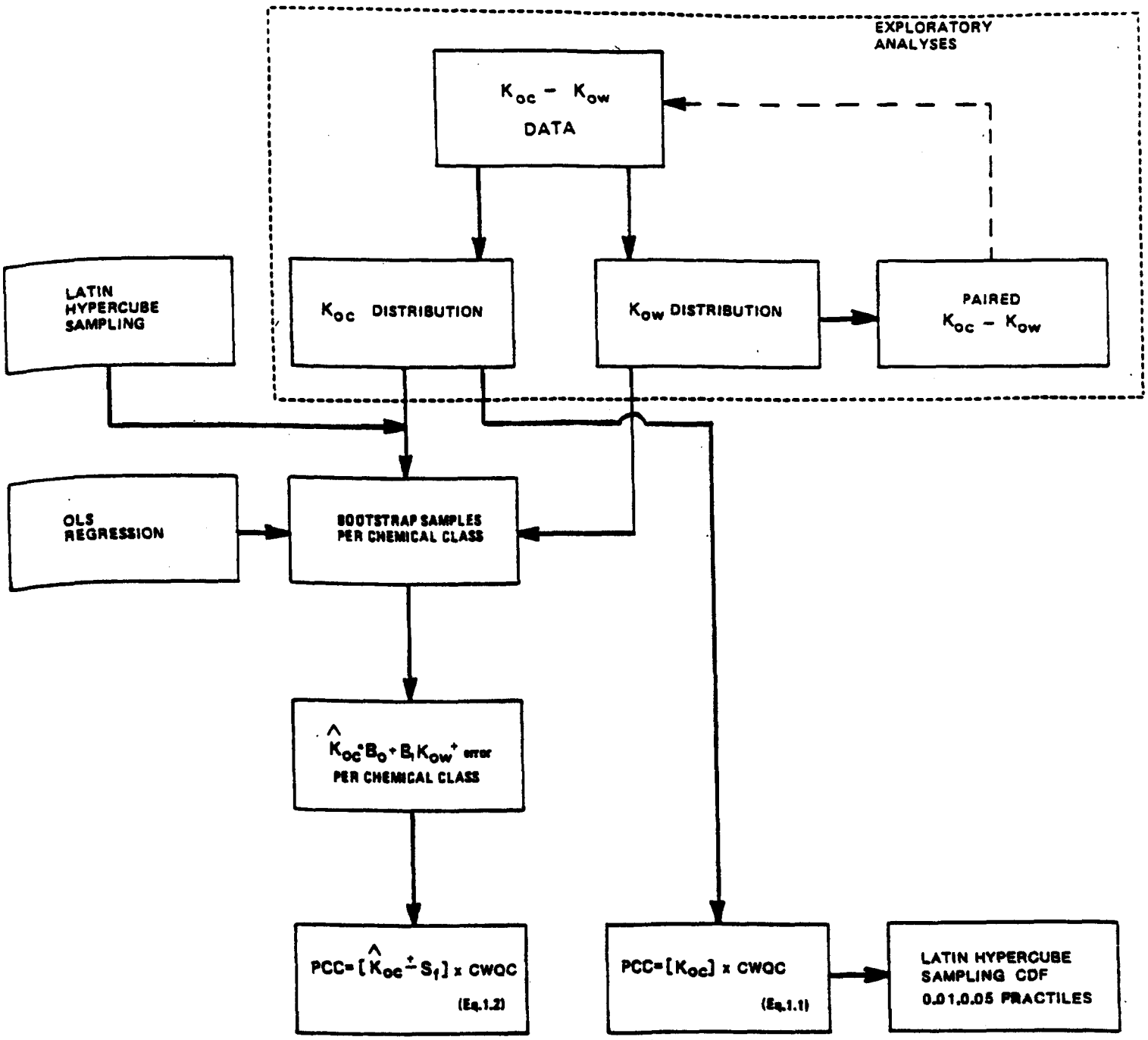


FIGURE 1.1 Analytical Sequence

The second approach was to apply nonparametric statistics to those compounds without measured K_{OC} values. The data were analyzed to determine their unique distributions, from which data sets were sampled. These data were used to develop multiple linear regression equations with associated confidence intervals (CI) for compounds with no K_{OC} values. The K_{OC} values were then used in equation (1.2) with the CI to define uncertainties on PCC values. This work is detailed in Appendix A.

The remainder of this report discusses the analytical methods and interprets the results. Chapter 2 describes the basic analytical/statistical methods and confidence interval calculation for both measured K_{OC} and regression-predicted K_{OC} values. The actual data analysis is presented in Chapter 3 together with results from exploratory analyses and the K_{OC}-K_{OW} distributions. Chapter 4 describes the development of PCC values and associated uncertainty. Chapter 5 presents overall conclusions and interpretation of the study results.

2.0 ANALYTICAL METHODS: DESCRIPTION/RATIONALE

This chapter provides the description and rationale for the analytical methods employed to define the uncertainty associated with the PCC values derived from equilibrium partitioning theory.

2.1 GENERAL APPROACH

As noted in the introduction, initial exploratory analyses were performed on the K_{OC} - K_{OW} data to evaluate chemical specific distributions. Details and results of these analyses are presented in Appendix B. Previous work (Kadeg et al. 1986) on these data sets verified that the log-transformed data for the group of chemicals were normally distributed. This was established using Kolomogorov-Smirnov (K-S) goodness-of-fit tests. The exploratory analyses indicated that chemical-specific data were normally or nearly normally distributed for larger data sets, but not necessarily normal for compounds with limited data. The trend was clear, however, that as the number of samples increased, the distributions tended more toward a normal or near-normal curve. Therefore, standard parametric statistics were applied to the chemical-specific measured K_{OC} data to determine the median value (μ), regardless of the number of observations, and the standard deviation (σ), defined as the median value times the maximum coefficient of variation (C_V), assuming normal distribution. This subsequently defined the characteristics/range of K_{OC} values to be employed in Equation (1.1). Latin Hypercube Sampling (LHS) as described in Section 2.2 was then employed to define the uncertainty of the PCC values associated with the corresponding measured K_{OC} values and a fixed CWQC value. Specific fractiles (0.01, 0.05) corresponding to the 99 percentile and 95 percentile of the cumulative distribution function, respectively, are the final PCC values.

For compounds for which EPA has not specified a CWQC value, a value was estimated from EPA acute water quality criteria (AWQC) using acute-to-chronic ratios (ACR) described by Kenaga (1982). If a compound-specific ACR value was not available, a range of CWQC values was determined using a range of ACR values from Kenaga (1982). In this case, the distribution of the range was considered to be uniform (equally probable), and the corresponding uncertainty

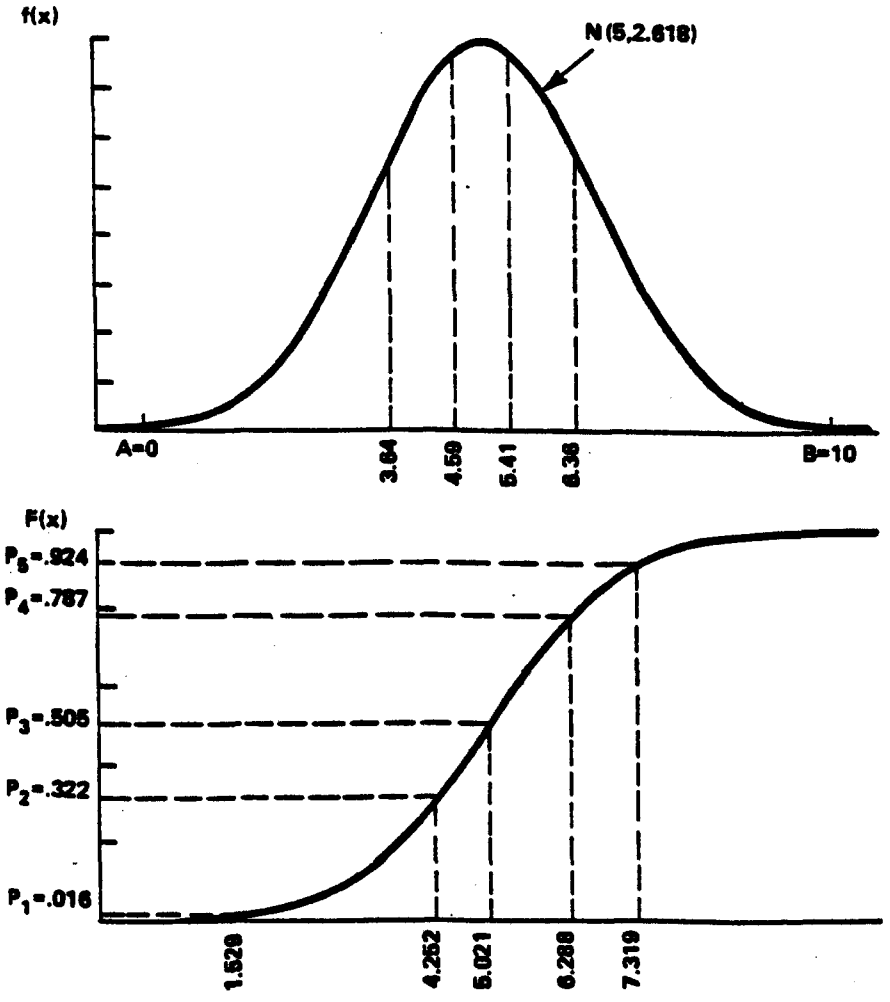
(i.e., CWQC uncertainty) was incorporated, using the LHS technique, into the cumulative probability distributions. The fractiles and recommended PCC values were then determined as described in the preceding paragraph.

To allow direct comparison of intermediate results (e.g., PCC distributions) without introducing CWQC uncertainty in only select cases, PCC values were also calculated assuming a fixed ACR value of 10 (order of magnitude) for all compounds. These results, however, were not incorporated into the final PCC values.

An alternative, nonparametric statistical approach was also investigated as presented in Appendix A. This approach is summarized as follows. The distributions developed during exploratory analyses (Appendix B) were treated as the raw data, although the relationship between the distributions for these small data sets and the distribution of the true populations is not known. Samples from these data were then used for all subsequent analyses: K_{ow}-K_{oc} pairs for all chemicals (having both measures) within each of three chemical classes (low-weight PAH, high-weight PAH and pesticides) were randomly selected by a Latin Hypercube sampling method. Regression analysis, using ordinary least squares, was performed on 100 samples for each chemical class. Resulting linear equations [of the form: $K_{oc} = B_0 + B_1 K_{ow}$] were applied to randomly sampled K_{ow} values for compounds within that class for which no K_{oc} measurements are available to predict the K_{oc} values needed to develop PCC values for those compounds. For each regression and K_{ow} value, the predicted K_{oc} value and the values defining the limits of the 95 percent confidence interval were multiplied by the CWQC for that compound to obtain a median value and confidence intervals for the PCC value.

2.2 LATIN HYPERCUBE SAMPLING

Latin Hypercube Sampling (LHS) is a constrained random-sampling technique which is used to transform distribution functions (e.g., normal or uniform) to cumulative probability functions or to select actual values for input variables. As shown in Figure 2.1, this technique generates a sample from a given distribution by first dividing the total distribution into a number of equal segments, and then sampling within each segment. This forces sampling of the tails of the distribution, resulting in a small sample being more



INTERVAL ENDPOINTS USED WITH A LHS OF SIZE 5 (TOP) AND SPECIFIC VALUES OF X SELECTED THROUGH THE INVERSE OF THE DISTRIBUTION FUNCTION (BOTTOM)

FIGURE 2.1 Illustration of LHS Sampling

representative of the distribution than unconstrained Monte Carlo sampling which may require several thousand samples to adequately represent the data, depending on the variance. Detailed description of the technique is found in McKay, Conover, and Beckman (1979).

2.3 CONFIDENCE INTERVALS ON PREDICTED VALUES OF K_{OC} and PCC

For compounds with a measured K_{OC} value, the only source of uncertainty in Equation (1.1) is the measured K_{OC}. The resulting confidence interval on PCC will be the same width as that associated with the K_{OC} value with the distribution shifted by multiplying the scalar CWQC. The distribution on the measured K_{OC} results from random error associated with the intra-laboratory variability and experimental bias resulting in inter-laboratory variability. The combination of both sources of uncertainty leads to a final estimate of the total uncertainty for measured K_{OC} values for a given compound.

For compounds without a measured K_{OC} value (Appendix A), the use of Equation (1.3) introduces several sources of measurable variance. First, the ability of regression equations to accurately predict values for K_{OC} is uncertain based on the ability of the regression to explain the variance in K_{OC}. If K_{OW} is a perfect predictor of K_{OC}, the variance introduced by use of the regression is zero. The study by Kadeg et al. (1986) indicates that there are other factors which probably affect K_{OC} that are not used in the regression due to lack of data (such as dissolved organic matter and particulate matter). Thus, for this study, it can be assumed that K_{OW} is not a perfect predictor for K_{OC} and that the error term will not be zero.

Since the error term and associated confidence interval is nonzero, any value of K_{OC} predicted from one of the regression equations will have some uncertainty associated with it. This uncertainty is caused purely by the use of the ordinary least squares (OLS) estimators B0 and B1. From the use of ordinary least squares criteria, it is possible to estimate the confidence interval (which reflects the error) on the estimated K_{OC}. This confidence interval is used to quantitatively measure the variance in the final sediment criteria values contributed by the use of a K_{OC} predicted from the linear regression model.

The error term in Equation (1.3) which defines the confidence interval is calculated as

$$\text{error} = T_c \times S_f \tag{2.1}$$

T_c is the critical value of the Student's t distribution (at $\alpha = 0.05$, 95 percent confidence interval) with n-k-1 degrees of freedom where n is the number of sample data points and k is the number of regressors used in the regression. S_f is the estimated standard error of the forecast, calculated as the positive square root of

$$S_f^2 = S_n^2 \left[1 + (1/n) + (X_f - X)^2\right]/SSQX \tag{2.2}$$

where

S_n^2 = the estimated variance of the error term in the regression
n = the number of data points in the regression
X_f = the measured K_{ow} used to predict K_{oc}
X = the average of the K_{ow} values used in the regression
SSQX = the sum of squares of the K_{ow} values used for the regression.

From Equation (2.2), it follows that the magnitude of the error term in Equation (1.2) increases as S_f^2 increases due to a poor fit of the data, or as n decreases, or as the value of K_{ow} used in Equation (2.2) moves away from the mean of the regressed K_{ow} values, or as the value of SSQX decreases due to a bunching of the K_{ow} values.

3.0 AVAILABLE K_{OC} - K_{OW} DATA

This chapter identifies the specific compounds under investigation, the associated available K_{OC} - K_{OW} summarized data, and the determined K_{OC} distributions to be applied to Equation (1.1).

3.1 COMPOUNDS AND K_{OC} - K_{OW} DATA

Table 3.1 identifies the representative hydrophobic organic chemical compounds for which K_{OW} and K_{OC} data were collected. Compounds in capital letters have common matched K_{OW} - K_{OC} data pairs. These data, taken from the available literature, were screened prior to analysis, limiting data to observations exhibiting internal consistency (Kadeg et al. 1986). Detailed evaluations and descriptions of these data are presented in Appendix B. Based on these evaluations, summary statistics, using a normal distribution, were developed for the compounds shown in Table 3.2.

3.2 K_{OC} DISTRIBUTION

The summary data presented in Table 3.2 were used to calculate K_{OC} values for the 5th, 25th, 50th, 75th, and 95th percentiles of the normal distribution from which each chemical specific K_{OC} is drawn. The percentiles were calculated as follows:

$$\text{5th percentile} = K_{OC} - 1.64 \times SD$$
$$\text{25th percentile} = K_{OC} - 0.67 \times SD$$
$$\text{50th percentile} = K_{OC}$$
$$\text{75th percentile} = K_{OC} + 0.67 \times SD$$
$$\text{95th percentile} = K_{OC} + 1.64 \times SD.$$

These results are presented in Table 3.3 and indicate the uncertainty (error) associated with the K_{OC} term in Equation (1.1). When the LHS technique is employed to develop the CDF curves, the information in Table 3.3 is internally generated from the data in Table 3.2 and by specification of a normal distribution.

TABLE 3.1 Representative Hydrophobic Organic Chemical Compounds[a/]

Polycyclic Aromatic Hydrocarbons (PAHs)

Low Molecular Weight PAHs (2 and 3 rings)

FLUORENE	Acenaphthylene
NAPHTHALENE	ANTHRACENE
Acenaphthylene	PHENANTHRENE

High Molecular Weight or "Combustion" PAHs (3 to 6 rings)

FLUORANTHENE	Benzo(b)flouranthene
PYRENE	Benzo(k)flouranthene
CHRYSENE	Indeno(1,2,3-cd)pyrene
BENZO(A)ANTHRACENE	DIBENZO(A,H)ANTHRACENE
BENZO(A)PYRENE	Benzo(ghi)perylene

Pesticides

DDD	
DDE	HEPTACHLOR
DDT	Heptachlor Epoxide
Acrolein	α-Hexachlorocyclohexane
ALDRIN	β-Hexachlorocyclohexane
CHLORDANE	γ-Hexachlorocyclohexane
DIELDRIN	δ-Hexachlorocyclohexane
α-Endosulfan	Isophorone
β-Endosulfan	TOXAPHENE
ENDRIN	

Polychlorinated Biphenyls (PCBs)

Aroclor 1016
Aroclor 1221
Aroclor 1232
Aroclor 1242
Aroclor 1248
Aroclor 1254
Aroclor 1260

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a/ Compounds in capital letters have common matched K_{ow} - K_{oc} data pairs.

TABLE 3.2 Summary of K_{ow} and K_{oc} Data for Selected Hydrophobic Organic Chemical Compounds

Compound	Log K_{ow}		Log K_{oc}	
	Mean	SD	Mean	SD
High Weight PAHs				
Benzo(a)anthracene	5.76	0.66	6.27	0.82
Benzo(a)pyrene	6.02	0.55	6.75	0.74
Chrysene	5.70	0.65	5.77	0.76
Dibenzo(a,h)anthracene	6.25	0.71	6.36	0.56
Fluoranthene	5.26	0.60	5.31	0.70
Pyrene	5.11	0.58	4.88	0.43
Low Weight PAHs				
Anthracene	4.45	0.51	4.42	0.58
Fluorene	4.27	0.49	4.01	0.53
Napthalene	3.37	0.31	3.52	0.39
Phenanthrene	4.49	0.51	4.22	0.55
Pesticides				
Aldrin	5.66	0.77	4.79	0.52
Chlordane	3.32	0.45	5.15	0.68
DDD	5.99	0.68	5.38	0.71
DDE	5.69	0.65	5.17	0.68
DDT	6.13	0.57	5.52	0.48
Dieldrin	4.95	0.68	3.81	0.50
Endrin	4.48	0.51	3.55	0.47
Heptachlor	4.48	0.61	4.00	0.53
Toxaphene	3.27	0.45	3.00	0.39

TABLE 3.3 Log K_{oc} Distribution (l/kg)

Compound	Percentile				
	5	25	50	75	95
High Weight PAHs					
Benzo(a)anthracene	4.925	5.720	6.27	6.823	7.615
Benzo(a)pyrene	5.536	6.254	6.75	7.246	7.964
Chrysene	4.524	5.261	5.77	6.279	7.016
Dibenzo(a,h)anthracene	5.442	5.985	6.36	6.735	7.278
Fluoranthene	4.162	4.841	5.31	5.779	6.458
Pyrene	4.175	4.592	4.88	5.168	5.585
Low Weight PAHs					
Anthracene	3.469	4.031	4.42	4.809	5.371
Fluorene	3.141	3.655	4.01	4.365	4.879
Naphthalene	2.880	3.259	3.52	3.781	4.160
Phenanthrene	3.318	3.852	4.22	4.588	5.122
Pesticides					
Aldrin	3.937	4.442	4.79	5.138	5.643
Chlordane	4.035	4.694	5.15	5.606	6.265
DDD	4.216	4.904	5.38	5.856	6.544
DDE	4.055	4.714	5.17	5.626	6.285
DDT	4.733	5.198	5.52	5.842	6.307
Dieldrin	2.990	3.475	3.81	4.145	4.630
Endrin	2.779	3.235	3.55	3.865	4.321
Heptachlor	3.131	3.645	4.00	4.355	4.869
Toxaphene	2.360	2.739	3.00	3.261	3.640

4.0 DEVELOPMENT OF SEDIMENT PERMISSIBLE CONTAMINATION CONCENTRATIONS AND ASSOCIATED UNCERTAINTY

This chapter presents the results of applying the determined K_{OC} distributions to Equation (1.1), using either EPA provided chronic water quality criteria (CWQC) or CWQC derived from acute-to-chronic ratios (ACR). Subsequent cumulative probability distribution (CDF) curves are presented, together with 0.01 and 0.05 probability fractiles which correspond to the 99th and 95th percentile protection levels and form the basis for the PCC final values.

4.1 CWQC VALUES

To apply water quality criteria to Equation (1.1), the appropriate water quality values must be selected. As noted in Section 1.0, chronic water quality criteria are most appropriate because of the long-term exposure of benthic organisms to sediment contaminants. This study estimates PCCs for the marine environment. A parallel analysis employing freshwater chronic criteria could be performed to develop PCC values for freshwater environments. The effects of salinity on K_{OC} values have been discussed previously (Kadeg et al. 1986). The ACR values employed were developed primarily from non-benthic, freshwater organisms. Due to the paucity of saltwater CWQCs and the absence of saltwater ACR values, the freshwater data were used. Furthermore, it is assumed that the freshwater species used in developing both CWQCs and ACRs have the same sensitivity as marine benthic organisms. The errors associated with these assumptions are mitigated through the uncertainty analyses performed on the data and the use of a range of ACR values.

