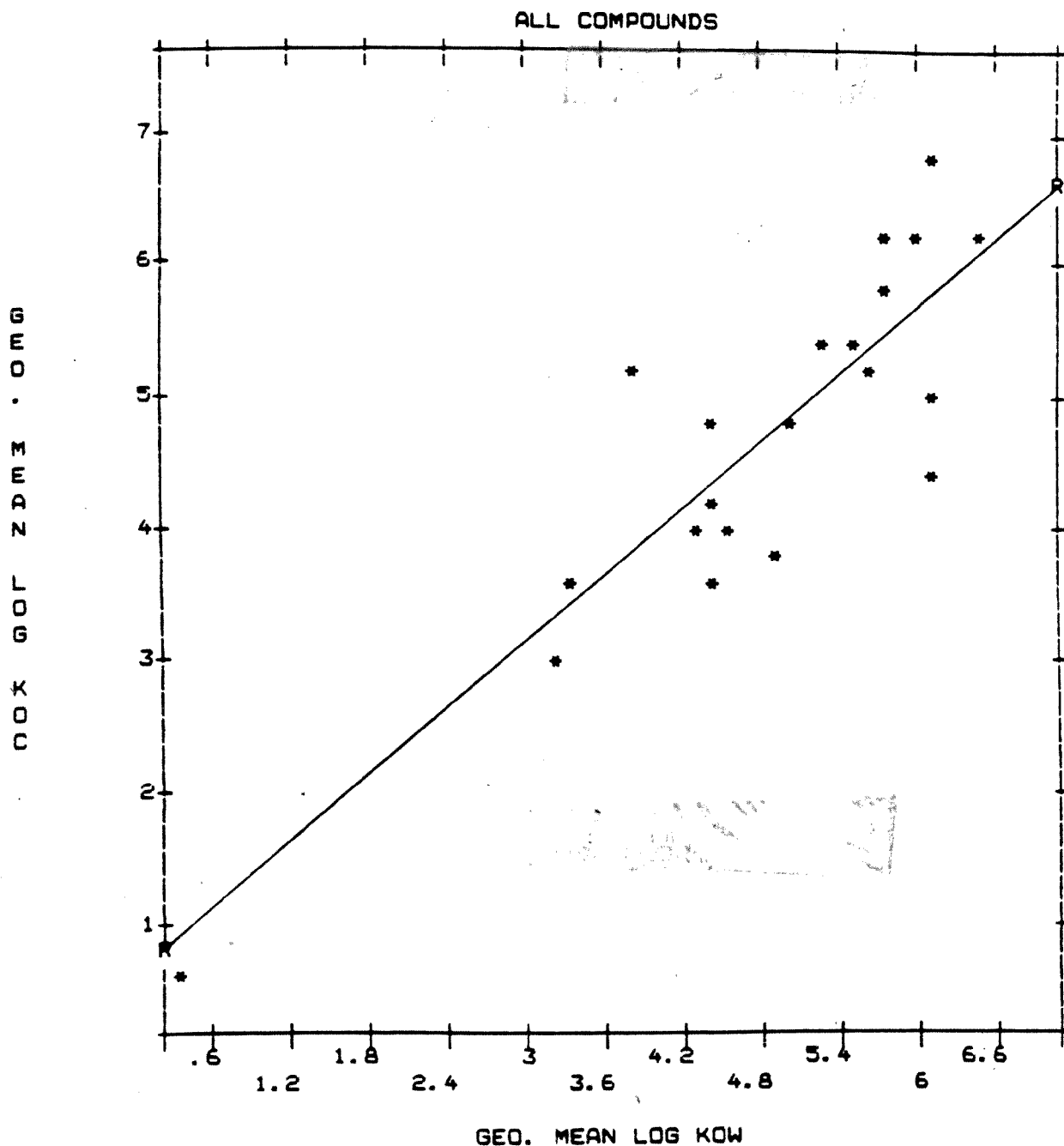


Water



## ELABORATION OF SEDIMENT NORMALIZATION THEORY FOR NONPOLAR ORGANIC CONTAMINANTS



SEDIMENT CRITERIA METHODOLOGY VALIDATION  
WORK ASSIGNMENT 37 TASK II  
ELABORATION OF SEDIMENT NORMALIZATION THEORY FOR  
NONPOLAR HYDROPHOBIC ORGANIC CHEMICALS

FINAL REPORT

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## ABSTRACT

The U.S. Environmental Protection Agency, under the criteria and Standards Division, is developing and evaluating sediment criteria methodologies. This study investigates aspects of the equilibrium partitioning methodology related to specific nonpolar, hydrophobic organic contaminants. Included for this class of compounds are: 1) an update of pertinent partitioning literature, 2) a refinement and analysis of empirical  $K_{oc}/K_{ow}$  regression equations, 3) an evaluation of environmental variables influencing partitioning and 4) estimated permissible sediment contamination concentrations (PCCs) based on results from refined equations.

Results from the investigation indicate that 1) percent organic content of the sediment is a significant normalization parameter, 2) other parameters, including salinity, temperature, dissolved organic carbon, sediment particle size and suspended particulate matter influence partitioning to a varying degree, 3) there is insufficient data to quantify these effects, 4) use of chemical class-specific regression equations is preferred for the nonpolar, hydrophobic organics, 5) these relationships represent a usable simplification of actual theoretical sorption mechanisms, 6) the calculated PCCs are higher (less stringent) than those previously estimated, based on the refined equations.

The study shows the need for additional uncertainty analysis on the empirical equations and for the development of additional laboratory and field data to verify and further refine the predictive equations.

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1.0 INTRODUCTION

The U. S. Environmental Protection Agency (EPA) is currently investigating the feasibility of developing sediment-based criteria for the protection of aquatic life in a manner that parallels the existing water quality criteria. Sediment quality criteria are needed because national water quality criteria alone are not sufficient to ensure protection of aquatic ecosystems consistent with provisions of the Clean Water Act and subsequent amendments.

To meet this goal, EPA's Criteria and Standards Division is funding a program to develop and validate sediment criteria methodologies. Under EPA guidance, Battelle Memorial Institute is currently coordinating some components of this program. The program is divided into two major components: one addresses trace metals and the other nonpolar hydrophobic organic chemicals. This study, the elaboration of sediment normalization theory, was initiated under the second component and will be integrated with other tasks currently being performed by Battelle and subcontractors. These other tasks include the development of screening level concentration (SLC) and sediment bioassays. Results from all investigations will lead to the selection of an optimum methodology for the development of criteria.

Specifically, sediment normalization theory as applied to this work refers to the normalization of equilibrium sediment/water partition coefficients ( $K_d$ ) to the organic content of the sediment. The use of organic carbon-normalized partition coefficients to compute "first cut" safe levels of sediment contamination has been discussed to some extent

in previous publications (Pavlou, 1984; Pavlou and Weston, 1984). Screening-level concentrations are contaminant threshold concentrations (at which adverse effects are observed) in sediments estimated from synoptic benthic and contaminant field data. They provide an interim measure of a probable no-effect level. These values can be compared to no-effect levels determined by laboratory bioassays and to "first cut" safe levels predicted by equilibrium partitioning theory. These three approaches comprise an integrated methodology for estimating sediment criteria. In order to better understand the rationale for performing the calculations presented in this report, the basic concept of equilibrium partitioning and the need for proper normalization of sediment contaminant concentrations is summarized below.

In the equilibrium partitioning approach, sediment/water equilibrium partition (distribution) coefficients are estimated for selected chemical contaminants. Corresponding acceptable contaminant concentrations for interstitial water are equated to the existing EPA water quality criteria. This approach permits the use of the large toxicological data base developed for the water quality criteria. The equilibrium partition coefficient is then multiplied by the water quality criteria to yield the permissible bulk sediment concentration value for the specific contaminant in question.

To obtain permissible sediment contamination concentrations (PCCs) that approximate the contaminant accumulation mechanism as well as account for site- (or area-) specific changes in ambient environmental conditions, the physical/chemical variables that influence the partitioning process must be determined and used to normalize the bulk sediment concentrations. In this manner parity and transferability of PCCs to a variety of sites can be established. Pavlou and Weston (1984), reviewed the literature and found that sediment organic carbon content is the primary environmental variable influencing partitioning. They recommended that partition coefficients be normalized to organic content. They also developed a preliminary predictive equation that relates organic carbon-normalized



sediment/water partition coefficients ( $K_{oc}$ ) to octanol/water partition coefficients ( $K_{ow}$ ). These equations, which depicted a linear relationship, estimate the PCC values for groups of nonpolar hydrophobic organic compounds. The predictive relationships are used to estimate partition coefficients for contaminants for which  $K_{oc}$  data was not available.

The objectives of this study are 1) to update the pertinent literature containing partitioning data for nonpolar, hydrophobic chemicals; 2) to refine the empirical  $K_{oc}/K_{ow}$  equations presented by Pavlou and Weston (1984), 3) to evaluate the effects of environmental variables which may influence equilibrium partitioning; and 4) to compute PCC values and compare with "first-cut" safe level values presented by Pavlou and Weston (1984) based on the updated information and new  $K_{oc}/K_{ow}$  relationships. The PCC values were not compared to the SLC and bioassay-determined safe levels because the latter data were not available at the time this report was prepared.

Following is a synopsis of the report contents:

Chapter 1, Introduction - includes introductory material, a brief description of methodology, and study objectives.

Chapter 2, Literature Search and Compilation of Information - contains the scope and review of the scientific literature together with a preliminary compilation of data. The chapter includes a list of specific nonpolar, hydrophobic organic chemicals investigated.

Chapter 3, Data Entry and Reduction - discusses the approach used to summarize the specific numerical partitioning data into a common format.

Chapter 4, Results and Discussion - describes the analysis of the data and the results of the investigation. It includes summary statistics, the  $K_{oc}/K_{ow}$  correlation approach, statistical analyses (predictive

regression relationships), a qualitative discussion of other factors influencing partitioning, and a discussion of current theoretical concepts regarding sorption phenomena. The computed PCC values and a comparison with previous results are also included.

Chapter 5, Summary and Conclusions - consists of a brief summary and conclusions. Areas for future investigation are also recommended.

Chapter 6, References - contains the literature cited.

The Appendices include a listing of researchers who provided information, the updated  $K_{OC}/K_{OW}$  partitioning data, plots of the predictive regression relationships by chemical classes, and the Bibliography.

## 2.0 LITERATURE SEARCH AND COMPILATION OF INFORMATION

To perform an effective review of the published and unpublished literature covering the partitioning of nonpolar, hydrophobic organics, it was necessary to restrict the data collection effort to a representative subset of compounds. The compounds chosen are listed in Table 1. This list also includes representative chemical classes such as low and high molecular weight polynuclear aromatic hydrocarbons (PAHs), pesticides, and polychlorinated biphenyls (PCBs).

A computerized literature search was performed through the Dialog Information Retrieval Service. Data bases searched included Water Resources Abstracts, Pollution Abstracts, Aqualine, Environmental Bibliography, Oceanic Abstracts, Scisearch, CA Search (Chemical Abstracts), and Dissertation Abstracts. Input to these data base searches included individual compound and class names from Table 1, and additional key words and symbols such as sediment, partitioning, octanol,  $K_{ow}$ ,  $K_{oc}$ , hydrophobic, and solubility.

The computer search identified approximately 700 to 1,000 references. These citations were carefully reviewed and approximately 140 articles were identified as potentially useful for this study. Copies of these articles, with a few exceptions, were obtained. The exceptions were obscure articles in a foreign language (eg., Japanese or Russian), or dissertations of limited distribution which duplicated later published work by the same author.