For the compounds with sufficient data to develop K_{OC} distributions (Table 3.3), a matrix of available water quality data was developed (Table 4.1). Based on this matrix, three approaches were taken. For those compounds with specified CWQC, the CWQC values were combined with the K_{OC} distributions directly in Equation (1.1), from which CDF curves were developed. For those compounds without specified CWQC but with specific ACR values (naphthalene and toxaphene), the ACR values were applied to acute

TABLE 4.1 Matrix of Available Water Quality Criteria Data

Compound	Criteria, µg/l				
	Fresh Acute	Fresh Chronic	Marine Acute	Marine Chronic	Specific ACR[a/]
Benzo(a)anthracene	--	--	300[b/]	--	--
Benzo(a)pyrene	--	--	300[b/]	--	--
Chrysene	--	--	300[b/]	--	--
Dibenzo(a,h)anthracene	--	--	300[b/]	--	--
Fluoranthene	3,980[c/]	--	40[c/]	16[c/]	3
Pyrene	--	--	300[b/]	--	--
Anthracene	--	--	300[b/]	--	--
Fluorene	--	--	300[b/]	--	--
Naphthalene	2,300[c/]	620[c/]	2,350[c/]	--	29
Phenanthrene	--	--	300[b/]	--	--
Aldrin	3.0	--	1.3	--	--
Chlordane	2.4	0.0043	0.09	0.004	2
DDD	--	--	--	--	--
DDE	1,050[c/]	--	14[c/]	--	--
DDT	1.1	0.001	0.13	0.001	53
Dieldrin	2.5	0.0019	0.71	0.0019	--
Endrin	0.18	0.0023	0.037	0.0023	2
Heptachlor	0.52	0.0038	0.053	0.0036	4
Toxaphene	1.6	0.013	0.07	--	100

a/ As reported by Kenaga (1982).

b/ Insufficient data for criteria. Based on lowest-observed-effect level for compound class.

c/ Insufficient data for criteria. Based on lowest-observed-effect level.

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criteria values to generate a calculated CWQC value, which was then treated as the specified CWQC value above. For the balance of the compounds, for which no specific CWQC or ACR values exist, a range of ACR values (3-29) was applied to the CDF based on Kenaga (1982), assuming a uniform distribution. This range portrays the effect of introducing uncertainty into the CWQC. Alternatively, for comparison purposes in the PCC distributions, the general assumption was made for this group of compounds that the chronic criteria would be an order of magnitude less than the acute criteria (i.e., ACR equals 10). This assumption appears to be a reasonable first-order estimate based on compound-specific ACR values presented by Kenaga (1982). The fixed ACR value of 10 was then used as before to generate a calculated CWQC for which a second set of CDF curves were generated. This alternate approach had the effect of eliminating the uncertainty in these curves associated with water quality criteria uncertainty. For calculation of the final PCC values, the curves generated from the uniform distribution of ACR values were selected over the curves generated from this alternate approach. Both sets of curves are presented in Appendix C. Compounds with specific CWQC values, or specific ACR values and associated calculated CWQC values, are presented in Table 4.2 together with the corresponding values. It is apparent that the chronic criteria values estimated from ACR values are generally higher than the EPA measured chronic criteria values. This reflects the limitation of the ACR as a good predictor of CWQC, but in view of the absence of measurements for chemicals for which only acute data were available, the ACR was the only method by which CWQC could be estimated. Furthermore, it should be recognized that the similarity of a saltwater ACR to the freshwater ACR is also an underlying assumption in these computations. This may warrant further investigation; however, for the present study, an adjustment factor is not recommended.

4.2 DISTRIBUTION OF PCC VALUES AND ASSOCIATED UNCERTAINTY

The CWQC values as determined above were combined with the K_{OC} distributions as described in Chapter 3 (Table 3.3) in Equation (1.1) to develop PCC distributions and define the uncertainty range. Table 4.3 presents the resulting distributions for the compounds under investigation.

TABLE 4.2 Specific Chronic Water Quality Criteria and Acute to Chronic Criteria Ratios for Selected Compounds

Compound	EPA Marine Chronic Criteria (ug/l)	ACR (species)[a/]	Calculated Marine Chronic Criteria (ug/l)[b/]
Fluoranthene	16	3 (MS)	13.3
Naphthalene	-	29 (CS)	81.0
Chlordane	0.004	2 (DM)	0.045
DDT	0.001	53 (FHM)	0.0025
Dieldrin	0.0019	-	-
Endrin	0.0023	2 (SHM)	0.0185
Heptachlor	0.0036	4 (DM)	0.0133
Toxaphene	-	100 (DM)	0.0007

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a/ Based on Kenaga (1982). Species upon which ACR is based is as follows:
MS = mysid shrimp
CS = coho salmon
DM = Daphnia magna
FHM = fathead minnow
SHM = sheepshead minnow

b/ Calculated marine chronic criteria were only used in subsequent calculations for those compounds without specific EPA chronic criteria (napthalene and toxaphene).

For those compounds with no specific CWQC or ACR value, the assumption of one order of magnitude difference between acute and chronic criteria (i.e., ACR equals 10) was used to permit comparison.

The LHS technique was applied to the PCC distributions (the K_{OC} distributions times the scaler CWQC value) to determine the resulting CDF curves for each chemical compound, as described above. These results are shown in Appendix C (Figures C.1 through C.19). For those compounds without specific CWQC or ACR values, the plots incorporating a uniform distribution of ACR values are also given. Table 4.4 presents the recommended PCC values (first cut criteria) based on the CDF curves using the 0.01 and 0.05 probability fractiles, which correspond to the 99th and 95th percentile levels of protection, respectively.

TABLE 4.3 Distribution of Permissible Sediment Contaminants Concentrations (ug/goc) Derived from Existing or Estimated Chronic Water Quality Criteria

Compound	Percentile				
	5	25	50	75	95
High Weight PAHs					
Benzo(a)anthracene	1.24E+03	7.83E+03	2.79E+04	9.96E+04	3.27E+05
Benzo(a)pyrene	5.18E+03	2.70E+04	8.44E+04	2.64E+05	1.37E+06
Chrysene	5.05E+02	2.74E+03	8.83E+04	2.84E+04	1.55E+05
Dibenzo(a,h)-anthracene	4.19E+03	1.46E+04	3.44E+04	8.11E+04	2.82E+05
Fluoranthene	2.32E+02	1.11E+03	3.27E+03	9.52E+03	4.89E+04
Pyrene	2.27E+02	5.89E+02	1.14E+03	2.20E+03	5.71E+03
Low Weight PAHs					
Anthracene	4.40E+01	1.61E+02	3.95E+02	9.67E+02	3.54E+03
Fluorene	2.10E+01	6.81E+01	1.53E+02	3.46E+02	1.12E+03
Naphthalene	6.14E+01	1.47E+02	2.68E+02	4.89E+02	1.17E+03
Phenanthrene	3.06E+01	1.06E+02	2.49E+02	5.86E+02	2.02E+03
Pesticides					
Aldrin	1.1	3.6	8.0	1.80E+01	5.82E+01
Chlordane	4.34E-02	1.98-01	5.65E-01	1.61	7.36
DDD	3.0	1.45E+01	4.32E+01	1.29E+02	6.23E+02
DDE	8.0	3.63E+01	1.04E+02	2.95E+02	1.34E+03
DDT	5.41E-02	1.58E-01	3.31E-01	6.95E-01	2.03
Dieldrin	1.86E-03	5.67E-03	1.23E-02	2.65E-02	8.11E-02
Endrin	1.38E-03	3.95E-03	8.16E-03	1.69E-02	4.82E-02
Heptachlor	4.87E-03	1.59E-02	3.60E-02	8.15E-02	2.66E-01
Toxaphene	1.60E-04	3.83E-04	7.00E-04	1.28E-03	3.06E-03

TABLE 4.4 PCC Values for Tested Fractiles

Compound	PCC (ug/goc) for Probability Fractile 0.01	0.05	Basis[a/]
High Weight PAHS			
Benzo(a)anthracene	160	2,100	est.
Benzo(a)pyrene	1,800	4,500	est.
Chrysene	120	440	est.
Dibenzo(a,h)anthracene	1,200	3,500	est.
Fluoranthene	160	310	CWQC
Pyrene	85	190	est.
Low Weight PAHs			
Anthracene	19	38	est.
Fluorene	5.9	16	est.
Naphthalene	50	72	calc.
Phenanthrene	11	24	est.
Pesticides			
Aldrin	0.43	0.84	est.
Chlordane	0.03	0.06	CWQC
DDD	0.6	2.2	est.
DDE	2.7	6.0	est.
DDT	0.04	0.07	CWQC
Dieldrin	0.001	0.002	CWQC
Endrin	0.001	0.002	CWQC
Heptachlor	0.004	0.006	CWQC
Toxaphene	0.0001	0.0002	calc.

a/ CWQC = based on existing EPA marine chronic water quality criteria value.
Calc. = based on calculation from compound-specific ACR value.
Est. = based on an estimate using a uniform distribution of a range of ACR values.

5.0 SUMMARY AND CONCLUSIONS

This study has investigated the uncertainty associated with the equilibrium partitioning (EP) approach to developing sediment criteria for hydrophobic organic chemicals, thereby allowing the uncertainty associated with a criterion value to play a role in the regulatory decision-making process. This method assumes that the concentration of a contaminant at the water/sediment interface is at equilibrium, that the bioavailable form is the free concentration of the contaminant in the aqueous phase, and that the sorption is controlled by the physical and chemical properties of the sorptive matrix and the chemical constituency of the aqueous phase. Hence, proper normalization of the contaminant concentration to these parameters is required. Previous studies together with the analyses presented have indicated that, for the hydrophobic organic chemicals, the key normalization parameter is organic carbon.

Permissible sediment contamination concentrations (PCCs) were estimated by multiplying measured or predicted organic carbon-normalized partitioning coefficients (K_{OC}) by EPA specified chronic water quality criteria (CWQC) values. The uncertainty associated with the PCC values can be quantified by use of parametric statistics on measured K_{OC} values or nonparametric analyses (Appendix A) on K_{OC} values determined from K_{OC}/K_{OW} regressions. These later evaluations confirmed the need to use the experimental data rather than the regression-predicted data because of the larger error associated with the predicted information. Furthermore, employing a quantitative uncertainty analysis technique, probability of exceedance curves are generated which measure the risk of exceeding an acceptable level of a given contaminant in sediments as a fraction of sediment contaminant concentration. PCC values for 10 PAHs and 9 chlorinated pesticides were computed for two levels of exceedance probability, 1 percent and 5 percent (which are within the range of current regulatory stipulations). These analyses were performed using water quality criteria values reflecting marine chronic effects.

In the absence of chronic water quality criteria, estimates were based on a uniform distribution on a range of acute-to-chronic ratios (ACR) or from a compound-specific ACR value. Uncertainties associated with ACR estimates were also incorporated into the probability of exceedance curves.

Table 5-1 summarizes the results of these analyses and compares the computed PCC values to similar quantities estimated in other studies. A 5 percent increase in the probability of exceedance induces approximately a two-fold increase in the estimated PCC value. It is apparent that in certain cases there is consistency in the estimated values among the different methods. For the majority of the pesticides, the values based on equilibrium partitioning (EP) agree with screening level concentration (SLC) values reported by Neff et al. (1986). The Apparent Effect Threshold (AET) values for benthic population data are, in general, higher for most of the compounds, but the amphipod equivalent AET appears to be lower. These discrepancies cannot be rationalized at this point because of the databases selected and the inherent assumptions and limitations of all three methods. However, this range of values provides a useful guide for regulatory decisions and argues for more field and laboratory experimentation to reduce the ranges. The EP-based criteria also demonstrate a variability between compounds that is expected based on their diverse K_{OC} values (e.g., the PAHs tend to have higher criteria values than the pesticides).

In review of the above results, it is obvious that for the EP approach there is need for field and laboratory measurements of K_{OC} values, both to verify and refine the PCC values. Also, marine-based chronic water quality criteria should continue to be developed and additional ACR data compiled.

TABLE 5-1 PCC Values From Equilibrium Partitioning Methodology and Other Preliminary Criteria Values

Compound	PCC (µg/goc) for probability fractile 0.01	0.05	Fractile ratio [a]	Other Studies AET Benthic (µg/goc) [b]	AET Amphipod (µg/goc) [b]	SLC µg/goc) [c]	CI
EPA CWQA [d]							
Fluoranthene	160	310	1.9	>6,300	160	43.2	(0.0-64.3)
Chlordane	0.03	0.06	1.9	--	--	0.098[e]	(0.0-0.136)
DDT	0.04	0.07	1.6	>3.7	>1.2	42.8	(0.0-113.7)
Dieldrin	0.001	0.002	1.6	--	--	0.021[e]	(0.0-0.084)
Endrin	0.001	0.002	1.6	--	--	--	
Heptachlor	0.004	0.006	1.6	--	--	0.008[e]	(0.0-0.029)
Est. CWQA [f]							
Benzo(a)anthracene	160	2,100	12.6	>4,500	110	26.1	(0.0-41.0)
Benzo(a)pyrene	1,800	4,500	2.4	>6,800	99	39.6	(0.0-46.8)
Chrysene	120	440	3.7	>6,700	110	38.4	(0.0-60.5)
Dibenzo(a,h)-anthracene	1,200	3,500	2.8	--	--	--	
Pyrene	85	190	2.2	>7,300	>210	43.4	(0.0-74.4)
Anthracene	19	38	2.0	--	--	--	
Fluorene	5.9	16	2.6	--	--	--	
Naphthalene.	50	72	1.4	>330	>200	36.7	(0.0-41.4)
Phenanthrene	11	24	2.2	>3,200	180	25.9	(0.0-38.4)
Aldrin	0.43	0.84	2.0	--	--	--	
DDD	0.6	2.2	3.5	--	--	--	
DDE	2.7	6.0	2.2	--	--	--	
Toxaphene	0.0001	0.0002	1.4	--	--	--	

a/ Determined prior to rounding of fractile values.

b/ Tetra Tech 1986.

c/ Neff et al. 1986.

d/ PCC values based on EPA CWQC or EPA suggested value.

e/ Freshwater value.

f/ PCC values based on chronic water quality criteria estimated from acute criteria.

6.0 REFERENCES

Kadeg, R. D., S. P. Pavlou and A. S. Duxbury. 1986. Elaboration of sediment normalization theory for nonpolar hydrophobic organic chemicals. Envirosphere Company, Bellevue, Washington.

Kenaga, E. E. 1982. Predictability of chronic toxicity from acute toxicity of chemicals in fish and aquatic invertebrates. Environmental Toxicology and Chemistry 1:347-358.

Mackay, M. D., W. J. Conover and R. J. Beckman. 1979. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. Technometrics 21:239-245.

Neff, J. M., D. J. Bean, B. W. Cornaby, R. M. Vaga, T. C. Gulbransen, and J. A. Scanlon. 1986. Sediment quality criteria methodology validation: calculation of screening level concentrations from field data. U.S. Environmental Protection Agency, Criteria and Standards Division, Washington, D.C.

Pavlou, S. P. The use of the equilibrium partitioning approach in determining safe levels of contaminants in marine sediments. Paper presented at the 6th Pellston Conference on the Role of Sediments in Regulating the Fate and Effects of Chemicals in Aquatic Environments, August 12-17, 1984, Florissant, Colorado.

Pavlou, S. P., and D. P. Weston. 1984. Initial evaluation of alternatives for development of sediment related criteria for toxic contaminants in marine waters (Puget Sound) phase II: development and testing of the sediment water equilibrium partitioning approach. JRB Associates, Bellevue, Washington.

Tetra Tech. 1986. Tasks 4 and 5a - Application of selected sediment quality value approaches to Puget Sound data. Draft report prepared for Resource Planning Associates for U.S. Army Corps of Engineers, Seattle District. Bellevue, Washington.

APPENDIX A

ALTERNATIVE NONPARAMETRIC APPROACH TO DETERMINE UNCERTAINTIES

CONTENTS

TABLES

FIGURES

A.0 INTRODUCTION

As described in Chapters [1] and 2 of the main report, an alternative approach using nonparametric statistics to determine uncertainties on K_{ow} and K_{oc} and subsequent PCC values was evaluated. This appendix provides background information on the approach (bootstrap method), and summarizes the K_{ow} and K_{oc} distributions and development of bootstrap method sampling space, the results, and conclusions of this evaluation.

A.1 BACKGROUND

A common problem in applied statistics involves estimating a statistic based on a finite number of observations or a sample taken from an unknown population of observations. Typically, the estimated statistic carries meaning only within the context of an interval surrounding that estimate. Classical point-interval estimation statistics handled this problem satisfactorily by assuming that sample estimates, such as the mean and variance reflected the true mean (u) and variance (σ^2) of the population from which the sample was taken. Classical distribution theory, confidence intervals and hypothesis testing tacitly assume that data follow a specific distribution, most commonly the normal distribution; these are called parametric methods. For the typical problem, applied data are rarely adequate to define the distribution of available data. Therefore, unless data exhibit completely anomalous behavior, it is commonly assumed that the data approximate the normal distribution, and investigators proceed to apply classical methods. Most classical parametric statistical methods are fairly robust; i.e., insensitive to bias, etc., when derived from nonnormal data. However, many applied statisticians have become increasingly uncomfortable in making this 'leap of faith' and have developed alternative estimation methods.

In the mid-1970s, increasing interest resulted in development of what have been designated as 'nonparametric' methods. These methods typically use ranked or ordered data (as defined by the raw data), rather than the raw data itself for which no true distributional characteristics could be defined. The methods make no assumptions about the distribution of the observations, and

methodological development has relied on exhaustive specification of the probability of the specific value found for a test, given a specific sample size. Examples of nonparametric methods and their corresponding parametric methods include: Wilcoxon's test as an alternative to the classical T-test; Kruskall-Wallis and Friedman tests as alternatives to classical analysis of variance; and Kendall's 'tau' statistic as an alternative to the classical correlation coefficient.

With decreasing costs for computer time and developments in exploratory data analysis, the approach applied to develop nonparametric methods was expanded. The conceptual approach of bootstrapping, developed by Efron and Tibshirani (1985), empirically defines the distributional attributes of the estimated statistic by replacing the distribution assumptions with the observed distribution of the estimated statistic when the sample is expanded into a population. The actual method involves iteratively sampling the observations, with replacement; each sample so derived is called a 'bootstrap' sample. The statistic of interest is then calculated for each bootstrap sample. The resulting empirical distribution of the statistic, from all possible estimates of the statistic given sample size and noted observations, provides both an estimate of the statistic and a context within which that estimate can be evaluated. Briefly stated, the bootstrapping method replaces the classical, assumed 'population' (from which the observed sample has been collected) with the bootstrap 'universe' of samples of which the observed sample is a single example. Bootstrap methods have been applied to define standard error, bias and precision errors for the one-sample situation, as well as to more complicated data structures such as time series and censored data. Usefulness of the method is evidenced in its application by widely divergent areas of research.

Given the limitations to the available data on which sediment PCC values were to be based (detailed in Appendix B), it was felt that the bootstrapping method could be an extremely powerful tool to quantify the variability of the possible regression models defining the relationship between K_{oc} and K_{ow} values for each chemical class.

A.2 DEVELOPMENT OF K_{oc} and K_{ow} DISTRIBUTIONS AND THE BOOTSTRAP SAMPLING SPACE

Given the results of the exploratory analysis (Appendix B), it was concluded that although the data are very limited, the distribution of the logarithmic transformation of both K_{ow} and K_{oc} values will be assumed to follow a normal distribution. To develop a balanced set of K_{ow}-K_{oc} data for the bootstrap regressions, normal distributions for the K_{ow} and K_{oc} values of each chemical were constructed. The mean of the normal distribution was chosen as the median value of all observed values. The standard deviation was slightly more difficult to determine because no estimates (parametric or nonparametric) of dispersion (on the observed data) were available for sets in which the number of observations was less than three. To determine the standard deviation for the K_{ow}-K_{oc} sets, the maximum coefficient of variation (C_v) observed in all the K_{ow} and the K_{oc} sets where the number of observations was greater than 10 were examined (Tables B.2 through B.4, Appendix B). The maximum C_v in the three K_{ow} sets with greater than 10 data points was 9.12 percent and in the four K_{oc} sets was 8.76 percent. The close agreement in the C_v values was unexpected because of the sediment variability included in the measured variability of K_{oc}.

To estimate the standard deviation, the maximum C_v was held constant for all K_{ow} and K_{oc} classes. Then, using the relationship C_v = 100 x (standard deviation)/(mean), the mean, and C_v value, the appropriate standard deviation for the normal distributions could be calculated. For N less than 4 but greater than 1, the calculated standard deviation (SD) was multiplied by 1.5 to derive an adjusted SD value; for K_{oc} or K_{ow} sets with less than 10 but more than 5 observations, the SD was multiplied by 1.25; for K_{ow} sets with greater than 10 observations, the calculated standard deviation (multiplied by 1) was used. The objective of this adjustment to the calculated SD was to increase the dispersion of the K_{ow} and K_{oc} distributions for which minimal data were available.

Table A.1 summarizes the mean and adjusted SD values used to generate the normal distributions of K_{oc} and K_{ow} for each chemical compound which had both K_{oc} and K_{ow} measures. The parameters in Table A.1 were used to

TABLE A.1 Summary Statistics for Normal Distributions of Low/High Weight PAH and Pesticides, Based on Median Observed K_{ow}/K_{oc} and Calculated SD Given Fixed Maximum N

	Log K_{ow}			Log K_{oc}	
Compound	Mean	SD	Adjusted SD	Mean	SD
Low Weight PAH					
Benzo(a) anthracene	5.76	0.53	0.66	6.27	0.58
Benzo(a)pyrene	6.02	0.55	0.55	6.75	0.55
Chrysene	5.70	0.52	0.65	5.77	0.58
Dibenzo(a,h) anthracene	6.25	0.57	0.71	6.36	0.56
Fluoranthene	5.26	0.48	0.60	5.31	0.44
Pyrene	5.11	0.47	0.58	4.88	0.48
High Weight PAH					
Anthracene	4.45	0.41	0.51	4.42	0.38
Fluorine	4.27	0.39	0.49	4.01	0.34
Naphthalene	3.37	0.31	0.31	3.52	0.30
Phenanthrene	4.49	0.41	0.51	4.22	0.38
Pesticides					
Aldrin	5.66	0.52	0.77	4.79	0.45
Chlordane	3.32	0.31	0.45	5.15	0.40
DDD	5.99	0.55	0.68	5.38	0.42
DDE	5.6[a]	0.52	0.65	5.17	0.48
DDT	6.13	0.56	0.56	5.52	0.42
Dieldrin	4.95	0.45	0.68	3.81	0.34
Endrin	4.48	0.41	0.51	3.55	0.30
Heptachlor	4.48	0.41	0.61	4.00	0.30
Toxaphene	3.27	0.30	0.45	3.00	0.20

generate 100 random observations (for both K_{oc} and K_{ow}) for each chemical. These 100 values per partition coefficient and per chemical represented the balanced data sets from which bootstrap samples were taken. To assess the reliability of the generated data sets given the limited data and the many assumptions that were made, random pairs of K_{oc} and K_{ow} values generated for each chemical compound were plotted along with the 'true' pairs available from the literature. A sample of these plots is presented in Figure A.1. To further corroborate the realism of data pairs selected from the hypothetical distributions, descriptive statistics were calculated from the bootstrap samples. Tables A.2 through A.4 document the desired statistics for K_{ow} and K_{oc} data for each chemical per compound (based on exploratory analyses) and the actual statistics calculated from the randomly assigned pairs. The agreement between the two sets of data is quite good.

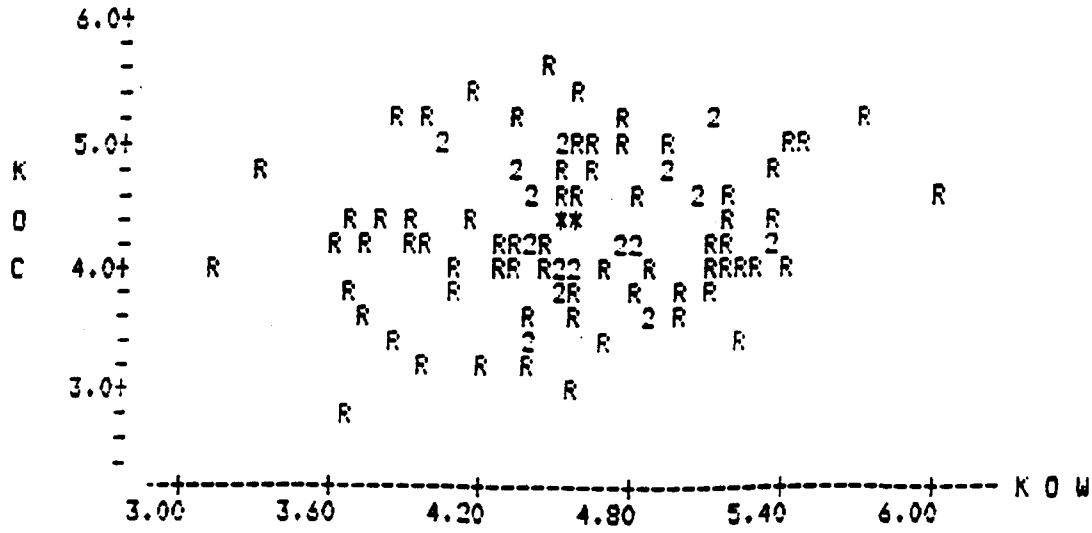
The plots presenting the simulated data pairs and the observed data pairs fell into three general cases as follows:

Case i: Many true pairs fell within the center of the simulated distribution (10 plots).

Case ii: Occasional true pairs exhibited mildly anomalous behavior; i.e., occurred at the fringes of the simulated data (4 plots).

Case iii: On rare occasions, observed pairs were highly anomalous within the simulated distributions (3 plots).

These results indicate that while available data were inadequate to accurately describe the actual distributions of the K_{oc} and K_{ow} data, the simulated distributions did not erroneously describe possible paired points. The existence of centered as well as anomalous pair behavior indicates that, overall, the simulated data is representative of the observed K_{oc} and K_{ow} data.



PHENANTHRENE: 2 PAIRS

R = RANDOM BINORMAL KOC-KOW PAIRS
* = PAIRED KOC-KOW POINT[S] FROM LITERATURE
INTEGER = NUMBER OF COINCIDENT OBSERVATIONS

FIGURE A.1 Example Figure - Comparison of Simulated and Observed Data Pairs for Phenanthrene.

TABLE A.2 Normal Distribution Parameters for K_{ow} and K_{oc}: Calculated[a/] and Observed [b/] High Weight Polynuclear Aromatic Hydrocarbons

Compound	K_{ow} Mean	K_{ow} SD	K_{oc} Mean	K_{oc} SD
Dibenzo(a,h)anthracene				
Observed	6.25	0.71	6.36	0.56
Calculated	6.26	0.71	6.45	0.60
Benzo(a)pyrene				
Observed	6.02	0.55	6.75	0.74
Calculated	5.91	0.63	6.76	0.75
Benzo(a)anthracene				
Observed	5.76	0.66	6.27	0.82
Calculated	5.73	0.76	6.09	0.79
Chrysene				
Observed	5.70	0.65	5.77	0.76
Calculated	5.78	0.76	5.63	0.74
Fluoranthene				
Observed	5.26	0.60	5.31	0.70
Calculated	5.22	0.64	5.28	0.75
Pyrene				
Observed	5.11	0.58	4.88	0.43
Calculated	5.08	0.60	4.93	0.44

a/ Calculated distribution parameters (X, s) were calculated from the random samples constrained to the expected distribution (μ,σ).

b/ Observed distribution parameters (μ,σ) were determined from available data and defined as follows:
μ = median value of observed K_{ow} or K_{oc} data, regardless of the number of observations and
σ = (median value) x (max coefficient of variation)
where max C_v (K_{ow}) = 0.0912
max C_v (K_{oc}) = 0.0876.

TABLE A.3 Normal Distribution Parameters for K_{ow} and K_{oc}: Calculated[a/] and Observed[b/] Low Weight Polynuclear Aromatic Hydrocarbons

	K_{ow}		K_{oc}	
Compound	Mean	SD	Mean	SD
Phenanthrene				
Observed	4.49	0.51	4.22	0.55
Calculated	4.56	0.54	4.31	0.59
Anthracene				
Observed	4.45	0.51	4.42	0.58
Calculated	4.52	0.54	4.44	0.58
Fluorene				
Observed	4.27	0.49	4.01	0.53
Calculated	4.24	0.48	4.00	0.51
Naphthalene				
Observed	3.37	0.31	3.52	0.39
Calculated	3.29	0.33	3.49	0.38

a/ Calculated distribution parameters (X, s) were calculated from the random samples constrained to the expected distribution (μ,σ).

b/ Observed distribution parameters (μ,σ) were determined from available data and defined as follows:
μ = median value of observed K_{ow} or K_{oc} data, regardless of the number of observations and
σ = (median value) x (max coefficient of variation)
where max C_v (K_{ow}) = .0912
max C_v (K_{oc}) = .0876.

TABLE A.4 Normal Distribution Parameters for K_{ow} and K_{oc} Distributions Calculated [a] and Observed [b] Pesticides

Compound	K_{ow} Mean	K_{ow} SD	K_{oc} Mean	K_{oc} SD
DDT				
Observed	6.13	0.57	5.52	0.48
Calculated	6.10	0.60	5.50	0.44
DDD				
Observed	5.99	0.68	5.38	0.71
Calculated	6.20	0.74	5.38	0.67
DDE				
Observed	5.69	0.65	5.17	0.68
Calculated	5.57	0.67	5.08	0.70
Aldrin				
Observed	5.66	0.77	4.79	0.52
Calculated	5.67	0.82	4.76	0.50
Dieldrin				
Observed	4.95	0.68	3.81	0.50
Calculated	5.02	0.67	3.80	0.46
Heptachlor				
Observed	4.48	0.61	4.00	0.53
Calculated	4.41	0.61	4.03	0.53
Endrin				
Observed	4.48	0.51	3.55	0.47
Calculated	4.39	0.55	3.61	0.47
Chlordane				
Observed	3.32	0.45	5.15	0.68
Calculated	3.34	0.43	5.11	0.60

TABLE A.4 (Continued)

Compound	K_{ow} Mean	K_{ow} SD	K_{oc} Mean	K_{oc} SD
Toxaphene				
Observed	3.27	0.45	3.00	0.39
Calculated	3.24	0.92	2.95	0.41

a/ Calculated distribution parameters (X, s) were calculated from the random samples constrained to the expected distribution (μ,σ).

b/ Observed distribution parameters (μ,σ) were determined from available data and defined as follows:
μ = median value of observed K_{ow} or K_{oc} data, regardless of the number of observations and
σ = (median value) x (max coefficient of variation)
where max C_v (K_{ow}) = .0912
max C_v (K_{oc}) = .0876.

Through the extensive exploratory analysis of measured K_{OC} and K_{OW} values, the above distributions were derived which describe the observed variability in the data sets. Although the data from which these distributions were generated were very limited, simulated data sets generated from these distributions using Latin Hypercube sampling were generally consistent with the observed data pairs. As a result, it appeared that such a sampling method might be adequate to derive a sample space for estimating the uncertainty in the PCC values.

A.3 ANALYSIS AND RESULTS

For compounds with a measured K_{OW} value but no measured K_{OC} value, the uncertainty in the sediment criterion increases because of the need to use a K_{OW}-K_{OC} regression relationship to calculate the K_{OC} value. For each class of compounds, the bootstrapping method was used to generate a sample of 100 possible regression equations. For each regression equation generated using the bootstrap method, a random value of K_{OW} was selected from the K_{OW} distribution based upon measured K_{OW} values. Then, using Equations (1.3) (i.e., the regression equation), (2.1), and (2.2) as discussed in the main report, a median PCC value and associated 95 percent confidence interval values were determined. Combining these results for the 100 equations permitted derivation of a distribution for the median and confidence intervals for the PCC values.

To evaluate these distributions, linear plots of the bootstrap samples were plotted which represent random and independent selections of K_{OW} and K_{OC} values (from the distributions described in Table A.1) for the chemical classes. These plots were elliptical and the shape of the distribution is the direct result of the uncertainty associated with K_{OC}-K_{OW} values for the chemical within each chemical class as well as the result of the assumptions made about the distribution of the data to compensate for the 'unpairedness' of the available data.

Additional plots of the chemical class-specific 100 regressions lines (predicted K_{OC} vs. observed K_{OW}) resulted in plots approaching the theoretical confidence intervals about the regression. The distributions were

generally parabolic, centered at the mean. These results suggest that 100 bootstrap samples will result in an adequate estimate of the variability in the regression lines derived from the simulated data.

Residual plots were also constructed for the chemical class-specific groups (i.e., high and low weight PAHs, pesticides). Residuals, which are the differences between simulated K_{oc} and predicted K_{oc} (based on the observed K_{ow} values) are the basis by which the success (or failure) of the linear model can be assessed. Plots of the residuals against the predictor or carrier variable (here simulated K_{ow} values) which exhibit random, homoscedastic behavior (across the predictor) support the model. For example, such a plot indicates that the effect on the predicted variable (here, K_{oc}) of the predictor has been accounted for by the model and no additional effect (such as an X^2 term) is required. The plots appeared to support such a conclusion.

Plots of the residuals against the predicted values can also be used to indicate the variability of the residuals with respect to the model predictions. Systematic nonrandom behavior suggests that some systematic variability in the predicted variable has not been accounted for by the linear model. The plots exhibited no such cumulative behavior in the regressed bootstrap samples, again supporting the model.

Finally, plots of the residuals against the observed values can and must exhibit nonrandom behavior due to the correlation between the observed and residual values. (Recall that the residual equals the observed minus the predicted value.) The absolute value of the slope of the residual vs. the observed K_{oc} plot equals zero only when the model is a perfect fit. The plots indicated that there is a less than perfect fit for each of the three chemical classes.

Examples of the above plots are presented in Figures A.2 through A.4. The results of this graphic evaluation suggested that, although the model appeared to be meeting the general constraints for its application, the underlying assumptions concerning the distribution of the data together with the limited real (measured) data sets (Appendix B) would ultimately lead to

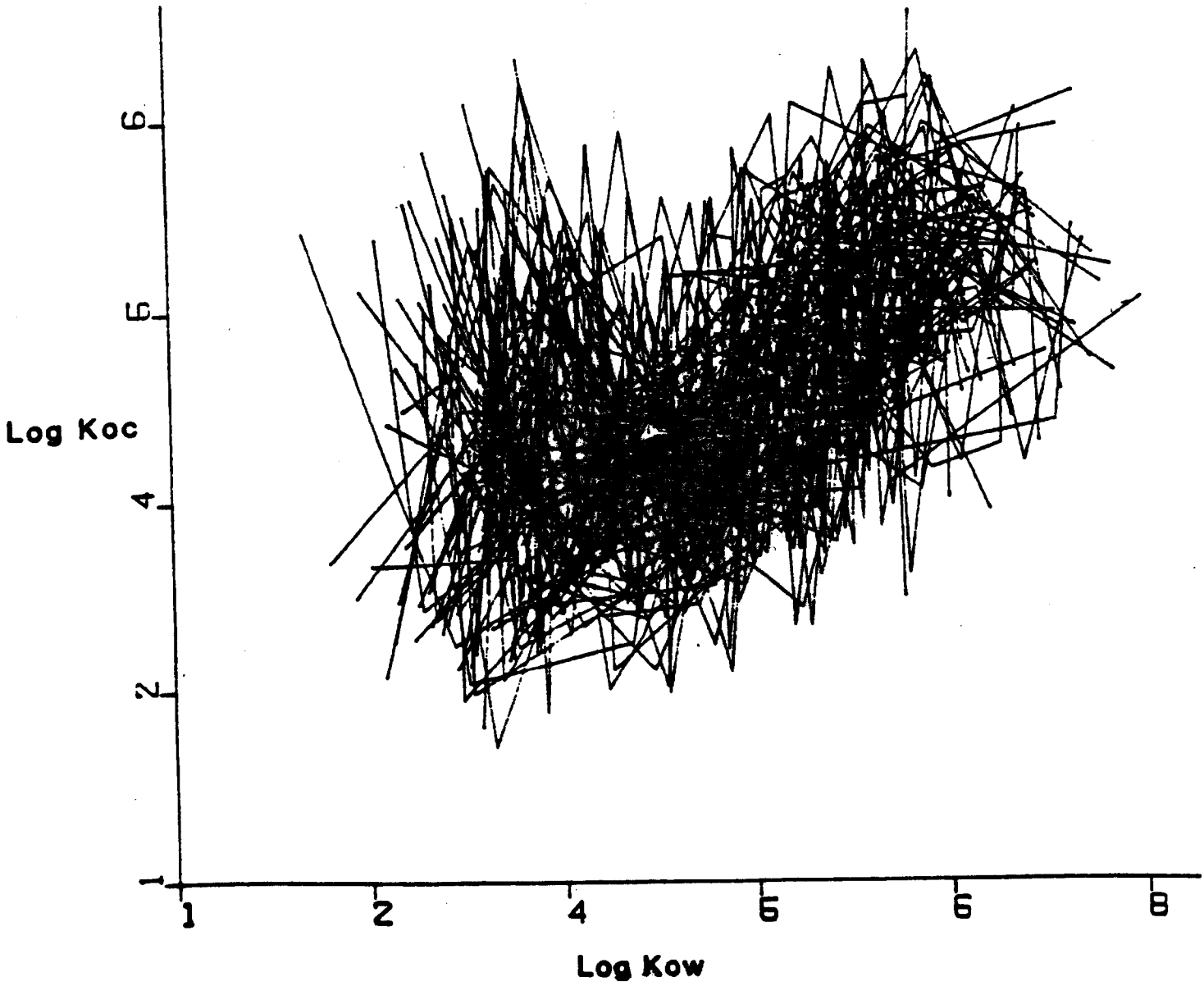


FIGURE A.2 Example Linear Plot of Bootstrap Sample - Simulated K_{ow} VS K_{oc} for Pesticides.

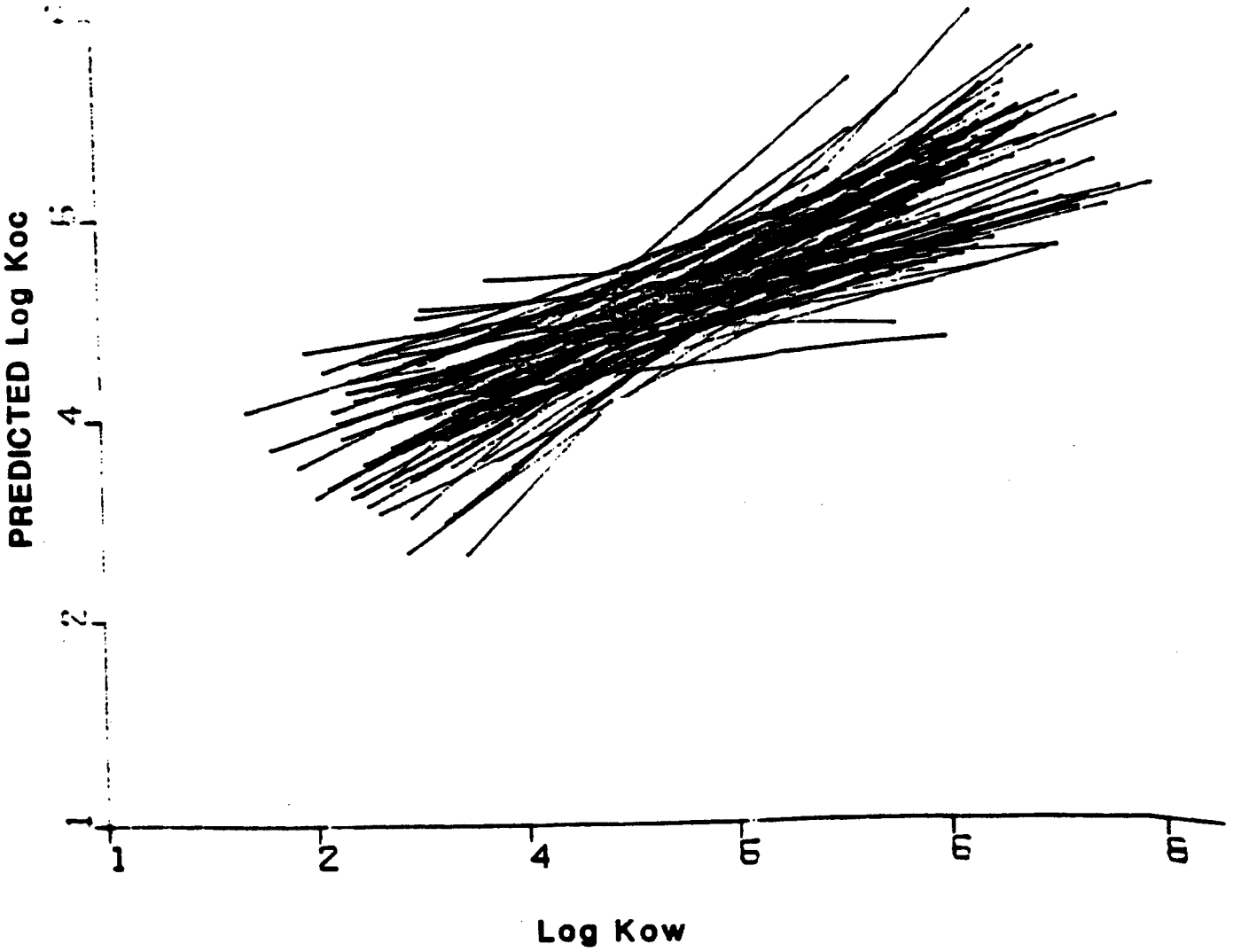


FIGURE A.3 Example Cross - Specific Plot - Predicted K_{oc} VS Simulated K_{ow} for Pesticides.

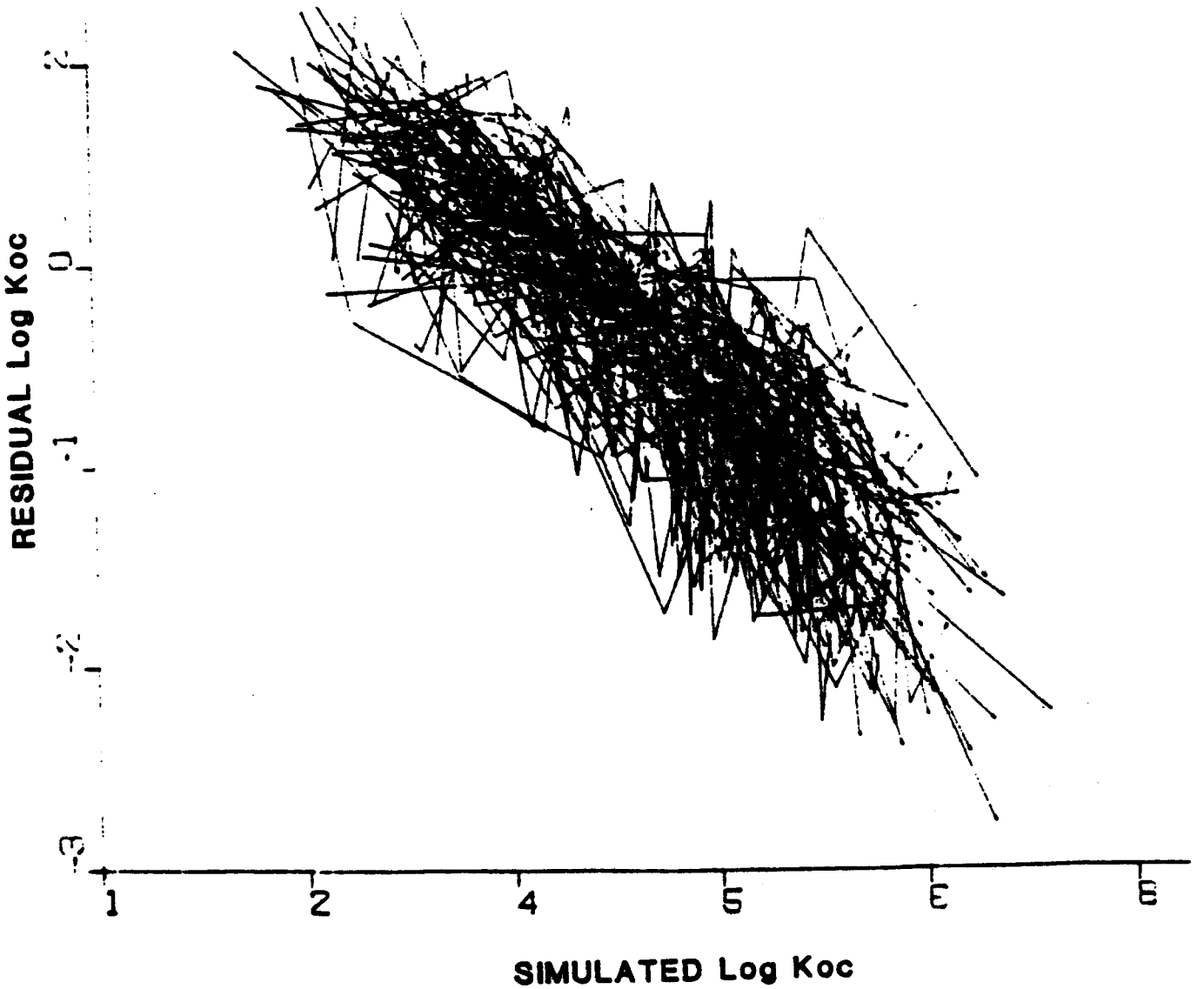


FIGURE A.4 Example Residual Plot - Residual K_{oc} VS Simulated K_{oc} for Pesticides.

unrealistically high uncertainties due to the scatter in the simulated data sets and resulting regression lines (as supported by the elliptically shaped plots of the bootstrap samples). In simplest terms, it appeared that the measured K_{oc} and K_{ow} data sets may have been too small to infer true "real world" distributions, as opposed to perceived, artificial distribution patterns indicated by the simulated data sets.