Concurrent with the computer literature search, key researchers known to be working on contaminant sediment partitioning were contacted to obtain additional unpublished information. Approximately 30 individuals, in the United States and other countries, were contacted. Nine responses and two unpublished manuscripts were obtained; the balance of material received had already been identified from the computer search. The extensive collection of the University of Washington libraries was also manually reviewed. One or two additional articles were identified and obtained.

TABLE 1

## REPRESENTATIVE HYDROPHOBIC ORGANIC CHEMICAL COMPOUNDS

Polycyclic Aromatic Hydrocarbons (PAHs)

## Low Molecular Weight PAHs (2 and 3 rings)

Fluorene	Acenaphthylene
Naphthalene	Anthracene
Acenaphthene	Phenanthrene

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

Fluoranthene	Benzo(b)fluoranthene
Pyrene	Benzo(k)fluoranthene
Chrysene	Indeno(1,2,3-cd)pyrene
Benzo(a)anthracene	Dibenzo(a,h)anthracene
Benzo(a)pyrene	Benzo(ghi)perylene

Pesticides

DDD	Endrin Aldehyde
DDE	Heptachlor
DDT	Heptachlor Epoxide
Acrolein	$\alpha$ -Hexachlorocyclohexane
Aldrin	$\beta$ -Hexachlorocyclohexane
Chlordane	$\gamma$ -Hexachlorocyclohexane
Dieldrin	$\delta$ -Hexachlorocyclohexane
$\alpha$ -Endosulfan	Isophorone
$\beta$ -Endosulfan	2,3,7,8-Tetrachlorodibenzo-p-dioxin
Endosulfan Sulfate	(TCDD)
Endrin	Toxaphene

Polychlorinated Biphenyls (PCBs)

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

All of the data used in this study were derived from the citations listed in the collected Bibliography. Emphasis was placed on obtaining publications that contained quantitative data: for example, values for  $K_{oc}$  and  $K_{ow}$ , percent carbon content of sediments, or discussions especially relevant to the measurement of sorption parameters and coefficients.

### 3.0 DATA ENTRY AND REDUCTION

The articles collected were reviewed to determine the level of quantification. Values for octanol/water partition coefficients ( $K_{ow}$ ), dry weight-normalized sediment/water partition coefficients ( $K_d$ ), organic carbon-normalized sediment/water partition coefficients ( $K_{oc}$ ), and organic carbon content of sediments (percent OC) were compiled. Data for solubility, salinity, temperature, dissolved organic matter, particle size, particulate matter, Eh, and pH were also sought. The data were reduced into a uniform format to enable a quick review and provide input for statistical analysis. Only a few citations in the Bibliography contained matched data sets ( $K_{oc}$  and  $K_{ow}$ ); none were extensive. Organic carbon content was rarely reported with individual  $K_{oc}$  values. Other supporting data for the parameters noted above were not adequate to perform any statistical analysis of their influence on partitioning.

Appendix I contains in tabular form the results of the data collection. Included are the  $K_{ow}$ ,  $K_{oc}$ , percent OC,  $K_d$ , and solubility data contained in the references for the compounds listed in Table 1. When available, the error ranges or uncertainties (one standard deviation) were included. No attempt was made to interpolate data points from graphical presentations of results; only reported numerical values were used. Not all compounds listed in Table 1 are presented in Appendix I because some compounds lacked matched data sets.

## 4.0 RESULTS AND DISCUSSION

This section presents the results of the descriptive statistics, the update and refinement of chemical class-specific relationships between  $K_{oc}$  and  $K_{ow}$ , and a discussion of additional physical/chemical factors affecting partitioning. Current concepts regarding physical/chemical aspects of sorption processes as related to sediment normalization theory are also discussed. Finally, the permissible contaminant concentration values calculated using the updated  $K_{oc}/K_{ow}$  relationships are presented.

### 4.1 DESCRIPTIVE STATISTICS

The data presented in Appendix I were used to refine the  $K_{oc}/K_{ow}$  relationships and estimate uncertainties. First, simple descriptive statistics were performed on the data. Arithmetic means, standard deviations, and geometric means were determined for the  $K_{oc}$  and  $K_{ow}$  values. In most cases, no estimates of uncertainty were reported. Therefore these values were taken as absolute when determining the standard deviation for a given compound set. In those instances where uncertainty was reported, mean upper and lower ranges were determined. The results of the descriptive statistics are shown in Table 2. Certain values were not incorporated into these statistics due to theoretical inconsistency and incompatibility with other reported data. The regression analyses discussed below were performed using paired (matched) data sets.

### 4.2 DEVELOPMENT OF $K_{oc}/K_{ow}$ RELATIONSHIPS

#### 4.2.1 Approach

The data (Appendix I), together with the descriptive statistics summarized in Table 2, were examined to determine the appropriate method for refining the relationships between  $K_{oc}$  and  $K_{ow}$  developed by Pavlou and Weston (1984).

TABLE 2  
DESCRIPTIVE STATISTICS

COMPOUND CLASS	COMPOUND NAME	KLM					NLC				
		NO. OF VALUES	ARITHMETIC MEAN	SD OF ARITHMETIC MEAN	GEOMETRIC MEAN (LOG)	MEAN ERROR RANGE	NO. OF VALUES	ARITHMETIC MEAN	SD OF ARITHMETIC MEAN	GEOMETRIC MEAN (LOG)	MEAN ERROR RANGE
HIGH WT. PAH	BENZODIANTHRENE	6	648267	387851	5.74		1	1737801		6.24	LOW FAIR
								1862987		6.27	MIDDLE
								1955262		6.30	HIGH
	BENZODIAPYRENE	24	1298256	743292	6.07		4	6831375	9231354	6.74	LOW FAIR
								10033258	11597986	6.89	MIDDLE
								15132782	14254847	7.04	HIGH
	BENZODIFLUDRANTHENE	2	2538775	2839716	6.32		0				
	BENZODI6,11FLUORENE	5	10457426	2772908	7.00		0				
	BENZODI11FLUDRANTHENE	2	4007968	4238686	6.45		0				
	CHRYSENE	6	577856	388867	5.71		1	588844		5.77	FAIR
	DIBENZODI6,11ANTHRENE	4	4928872	7867737	6.38	LOW	15	1957853	918726	6.23	FAIR
			5145925	6972137	6.42	MIDDLE					
			5446645	6883437	6.45	HIGH					
	FLUDRANTHENE	6	193163	84931	5.25		1	204174		5.31	FAIR
	INDEN(1,2,3-C)DIPYRENE	1	50118724		7.70		0				
	PYRENE	6	126996	44784	5.08	LOW	31	81657	31516	4.87	FAIR
			128888	44283	5.09	MIDDLE					
			138778	44158	5.10	HIGH					
LOW WT. PAH	ACENAPHTHENE	7	17332	9431	4.18	LOW	0				
			17351	9409	4.18	MIDDLE					
			17370	9386	4.18	HIGH					



TABLE 2 (cont.)  
DESCRIPTIVE STATISTICS

COMPOUND CLASS	COMPOUND NAME	NDM					KOC				
		NO. OF VALUES	SD OF ARITHMETIC: MEAN	ARITHMETIC: MEAN	GEOMETRIC MEAN (LOG)	MEAN ERROR RANGE	NO. OF VALUES	SD OF ARITHMETIC: MEAN	ARITHMETIC: MEAN	GEOMETRIC MEAN (LOG)	MEAN ERROR RANGE
	ACENAPHTHYLENE	2	10367	2343	4.01		0				
	ANTHRACENE	7	27839	13709	4.40		3	185004	283500	4.70	PAIR
	FLUORENE	7	20400	5462	4.30		1	10233		4.01	PAIR
	NAPHTHALENE	20	2297	207	3.36	LOW	0	6467	6502	3.55	PAIR
			2619	331	3.30	MIDDLE					
			2540	453	3.40	HIGH					
	PHENANTHRENE	6	29906	12000	4.43		2	17466	7690	4.22	PAIR
PCBS	AROCOR 1016	1	19953	-	4.30	LOW	0				
			301995	-	5.40	HIGH					
	AROCOR 1221	1	603	-	2.70	LOW	0				
			10000	-	4.00	HIGH					
	AROCOR 1232	1	1514	-	3.10	LOW	0				
			30200	-	4.40	HIGH					
	AROCOR 1242	1	10000	-	4.00	LOW	0				
			396107	-	5.60	HIGH					
	AROCOR 1240	1	1000000	-	6.00		0				
	AROCOR 1254	2	1035760	50572	6.02		14	3800650	5327463	6.25	PAIR
	AROCOR 1260	1	1000000	-	6.00		0				
PESTICIDES	ACROLEIN	2	4.365	5.056	0.40		1	5.01	-	0.70	PAIR
	ALDRIN	3	8591026	14313414	6.12		4	56311	42700	4.30	PAIR

TABLE 2 (cont.)  
DESCRIPTIVE STATISTICS

COMPOUND CLASS	COMPOUND NAME	KOW					KOC				
		NO. OF VALUES	ARITHMETIC MEAN	SD OF ARITHMETIC MEAN	GEOMETRIC MEAN (LOG)	MEAN ERROR RANGE	NO. OF VALUES	ARITHMETIC MEAN	SD OF ARITHMETIC MEAN	GEOMETRIC MEAN (LOG)	MEAN ERROR RANGE
	CHLORDANE	3	101562	173581	3.86		1	141254	-	5.15	PAIR
	DOD	5	639659	505715	5.56		1	239883	-	5.38	PAIR
	DDE	7	477837	211807	5.60		1	147911	-	5.17	PAIR
	DDT	10	3111716	6980374	6.07		17	670204	968288	5.48	PAIR
	DIELDRIN	2	794896	1117225	4.95		2	8097	6768	3.82	PAIR
	ENDOSULFAN	1	3981	-	3.60		0				
	ENDRIN	6	113984	161546	4.44		2	4642	4163	3.56	PAIR
	HEPTACHLOR	3	74634	97301	4.54		1	10000	-	4.00	PAIR
	HEXACYCLOCHLOROCYCLOHEXANE	1	10000	-	4.00		0				
	ISOPHORONE	3	50.197	3.466	1.70		0				
	TCDD	1	7943282	-	6.90		0				
	TOXAPHENE	2	1847	210	3.27		1	1000	-	3.00	PAIR

Kolmogorov-Smirnov (K-S) goodness-of-fit tests were performed to determine whether the data were normally distributed and whether transformations were required. The K-S tests were performed on untransformed and log-transformed data. These tests indicated that only the log-transformed data were normally distributed. The transformed geometric mean data best fit the normal curve and were selected for the regressions.

Mean values for each compound rather than individual data points were used in the regression analyses. Mean data values were used because of the limitations of the data reported in the literature. A few researchers presented all data collected, some provided summary data, and some single values. Sample sizes were not always reported, and in certain cases it was evident that single values were based upon more extensive data sets, but no reference was given in the publication. It was therefore not possible to perform weighted regressions. If one compound has more individual data points than others in a chemical-class regression, the resulting regression would be skewed toward the compound with the most data points. Use of a representative value (eg. mean) for each compound, results in a one-to-one correspondence between compounds and data points. Also, the use of mean values permits the incorporation of reported summarized data.

The use of median values versus mean values was also examined. Recomputation of the statistics using median values was not justified because the differences between the mean and median values were negligible (typically 0.01 log unit or less), primarily because of the small data sets.

In this study, an effort was made to collect all reported  $K_{ow}$  values by compound instead of selecting them from a single literature or experimental value. To test the difference between these methods, one regression was run that incorporated all raw  $K_{oc}$  data and also used the corresponding  $K_{ow}$  values selected by the individual researchers.

The resulting regression agrees well with several  $K_{oc}/K_{ow}$  regression equations previously reported in the literature (Kenaga and Goring, 1980; Lyman et al., 1982). The resulting equation, however, contains the inherent weaknesses associated with biasing and skewing, as noted previously.