Table A.5 summarizes the range in PCC values. The range is defined as the difference between the log values of the PCC. The range in all values is the difference between the absolute minimum and maximum PCC values calculated in 100 samples including confidence intervals on the predicted K_{oc}. The 80 percent range is the difference between minimum and maximum values in the range of the 10th to 90th percentiles on the median PCC. The minimum and maximum confidence intervals are from those generated in the analysis for any one sample observation. As these values indicate, there is substantial variability across both the distribution of median PCC values and of confidence intervals for each median PCC.

From columns 3 and 4 of Table A.5, it can be seen that the 80 percent confidence interval contributes from 40 to 48 percent of the range in the PCC variability for the median values of the PCC. Columns 1 and 2 (which include the confidence intervals) show a similar decrease in overall variability when comparing the 80 percent range to the 100 percent range. This decrease in range is probably due to the elimination of some poorly-fit regression lines which were used to calculate the PCC values in the tails of the distribution on the median PCC. This reduction in range would indicate that such ill-fit regression lines are not predominant, but do occur.

Columns 5 and 6 on Table A.5 show the range in the width of the confidence intervals. This variability in the width of the confidence intervals corresponds to the wide range in slope and intercept terms reported in the results of the bootstrapping method and shows the resulting impact on the range of PCC values (i.e., uncertainty). As discussed in Section 2.3 of the main text, the width of the confidence interval is dependent on several factors including the fit of the regression (as typically measured by the R-square term), the number of data points, and the spread of the data used in the regression.

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TABLE A.5 Summary of Calculated Ranges in PCC Values for Compounds without Measured K_{oc}

Compound	Range of Values [a]				Range in C.I. [d]	
	All Values [b]		Medians [c]			
	100Δ	80Δ	100Δ	80Δ	Max.	Min.
High Weight PAHs						
Benzo(b)fluoranthene	14.44	9.92	4.68	2.20	13.23	1.13
Benzo(g,h,i)pyrene	18.72	10.75	5.27	2.49	16.91	1.36
Benzo(k)fluoranthene	15.37	10.59	4.73	2.28	13.90	1.16
Indeno(1,2,3,c,d)pyrene	23.94	15.27	7.61	3.44	22.19	1.65
Low Weight PAHs						
Acenaphthene	19.55	4.26	1.92	0.93	19.55	0.23
Acenaphthylene	40.00	18.90	11.03	4.60	40.00	0.52
Pesticides						
Endosulfan	7.43	5.68	1.79	0.76	7.17	1.58
Hexacyclochlorohexane	6.95	4.81	1.50	0.72	6.92	1.53
Isophorone	10.72	8.29	3.57	1.41	9.26	1.95

a/ Range is defined as the difference of the log values of the PCC.
b/ The range in all values is the difference between the absolute minimum and maximum values calculated in 100 samples. The 80 percent range is the difference between minimum and maximum values in the 10th to 90th percentiles on the median PCC.
c/ The range is calculated as the difference between median values of the PCC, excluding confidence intervals on the PCC.
d/ Minimum and maximum confidence intervals from those generated in the analysis of 100 samples for any one sample observation.

Tables A.6 and A.7 show the results of a parametric sensitivity analysis using three regression equations, three values for K_{ow}, and the 80 percent confidence interval on the predicted value of K_{oc}. Table A.6 lists the regression equations and K_{oc} values used. For each chemical class, three regression equations were chosen based on the distribution of the calculated slope term. From the values of B1 generated by the bootstrapping method, regression equations were chosen for the median, upper, and lower quartile values of B1. For these analyses, the CWQC value in Equation (1.3) of the main report was uniformly defined as an order of magnitude less than the acute water quality criteria (i.e., acute to chronic ratio of 10). These results show that there is a substantial range in the calculated PCC values when the K_{oc}-K_{ow} regression relationship is used to calculate the PCC value. Much of this range is due to confidence intervals on the predicted value of K_{oc} with some contribution from variance in B0 and B1 regression terms and the value of K_{ow} used in the regression.

The range in PCC values due to the confidence intervals on K_{oc} varies between compound classes. As would be expected, the confidence intervals for the pesticides are more uniform because of the larger sample sizes used. The largest width in the PCC confidence interval is seen for the low weight PAH compounds, which have the fewest data points.

Due to the instability of the regression lines generated by the bootstrapping method, it is not feasible to define a single probability function for the PCC distribution for compounds without a measured K_{oc}. It is certain, however, that a great deal of confidence can be gained by measuring the K_{oc} value.

A.4 CONCLUSIONS

Based on the above analysis, the uncertainty associated with the PCC values in Table A.6 is very broad. The application of the nonparametric bootstrapping techniques, while technically correct, has resulted in an overstatement of these uncertainties. This is directly attributed to the assumptions required to generate a data set of suitable size to employ this method. It is apparent that the selection of distributions (data patterns)

TABLE A.6 Regression Statistics Used in Parametric Sensitivity Analyses

	Regression Equation Parameters [a]				
Compound Class	B0	B1	S2	XBAR	SSQX
High Weight PAH	4.30	0.2400	0.54	5.90	9.62
	3.50	0.4400	0.39	5.20	2.72
	0.18	0.9600	0.15	5.70	0.94
Low Weight PAH	3.00	0.1800	0.42	4.50	13.60
	2.20	0.5100	0.95	3.80	6.54
	0.57	0.7900	0.06	4.30	20.60
Pesticides	3.10	0.2800	0.54	4.80	3.11
	2.30	0.3900	0.28	4.90	0.77
	1.90	0.5400	0.62	4.70	1.43

	Log K_{oc}		
Compound	Q1	Median	Q3
High Weight PAH			
Benzo(b)fluoranthene	5.732	6.320	6.908
Benzo(g,h,i)pyrene	6.503	7.050	7.597
Benzo(k)fluoranthene	5.850	6.450	7.050
Indeno(1,2,3,c,d)pyrene	6.986	7.700	8.414
Low Weight PAH			
Acenaphthene	3.893	4.150	4.407
Acenaphthylene	3.761	4.010	4.259
Pesticides			
Endosulfan	3.377	3.600	3.823
Hexacyclochlorohexane	3.752	4.000	4.248
Isphorene	1.595	1.700	1.805

---

[a] B0 = regression equation intercept
B1 = regression equation slope
S2 = estimated variance of error term in regression
XBAR = average of log K_{ow} values used in regression
SSQX = sum of the squares of the log K_{ow} value used for the regression
Q1 = lower quartile value
Q3 = upper quartile value

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TABLE A.7 Permissible Sediment Contaminant Concentration Values (ug/goc) by K_{OW} Values

Compound	Regr	25th Percentile Predicted Confidence Interval			Median Predicted Confidence Interval			75th Percentile Predicted Confidence Interval		
		Low	Med	High	Low	Med	High	Low	Med	High
Benzo(b)fluoranthene	Q1	5.76E+02	7.11E+03	8.78E+04	7.82E+02	9.84E+03	1.24E+05	9.74E+02	1.36E+04	1.90E+05
	Q2	1.68E+03	1.58E+04	1.48E+05	2.18E+03	2.86E+04	3.76E+05	2.43E+03	5.20E+04	1.11E+06
	Q3	1.92E+03	7.22E+03	2.71E+04	5.52E+03	2.65E+04	1.27E+05	1.18E+04	9.73E+04	8.01E+05
Benzo(g,h,i)pyrene	Q1	8.45E+02	1.09E+04	1.40E+05	1.01E+03	1.47E+04	2.14E+05	1.14E+03	1.99E+04	3.47E+05
	Q2	2.29E+03	3.45E+04	5.20E+05	2.45E+03	6.00E+04	1.47E+06	2.45E+03	1.04E+05	4.44E+06
	Q3	7.15E+03	3.97E+04	2.21E+05	1.39E+04	1.33E+05	1.28E+06	2.46E+04	4.46E+05	8.08E+06
Benzo(k)fluoranthene	Q1	6.17E+02	7.59E+03	9.34E+04	8.26E+02	1.06E+04	1.35E+05	1.01E+03	1.47E+04	2.14E+05
	Q2	1.80E+03	1.78E+04	1.76E+05	2.26E+03	3.27E+04	4.72E+05	2.45E+03	6.00E+04	1.47E+06
	Q3	2.46E+03	9.38E+03	3.58E+04	6.65E+03	3.53E+04	1.88E+05	1.39E+04	1.33E+05	1.28E+06
Indeno(1,2,3,c,d)pyrene	Q1	9.96E+02	1.42E+04	2.03E+05	1.16E+03	2.11E+04	3.83E+05	1.24E+03	3.13E+04	7.87E+05
	Q2	2.44E+03	5.62E+04	1.29E+06	2.44E+03	1.16E+05	5.50E+06	2.28E+03	2.39E+05	2.51E+07
	Q3	1.29E+04	1.16E+05	1.03E+06	2.72E+04	5.60E+05	1.15E+07	5.39E+04	2.71E+06	1.37E+08
Acenaphthene	Q1	1.98E+01	2.38E+02	2.87E+03	2.25E+01	2.65E+02	3.13E+03	2.53E+02	2.95E+02	3.44E+03
	Q2	1.81E+01	7.28E+02	2.94E+04	2.37E+01	9.84E+02	4.10E+04	2.99E+01	1.33E+03	5.93E+04
	Q3	8.27E+01	2.10E+02	5.33E+02	1.32E+02	3.35E+02	8.48E+02	2.11E+02	5.35E+02	1.35E+03
Acenaphthylene	Q1	5.8	7.13E+01	8.73E+02	6.6	7.90E+01	9.42E+02	7.5	8.76E+01	1.03E+03
	Q2	4.9	1.97E+02	7.92E+03	6.5	2.64E+02	1.07E+04	8.3	3.53E+02	1.51E+04
	Q3	2.05E+01	5.22E+01	1.33E+02	3.24E+01	8.20E+01	2.08E+02	5.10E+01	1.29E+02	3.26E+02
Endosulfan	Q1	1.79E-02	3.8E-03	0.79	2.47E-03	4.4E-02	0.77	3.34E-03	5.0E-02	0.76
	Q2	4.66E-03	1.4E-04	0.42	8.21E-04	1.7E-02	0.36	1.42E-03	2.1E-02	0.31
	Q3	4.08E-03	1.8E-04	0.79	7.53E-04	2.4E-02	0.75	1.34E-03	3.1E-02	0.73
Hexacyclochlorohexane	Q1	7.16E-03	0.11	1.8	9.80E-03	0.13	1.8	1.3E-02	0.16	1.9
	Q2	2.81E-03	4.6E-02	0.77	5.05E-03	5.8E-02	0.67	8.65E-03	7.2E-02	0.61
	Q3	2.64E-03	6.7E-02	1.7	4.83E-03	9.2E-02	1.7	8.24E-03	0.13	1.9
Isophorone	Q1	1.67E+01	2.27E+03	3.08E+05	2.03E+01	2.43E+03	2.91E+05	2.45E+01	2.60E+03	2.76E+05
	Q2	0.72	5.39E+02	4.04E+05	0.96	5.92E+02	3.65E+05	1.3	6.51E+02	3.30E+05
	Q3	0.32	3.72E+02	4.30E+05	0.45	4.24E+02	3.98E+05	0.63	4.84E+02	3.69E+05

inferred from the original raw data sets resulted in K_{oc} ranges beyond those which are chemically and physically feasible for a characteristic marine environment. Therefore, the PCC values and associated ranges reported in this appendix are not recommended, but are rather included for illustrative purposes. While the overall nonparametric approach is still suitable to determine uncertainties, it is clear that more field K_{oc} and K_{ow} data are required.

A.5 References

Efron, B., and R. Tibshirani. 1985. The bootstrap method for assessing statistical accuracy. Tech. Rept. 101, Division of Biostatistics, Stanford University, Palo Alto, California.

APPENDIX B

ANALYSIS OF AVAILABLE K_{OC} - K_{OW} DATA

CONTENTS

TABLES

FIGURES

APPENDIX B
AVAILABLE K_{OC}-K_{OW} DATA

This appendix describes the detailed review and analysis of the K_{OW} and K_{OC} data previously collected (Kadeg et al. 1986) and used for the uncertainty analysis of sediment normalization theory.

B.0 DESCRIPTION/LIMITATIONS

K_{OW} and K_{OC} data taken from available literature were screened prior to analysis, limiting data to observations exhibiting internal consistency (Kadeg et al. 1986). Internally consistent, acceptable data are summarized in Table B.1. The table indicates (by chemical compound within the four chemical classes) the following: the number of K_{OW} and K_{OC} measurements; the number of individual laboratories which made the measurements; and the number of true common pairs, i.e., paired K_{OW}-K_{OC} values for a specific compound, generated by the same research laboratory. Compounds are ordered within chemical class in the table, on the basis of the number of observed measures on K_{OW} and K_{OC}. Compounds at the top of the class influenced all subsequent analyses/conclusions by virtue of the relatively greater information available on their partitioning behavior.

Several features of the available chemical partitioning data are immediately apparent:

- Available data are unbalanced in terms of information on partitioning behavior. This imbalance is indicated by the different number of both measurements (ranging from 1 to 24 for K_{OW} coefficients and 1 to 31 for K_{OC} coefficients) and researchers (ranging from a single laboratory to 15 laboratories in K_{OW} and a single laboratory to 8 laboratories in K_{OC}).

- Detailed information indicative of the distribution of K_{OW} measurements is limited to three compounds:

TABLE B.1 K_{ow} and K_{oc} Data: Summary by Chemical Class and Compound Number of Observations[N/], Labs, and Common Pairs

Compound	K_{ow} N	K_{ow} No. Labs	K_{oc} N	K_{oc} No. Labs	Common Pairs
High Weight PAH					
Benzo(a)pyrene	24	7	4	1	0
Pyrene	6	6	31	3	2
Dibenzo(a,h)anthracene	4	4	15	2	2
Chrysene	5	6	1	1	1
Fluoranthracene	6	6	1	1	1
Benzo(a)anthracene	6	6	1	1	0
Benzo(g,h,i)perylene	5	5	0	0	0
Benzo(b)fluoranthene	2	2	0	0	0
Benzo(k)fluoranthene	2	2	0	0	0
Indeno(1,2,3,c,d)pyrene	1	1	0	0	0
Low Weight PAH					
Naphthalene	20	11	8	6	4
Fluorene	7	7	1	1	1
Anthracene	7	5	3	2	2
Phenanthrene	6	5	2	1	2
Acenaphthylene	2	2	0	0	0
Polychlorinated Biphenyl Compounds					
Arochlor 1254	2	2	14	1	0
Arochlor 1248	1	1	0	0	0
Arochlor 1260	1	1	0	0	0
Pesticides					
DDT	18	15	14	8	6
DDE	7	7	1	1	1
Endrin	6	6	2	2	1
DDD	5	5	1	1	1
Aldrin	3	3	4	4	2
Chlordane	3	3	1	1	1
Heptachlor	3	3	1	1	1
Dieldrin	2	2	2	2	1
Toxaphene	2	2	1	1	1
Acrolein	1	1	1	1	0
Isophorone	3	2	0	0	0
Endosulfan	1	1	0	0	0
Hexacyclochlorohexane	1	1	0	0	0
TCDD	1	1	0	0	0

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1) Benzo(a)pyrene (n=24)
2) Naphthalene (n=20)
3) DDT (n=18).

- Distributional attributes of K_{oc} measures are limited to four compounds:

1) Pyrene (n=31)
2) Dibenzo(a,h)anthracene (n=15)
3) Arochlor 1254 (n=14)
4) DDT (n=14).

- The number of true paired measurements is severely limited. Of the ten high weight PAHs, four chemicals have one to two sets of paired observations. Four of the six low weight PAHs are paired, as are 9 of the 14 pesticides. No pairs are available for any of the PCB compounds, thereby eliminating this class from analysis.

The inherent structure of available K_{ow}-K_{oc} data sets presents several analytical difficulties due to the assumptions associated with statistical methods used to predict values of a response variable (K_{oc}) on the basis of observed values of a predictor variable (K_{ow}). Ordinary least squares (OLS) regression assumes that response and predictor variables are multivariate normal in distribution. It further assumes that the predictor variable is measured without error. Finally, and most importantly, OLS regression tacitly assumes that the measures on predictor and response are paired observations.

The K_{ow}-K_{oc} data sets met few if any of the above criteria. Deficiencies are due, primarily, to the observational nature of the study and the uncontrolled nature of experimentation. Several of the limitations can be compensated for by variations to OLS. Imbalance in the number of K_{ow} and K_{oc} values can be compensated by analyzing summary statistics, i.e., mean and variance of the K_{ow} and K_{oc} values. The variance associated with the estimated mean must be included in the overall error estimate to ensure that the sum of squares is not artificially deflated, resulting in an overly optimistic estimate of the fit of the data. When the number of observations

representing each mean value varies or the variances associated with the mean values differ, weighted least squares (WLS) regression which 'weight' observations on the basis of data 'reliability' is typically used. When the measurement error of the predictor variable is much greater than that of the response variable, Draper and Smith (1981) indicate that error in the predictors may be effectively ignored without serious implications to the OLS regression results. When the measurement errors (in predictor and response variables) are of the same order of magnitude, Action (1966) has presented analytical solutions for correcting the variance estimates.

None of the variations to the OLS regression solution are adequate to address all the difficulties posed by the K_{ow}-K_{oc} data, and none of the methods described above can deal with the minimal number of pairings in the available data. Because the assumption that the predictor and response variables are paired is basic to regression analysis and because the available data are very limited in paired observations, the bootstrapping method was applied (Appendix A).

Application of the bootstrapping method typically involves

- Randomly sampling reported K_{ow} and K_{oc} values for each chemical for data from each chemical class.

- Determining the slope and intercept estimates of the K_{ow} and K_{oc} relationship (for each chemical class) from this random sampling using the least squares regression algorithm.

- Using the distribution of the slope and intercept estimates to define the distribution of these estimates (e.g., the median or average slope and intercept; and the first and third quartiles of each estimate) and to define a chemical class-specific distribution of the resulting K_{oc} values.

However, given the available data, this classical approach for applying the bootstrapping method would have given greater influence to chemicals for which the least amount of information is available. If only a single K_{oc}

value is available for a specific chemical (as occurred for many of the chemicals, Table B.1), that value would necessarily be included in each bootstrap sample and in each regression solution because randomly selecting one from a single valued distribution implies selection of that value. This situation is different from the situation in which multiple observations or measurements coincide. In this case, the phenomenon is considered to be known. To eliminate the sample-biasing due to 'lack of information' in the data included in the bootstrap samples, exploratory analyses of the available data were made to

- Define the distributional structure of available data (within and across chemical classes).
- Evaluate the laboratory factor as it affects apparent distributions (defining inter- and intra-laboratory variability).
- Develop a balanced set of observations which would be iteratively sampled by the bootstrapping algorithm.

The results from these exploratory analyses are discussed below.

B.1 Distributions of K_{OC} and K_{OW}

Tables B.2 through B.4 describe all available data per individual chemical compound within the high weight PAH, low weight PAH, and pesticide classes. The tables present the median value, i.e., the natural log-transformed value of the K_{OW} or K_{OC} which is in the center of the range; N, the number of measured values; a brief descriptive summary of the type of frequency distribution of the available data (approximately normal, bimodal, uniform, etc.); and the coefficient of variation (C_v). The C_v is the standard deviation normalized by the mean value multiplied by 100 and gives a percentage ratio of data variability to an average value. The median is the most appropriate measure of central tendency for these data because it truly reflects the center of the observed values. In normally distributed data, the median and mean values will coincide. Given the sensitivity of the mean to

TABLE B.2 Summary Statistics of K_{ow} and K_{oc} Distributions: High Weight PAH Compounds

Compound	Log K_{ow}	Log K_{oc}	Pairs
Phenanthrene			
Median	4.49	4.22	
N	6	2	
Histogram	Right skew	Uniform	2
C_v (%)	5.8	4.7	
Anthracene			
Median	4.45	4.42	
N	7	3	
Histogram	Sparse normal	Uniform	2
C_v(%)	4.7	17.1	
Fluorene			
Median	4.27	4.01	
N	7	1	
Histogram	Uniform	Undefined	1
C_v(%)	2.6	--	
Naphthalene			
Median	3.37	3.52	
N	20	8	
Histogram	Normal	Uniform	4
C_v(%)	1.8	15.7	

N is the number of observations.
C_v is the coefficient of variance.