#### 4.2.2 Detailed Analyses

A review of the descriptive statistics summarized in Table 2 yields some additional information to that determined from examining the raw data presented in Appendix I.

- o Variation of reported  $K_{oc}$  values is quite high; of the 11 compounds for which more than one  $K_{oc}$  value is reported, five exhibited a standard deviation about the mean exceeding the arithmetic mean.
- o For sample sets of four or more  $K_{oc}$  values, the geometric mean is from approximately 10 to 50 percent lower than the arithmetic mean, which indicates high data scatter. This variation in  $K_{oc}$  is not surprising, and can be attributed to a number of factors, including sorbent concentration effects (Voice and Weber, 1985), particle effects (Di Toro, in press; Di Toro and Horzempa, 1982), physical/chemical effects (Versar, 1984) or differing experimental and laboratory techniques.
- o The variability in  $K_{ow}$  for a given compound is also large in many cases. For example, the standard deviation of the mean compound value is greater than the arithmetic mean compound value for 3 out of 27 compounds. This variability could be due in part to the lack of standardized methodologies for determining  $K_{ow}$  (Karickhoff and Brown, 1979), as well as to some of the factors noted above for  $K_{oc}$  variability, i.e., particle effects and dissolved organic matter.

The results of the  $K_{oc}/K_{ow}$  regression analyses are summarized in Table 3 and are discussed below. These relationships and the individual data points are also presented graphically in the figures included in Appendix II.

All of the regression equations, except the low-weight PAH equation, are significant at the 0.05 (95 percent confidence) level, based on analysis of variance (ANOVA) statistics. The relationship implies that a unique regression line of non-zero slope may be determined for the given data set for a high degree of probability ( $\geq 0.95$ ). In the case of the low-weight PAHs, there are too few data points (four), and with the data scatter, the regression equation is not statistically significant and should not be used.

In all cases, the correlation coefficients ( $r$ ) are greater than 0.8 indicating strong correlations between the two variables. The coefficient of variation,  $r^2$ , is typically greater than 0.7, indicating that varying  $K_{ow}$  explains over 70 percent of the corresponding change in  $K_{oc}$ . The coefficient of variation is not ideal ( $r^2 = 1.0$ ), but is acceptable for using  $K_{ow}$  values to predict  $K_{oc}$  in the absence of empirical data.

The standard error of estimate (SE) is a measure of deviation from the value given by the regression line. For the regression equations in Table 3, SE ranges from about 0.4 to 0.7 log units and averages about half a log unit. The standard error of estimate defines the characteristic uncertainty of the regression. By definition, about two-thirds of the data will lie within one standard error of the regression line, while about 95 percent of the points will lie within two standard errors of the line. Given the small sample size of the database, however, these boundaries cannot be strictly imposed. Thus, for any point predicted by the equations in Table 3, the 95 percent confidence interval ranges from about 0.8 to 1.4 log units, depending upon the SE for the specific equation. It is important to note that this error measurement is only for the regression equations, and does not incorporate the intrinsic uncertainty of the individual data points, which are representative mean compound values.

TABLE 3

REGRESSION RELATIONSHIPS OF  $K_{ow}$  AND  $K_{oc}$  DEVELOPED FROM COLLECTED DATA

Compound Family	Data Type	Regression Equation	correlation r	$r^2$	Standard Error (SE) of Estimate	F Significance	no. of pts
All Compounds	Geometric Mean	$\log K_{oc} = 0.881 \log K_{ow} + 0.419$	0.874	0.764	0.689	0.0000	21
All PAHs	Geometric Mean	$\log K_{oc} = 1.10 \log K_{ow} - 0.376$	0.945	0.893	0.379	0.0000	10
Low Weight PAHs	Geometric Mean	$\log K_{oc} = 0.818 \log K_{ow} + 0.763$	0.804	0.647	0.371	0.1959	4
High Weight PAHs	Geometric Mean	$\log K_{oc} = 1.23 \log K_{ow} - 1.13$	0.837	0.701	0.445	0.0376	6
Pesticides	Geometric Mean	$\log K_{oc} = 0.717 \log K_{ow} + 0.802$	0.869	0.755	0.742	0.0011	10
All Compounds	Raw Data Points	$\log K_{oc} = 0.988 \log K_{ow} - 0.087$	0.818	0.670	0.583	0.0000	83

To generally characterize the intrinsic uncertainty in individual compound data points, reported error ranges for the individual compound data, where available, were determined by calculating the mean high and low values from the literature. These results are given in Table 2. Regression equations were determined with these high and low values, using the same methods as above. An analysis of covariance test, which compares lines of regression, indicated no statistically significant difference between these regression equations and the ones presented in Table 3. These results suggest that, given the limited size of the data sets, the characteristic uncertainty of the regression lines may overshadow the uncertainty associated with the data measurement. This uncertainty may be a point for further investigation in supporting studies, and underlines a need for additional data.

Residuals are defined as the differences between the observed values (in this case, the log-transformed geometric mean  $K_{OC}$  data) and the values predicted by the regression line. They are a measure of the amount of variability not explained by the model, and when plotted can be used to evaluate the suitability of the underlying model assumptions. Ideally, the variance should be constant and the plot of residuals against  $K_{OC}$  will leave the impression of a horizontal band. Deviations from this pattern (e.g. expanding, sloping, or curved bands) give identifiable inadequacies in the model assumptions (Draper and Smith, 1966).

For the three regression equations with the largest data sets (all compounds, all PAHs, and pesticides), the residuals were determined and plotted against the corresponding  $K_{OC}$  value predicted by the respective regression model. These plots are presented in Appendix II.

The residuals plot for the "all compounds" regression has an increasing variance (expanding band) with increasing magnitude of  $K_{OC}$ . This increase in variance indicates the need for a weighted regression (i.e. a weighting of the data before regression analysis). If a weighted analysis is called for, but an ordinary (linear) analysis is performed

as in this case, the estimates obtained are still unbiased but do not have minimum variance (Draper and Smith, 1966). Therefore, it is not desirable to use this predictive relationship because it violates one of the implicit model assumptions, constant variance. This statistical result supports the intuitive physical/chemical weakness of combining data from several chemical families to derive a single regression equation. Further evidence supporting segregation into specific compound classes comes from a closer examination of the individual residuals from this plot. There is a clear separation of the PAH and pesticide data; most of the PAH residuals are positive, while most of pesticide residuals are negative.

In contrast, the residuals plot of the PAH regression indicates a more nearly constant variance. In addition, the magnitude of the variance is smaller than that for the "all compounds" regression. Given the limited number of data points, this plot indicates that underlying model assumptions have not been violated, and there is a noticeable improvement by providing a separate regression for this class of compounds.

The results of the residuals plot for the pesticides regression are not as clear. The magnitude of the variances is greater than that of the PAH residuals, and one or two points influence the perception of the plot. Data are not sufficient, particularly for log K<sub>oc</sub> values between 1.5 and 3.5, to draw conclusions on the appropriateness of the underlying regression assumptions. However, given the great physical/chemical differences of some of these pesticides, one would intuitively expect the variance to be high when combining them in a single pesticide regression.

From a physical/chemical perspective and as supported by the above analysis, it is preferable to employ compound or family-specific regression equations for K<sub>oc</sub> estimation, where possible. Effects on partitioning of chemical characteristics unique to each chemical class



will be masked if equations developed from data for all compounds are used. This need for specific equations has been acknowledged by the investigators identified in Table 4, who have noted the compound classes of the data bases from which regression equations were developed.

Selected regression equations reported in previous investigations are presented in Table 4. Although insufficient information is given in these studies to perform an analysis of covariance, some general comparisons can be made. The slopes from the previous studies are in the same general range (0.8 - 1.0) as the slopes determined in this study. The slope of the pesticide regression is lower than for the other regressions in this study; this observation follows the same pattern as the previous studies. The intercepts tend to be higher than those previously reported, perhaps an indication of cumulative error effect from combining results from numerous studies. The correlation coefficients are comparable, and in some cases are slightly higher than those previously reported for corresponding chemical classes. Since this study is an analysis and compilation of data from numerous researchers, the slightly improved correlation coefficients were unexpected, and thus support the approach used to summarize and analyze the data.

Insufficient data existed to perform a statistical analysis for nonlinearity in the relationship between  $K_d$  and sediment organic content. One would expect, for example, that in sediments of low organic carbon content (e.g., < 1 percent), departures from the linear relationship between  $K_{oc}$  and  $K_{ow}$  would occur. These departures can be attributed to a number of other physical/chemical factors influencing the partitioning process. On the other hand, for sediments of organic content in excess of 25 to 30 percent, one would expect different kinetics, surface/surface interactions, and affinity effects to cause departures from the linear relationship.

TABLE 4  
SELECTED REGRESSION EQUATIONS FROM THE LITERATURE FOR THE ESTIMATION OF  $K_{OC}$  FROM  $K_{OW}$

Regression Equation	Number of Compounds Considered	Correlation Coefficient	Chemical Class	Reference
$\log K_{OC} = 0.544 \log K_{OW} + 1.377$	45	0.86	Pesticides	Kenaga and Goring, 1980
$\log K_{OC} = 0.937 \log K_{OW} - 0.006$	19	0.97	Aromatics, polynuclear aromatics, triazines, dinitroaniline herbicides	Brown and Flagg, 1981
$\log K_{OC} = 1.000 \log K_{OW} - 0.210$	10	1.00	Mostly aromatic and polynuclear aromatics	Karickhoff et al., 1979
$\log K_{OC} = 0.940 \log K_{OW} + 0.020$	9	--	Triazines and dinitroaniline herbicides	Lyman et al., 1982
$\log K_{OC} = 1.029 \log K_{OW} - 0.180$	13	0.95	Variety of herbicides, insecticides, and fungicides	Rao and Davidson, 1980
$\log K_{OC} = 0.524 \log K_{OW} + 0.855$	30	0.92	Substituted phenyl ureas and alkyl N-phenylcarbamates	Briggs, 1973
$\log K_{OC} = 0.989 \log K_{OW} - 0.346$	5	1.00	Aromatic and polynuclear aromatic hydrocarbons	Karickhoff, 1981
$\log K_{OC} = 0.843 \log K_{OW} + 0.158$	19	0.96	Priority pollutants	Pavlou and Weston, 1984

Source: Pavlou and Weston, 1984

To further support the above findings, some alternate nonparametric statistics were run on a small subset of the summary data. For six high-weight PAH compounds (benzo(a)anthracene, benzo(a)pyrene, chrysene, dibenzo(a,h)anthracene, fluoranthene, and pyrene), with matched  $K_{OC}$  and  $K_{OW}$  data, Efron's Bootstrap Technique (Efron and Tibshirani, 1985) was employed. This method consists of running all possible regressions between data points, and determining the asymptotic value for the intercept and slope. This method is theoretically desirable because no assumptions concerning the distribution of the data or coefficients are made; rather, the distribution is determined on the basis of the observations. For the six compounds, using the mean and mean range data sets, use of this method would require nearly  $4 \times 10^8$  regressions. However, a small representative subset of these combinations typically is chosen, and in this case nine regressions were selected. Although too limited to be definitive, the analysis revealed several things. There was not a great deal of stability in slopes and intercepts between data sets. This lack of stability accounts for the variability associated with the observed values. Additionally, there were some nonlinearity problems (non-normal distribution) and residuals were not random across almost all variables. All of these observations suggest that there are other factors in the data that are not accounted for by the regression equations. In other words, while normalization of the partition coefficients to organic carbon content of the sediment produces usable regression equations, there are some other factors which influence partitioning. Other influencing factors are also possible based on the correlation coefficients of the regression equations from the parametric statistics which yield  $r^2$  values of approximately 70 percent, leaving 30 percent of the variation unexplained. Recent findings, which are discussed in the following sections, may explain the variation not accounted for by normalization to organic carbon content.

General inspection of the regression plots in Appendix III also indicates another important factor. There are several points of high leverage, i.e., data which disproportionately influence the location of the regression line. Also, in some cases only one or two points define a broad range (two or three log units) on the plot. Thus, the regressions are sensitive to the deletion (or addition) of data points. The small data sets do not warrant the statistical rejection of outlying data points, however. In addition, there may be a basis for such data because an individual compound within a chemical class may partition differently than other compounds within the class as a result of compound-specific physical/chemical characteristics.

From the above discussion of the detailed analyses, the following key points are noted:

- The reported partitioning data vary noticeably. Such variation implies the need for care in and standardization of measurements.
- Chemical-class specific regressions are preferred over a single regression combining all data.
- The regression equations presented in this study for all PAHs and pesticides are suitable for predictive use.  $K_{ow}$  accounts for approximately 70 percent of the variability when predicting  $K_{oc}$ .
- Other physical/chemical parameters as well as pure error account for the balance of variability in the regression equations. Additional detailed analyses are needed to segregate these factors and further define uncertainties.
- Additional data are needed to verify and/or refine the regressions. The additional data would also serve to better define uncertainties.

#### 4.3 INFLUENCE OF OTHER PHYSICAL/CHEMICAL PARAMETERS ON $K_{OC}$

It was immediately evident after the review of the collected literature that the information was insufficient to quantitatively or statistically evaluate the effects of parameters other than sediment organic content. Some of these parameters have been discussed in the literature, however, together with other factors relating to sediment normalization theory. These discussions are characteristically qualitative, although quantitative values are occasionally presented. In some instances researchers either did not report the supporting data or are employing professional judgment to derive qualitative relationships. Although a thorough review of the literature is beyond the scope of this study, a brief analysis of some of the key points that would support the statistical analyses are presented.

##### 4.3.1 Additional Parameters Influencing Partitioning

Parameters such as pH, salinity, temperature, dissolved organic matter concentration, and redox potential, as well as sediment composition and particle size may have some effect on the partitioning relationship. The literature discussing these parameters was recently reviewed by Versar (1984) in a draft study of selected contaminants at a large marine Superfund site. Their findings, together with additional information, are summarized below.

pH - The pH may significantly affect sediment adsorption of some organic chemicals (for example, acidic compounds such as phenols and basic organic compounds like amines). Some of the organic acids also form strong associations with clays, particularly when the pH of the water is about 1.0 unit above the  $pK_a$  value of the acid (Lyman et al., 1982). The effect of pH on highly hydrophobic neutral organics, however, appears minimal. The pH is not expected to have an effect on the environmental fate of aldrin or the PAHs and should have no effect on the fate of PCBs because they are highly lipophilic molecules with little tendency toward ionization (Versar, 1984).

Salinity - The salinity of a solution may affect the solubility of organic compounds, and thus the adsorption of these compounds on sediments. As the salinity of a solution increases, the solubility of hydrophobic compounds can either decrease or increase. Increased salinity also affects the adsorption of organic cations by increasing the rate at which inorganic cations replace organic cations on the sediments (Lyman et al., 1982).

The solubility of aromatic hydrocarbons is typically reduced by the presence of most inorganic salts in solution (Sutton and Calder, 1975; Eganhouse and Calder, 1976). These studies suggest that the relationship for the effect of salinity on hydrocarbon solubility be expressed as

$$\log S_0/S_s = K_s C_s$$

where  $S_0$  and  $S_s$  are the solute solubilities in fresh and salt water, respectively,  $C_s$  is the salt molarity, and  $K_s$  is the salting constant.  $K_s$  values for some compounds are available from May (1980). The effect of inorganic salts on the solubilities of the aromatic hydrocarbons appears to be the same whether they exist in pure or multicomponent solutions (Eganhouse and Calder, 1976); hence, this effect could easily be accounted for if the  $K_{ow}$  values were determined in a saltwater/octanol system.

The presence of electrolytes (salts) in solution also increases the sorption of PCB by sediments, a "salting out" effect; the solubility of PCB in water decreases as salinity increases (Sayler and Colwell, 1976; Dexter and Pavlou, 1978; Wildish et al., 1980). Dexter and Pavlou (1978) experimentally determined that the solubilities of PCB isomers at a salinity of 30 parts per thousand are up to 5 times lower than those in fresh water.

A similar sorption effect is seen with DDT. Picer et al. (1977) found an 11 to 53 percent increase in adsorption of DDT on different sediments when salinity was increased from 3.7 to 37 percent. Although there are numerous studies of DDT distribution and behavior in the freshwater environment, no data on the solubility of DDT in the marine environment have been published (Versar, 1984).

Normally, the presence of electrolytes in water reduces the solubility of hydrophobic compounds. However, Yaron et al. (1967) found that varying the salinity over a range of 3 to 63 ppt did not affect the quantity of aldrin adsorbed from aqueous-solution onto soils. Therefore, salinity is not considered an important parameter in the adsorption/desorption determinations for aldrin.

Temperature - Solubility of some organic compounds, and therefore their adsorption to sediments, may be affected by the ambient temperature. An 18 percent increase in the adsorption coefficient was measured with a temperature drop from 20°C to 5°C (Lyman et al., 1982). The effect of temperature on absorption varies with the compound under consideration, and for some compounds no appreciable effect is seen. Biggar and Riggs, (1974) observed a strong nonlinear relationship between temperature and aldrin solubility. Aldrin solubility decreased from 13.5 ppb to 5.5 ppb with a drop in temperature from 25°C to 15°C.

Studies have determined that temperature is an important parameter in determining PAH solubility. May (1980) used a dynamic, coupled-column liquid chromatographic procedure to obtain solubility data on 12 PAHs over a 30°C temperature range and developed quadratic equations describing the relationship between temperature and solubility for each

compound. The solubility data of May (1980) at typical water temperatures indicated that the decreased solubility at lower temperatures results in an increased affinity of compounds for the solid organic phase (Versar, 1984). Herbes (1977) observed a threefold increase in adsorption of anthracene on autoclaved yeast cells when the temperature was decreased from 42°C to 4.5°C. Meyers and Quinn (1973) reported the same effect for anthracene adsorbing on bentonite in sea water.

Little information was available on the effect of temperature on solubility and partitioning behavior of PCBs. However, the effect is not expected to be significant for the 20°C range of temperatures found in most aquatic environments (Versar, 1984).

Changes in temperature affect the solubilities and thus the partitioning between water and sediment of DDT, DDD, and DDE. Biggar and Riggs (1974) found that a temperature decrease from 25°C to 15°C results in an approximately two-fold lowering of DDD and DDE solubilities; with DDT, a 1.5-fold lowering occurs. They noted that the relationship between pesticide solubilities and temperature is not linear. From adsorption studies of DDT on humic acid, Weil et al. (1973) calculated that its heat of adsorption is 2.5 kcal/mol. Using the Van't Hoff equation, Versar (1984) estimated that the adsorption coefficient at 10°C is approximately 3 orders of magnitude greater than that at 25°C. However, this effect was only for DDT adsorption on humic acid. The temperature effect for adsorption on less organic sediments should be similar, but perhaps not as large. Unfortunately, the reliable solubility and octanol/water partitioning data for DDT, DDD, and DDE were determined solely at room temperature (Biggar and Riggs, 1974; O'Brien, 1974).



Dissolved organic matter - Equilibrium partitioning of organic contaminants between sediment and water is affected by the concentration of organic matter dissolved in the water. A greater concentration of dissolved organic matter favors a greater equilibrium concentration of contaminant in the aqueous phase through two mechanisms: first through the increased solubility of organic contaminants in water of high dissolved organic material concentration; and second through increased competition for sediment adsorption sites among the organic material present (Hassett and Anderson, 1978). Low concentrations of dissolved organic carbon (1 to 2 mg C/l) are not considered sufficient to significantly shift the sediment/water partitioning equilibrium towards a higher pollutant concentration in the water (Versar, 1984). Boehm and Quinn (1973) discovered that the removal of dissolved organic matter from Narragansett Bay water samples had no effect on the solubility of aromatic hydrocarbons; however, aliphatic hydrocarbon solubilities were significantly affected. It therefore appears from these experiments that the presence of dissolved organic matter has no effect on the solubilities or the partitioning behavior of PAHs. Partitioning of PCBs between water and the dissolved organic phase can decrease the quantity of PCB available for partitioning between water and the sediment organic phase. Sayler and Colwell (1976) demonstrated partitioning of PCBs between water and crude oil as an organic phase as well as sediment. Picer et al. (1977) performed DDT adsorption experiments in seawater contaminated with crude oil and detergent. The presence of these organic compounds in the water column seemed to produce a decrease in the rate of DDT adsorption, but a shift in the final equilibrium toward the sediment phase (increasing K). The effect should not be noticed at low dissolved organic carbon concentrations (Versar, 1984).

Sediment particle size - Size fractionation may be important as a secondary factor in the determination of sediment/water partitioning because it indicates sediment composition and the amount of surface area available for sorption. Large variations in sediment size fractions at different sites within an embayment may result in geographical variability in adsorption of organic compounds. The adsorption coefficient has been reported to increase by a factor of ten with a 100  $\mu\text{m}$  decrease in sediment particle size (Pavlou and Dexter, 1979). Sorption of organics to inorganic clays can be significant when the particle size is small and the surface area is large (Lyman et al., 1982). The total surface of the sediments significantly affects the amount of contaminant being adsorbed. Karickhoff and Brown (1978) demonstrated the variation in adsorption coefficients for pesticides on coarse and fine sediment, and recommended that  $K_{oc}$  be determined on finer sediment particles, i.e.,  $\leq 50 \mu\text{m}$  in diameter (the size/class of silt and clay). Karickhoff et al. (1979) measured the sorption of anthracene, 9-methylanthracene, naphthalene, 2-methyl-naphthalene, phenanthrene, and pyrene on sediments with different size compositions. Their results showed that the  $K_{oc}$  values of the compounds sorbed on the sand fraction ( $\geq 50 \mu\text{m}$ ) were considerably less than those on smaller size fractions ( $\leq 50 \mu\text{m}$ ). Similarly, May (1980) found that phenanthrene adsorption on silica gel is an inverse function of particle surface area. Working with samples from the continental shelf off Washington State, Prah and Carpenter (1983) discovered disproportionately high concentrations of PAHs associated with low-density, carbon-rich sediment particles composed mostly of plant detritus and charcoal. These low-density particles made up only about 1 percent of bulk dry sediments, but accounted for 10 to 35 percent of the total sediment PAH. The rest of the PAHs (50 to 78 percent) remained in the silt/clay fraction (Versar, 1984).

The particle size and resulting surface area of the sediments may be an important factor in the adsorption of PCBs to sediments (Haque et al., 1974; Steen et al., 1978; Hiraizumi et al., 1979). Hiraizumi et al. (1979) demonstrated a positive linear relationship between PCB concentration factors and specific surface area of adsorbing agents such as sand, mud, clay, and plankton. The effects of sediment surface area and organic content on the extent of PCB adsorption, however, are difficult to separate. Choi and Chin (1976) showed that smaller particle size fractions of marine sediments tend to have a higher organic content.

Dissolved inorganic compounds - The presence or absence of dissolved inorganic compounds appears to have little effect on the partitioning of hydrophobic organic compounds. There are, perhaps, one or two exceptions. There is no evidence that dissolved inorganic compounds influence the fate of aldrin, the PAHs, or PCBs. However, DDT sorption can be reduced if metals are present (Callahan et al., 1979) because the presence of Fe II in soil of high organic content can facilitate reduction of DDT to DDE. Porphyrins also can reduce DDT to DDD under anaerobic conditions (Versar, 1984). These reactions in sediments are difficult to quantify because they occur only under anaerobic conditions and depend on the concentrations of metals or porphyrin reducing agents in the water and sediment. In most cases, dissolved inorganic compounds are not expected to affect sorption significantly.