TABLE B.3 Summary Statistics of K_{ow} and K_{oc} Distributions: Low Weight PAH Compounds

Compound	Log K_{ow}	Log K_{oc}	Pairs
Dibenzo(a,h)anthracene			
Median	62.5	6.36	
N	4	15	
Histogram	Sparse normal	Bimodal	2
C_v(%)	8.9	4.1	
Benzo(a)pyrene			
Median	6.02	6.75	
N	24	4	
Histogram	Left skew	Unimodal	0
C_v(%)	3.1	5.6	
Benzo(a)anthracene			
Median	5.76	6.27	
N	6	1	
Histogram	Approx normal	Undefined	1
C_v(%)	5.0	--	
Chrysene			
Median	5.70	5.77	
N	6	1	
Histogram	Sparse normal	Undefined	1
C_v(%)	4.4	--	
Fluoranthene			
Median	5.26	5.31	
N	6	1	
Histogram	Sparse normal	Undefined	1
C_v(%)	3.9	--	
Pyrene			
Median	5.11	4.88	
N	6	31	
Histogram	Sparse normal	Bimodal	2
C_v(%)	3.0	4.6	

N is the number of observations.
C_v is the coefficient of variance.

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TABLE B.4. Summary Statistics of K_{ow} and K_{oc} Distributions: Pesticide Compounds

Compound	Log K_{ow}	Log K_{oc}	Pairs
DDT			
Median	6.13	5.52	
N	18	14	
Histogram	Normal	Normal	6
C_v(%)	9.1	8.8	
DDD			
Median	5.99	5.38	
N	5	1	
Histogram	Right skew	Undefined	1
C_v(%)	11.0	--	
DDE			
Median	5.69	5.17	
N	7	1	
Histogram	Sparse normal	Undefined	1
C_v(%)	6.0	--	
Aldrin			
Median	5.66	4.79	
N	3	4	
Histogram	Uniform	Uniform	2
C_v(%)	18.3	26.3	
Dieldrin			
Median	4.95	3.81	
N	2	2	
Histogram	Undefined	Undefined	1
C_v(%)	35.9	10.9	
Heptachlor			
Median	4.48	4.00	
N	3	1	
Histogram	Uniform	Undefined	1
C_v(%)	15.5	--	

TABLE B.4 (Continued)

Compound	Log K_{ow}	Log K_{oc}	Pairs
Endrin			
Median	4.48	3.55	
N	6	2	
Histogram	Sparse normal	Undefined	1
C_v(%)	21.4	13.0	
Chlordane			
Median	3.32	5.15	
N	3	1	
Histogram	Uniform	Undefined	1
C_v(%)	37.0	--	
Toxaphene			
Median	3.27	3.00	
N	2	1	
Histogram	Undefined	Undefined	1
C_v(%)	1.52	--	

N is the number of observations.
C_v is the coefficient of variance.

extreme values and the limited number of observations available for most of the chemicals, the median, above and below which half of the observed values lie, is a better summary statistic than the mean.

The C_v uses two statistics that are only relevant in the context of a normal distribution. For purposes of comparison, an alternative, nonparametric analog to the C_v was also examined. This alternative nonparametric C_v value is the difference between the first and third quartile value divided by the median value, multiplied by 100. The denominator represents the nonparametric analog to the mean. The numerator represents the absolute range in variable values which includes the mid-lying 50 percent of the observations and serves as the nonparametric analog to the dispersion of a normal distribution, i.e., standard deviation. Differences between the parametric and nonparametric estimates of the coefficient of variation were found to be negligible. The parametric estimate is presented in the tables because it is the more commonly used statistic.

The limited number of K_{ow} and K_{oc} measures constrained the investigation of the distributional structures to three and four chemicals, respectively. The chemicals are benzo(a)pyrene, napthalene, and DDT for K_{ow}; and dibenzo(a,h)anthracene, pyrene, arochlor 1254 and DDT for K_{oc}.

K_{ow}

As discussed in Section 1.2 of the main report, any reported K_{ow} measure carries with it the true value of the coefficient, any laboratory bias in the estimate of the true value, and analytical error. The extent to which laboratory bias affected tne reported values is of particular interest for those chemicals for which only a single laboratory's measurements are available. The following discussion focuses on this factor as it appears to affect the distribution of K_{ow} measurements, for those chemicals for which more than ten measurements are available.

- Twenty four measurements, determined by seven different analytical laboratories, are available for the high weight PAH benzo(a)pyrene. Figure B.1 shows the frequency distribution (histogram) for the available data. Mallon and Harrison (1984) determined 18 of the data entries; the remaining six were results from six other laboratories. In Figure B.1 the Mallon results are coded with an 'M' and the other laboratories' results are coded with an 'O'. Numerical values indicate multiple data points, the value corresponding to the number of points. The plot suggests that anomalously high K_{ow} values were reported by some of the laboratories; specifically, MacKay et al. (1980), Rapport and Eisenreich (1984), and Rapport and Eisenreich (op. cit., 1984). Data from the other three laboratories fall well within the range of benzo(a)pyrene measures reported by MacKay et al. (1980).

- The frequency distribution of the 20 measured K_{ow} values for naphthalene is presented in Figure B.2. While the data are sparse, there appear to be two peaks in the distribution (at log K_{ow} of 3.36 and 3.44). The figure also indicates that nine of the values are from a single laboratory, Garst and Wilson (1984), coded with a "G" while the remaining 11 values are from 11 individual laboratories coded with an "O." The Garst results span the entire range of observed naphthalene K_{ow} values, and the peak in the distribution at 3.44 is due primarily to Garst's observations while the peak at 3.36 represents the data from the other laboratories.

- The 17 measurements of DDT K_{ow} values represent results from 15 individual laboratories. Figure B.3 which exhibits the frequency distribution of DDT K_{ow} measurements indicates that the data follow a normal distribution.

Examination of the K_{ow} data for the three chemicals for which an adequate number of K_{ow} measurements are available indicates that inter-laboratory variability is substantial. Although the distribution of observations is relatively uniform among analytical laboratories, the distribution of K_{ow} values appears to approximate a normal distribution.

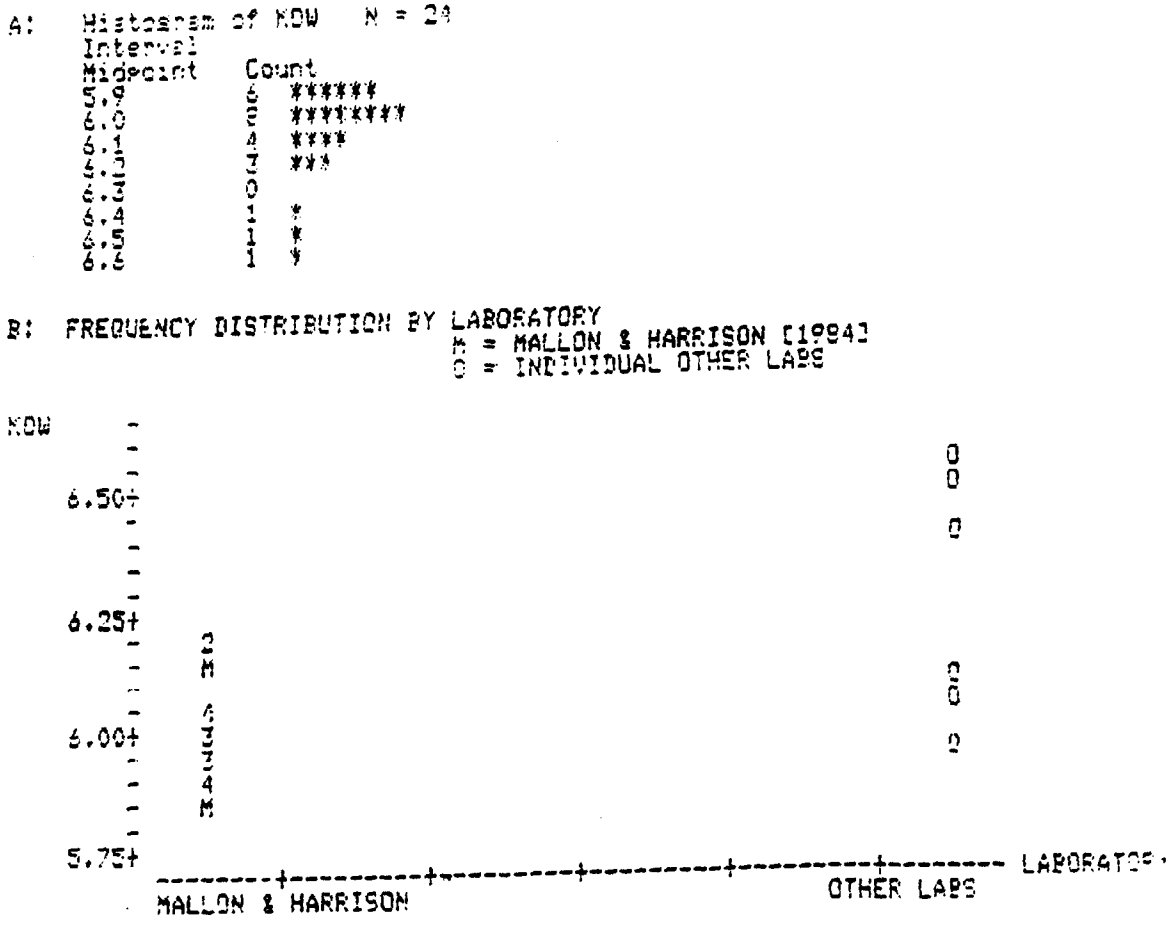


FIGURE B.1 Benzo(a)pyrene K_{ow} Data: Frequency Distribution.

A: Histogram of KOW N = 20

Interval Midpoint	Count	
3.26	1	*
3.28	0	
3.30	2	**
3.32	1	*
3.34	0	
3.36	5	*****
3.38	3	***
3.40	1	*
3.42	0	
3.44	4	****
3.46	2	**
3.48	1	*

B: FREQUENCY DISTRIBUTION BY LABORATORY
G = GARST & WILSON [1984]
O = INDIVIDUAL OTHER LABS

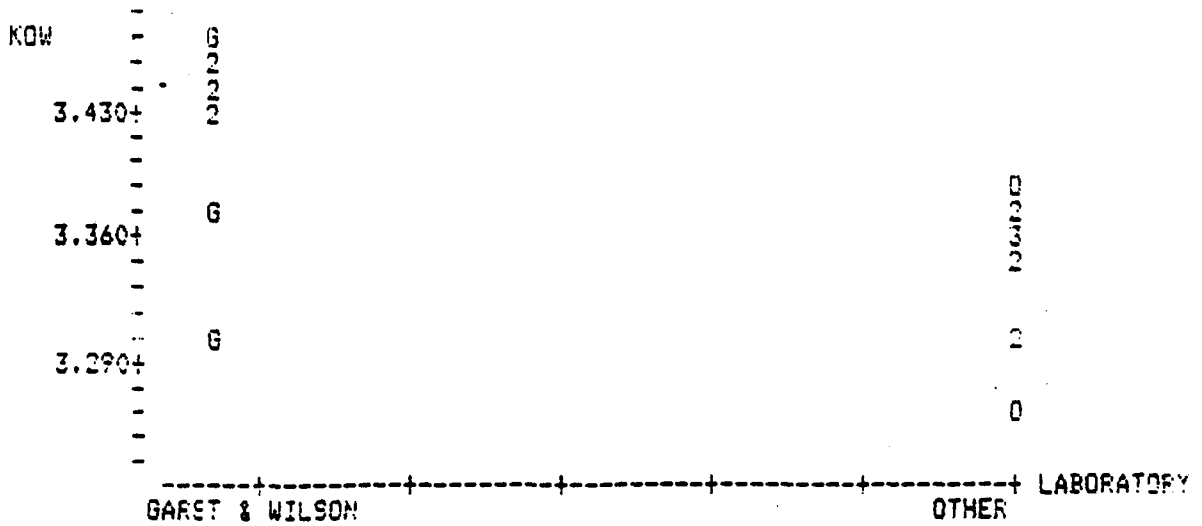


FIGURE B.2 Napthalene K_{OW} Data: Frequency Distribution.

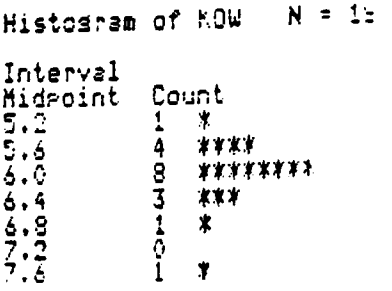


FIGURE B.3 DDT K_{OW} Data: Frequency Distribution.

These results are based on a very limited number of data points (maximum 24) and chemicals (3) and are therefore tentative.. Further data are required to validate these results for all the chemicals evaluated in this report.

K_{OC}

As discussed in Section 1.2 of the main report, K_{OC} measurements include analytical error and potential bias; additionally, they reflect the role of inter-laboratory variability in K_{OC} measurements for chemicals. The effect of inter-laboratory variability will be evaluated for the four chemicals with greater than ten measurements of K_{OC}.

- Of the 15 K_{OC} values reported for dibenzo(a,h)anthracene, 14 of the measures are from Means et al. (1980) and one value is from Versar (1984). The frequency distribution for the data is shown in Figure B.4. The data do not appear to follow a normal distribution--rather, they exhibit either a bimodal distribution or a tendency to be skewed to the right. The figure also indicates that Versar's single result lies at the low end of the 14 measures made by Means et al.

- The 31 reported values for the K_{OC} of pyrene represent 17 values from Karickhoff and coworkers (1979, 1981, 1985) coded with a "K" and 14 values from Means et al. (1980) coded with an "M." The frequency distribution shown in Figure B.5 exhibits a highly right-skewed and/or bimodal distribution of the observed values.

- The measurements of Arochlor 1254 K_{OC} represent 14 observations from a single laboratory, Weber et al. (1983). These values indicate only replication (or analytical) error and cannot exhibit any effects due to inter-laboratory differences. The data as presented in Figure B.6 exhibit a near-normal distribution.

- The 14 values for the DDT K_{OC} represent data from eight laboratories: six values from Gerstl and Mingelgrin (1984), and with the remaining eight values from the seven other laboratories.

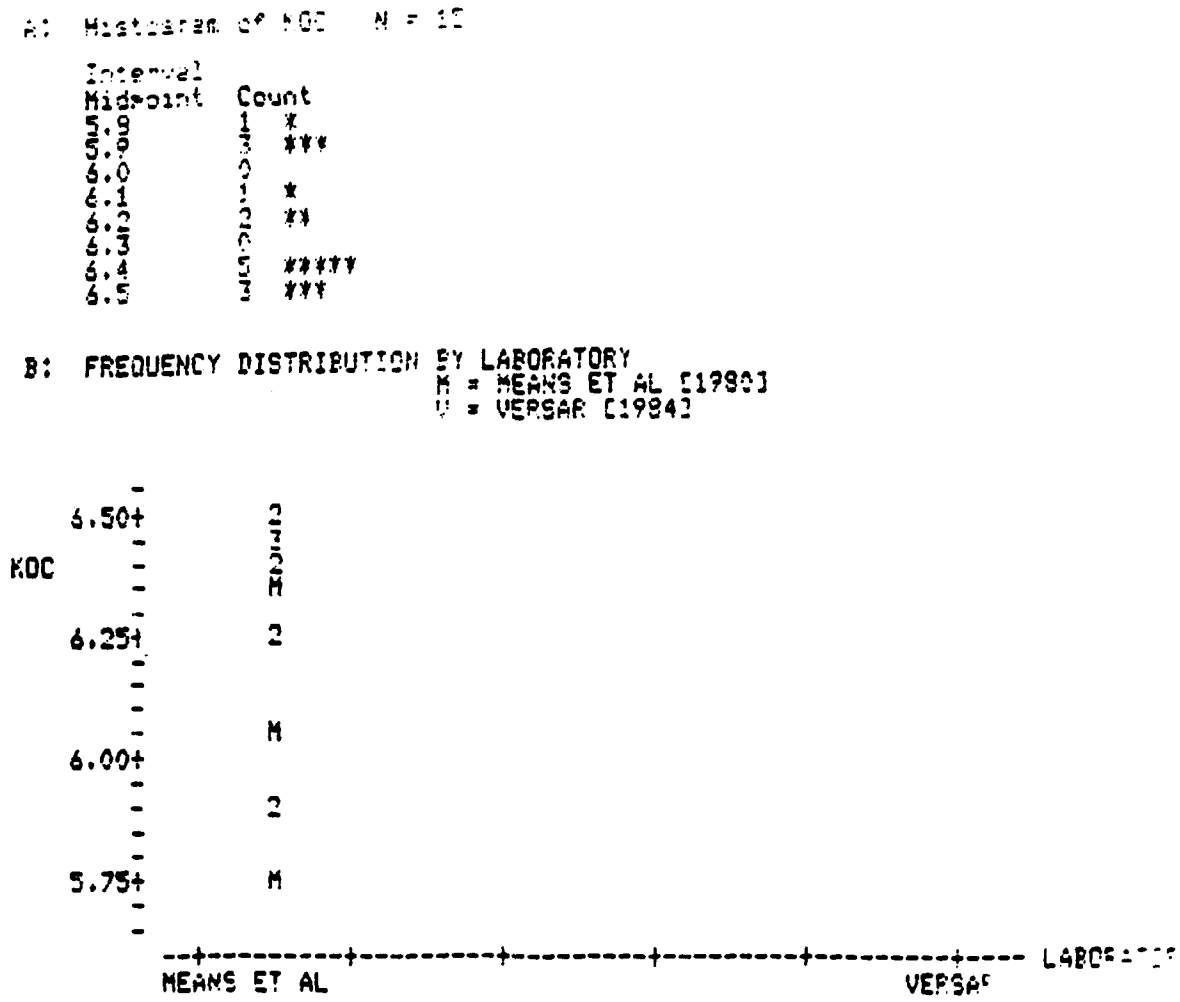


FIGURE B.4 Dibenzo(a,h)anthracene K_{oc} Data: Frequency Distribution.

A: Histogram of KOC N = 31

Interval Midpoint	Count	
4.0	1	*
4.1	0	
4.2	0	
4.3	0	
4.4	0	
4.5	1	*
4.6	1	*
4.7	3	***
4.8	8	********
4.9	5	*****
5.0	2	**
5.1	10	**********

B: FREQUENCY DISTRIBUTION BY LAB
K = KARICKHOFF ET AL [1979,1981,1985]
M = MEANS ET AL [1990]

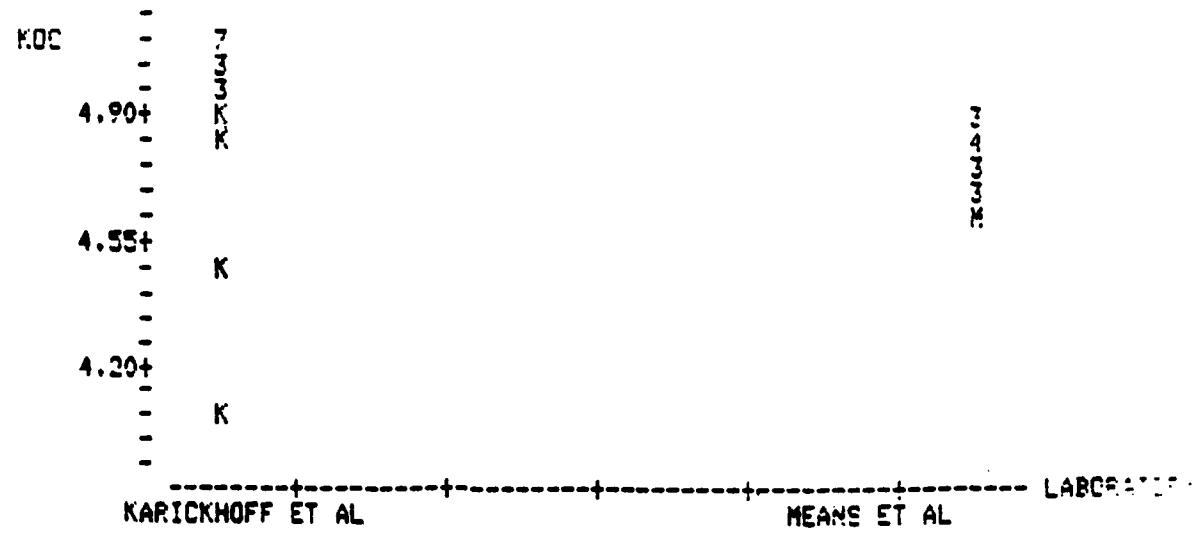


FIGURE B.5 Pyrene K_{oc} Data: Frequency Distribution.

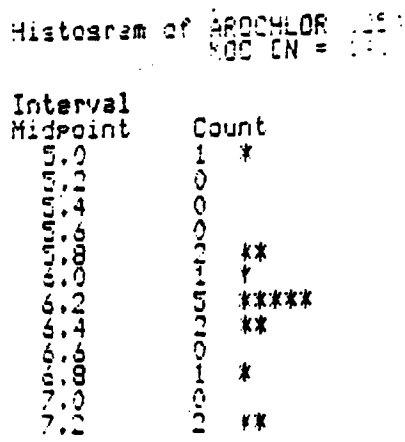


FIGURE B.6 Arochlor 1254 K_{oc} Data: Frequency Distribution.