Redox potential (Eh) - The redox potential, a measure of the oxidative state of the system, is a much more significant factor affecting inorganic sediment chemistry than it is for hydrophobic organics. The Eh does not affect the partitioning of PAHs between sediment and water, and because PCBs are not oxidized, no effect of Eh on these compounds is observed (Versar, 1984). It is not known whether the chemical

oxidation of aldrin to dieldrin is a major decomposition pathway. There is empirical evidence of aldrin oxidation under laboratory conditions (Callahan et al., 1979), but the rate of oxidation, either in the laboratory or in nature, is unknown (Versar, 1984). The effect of Eh is significant in the case of the DDT family, because of the effect described in the previous section. However, the magnitude is difficult to quantify.

Based on the above discussion and the general information contained in the literature, the unnormalized partition coefficient ( $K_d$ ) may be conceptually expressed as a function of sediment organic carbon (OC), pH (H), salinity (S), temperature (T), dissolved organic matter (D), sediment particle size (P), Eh (E), and suspended particulate matter (M) for most hydrophobic organic compounds. One possible form of this relationship is:

$$K_d = aOC + bS + cT^n + eD + fP^x + gM,$$

where a, b, c, e, f, g, n, and x are compound specific proportionality constants. This expression is conceptual, will vary between compounds and will likely require significant modification as additional information is obtained. Furthermore, field data will be required to refine the expression and to determine values for the environmentally based proportionality constants.

#### 4.3.2 Current Considerations

The recent interest in liquid-solid phase sorption or partitioning, resulting at least in part from the concern over the fate and effects of toxicants released to the environment, has led to studies containing some contradictory experimental evidence and in reconsideration of theoretical aspects of partitioning of hydrophobic compounds. Voice and Weber (1985) state that:

A notable apparent contradiction of experimental evidence with sorption theory has been cited in several reports that have described a 'solids effect' in laboratory isotherm measurements" (O'Connor and Connolly, 1980; Voice et al. 1983; DiToro and Horzempa 1982). "These works document a dependence of partition coefficients (ratios of individual phase concentrations) on the mass of the solid phase utilized in the experimental system, whereas simple phase equilibrium relationships predict no such dependence.

They go on to note that several explanations have been suggested for these observations.

DiToro and Horzempa (unpublished) have performed laboratory experiments in which, after a chemical constituent has come to equilibrium in the two phases, a portion of the aqueous phase is removed and the sorbent is resuspended and allowed to re-equilibrate. After phase separation, it was found that aqueous concentrations had increased in all cases. They also found similar effects when only local solids concentration (amount of material) was changed. They explain their results in the context of a reversible and resistant component equilibrium model and the role of particle-particle interactions on desorption equilibria. In other words, the sorption of the contaminants is not completely reversible and is influenced by suspended particulate concentration through particle collision kinetics. DiToro (in press) has developed a theoretical model which describes these observations. This model requires additional input data and results in the experimental values presented in the Appendix II table which do not fit the conventional regression models. Voice and Weber (1985) note that these results are not incompatible with a simpler theory, which is also explored in the work of Gschwend and Wu (1985). They suggest that these observations could be the result of a dynamic equilibrium between the distribution of organic material in the solid and in the liquid phase. When the solids concentration is increased, even locally, a driving force may be set up to transfer organic matter from the solid to the liquid phase. This additional organic carbon may act as a competing sorbent or carry sorbed contaminant as it leaves the solid phase. Voice and Weber

(1985) thus propose a model that relates the solid phase or particle phenomenon to the complexation (or binding) of the solute by nonseparable organic matter in the liquid phase, and the subsequent sorption of both free and bound solute. They proceed to show that linear partitioning in the resulting bisolute system can produce the nonlinear sorption anomalies that have been observed in previous isotherm studies.

Uncertainties in  $K_{ow}$  values are also a factor in the current considerations of partitioning theory. These uncertainties are important, because in the standard linear regression analyses of  $K_{ow}$  and  $K_{oc}$ ,  $K_{ow}$  is chosen as the independent variable, i.e., the variable measured without error. Halfon (1985) touches on this issue in his recent article discussing regression methods in ecotoxicology. He argues that a modified geometric mean rather than linear functional regression method should be used to compute slope and intercept coefficients to account for large variations within the independent variable for many predictive environmental regression relationships. However, unlike the examples selected by Halfon, the theoretical partitioning regression slope does not have to be exactly unity (see Lyman, 1982), and, as he admits, the correlation coefficient,  $r$ , does account for variability (error) in both variables. This discrepancy may become a point of contention between statisticians and researchers.

It is clear from the above discussion that the determination of  $K_{oc}$  from  $K_{ow}$  using a linear isotherm does not explicitly incorporate some of the more subtle factors that may influence partitioning. It is also apparent, however, that the above concepts are uncertain and researchers are not in agreement as to the theoretical considerations and mechanisms involved. Until such time as more complete data sets are available and there is a better understanding of physical/chemical mechanisms, the regression equations presented here provide a useful, predictive tool. These equations, incorporating one of the most

important variables affecting partitioning, organic carbon (Chiou et al., 1983; Lyman et al., 1982; Pavlou and Weston, 1984; Versar, 1984), are suitable to estimate preliminary permissible sediment contamination concentrations.

#### 4.4 RECOMPUTED PERMISSIBLE SEDIMENT CONTAMINATION CONCENTRATIONS

The compound-class regression relationships given in Table 3, using geometric mean  $K_{ow}$  values reported in Table 2, were employed to calculate revised  $K_{oc}$  values for the compounds listed in Table 2. These revised  $K_{oc}$  values were then combined with existing (or projected) water quality criteria to determine permissible sediment contamination concentrations. Results of these analyses, together with the results previously reported by Pavlou and Weston (1984), are presented in Table 5.

Comparing the previous results with the results of this study, significant differences in the projected permissible sediment contamination concentrations (PCCs) are observed. These differences cannot be attributed to the relatively minor differences in  $K_{ow}$ , which are typically within  $\pm 0.2$  log units between the two studies. Rather, the differences are attributed to the large variations in projected  $K_{oc}$  values, which differ by as much as 2 to 3 orders of magnitude. These variations result from the use of the refined regression equations. The relationships developed in this study and the corresponding revised PCC values represent a better estimation because the present study makes a distinction between compound classes. Thus several regression relationships apply rather than a single "universal" relationship, as employed by Pavlou and Weston (1984). In addition, this study draws on a broader data base in the development of the regression equations. The projected PCC values are generally less stringent than previously reported. The relatively minor differences in  $K_{ow}$  values between these two studies and the

TABLE 5

SUMMARY OF REVISED PERMISSIBLE SEDIMENT CONTAMINATION CONCENTRATIONS BASED UPON REVISED  $K_{oc}/K_{ow}$  RELATIONSHIPS

Compound	Water Quality Criteria ( $\mu\text{g/l}$ )		Pavlou and Weston <sup>a/</sup>		This Study <sup>b/</sup>		Pavlou and Weston PCC's <sup>a/</sup> ( $\mu\text{g/g}_{oc}$ )		PCC's This Study ( $\mu\text{g/g}_{oc}$ )	
	Acute <sup>c/</sup>	Chronic <sup>c/</sup>	$\log K_{ow}$	$K_{oc} \times 10^5$	$\log K_{ow}$	$K_{oc} \times 10^5$	Acute	Chronic	Acute	Chronic
<b>High Wt. PAHs</b>										
Benzo(a)anthracene	150 d/e/	--	5.61	0.370	5.74	8.51	5,500	--	128,000	--
Benzo(a)pyrene	150 d/e/	--	6.31	3.00	6.07	21.6	45,000	--	325,000	--
Benzo(b)fluoranthene	150 d/e/	--	6.57	5.00	6.32	44.0	75,000	--	660,000	--
Benzo(g,h,i) perylene	150 d/e/	--	7.23	18.00	7.00	302	270,000	--	4,530,000	--
Benzo(k)fluoranthene	150 d/e/	--	6.84	8.40	6.45	63.6	125,000	--	954,000	--
Chrysene	150 d/e/	--	5.61	0.770	5.71	7.82	11,500	--	117,000	--
Dibenzo(a,h)anthracene	150 d/e/	--	6.50	1.60	6.42	58.4	24,000	--	876,000	--
Fluoranthene	20 d/	--	5.33	0.450	5.25	2.1	900	--	4,250	--
Indeno(1,2,3,c,d)pyrene	150 d/e/	--	7.66	41.0	7.70	2,193	600,000	--	32,900,000	--
Pyrene	150 d/e/	--	5.18	0.330	5.09	1.35	4,950	--	20,000	--
<b>Low Wt. PAHs</b>										
Acenaphthene	475 d/	--	4.17	0.047	4.18	0.167	2,300	--	7,940	--
Acenaphthylene	150 d/e/	--	4.07	0.039	4.01	0.108	600	--	1,620	--
Anthracene	150 d/e/	--	4.40	0.074	4.40	0.291	1,100	--	4,370	--
Fluorene	150 d/e/	--	4.18	0.048	4.38	0.277	700	--	4,160	--
Naphthalene	1,175 d/	--	3.31	0.009	3.38	0.022	1,050	--	2,590	--
Phenanthrene	150 d/e/	--	4.52	0.093	4.43	0.314	1,400	--	4,710	--
<b>PCBs</b>										
Aroclor 1016	--	0.014 e/	--	--	4.89 f/	0.203	--	--	--	0.285
Aroclor 1221	--	0.014 e/	--	--	3.39 f/	0.017	--	--	--	0.0239
Aroclor 1232	--	0.014 e/	--	--	3.83 f/	0.035	--	--	--	0.0494
Aroclor 1242	--	0.014 e/	--	--	4.80 f/	0.175	--	--	--	0.245
Aroclor 1248	--	0.014 e/	--	--	6.00	1.27	--	--	--	1.78
Aroclor 1254	--	0.014 e/	--	--	6.02	1.31	--	--	--	1.84
Aroclor 1260	--	0.014 e/	--	--	6.00	1.27	--	--	--	1.78



TABLE 5 (Continued)

SUMMARY OF REVISED PERMISSIBLE SEDIMENT CONTAMINATION CONCENTRATIONS BASED UPON REVISED  $K_{OC}/K_{OW}$  RELATIONSHIPS

Compound	Water Quality Criteria ( $\mu\text{g/l}$ )		Pavlou and Weston <sup>a/</sup>		This Study <sup>b/</sup>		Pavlou and Weston PCC's <sup>a/</sup> ( $\mu\text{g/g}_{OC}$ )		PCC's This Study ( $\mu\text{g/g}_{OC}$ )	
	Acute <sup>c/</sup>	Chronic <sup>c/</sup>	$\log K_{OW}$	$K_{OC} \times 10^5$	$\log K_{OW}$	$K_{OC} \times 10^5$	Acute	Chronic	Acute	Chronic
<b>Pesticides</b>										
Acrolein	28 <u>d/</u>	--	--	--	0.40	0.00012	--	--	0.343	--
Aldrin	1.3	--	--	0.004	6.12	1.55	0.52	--	201	--
Chlordane	0.09	0.004	--	--	3.86	0.037	--	--	0.334	0.0148
DDD	1.8 <u>d/</u>	--	6.03	1.80	5.56	0.614	325	--	111	--
DDE	7 <u>d/</u>	--	5.74	0.990	5.60	0.656	700	--	460	--
DDT	0.13	--	5.98	1.60	6.07	1.42	21	--	18.5	--
Dieldrin	2.5	0.0019	--	--	4.95	0.224	--	--	56	0.0426
Endosulfan	0.034	0.0087	--	--	3.60	0.024	--	--	0.0822	0.0210
Endrin	0.037	0.0023	--	--	4.44	0.097	--	--	0.358	0.0222
Heptachlor	0.053	0.0036	--	--	4.54	0.114	--	--	0.604	0.0411
Hexachlorocyclohexane	0.08 <u>d/</u>	--	--	--	4.00	0.047	--	--	0.374	--
Isophorone	6,450 <u>d/</u>	--	1.67	0.00037	1.70	0.001	240	--	677	--
TCDD	--	--	--	--	6.90	5.61	--	--	--	--
Toxaphene	0.035 <u>d/g/</u>	--	--	--	3.27	0.014	--	--	0.0491	--

a/ As reported in Pavlou and Weston (1984), Table 7.