A: Histogram of KOC N = 14

Interval Midpoint	Count	
4.6	1	*
4.8	0	
5.0	0	
5.2	2	**
5.4	4	****
5.6	1	*
5.8	3	***
6.0	1	*
6.2	1	*
6.4	0	
6.6	1	*

B: FREQUENCY DISTRIBUTION BY LABORATORY
G = GERSTL & MINGELGRIN [1984]
O = OTHER INDIVIDUAL LAB

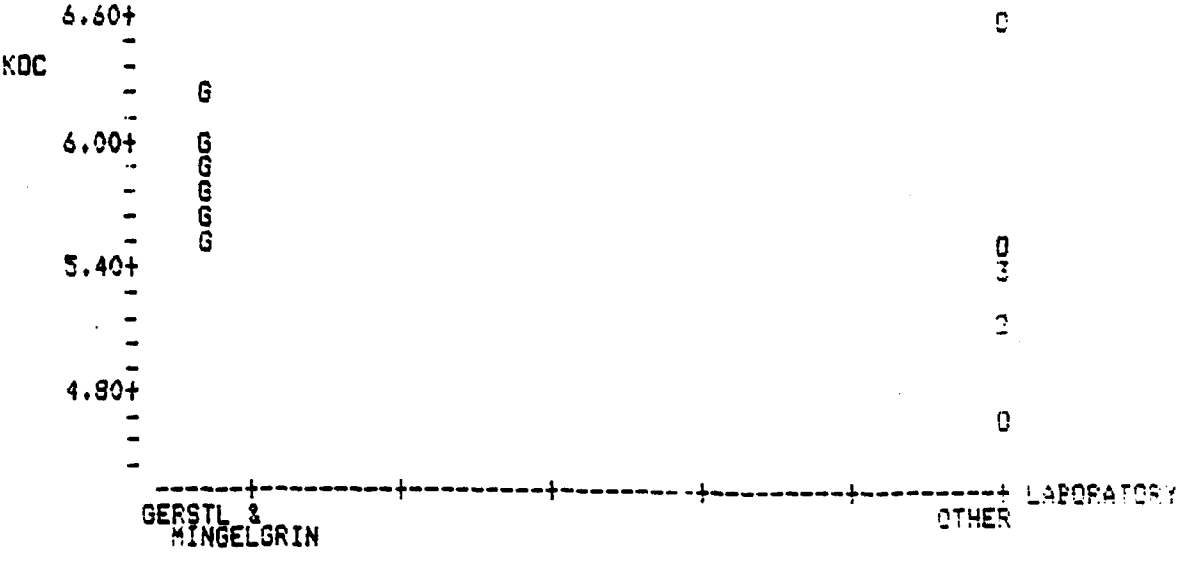


FIGURE B.7 DDT K_{OC} Data: Frequency Distribution.

The data exhibit a fairly normal distribution (Figure B.7) and, as expected, the range of K_{OC} values from the seven other laboratories is wider than that exhibited by the six observations from Gerstl and Mingelgrin (1984).

The K_{OC} data indicate that different laboratories give different estimates of the K_{OC} for a given compound. Whether these differences can be attributed to inter-laboratory differences or natural variability of the sediments sampled cannot be determined from the available data. However, the distribution of K_{OC} values tends to a more normal distribution as the number of laboratories that measured the K_{OC} increases and/or balances in contribution. As with the K_{OW} data, these results must be considered tentative because they are based on a limited number of data points. Further data are required to validate these results for all the chemicals in this report.

B.2 REFERENCES

Action, F. S. 1966. Analysis of straight line data. John Wiley and Sons, Inc. New York, New York.

Draper, N. R., and H. Smith. 1981. Applied regression analysis. John Wiley and Sons, Inc. New York, New York.

Garst, J. E., and W. C. Wilson. 1984. Acute, wide-range, automated, high performance liquid chromatographic method for the estimation of octanol/water partition coefficients I: Effect of chromatographic conditions and procedure variables on accuracy and reproducibility of the method. J. Pharm. Sci. 73(11):1616-1623.

Gerstl, Z., and U. Minglegrin. 1984. Sorption of organic substances by soils and sediments. J. Environ. Sci. Health 319(3):297-312.

Kadeg, R. D., S. P. Pavlou and A. S. Duxbury. 1986. Elaboration of sediment normalization theory for nonpolar hydrophobic organic chemicals. Envirosphere Company, Bellevue, Washington.

Karickhoff, S. W. 1981. Semi-empirical estimation of sorption of hydrophobic pollutants on natural sediments and soils. Chemosphere 10(8):833-846.

Karickhoff, S. W., and D. S. Brown. 1979. Determination of octanol/water distribution coefficients, water solubilities, and sediment/water partition coefficients for hydrophobic organic pollutants. EPA-600/4-79-032, National Technical Information Service, Springfield, Virginia.

Karickhoff, S. W., D. S. Brown and T. A. Scott. 1979. Sorption of hydrophobic pollutants on natural sediments. Water Res. 13:241-248.

Karickhoff, S. W., and K. R. Morris. 1985. Sorption dynamics of hydrophobic pollutants in sediment suspensions. Environ. Tox. Chem. 4:469-479.

Mackay, D., A. Bobra and W. Y. Shiu. 1980. Relationships between aqueous solubility and octanol-water partition coefficients. Chemosphere 9:701-711.

Mallon, B. J. and F. L. Harrison. 1984. Octanol-water partition coefficient of benzo(a)pyrene: measurement, calculation and environmental implications. Bull. Environ. Contam. Toxicol. 32:316-323.

Means, J. C., S. G. Wood, J. J. Hassett and W. L. Banwart. 1980. Sorption of polynuclear aromatic hydrocarbons by sediments and soils. Environ. Sci. Technol. 14(2):1524-1528.

Rapport, R. A. and S. J. Eisenreich. 1984. Chromatographic Determination of Octanol-Water Partition Coefficients for 58 Polychlorinated Biphenyl Congeners. Environ. Sci. Technol. 18(3):163-170.

Versar, Inc. 1984. Chemical and toxicological review of priority contaminants in nearshore tideflats and deepwater of Commencement Bay, Washington. Draft final report: Versar Inc., Springfield, Virginia.

Weber, W. J., Jr., T. C. Voice, Massoud-Pirbazari, G. E. Hunt and D. M Ulanoff. 1983. Sorption of hydrophobic compounds by sediments, soils and suspended soils - II. Water Res. 17(10):1443-1452.

APPENDIX C

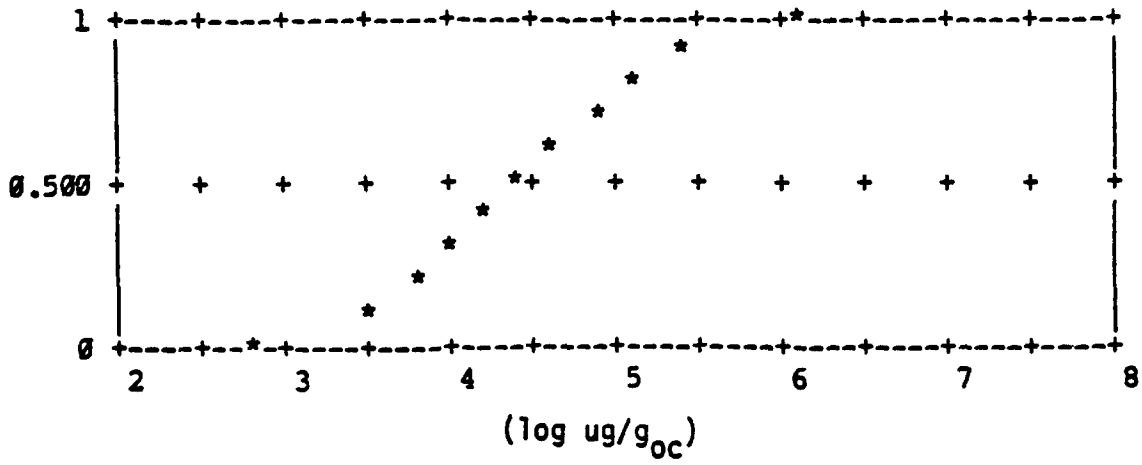
CUMULATIVE PROBABILITY DISTRIBUTION PLOTS

FIGURES

FIGURES (Continued)

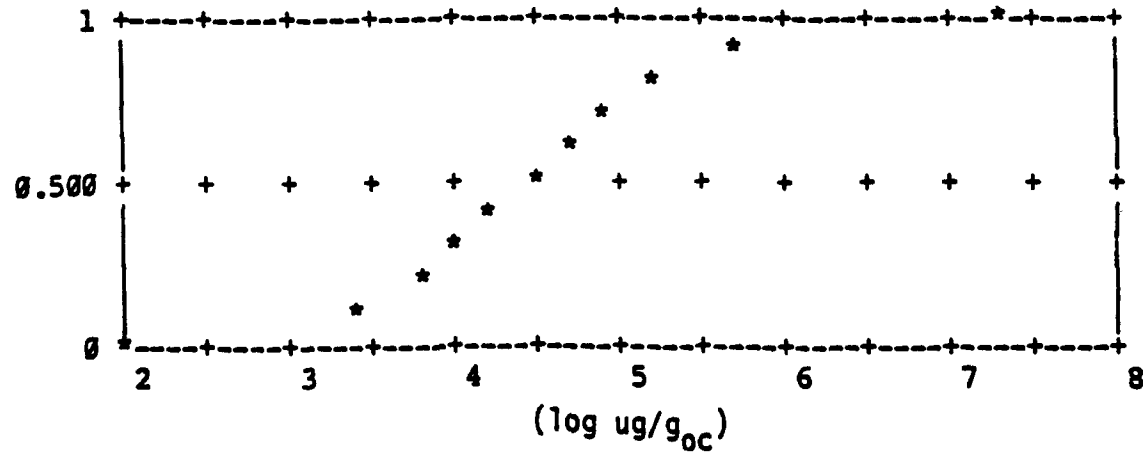
BENZO(A)ANTHRACENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	2.898	791
0.05	3.234	1,710
0.5	4.446	27,900

B

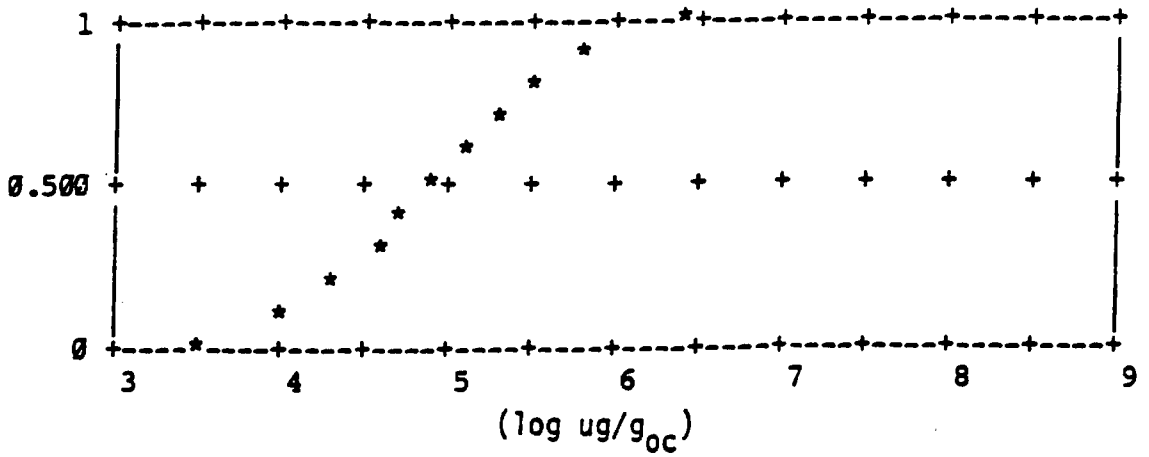


Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	2.213	163
0.05	3.314	2,060
0.5	4.461	28,900

FIGURES C.1A and C.1B Cumulative Probability Distribution Plots of Chronic Criteria Values for Benzo(a) anthracene for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

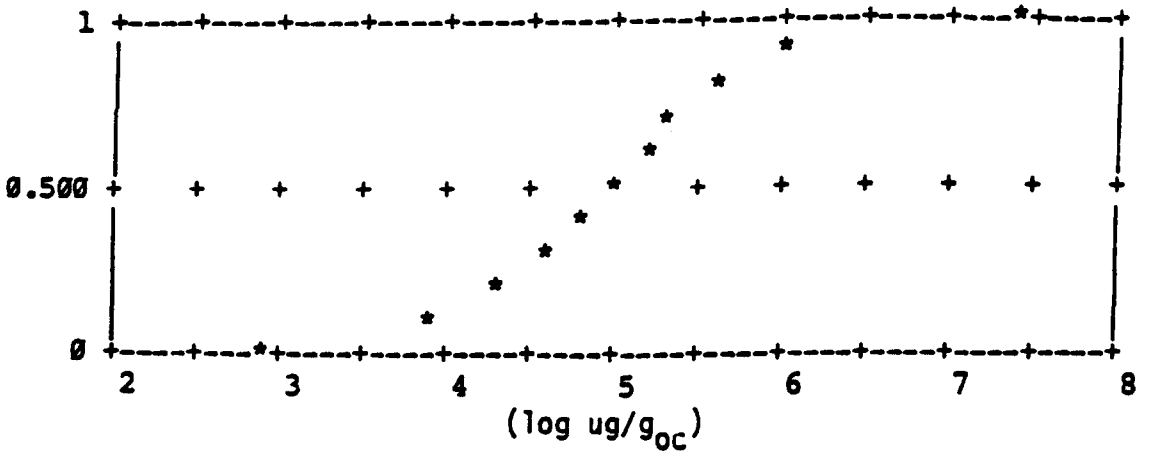
BENZO (A) PYRENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	3.539	3,460
0.05	3.840	6,920
0.5	4.926	84,300

B

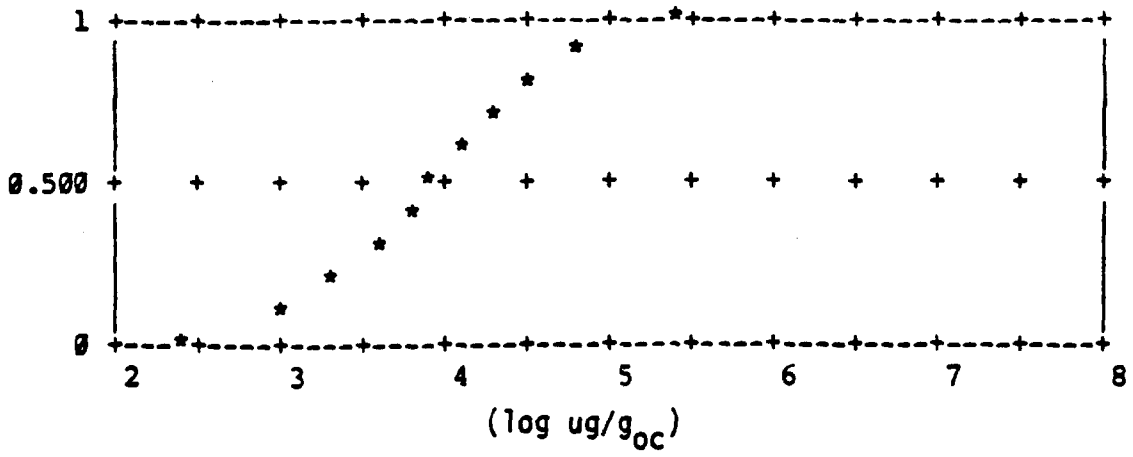


Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	3.259	1,820
0.05	3.648	4,450
0.5	4.996	99,100

FIGURES 4.2A and 4.2B Cumulative Probability Distribution Plots of Chronic Criteria Values for Benzo(a)pyrene for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

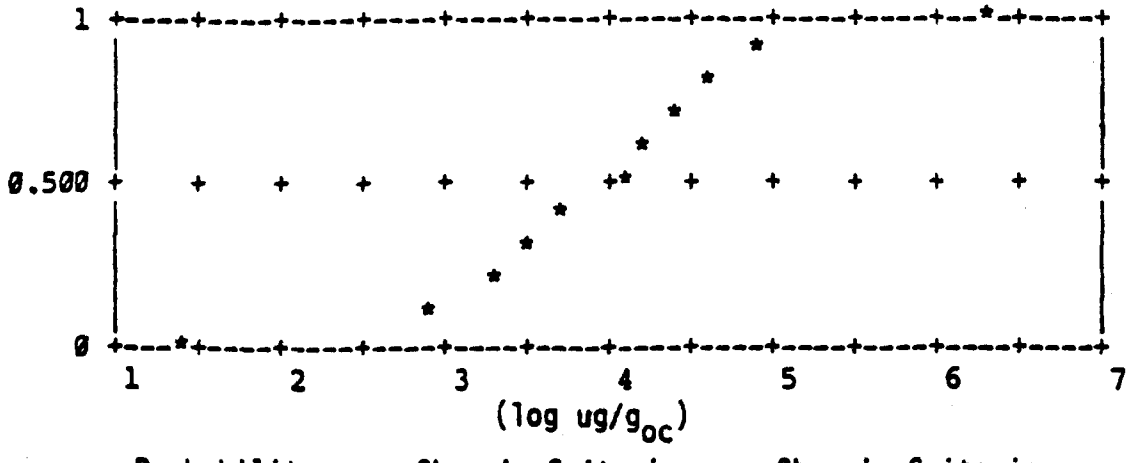
CHRYSENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	2.525	335
0.05	2.834	682
0.5	3.946	8,830

B

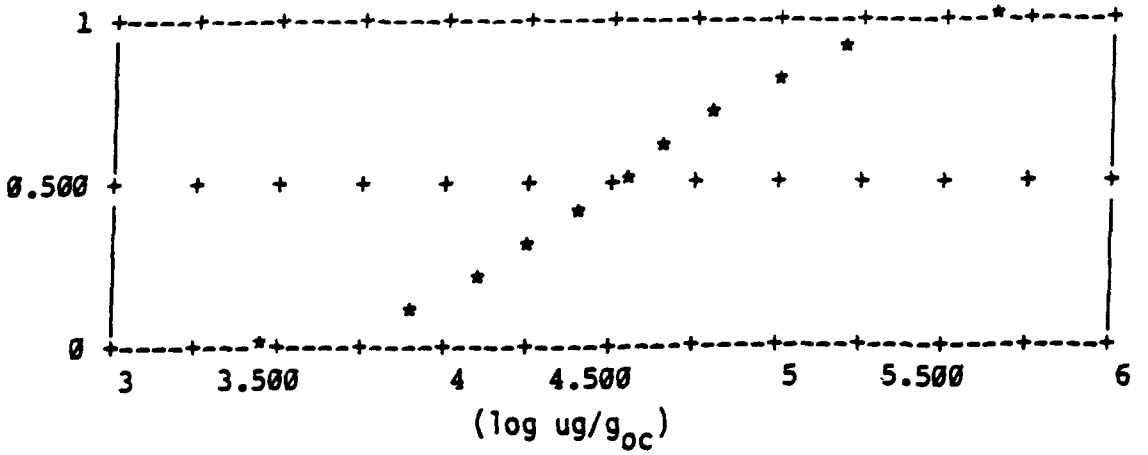


Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	2.084	121
0.05	2.647	444
0.5	3.975	9,440

FIGURES C.3A and C.3B Cumulative Probability Distribution Plots of Chronic Criteria Values for Chrysene for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

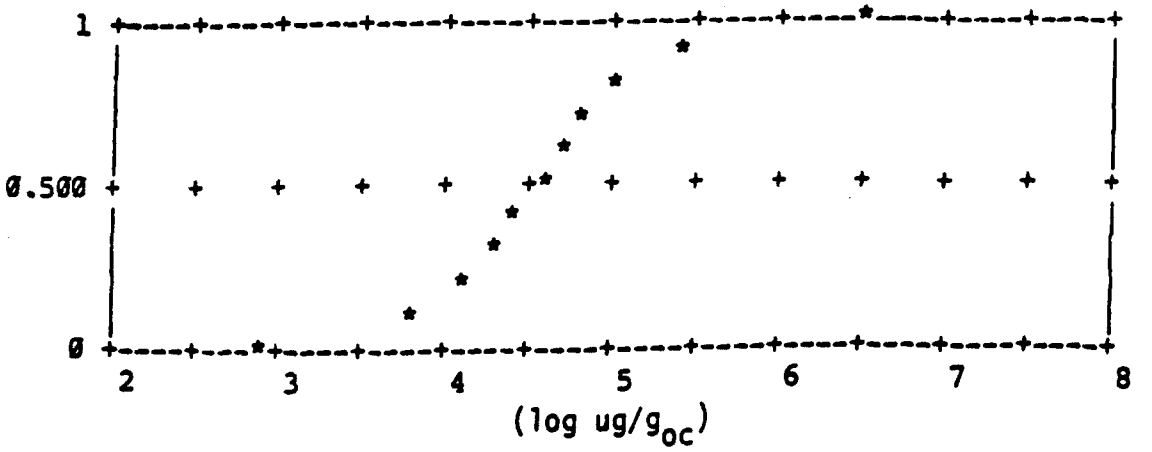
DIBENZO(A,H)ANTHRACENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	3.494	3,120
0.05	3.720	5,250
0.5	4.537	34,400

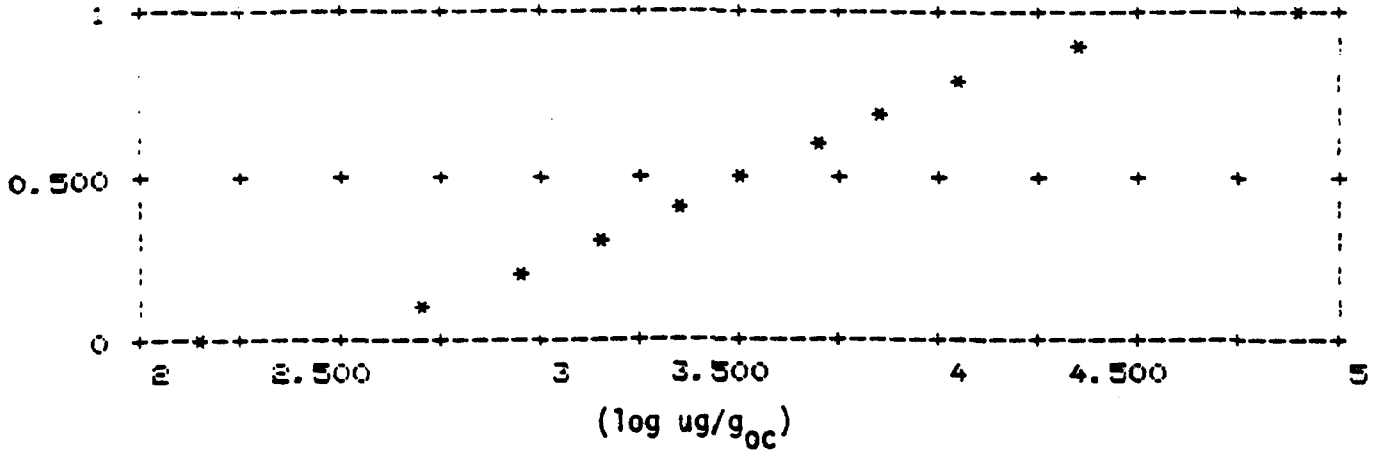
B



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	3.090	1,230
0.05	3.543	3,490
0.5	4.573	37,400

FIGURES C.4A and C.4B Cumulative Probability Distribution Plots of Chronic Criteria Values for Dibenzo(a,h)anthracene for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

FLUORANTHENE

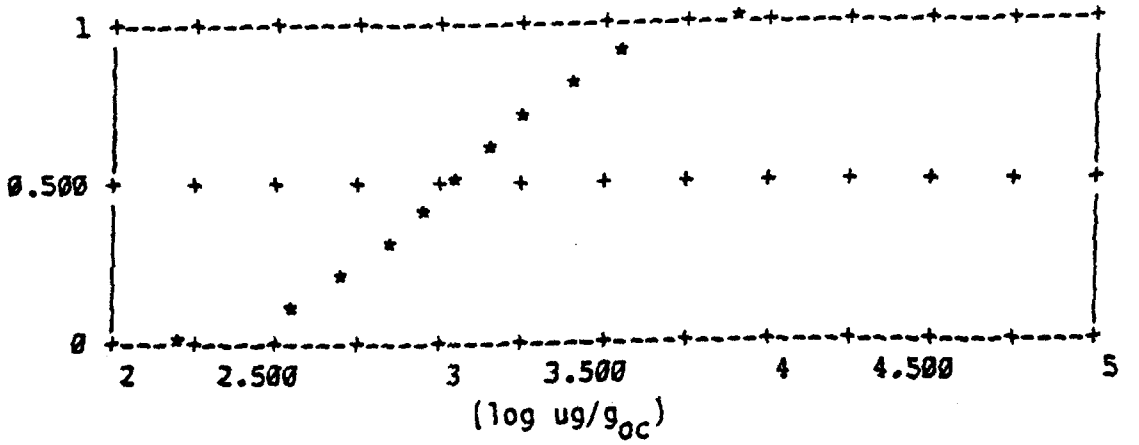


Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	2.201	159
0.05	2.486	306
0.5	3.514	3,270

FIGURE C.5 Cumulative Probability Distribution Plots of Chronic Criteria Values for Fluoranthene.

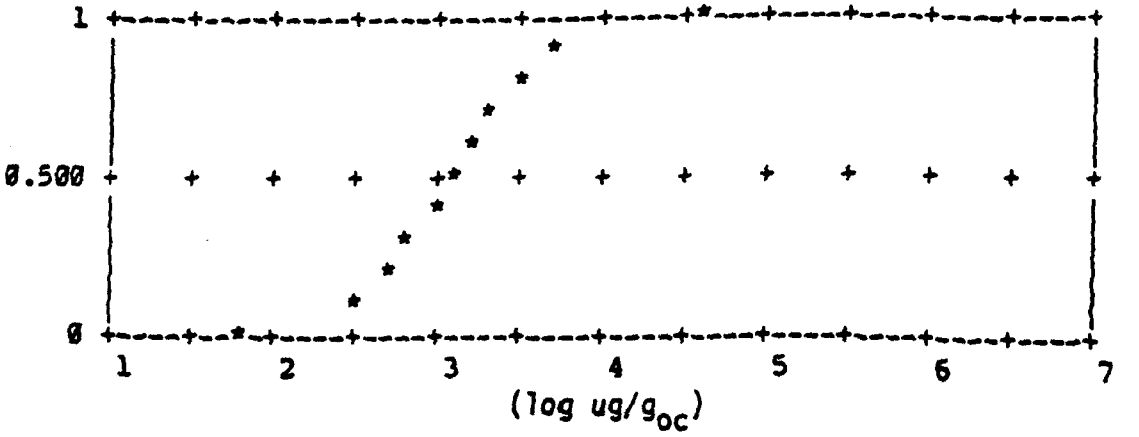
PYRENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	2.257	181
0.05	2.431	270
0.5	3.057	1,140

B

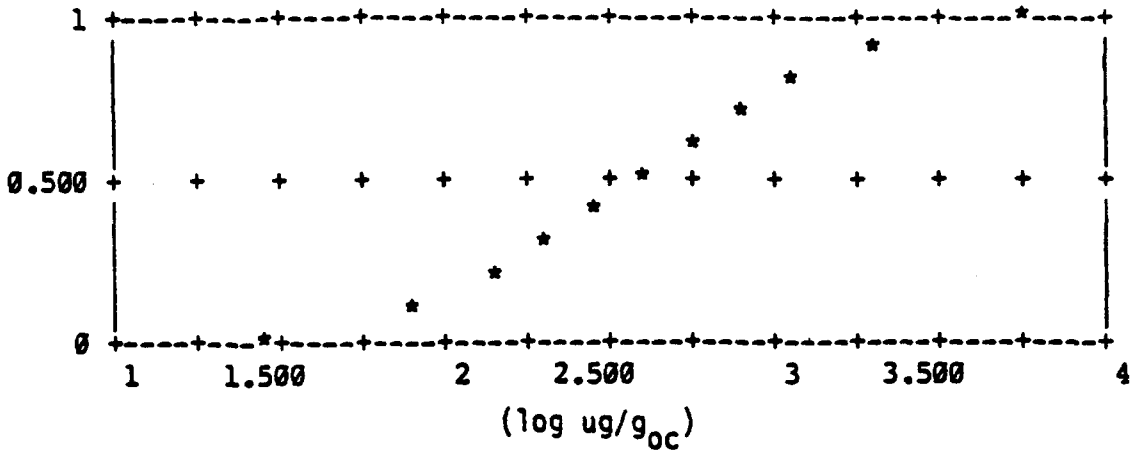


Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	1.928	84.7
0.05	2.272	187
0.5	3.078	1,200

FIGURES C.6A and C.6B *Cumulative Probability Distribution Plots of Chronic Criteria Values for Pyrene for:* (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

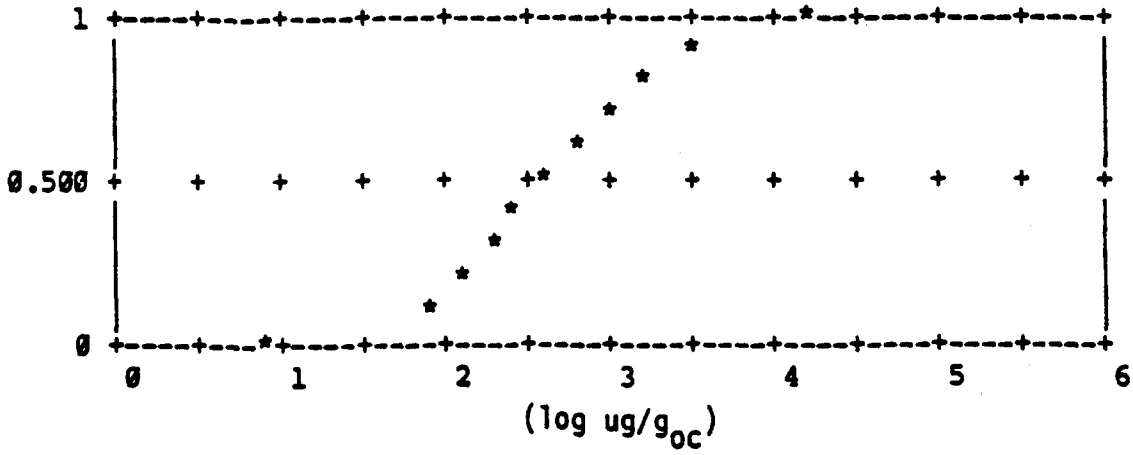
ANTHRACENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	1.508	32.2
0.05	1.744	55.5
0.5	2.597	395

B

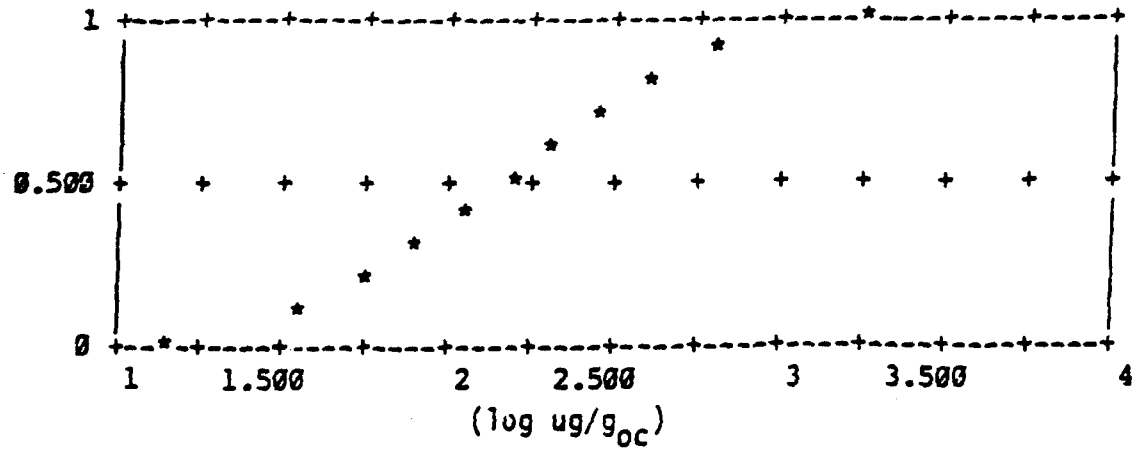


Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	1.277	18.9
0.05	1.579	37.9
0.5	2.645	442

FIGURES C.7A and C.7B Cumulative Probability Distribution Plots of Chronic Criteria Values for Anthracene for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

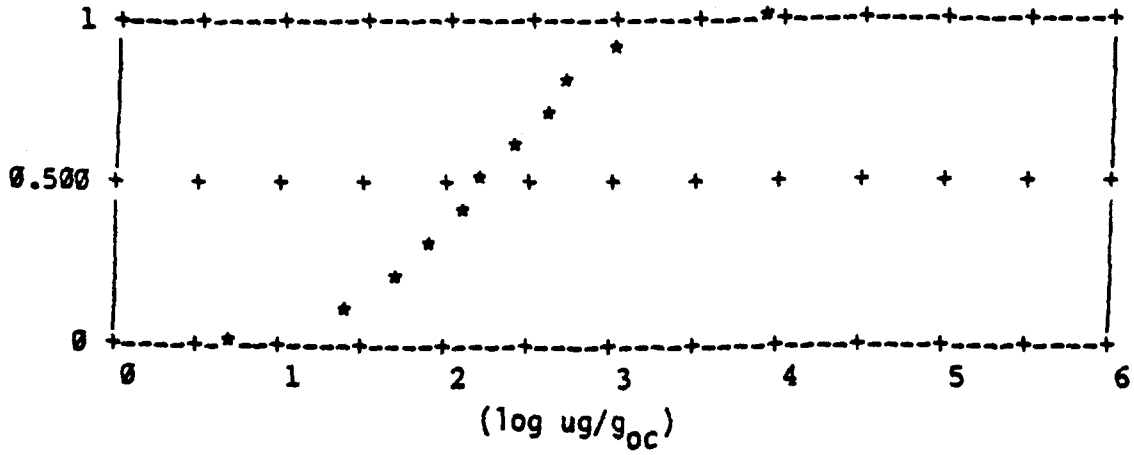
FLUORENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	1.192	15.6
0.05	1.408	25.6
0.5	2.185	153

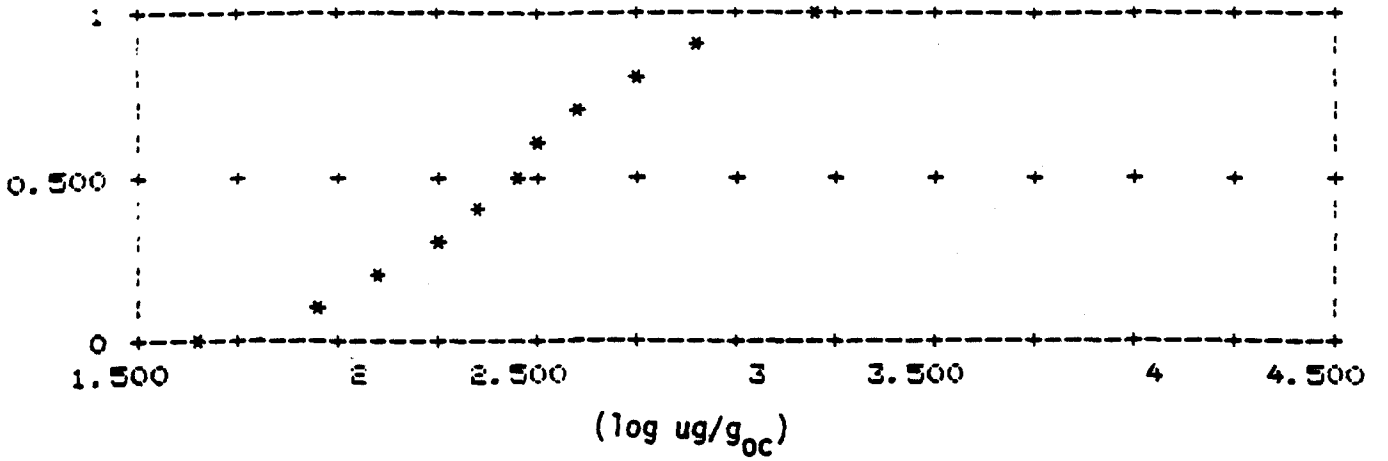
B



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	0.773	5.93
0.05	1.195	15.7
0.5	2.234	171

FIGURES C.8A and C.8B Cumulative Probability Distribution Plots of Chronic Criteria Values for Fluorene for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

NAPTHALENE

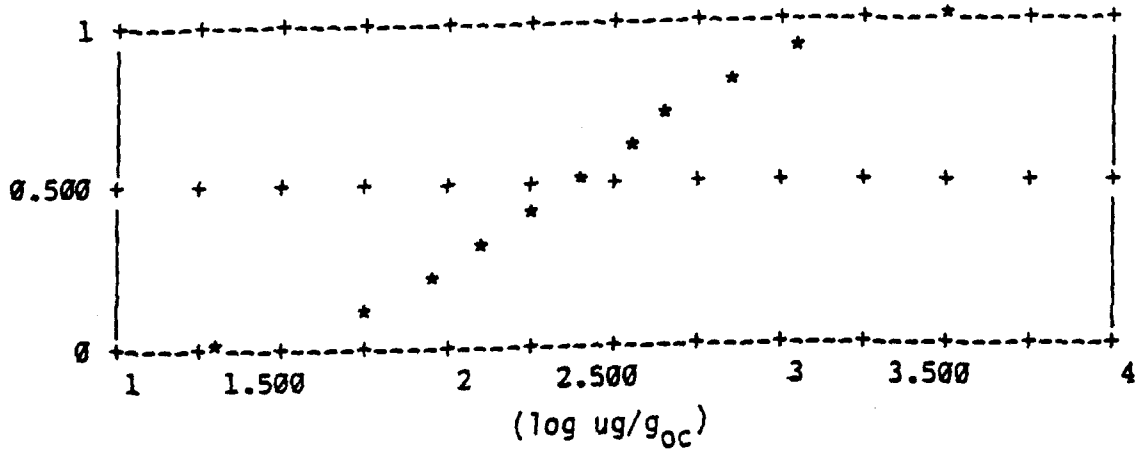


Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	1.697	49.7
0.05	1.856	71.7
0.5	2.429	268

Figure C.9 Cumulative Probability Distribution Plot of Chronic Criteria Values for Naphthalene for Fixed Acute to Chronic Toxicity Ratio of 29.

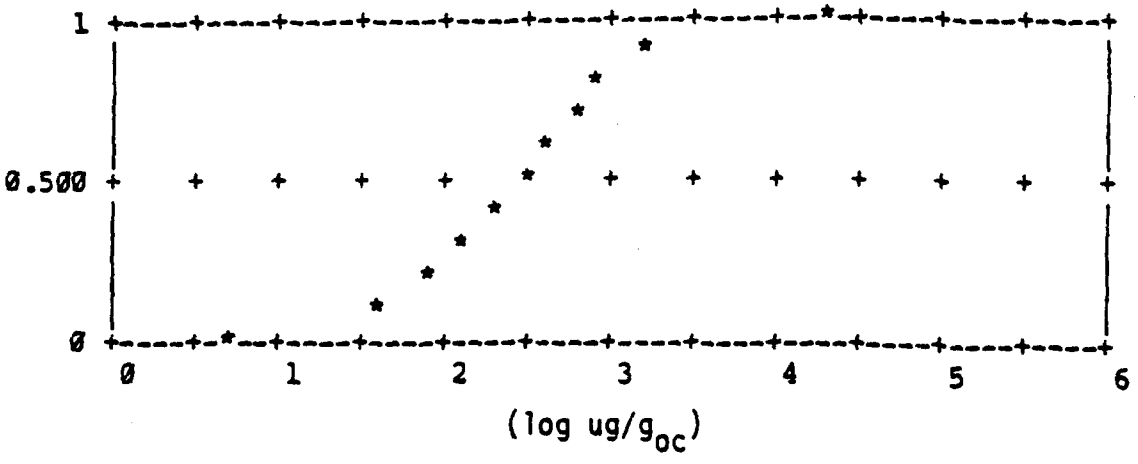
PHENANTHRENE

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	1.355	22.6
0.05	1.581	38.1
0.5	2.396	249

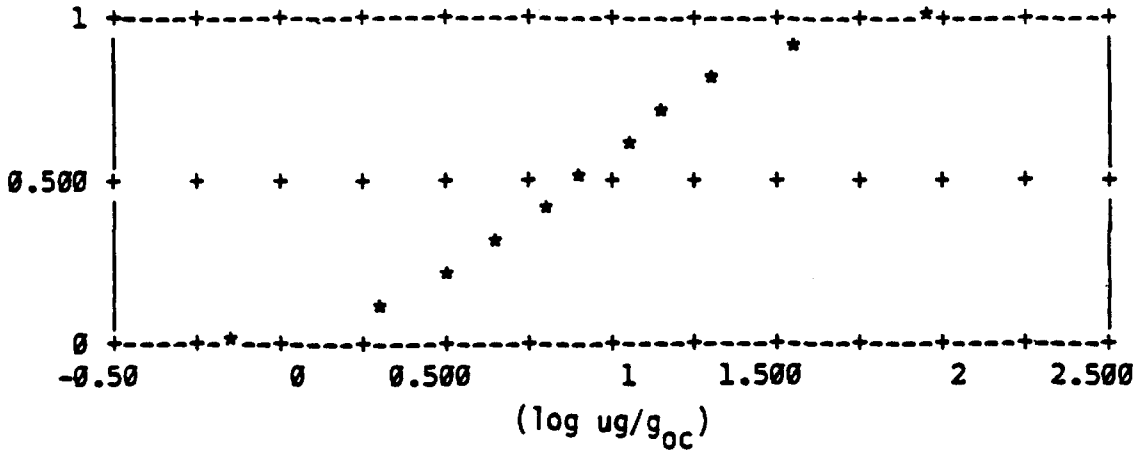
B



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	1.042	11.0
0.05	1.387	24.4
0.5	2.435	272

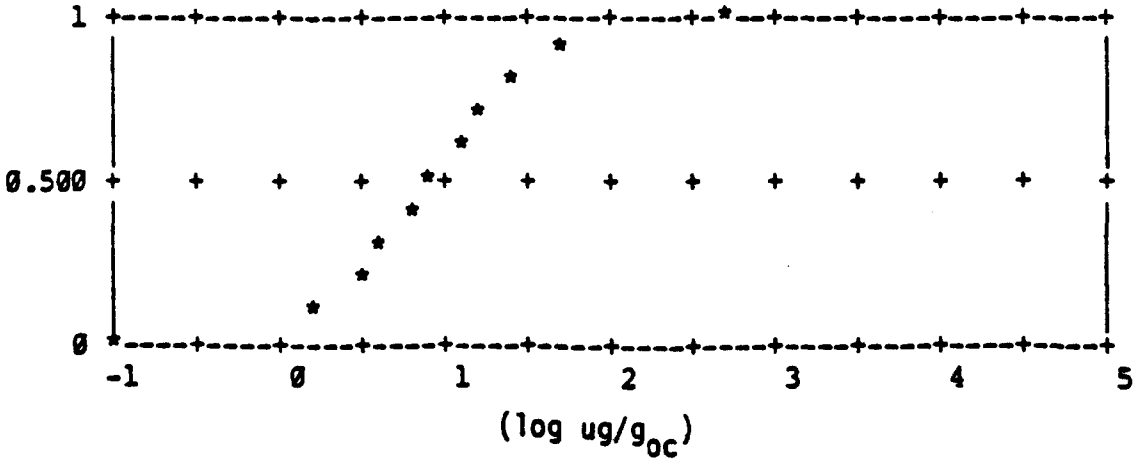
FIGURES C.10A and C.10B Cumulative Probability Distribution Plots of Chronic Criteria Values for Phenanthrene for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-0.0832	0.826
0.05	0.131	1.35
0.5	0.903	8.0

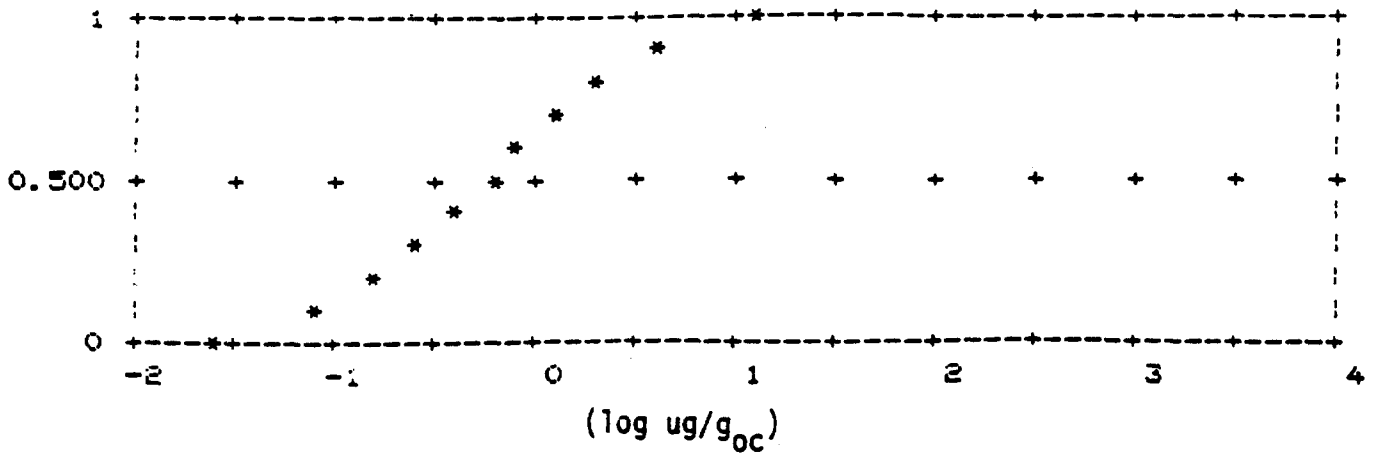
B



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-0.368	0.429
0.05	-0.074	0.843
0.5	0.932	8.55

FIGURES C.11A and C.11B Cumulative Probability Distribution Plots of Chronic Criteria Values for Aldin for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

CHLORDANE

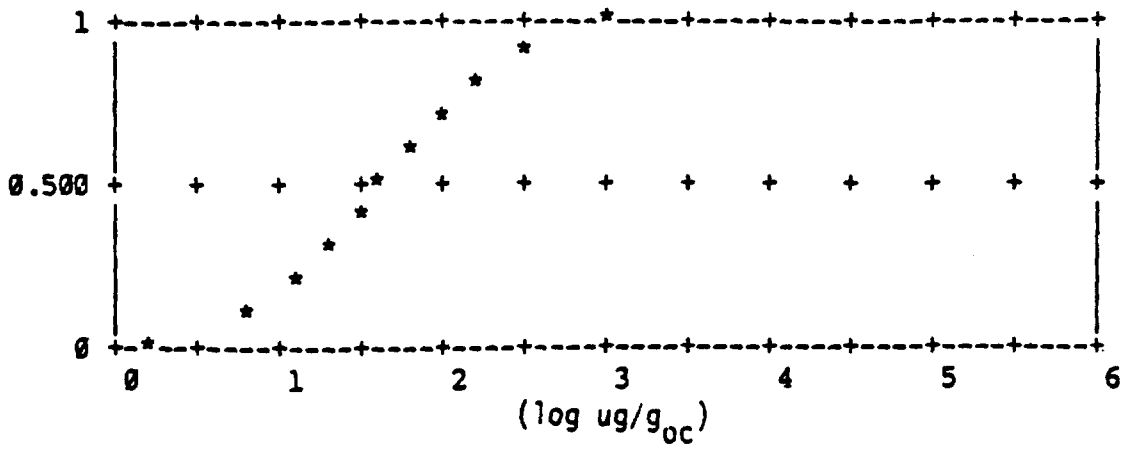


Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-1.524	0.0299
0.05	-1.247	0.0566
0.5	-0.248	0.565

FIGURES C.12 Cumulative Probability Distribution Plots of Chronic Criteria Values for Chlordane.

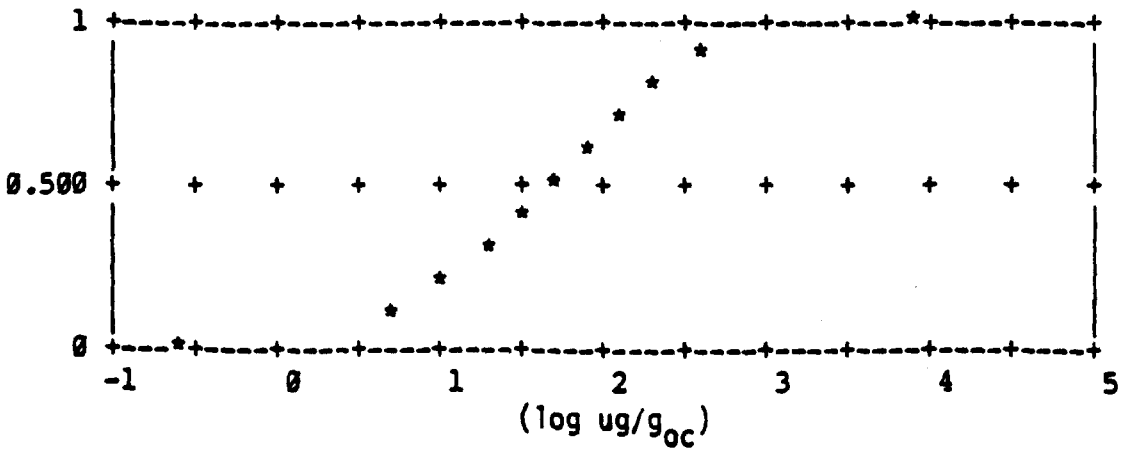
DDD

A



Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	0.305	2.02
0.05	0.594	3.93
0.5	1.636	43.3

B

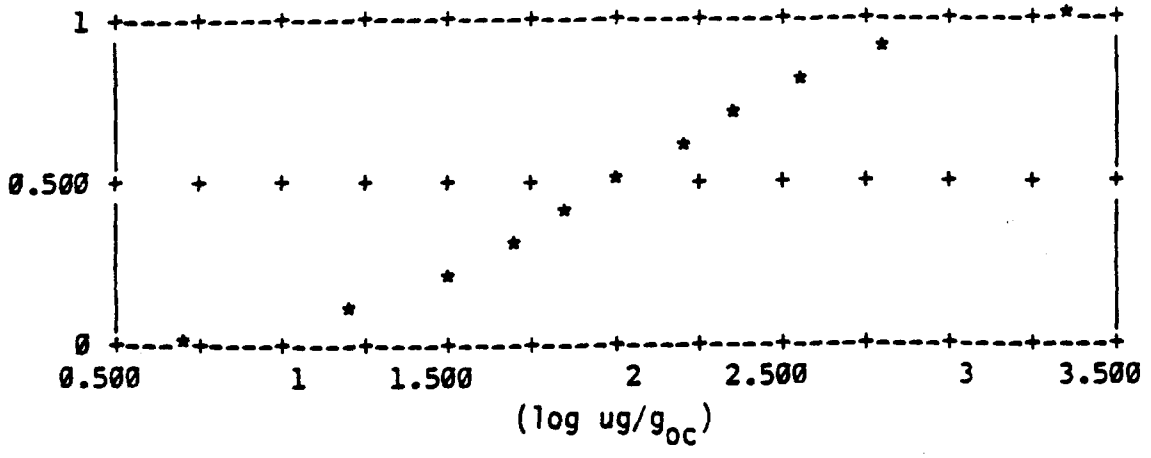


Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-0.207	0.621
0.05	0.336	2.17
0.5	1.690	49.0

FIGURES C.13A and C.13B Cumulative Probability Distribution Plots of Chronic Criteria Values for DDD for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.

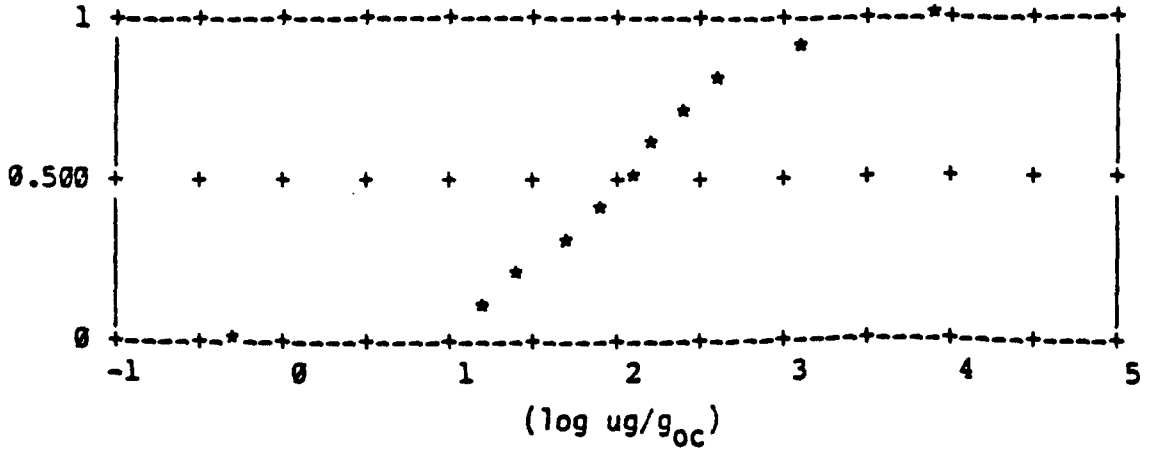
DDE

A



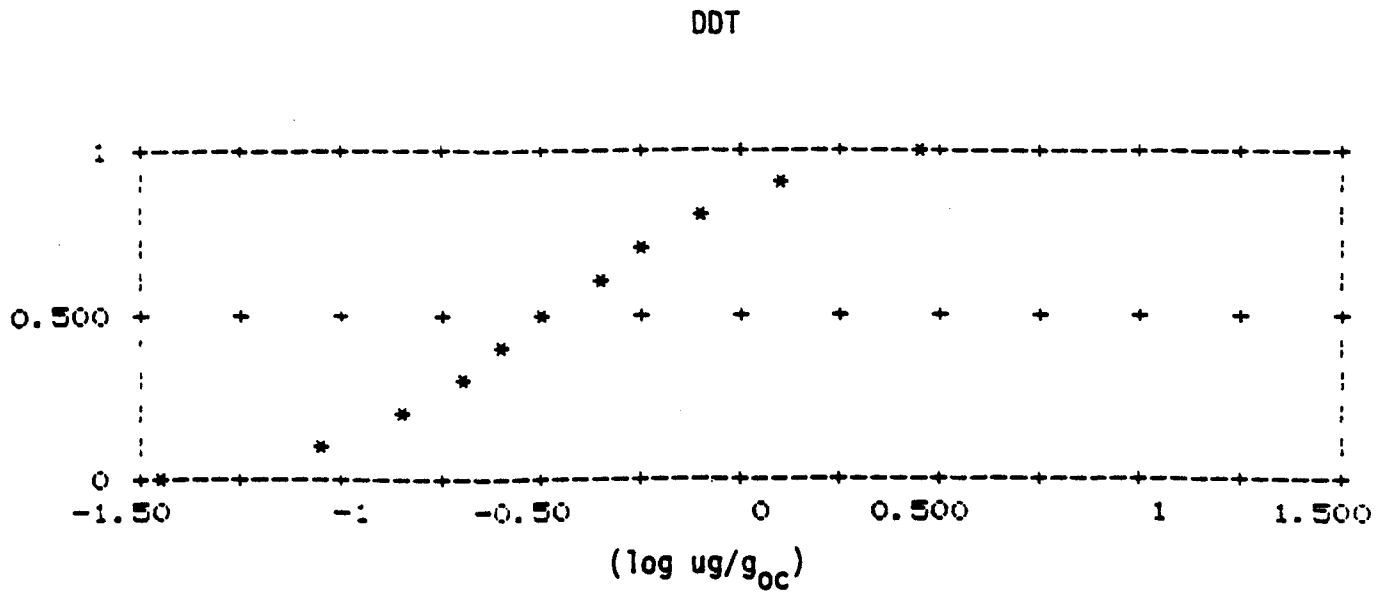
Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	0.749	5.61
0.05	1.024	10.6
0.5	2.017	104

B



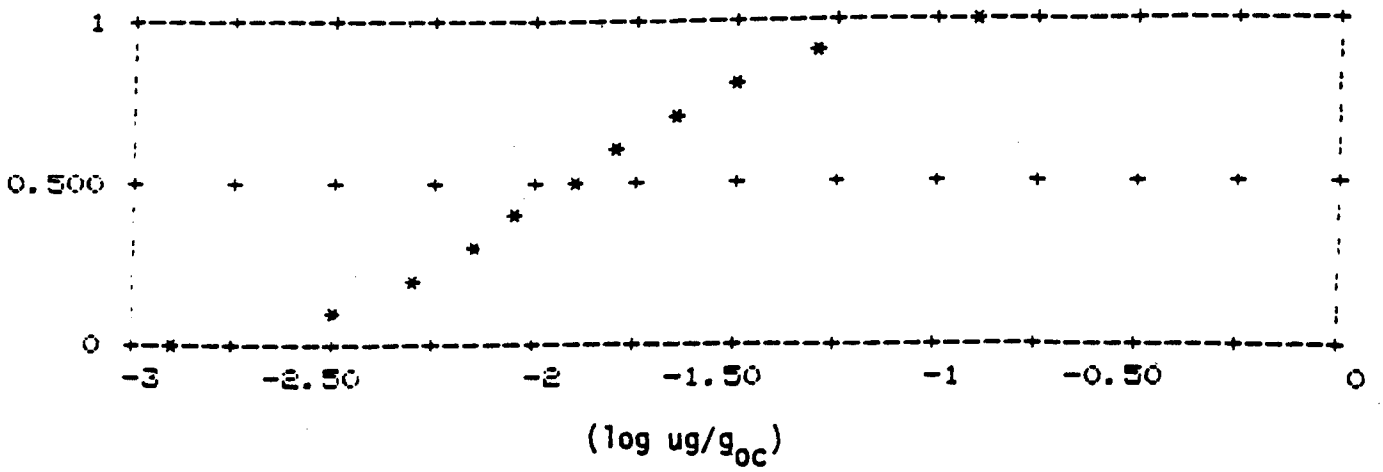
Probability Fractile	Chronic Criteria (log ug/g$_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	0.431	2.70
0.05	0.777	5.98
0.5	2.061	115

FIGURES C.14A and C.14B Cumulative Probability Distribution Plots of Chronic Criteria Values for DDE for: (A) Fixed Acute to Chronic Toxicity Ratio of 10 and (B) Uniform Distribution of Acute to Chronic Toxicity Ratio from 3 to 29.



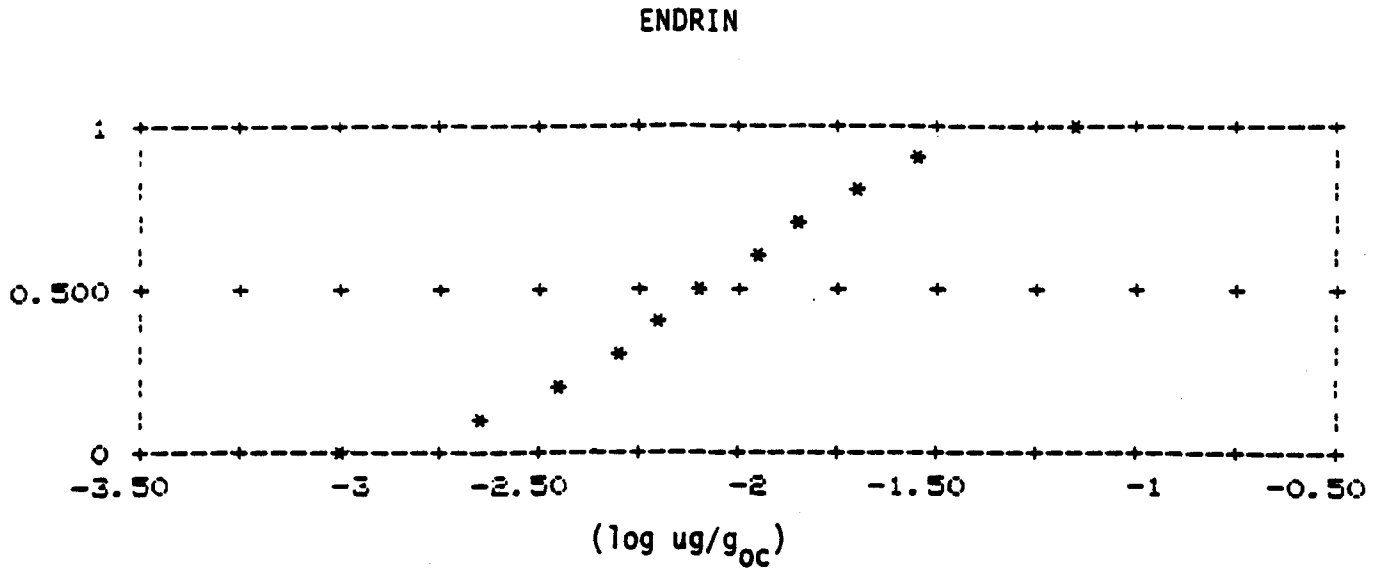
Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-1.381	0.0416
0.05	-1.185	0.0653
0.5	-0.480	0.331

FIGURE C.15 Cumulative Probability Distribution Plot of Chronic Criteria Values for DDT.



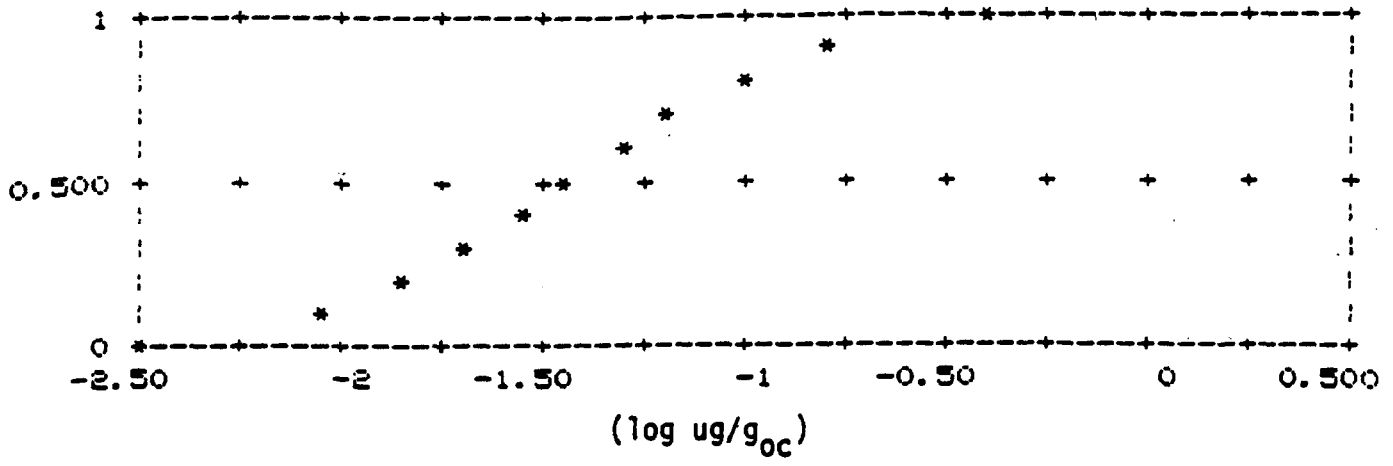
Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-2.849	0.00142
0.05	-2.646	0.00226
0.5	-1.911	0.0123

FIGURE C.16 Cumulative Probability Distribution Plot of Chronic Criteria Values for Dieldrin.



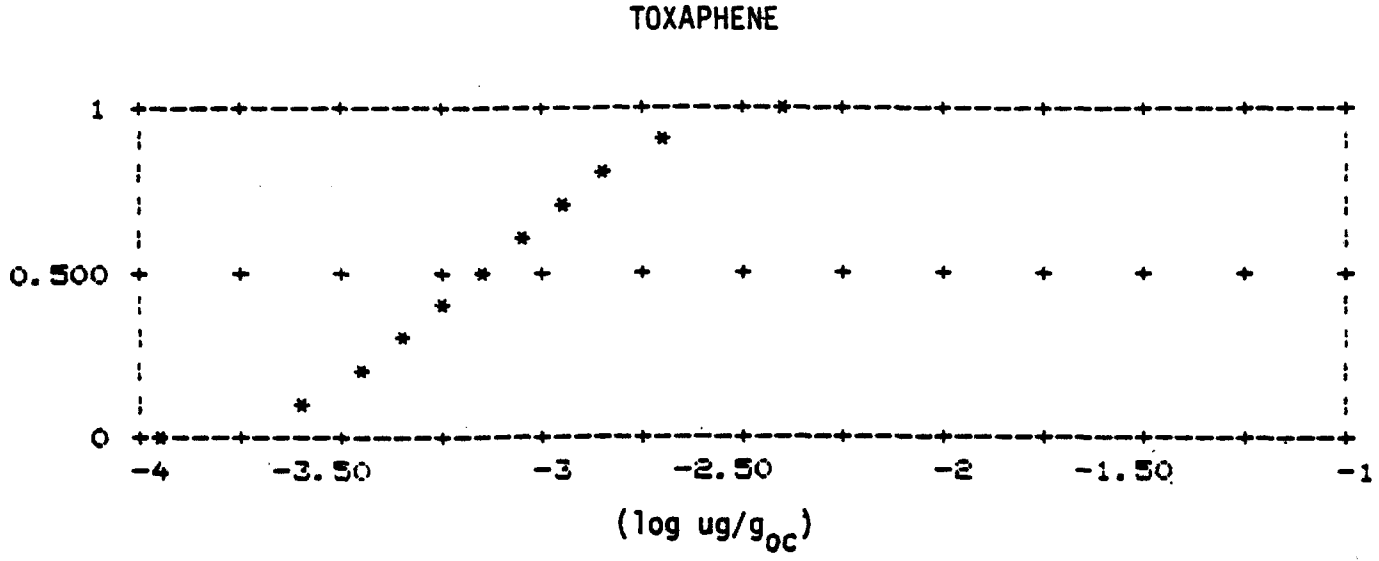
Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-2.970	0.00107
0.05	-2.779	0.00166
0.5	-2.088	0.00817

FIGURE C.17 Cumulative Probability Distribution Plot of Chronic Criteria Values for Endrin.



Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{oc}$)
0.01	-2.438	0.00365
0.05	-2.222	0.00600
0.5	-1.444	0.0360

FIGURE C.18 Cumulative Probability Distribution Plot of Chronic Criteria Values for Heptachlor.



Probability Fractile	Chronic Criteria (log ug/g $_{oc}$)	Chronic Criteria (ug/g$_{OC}$)
0.01	-3.887	0.000130
0.05	-3.728	0.000187
0.5	-3.155	0.000700

FIGURE C.19 Cumulative Probability Distribution Plot of Chronic Criteria Values for Toxaphene for Fixed Acute to Chronic Toxicity Ratio of 100.