b/  $\log K_{OW}$  based upon geometric mean values (Table 2).  $K_{OC}$  determined from presented  $K_{OW}$  values and appropriate compound class regression from Table 3. The equation for all PAHs was used to determine the low weight PAH values.

c/ Marine (saltwater) criteria as presented in Federal Register, Vol. 45, No. 231 (1980).

d/ Not nationally adopted water quality criteria, but rather one-half the lowest concentration at which toxic effects have been noted as reported in Federal Register, Vol. 45, No. 231 (1980). Actual criteria, when established, are likely to be different.

e/ Based on class criteria for polynuclear aromatic hydrocarbons (300  $\mu\text{g/l}$ ) or polychlorinated biphenyls (0.014  $\mu\text{g/l}$ )

f/ Based on median value of reported range.

g/ Freshwater criteria, no saltwater data available.

resulting large differences in  $K_{oc}$  values indicate the need to verify the regression equations and develop a broader base of measured  $K_{oc}$  values for specific compounds. A field verification program is recommended, together with a probabilistic uncertainty analysis, to ensure that the revised PCC values are appropriate.

## 5.0 SUMMARY AND CONCLUSIONS

A review of the scientific literature identified approximately 140 articles containing information related to the partitioning of selected nonpolar hydrophobic organic chemicals. Analysis of these data disclosed predictive, chemical class-specific  $K_{oc}/K_{ow}$  regression equations. Insufficient quantitative information was found to permit any additional physical/chemical parameters to be incorporated in these relationships. However, analysis of these equations together with a review of qualitative information from the literature indicates that the percent organic content of the sediment is a significant normalization parameter, and that the effects of other parameters, in general, are minor and are compound-specific. Other parameters which may have an effect on partitioning include salinity, temperature, dissolved organic carbon, sediment particle size, and suspended particulate matter. The use of class-specific  $K_{oc}/K_{ow}$  equations is preferred over the use of a single equation incorporating data from all compounds where possible.

The review verifies that the derived relationships represent a usable simplification of actual theoretical sorption mechanisms, that to date have not been totally resolved for the nonpolar hydrophobic organics in a sediment/water system. The chemical class-specific regression relationships are used to recalculate previous "first-cut" safe levels presented by Pavlou and Weston (1984). The resulting permissible sediment contamination concentrations are less stringent than those previously presented. This difference appears to be the direct result of applying the new refined, chemical class-specific regression relationships, rather than a result of other factors such as variation in reported  $K_{ow}$  values.

Based on the literature review and subsequent analyses and development of predictive relationships, two areas for future investigation are evident. Additional field and laboratory data are required to validate and possibly refine the predictive partitioning ( $K_{oc}/K_{ow}$ ) relationships. Also, an uncertainty analysis of the predicted criteria needs

to be performed to a greater level of detail than presented here. Sufficient data need to be collected to develop additional class-specific relationships and to narrow the ranges of uncertainty. This latter effort will permit comparison with SLC values developed in the other tasks.

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## APPENDIX I

SUMMARY OF ALL LOG  $K_{ow}$ , LOG  $K_{oc}$  AND RELATED DATA

SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
BENZO(A)ANTHRACENE	1985	DI TORO	SMITH ET. AL.	ADSORB	*		* 5.92 a	*			* 40 a		* 336000	1.21 a
				DESORB	*		* 5.30 a	*			* 40 a		* 80000	3.90 a
	1984	LANDRUM ET. AL.			* 5.30		*	*			*		*	
	1977	MACKAY & SHIU			*		*		* 0.014	0.0002	*		*	
	1984	MACKAY ET. AL.			* 6.10		*		* 0.0141		*		*	
	1984	MILLER ET. AL.			*		*		* 0.00057		*		*	
	1985	MILLER ET. AL.			* 5.91		*		*		*		*	
	1982	MILLS ET. AL.			* 5.60		*		*		*		*	
	1975	RADDING ET. AL.	HANSCH		* 5.61		*		*		*		*	
	1979	REINBOLD ET. AL.			*		* 6.27	0.03	*		* 1.4		* 26200	1700
	1984	WALTERS & LUTHY			*		*		* 0.0168	0.0011	*		*	
			MAY ET. AL.		*		*		* 0.0094	0.0001	*		*	
			VERSAR		*		*		* 0.014		*		*	
			WALCHOPE & GETZEN		*		*		* 0.010		*		*	
			YALKOWSKY & VALVANI		* 5.91		*		*		*		*	
BENZO(A)PYRENE	1985	DI TORO	SMITH ET. AL.	ADSORB	*		* 5.60 a	*			* 3.0 a		* 10200	1.25 a
					*		* 5.60 a	*			* 40 a		* 31100	1.21 a
				DESORB	*		* 4.89 a	*			* 3.0 a		* 10200	1.25 a
					*		* 4.89 a	*			* 40 a		* 31100	1.21 a
	1984	LANDRUM ET. AL.			* 5.95		*		*		*		*	
	1977	MACKAY & SHIU			*		*		* 0.0038	0.00031	*		*	
	1980	MACKAY ET. AL.			* 6.57		*		* 0.0038		*		*	
	1984	MALLON & HARRISON			* 6.12		*		*		*		*	
					* 5.93		*		*		*		*	
					* 5.96		*		*		*		*	
					* 6.00		*		*		*		*	
					* 5.85		*		*		*		*	
					* 5.91		*		*		*		*	
					* 6.05		*		*		*		*	
					* 6.06		*		*		*		*	
					* 6.05		*		*		*		*	
					* 5.92		*		*		*		*	
					* 6.19		*		*		*		*	
					* 6.15		*		*		*		*	
					* 5.89		*		*		*		*	
					* 5.97		*		*		*		*	
					* 6.22		*		*		*		*	

\* DATA POINTS NOT USED IN CALCULATIONS DUE TO INTERNAL INCONSISTENCIES

SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM ERROR	REP.	KD/KP	REP. ERROR
BENZO(A)PYRENE CONT.	1984	MALLON & HARRISON	LITERATURE HANSCH SMITH ET. AL.	a	6.04									
				a	5.88									
				a	5.99									
	1985	MILLER ET. AL.		a					0.00378					
	1982	MILLS ET. AL.		a	6.00									
	1984	RAPAPORT & EISENRICH		a	6.42									
				a	6.50									
	1975	RADDING ET. AL.		a	6.04									
	1982	READMAN ET. AL.		a					0.00172					
	1979	REINBOLD ET. AL.		a			7.45	0.11			0.06		17000	5000
				a			6.77	0.25			0.6		35000	27000
				a			6.73	0.18			1.4		76000	24000
				a			6.59	0.06			3.8		150000	20000
BENZO(B)FLUORANTHENE	1977	MACKAY & SHIU	EPA	a					0.045	0.0012				
	1982	MILLS ET. AL.		a	6.60									
	1982	READMAN ET. AL.		a	6.04									
BENZO(G,H,I)PERYLENE	1977	MACKAY & SHIU	LITERATURE	a					0.00026	0.00001				
	1980	MACKAY ET. AL.		a	6.77				0.00026					
	1985	MILLER ET. AL.		a	7.10									
	1982	MILLS ET. AL.		a	7.00									
	1984	RAPAPORT & EISENRICH		a	7.05									
				a	7.10									
BENZO(K)FLUORANTHENE	1977	MACKAY & SHIU	EPA	a					0.0020	0.00003				
	1982	MILLS ET. AL.		a	6.85									
	1982	READMAN ET. AL.		a	6.04									
CHRYSENE	1981	BRIGGS	MAY ET. AL.	a					0.0015					
				a					0.0118	0.0001				
				a					0.002	0.0002				
	1977	MACKAY & SHIU	HANSCH MABEY ET. AL.	a					0.002					
	1980	MACKAY ET. AL.		a	6.01									
	1984	MILLER ET. AL.		a					0.0012					
	1985	MILLER ET. AL.		a	5.79									
	1982	MILLS ET. AL.		a	5.60									
	1975	RADDING ET. AL.		a	5.61									
	1985	STAPLES ET. AL.		a					0.018					

## SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% DC OR OM	REP. ERROR	KD/KP	REP. ERROR
CHRYSENE CONT.	1984	VERSAR			5.32		5.77							
	1984	WALTERS & LUTHY							0.00327	0.00043				
			VERSAR						0.002					
			WAUCHOPE & GETZEN						0.006					
			YALKOWSKY & VALVANI		5.91									
DIBENZO(A,H)ANTHRACENE	1980	MEANS ET. AL.			6.50	0.14	6.23		0.00249	0.0001	1.21		20461	
							6.23				2.07		34929	
							5.91				2.20		18361	
							6.42				0.72		18882	
							6.07				0.15		1759	
							6.36				0.11		2506	
							6.48				0.48		14497	
							6.43				0.95		25302	
							6.49				0.66		20192	
							5.75				1.30		7345	
							6.47				1.88		55697	
							6.38				1.67		39809	
							5.91				2.38		19254	
							6.43				1.48		39840	
	1984	MILLER & WASIK							0.0005					
	1982	MILLS ET. AL.			6.00									
	1984	VERSAR			5.97		5.92							
	1984	WALTERS & LUTHY			7.19				0.00249					
FLUORANTHENE	1981	BRIGGS							0.29					
			MAY ET. AL.						0.206	0.002				
	1977	MACKAY & SHIU							0.260	0.020				
	1980	MACKAY ET. AL.			5.29				0.26					
	1985	MILLER ET. AL.			5.22									
	1982	MILLS ET. AL.			5.53									
	1982	READMAN ET. AL.	EPA		4.90									
	1984	VERSAR			5.33		5.31							
	1984	WALTERS & LUTHY							0.199	0.011				
			VERSAR						0.26					
			WAUCHOPE & GETZEN						0.265					
			YALKOWSKY & VALVANI		5.22									

SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
INDENO(1,2,3,C,D)PYRENE	1982	MILLS ET. AL.			7.70									
PYRENE	1981	BRIGGS							0.12					
			MAY ET. AL.						0.132	0.001				
	1985	DI TORO	KARICKHOFF ET. AL.	ADSORB			5.00 a				2.34 a		2820 a	1.07
				DESORB			4.54 a				2.34 a		816 a	1.53
	1981	KARICKHOFF					4.83							
	1985	KARICKHOFF & MORRIS					4.98				3.04		2900	
							4.94				1.48		1300	
	1979	KARICKHOFF ET. AL.			5.18		4.04				0.08		9.4	
							4.88				2.78		2100	
							5.11				2.34		3000	
							5.08				2.89		3600	
							5.08				3.29		3800	
							4.51				0.13		42	
							4.96				3.27		3000	
							5.11				1.98		2500	
							5.05				1.34		1500	
							5.08				1.20		1400	
							5.08				0.57		68	
							5.05				2.92		3200	
							5.08				1.99		2300	
							5.05				2.26		2500	
	1977	WACKAY & SHIU							0.135	0.005				
	1980	WACKAY ET. AL.			5.12				0.135					
			LITERATURE		4.88									
	1980	MEANS ET. AL.			5.09	0.04	4.80		0.135	0.013	1.21		760	
							4.71				2.07		1065	
							4.70				2.20		1155	
							4.93				0.72		614	
							4.83				0.15		101	
							4.81				0.11		71	
							4.76				0.48		277	
							4.92				0.95		783	
							4.88				0.66		504	
							4.78				1.30		723	
							4.77				1.88		1119	
							4.68				1.67		806	

a - DATA POINTS NOT USED IN CALCULATIONS DUE TO INTERNAL INCONSISTENCIES

## SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% DC OR OM	REP. ERROR	KD/KP	REP. ERROR
PYRENE CONT.	1980	NEANS ET. AL.					4.64				2.38		1043	
							4.83				1.48		994	
	1982	MILLS ET. AL.			5.30									
	1984	RAPAPORT & EISENRICH			4.96									
	1984	WALTERS & LUTHY							0.133	0.033				
			SCHWARZ						0.129					
			VERSAR						0.14					
			WAUCHOPE & GETZEN						0.148					
+++++														
ACENAPHTHENE	1980	BANERJEE ET. AL.			3.92	0.00			7.37	0.3				
	1977	MACKAY & SHIU							3.93	0.014				
	1980	MACKAY BOBBA & SHIU			4.15									
	1982	MILLS ET. AL.			4.32									
	1985	STAPLES ET. AL.	MABEY ET. AL.						3.42					
	1980	VEITH ET. AL.			4.49									
					4.45									
					3.92									
	1984	WALTERS & LUTHY							4.16	0.57				
			ARNOLD ET. AL.						3.47					
			VERSAR						3.47					
			WAUCHOPE & GETZEN						3.88					
			YALKOWSKY & VALVANI		4.03									
-----														
ACENAPHTHYLENE	1982	MILLS ET. AL.			4.00									
	1984	WALTERS & LUTHY							16.1	0.45				
			VERSAR						3.93					
			YALKOWSKY & VALVANI		3.94									
-----														
ANTHRACENE	1981	BRIGGS							0.07					
			MAY ET. AL.						0.0446	0.0002				
	1981	KARICKHOFF			4.54		4.20							
	1979	KARICKHOFF ET. AL.			4.34		4.42							
	1984	LANDRUM ET. AL.			4.15									
			BRUEGGEMAN ET. AL.						0.0724					
	1977	MACKAY & SHIU							0.073	0.0005				
	1980	MACKAY BOBBA & SHIU			4.73									
			LITERATURE		4.15									



SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
ANTHRACENE CONT.	1982	MILLS ET. AL.			4.45									
	1984	RAPOPORT & EISENRICH			4.45									
	1983	SHANN ET. AL.							0.03					
									0.051					
	1984	WALTERS & LUTHY							0.0698	0.0075				
			ISHOW						0.075					
			SCHWARZ						0.041					
			VERSAR						0.075					
			WALCHOPPE & GETZEN						0.075					
	1983	WASIK ET. AL.							0.0446	0.0002				
	1984	WIJAYARATNE & MEANS					5.71							
FLUORENE	1981	BRIGGS							1.5					
			RAY ET. AL.						1.685	0.005				
	1977	MACKAY & SHIU							1.98	0.004				
	1980	MACKAY ET. AL.			4.27									
			LITERATURE		4.18									
	1982	MILLS ET. AL.			4.38									
	1984	RAPOPORT & EISENRICH			4.23									
			LITERATURE		4.38									
	1984	VERSAR			4.18		4.01							
	1984	WALTERS & LUTHY							1.98	0.057				
			VERSAR						1.98					
			WALCHOPPE & GETZEN						1.98					
			VALKOWSKY & VALVANI		4.47									
	1983	WASIK ET. AL.							1.56	0.00				
NAPHTHOLENE	1981	BRIGGS			3.36		2.62		28.4					
			RAY ET. AL.						31.69					
	1977	CHIOU ET. AL.	CRC						38					
			HANSCH & FUJITA		3.37									
	1984	GARST & WILSON			3.44	0.02								
					3.47	0.04								
					3.46	0.03								
					3.43	0.02								
					3.46	0.03								
					3.38	0.02								
					3.44	0.02								

a - DATA POINTS NOT USED IN CALCULATIONS DUE TO INTERNAL INCONSISTENCIES

## SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM ERROR	KD/KP	REP. ERROR
NAPHTHALENE CONT.	1984	GARST & WILSON			3.43	0.02							
					3.30	0.02							
	1981	KARICKHOFF			3.36		3.43						
	1979	KARICKHOFF ET. AL.			3.31		3.11						
	1978	KRISHNAMURTHY & WASIK			3.39	0.14							
	1977	MACKAY & SHIU							31.7	0.26			
	1980	MACKAY ET. AL.			3.30								
	1984	MILLER ET. AL.			3.35								
	1982	MILLS ET. AL.			3.36								
	1984	RAPAPORT & EISENRICH			3.26								
	1985	SALEN					4.21				1.34		219
							3.97				1.34		125
							4.20				1.34		210
	1984	VERSAR			3.37		3.27						
	1984	WALTERS & LUTHY							32.9	1.2			
			ARNOLD ET. AL.						34.4				
			EGANHOUSE & CALDER						31.3				
			ISHOW						30				
			SCHWARZ						30.3				
			VERSAR						34.4				
			MAUCHOPE & GETZEN						31.2				
	1983	WASIK ET. AL.			3.35	0.04			30.64	0.00			
	1984	WIJAYARATNE & NEANS					3.61						
PHENANTHRENE	1981	BRIGGS							0.99				
			MAY ET. AL.						1.002	0.011			
	1981	KARICKHOFF			4.57		4.08						
	1979	KARICKHOFF ET. AL.			4.52		4.36						
	1984	LANDUM ET. AL.			3.92								
	1977	MACKAY & SHIU							1.29	0.07			
	1980	MACKAY ET. AL.			4.64				1.26				
			LITERATURE		4.46								
					4.46								
	1982	MILLS ET. AL.											
	1984	WALTERS & LUTHY							1.29	0.014			
			EGANHOUSE & CALDER						1.07				
			ISHOW						1.6				
			SCHWARZ						1.151				
			VERSAR						1.29				

SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
PHENANTHRENE CONT.	1984	WALTERS & LUTHY	WAUCHOPE & GETZEN		*		*		1.180		*		*	
	1983	MASIK ET. AL.			*		*		1.00	0.01	*		*	
*****														
AROCLO 1016	1982	MILLS ET. AL.			* 4.30 - 5.40a*				0.42		*		*	
AROCLO 1221	1982	MILLS ET. AL.			* 2.78 - 4.00a*				15		*		*	
AROCLO 1232	1982	MILLS ET. AL.			* 3.18 - 4.48a*				1.45		*		*	
AROCLO 1242	1982	MILLS ET. AL.			* 4.00 - 5.60a*				0.1 - 0.3		*		*	
AROCLO 1248	1982	MILLS ET. AL.			* 6.00				0.054		*		*	
AROCLO 1254	1985	DI TORO	EPA		* 6.03						*		*	
			WILBISH ET. AL.	ADSORB			* 4.98 a				* 0.6 a		* 570 a	
							* 4.93 a				* 3.00 a		* 2550 a	
				DESORB			* 3.00 a				* 0.6 a		* 5.97 a	
							* 1.69 a				* 3.00 a		* 1.48 a	
	1983	HORZEMPA & DI TORO		ADSORB			* 3.83 a				* 0.4 a(OM)		* 15.7 a	
							* 2.65 a				* 5.4 a(OM)		* 14.1 a	
							* 2.51 a				* 4.9 a(OM)		* 9.3 a	
							* 2.63 a				* 4.6 a(OM)		* 11.3 a	
							* 3.26 a				* 1.2 a(OM)		* 12.6 a	
							* 2.57 a				* 4.9 a(OM)		* 10.6 a	
				DESORB			* 4.05 a				* 0.4 a(OM)		* 26.0 a	
							* 3.05 a				* 5.4 a(OM)		* 35.2 a	
							* 2.89 a				* 4.9 a(OM)		* 22.06 a	
							* 3.04 a				* 4.6 a(OM)		* 29.3 a	
							* 3.29 a				* 1.2 a(OM)		* 13.6 a	
							* 2.71 a				* 4.9 a(OM)		* 14.6 a	
	1982	MILLS ET. AL.			* 6.00				0.01 - 0.06		*		*	
	1983	WEBER ET. AL.					* 6.17				* 0.11		* 1626	
							*				* 0.00		* 1654	
							* 6.16				* 1.82		* 26408	
							* 5.89				* 0.47		* 3626	
							* 5.84				* 3.45		* 23760	
							* 5.04				* 1.05		* 1152	

a - DATA POINTS NOT USED IN CALCULATIONS DUE TO INTERNAL INCONSISTENCIES

SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
AROCLO 1254 CONT.	1983	WEBER ET. AL.			*		* 6.31	*			* 2.61	*	53543	
					*		* 6.88	*			* 1.98	*	158686	
					*		* 6.29	*			* 1.84	*	35734	
					*		* 7.19	*			* 0.67	*	102841	
					*		* 6.34	*			* 3.51	*	76759	
					*		* 7.20	*			* 0.07	*	11143	
					*		* 6.10	*			* 9.25	*	116338	
					*		* 5.97	*			* 9.48	*	88981	
AROCLO 1260	1982	MILLS ET. AL.			*		* 6.15	*			* 8.30	*	117693	
					*									
					*									
					*									
					*									
					*									
					*									
					*									
ACROLEIN	1980	KENAGA			*									
					*		* 0.70	*						
					*									
					*									
ALDRIN	1981	BRIGGS			*									
					*									
					*									
					*									
CHLORDANE	1982	MILLS ET. AL.			*									
					*									
					*									
					*									
					*									
					*									
					*									
					*									
DDD	1982	MILLS ET. AL.			*									
					*									
					*									
					*									
					*									
					*									
					*									
					*									
DDE	1982	MILLS ET. AL.			*									
					*									
					*									
					*									
					*									
					*									
					*									
					*									

## SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
DOE CONT.	1977	CHIOU ET. AL.	O'BRIEN						0.040					
					5.69									
	1981	MC DUFFIE			5.89									
	1982	MILLS ET. AL.	RAO & DAVIDSON		5.70				0.0012 - 0.14					
					4.86									
	1983	SHARM ET. AL.			5.63				0.006					
									0.0011					
	1980	VEITH ET. AL.			5.77									
	1984	VERSAR			5.69		5.17		0.01					
DOT	1974	BIGGAR & RIGGS							0.0017					
	1981	BRIGGS			5.98		5.38		0.0039					
	1985	CHIOU			6.36									
	1981	CHIOU ET. AL.			6.19		5.14							
	1977	CHIOU ET. AL.	BIGGAR ET. AL.						0.0034					
			BOWMAN ET. AL.						0.0031					
	1985	DI TORO	PICER ET. AL.	ADSORB			6.07 a				0.04 a		9980 a	
				DESORB			4.62 a				0.04 a		351 a	
			SHARM ET. AL.	DESORB			4.15 a				1.45 a		203 a	
	1981	ELLENHUSEN ET. AL.			6.19									
					5.94									
	1984	GERSTL & MINGELGRIN			5.44		6.24		0.0045		0.45 (OM)		4546	
							5.95				1.25 (OM)		6468	
							5.70				2.82 (OM)		8121	
							5.46				5.82 (OM)		9637	
							5.87				7.95 (OM)		34504	
							5.77				4.35 (OM)		15012	
	1984	BEYER ET. AL.			6.28									
					6.36									
	1980	KENAGA			5.57									
	1980	KENAGA & GORTING	HAWKER & THOMPSON				5.38							
	1984	LANDRUM ET. AL.			5.44									
	1980	MACKAY ET. AL.			7.48				0.0031					
	1982	MILLS ET. AL.			4.00 - 6.00				0.002 - 0.005					
			RAO & DAVIDSON		5.57		5.38							
	1976	PLATFORD			5.1				2					
	1984	ROPAPORT & EISENRICH			6.16									
			LITERATURE		6.11									

a - DATA POINTS NOT USED IN CALCULATIONS DUE TO INTERNAL INCONSISTENCIES

## SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
DDT CONT.	1985	STAPLES ET. AL.	MABEY ET. AL.		* 6.90		* 6.60		* 0.0055					
	1983	SWANN ET. AL.			*		* 4.64		* 0.02					
					*		* 5.10		* 0.0023					
	1980	VEITH ET. AL.			* 5.98		*		*					
	1984	VERSAR			* 6.19		* 5.50		* 0.0017					
DIELDRIN	1974	BIGGAR & RIGGS	SHARM ET. AL.		*		*		* 0.022					
	1981	BRIGGS			* 6.20		* 4.11		* 0.0271					
	1985	DI TORO			*		* 3.52		*		* 1.45		* 48.3	
	1982	MILLS ET. AL.			*		*		* 0.186 - 0.200					
					* 3.69		*		*		*			
	1985	STAPLES ET. AL.	MAD & DAVIDSON MABEY ET. AL.		*		*		* 0.02					
ENDOSULFAN	1982	MILLS ET. AL.			* 3.60		*		* 0.100 - 0.260					
ENDRIN	1974	BIGGAR & RIGGS	SHARM ET. AL.		*		*		* 0.024					
	1985	DI TORO			*		* 3.80		*		* 1.45		* 109	
	1982	MILLS ET. AL.			* 5.60		*		* 0.220					
			MAD & DAVIDSON		* 3.20		*		*		*			
	1984	RAPOPORT & EISENRICH			* 4.40		*		*		*			
			LITERATURE		* 4.56		*		*		*			
	1985	STAPLES ET. AL.	MABEY ET. AL.		* 3.54		* 3.23		* 0.25					
HEPTACHLOR	1974	BIGGAR & RIGGS	MAD & DAVIDSON MABEY ET. AL.		*		*		* 0.030					
	1981	MCDUFFIE			* 5.27		*		*		*			
	1982	MILLS ET. AL.			*		*		* 0.056 - 0.10					
					* 3.87		*		*		*			
	1985	STAPLES ET. AL.			* 4.40		* 4.00		* 0.10					
HEPTACHLOR EPOXIDE	1982	MILLS ET. AL.			*		*		* 0.200 - 0.350					
HEXACHYCHLOROCYCLOHEXANE	1982	MILLS ET. AL.			* 4.00		*		* 0.70 - 21.3					
ISOPHORONE	1982	MILLS ET. AL.			* 1.70		*		* 12000					
	1980	VEITH ET. AL.			* 1.67		*		* 14500					
					* 1.73		*		*		*			

SUMMARY OF ALL LOG KOW, LOG KOC AND RELATED DATA

COMPOUND	YEAR	AUTHOR	CITATION	MISC.	LOG KOW	REP. ERROR	LOG KOC	REP. ERROR	SOLU- BILITY	REP. ERROR	% OC OR OM	REP. ERROR	KD/KP	REP. ERROR
TCDD	1981	BRIGGS			6.90	*	*		*		*		*	
	1982	MILLS ET. AL.			*		*		0.0002		*		*	
					*		*		*		*		*	
TOXAPHENE	1980	KENAGA & GORING	SANBORN ET. AL.		*		*		0.40		*		*	
	1982	MILLS ET. AL.			*		*		0.7 - 3.0		*		*	
			RAO & DAVIDSON		3.23		*		*		*		*	
	1985	STAPLES ET. AL.	MABEY ET. AL.		3.30		3.00		0.50		*		*	
					*		*		*		*		*	
					*		*		*		*		*	

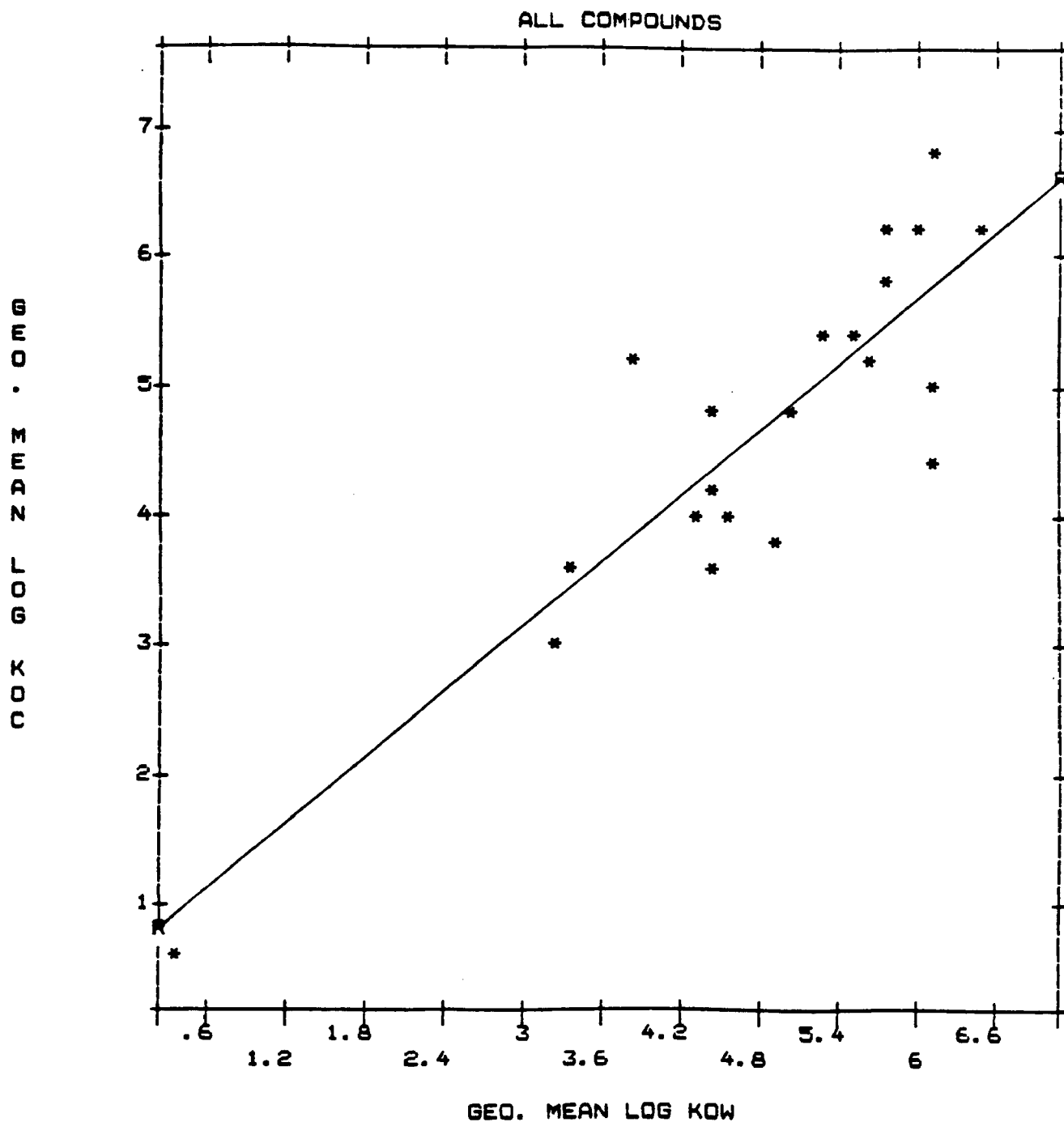
**APPENDIX IV (Continued)**

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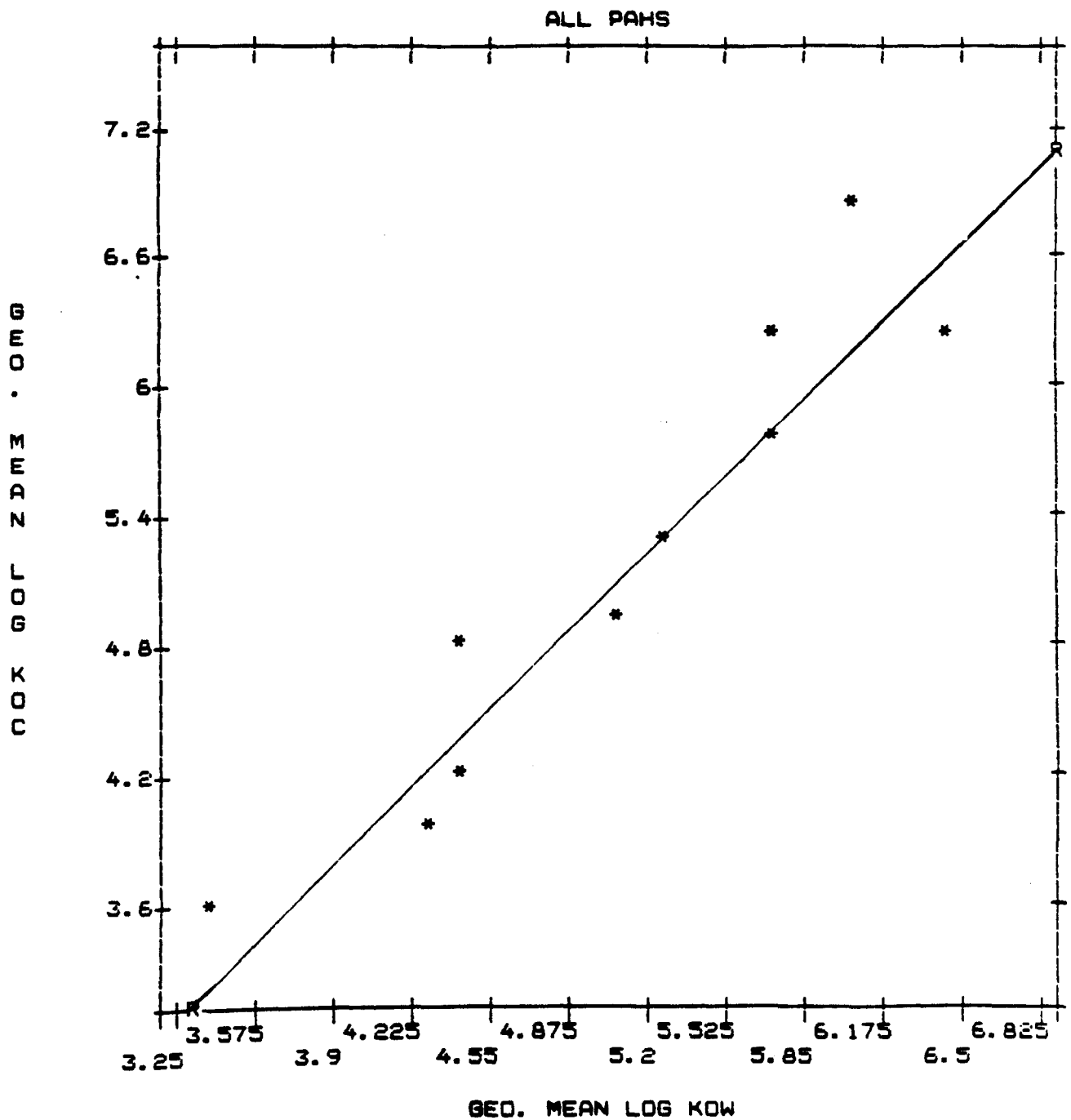
## APPENDIX II

PLOTS OF  $K_{oc}/K_{ow}$  REGRESSION ANALYSES



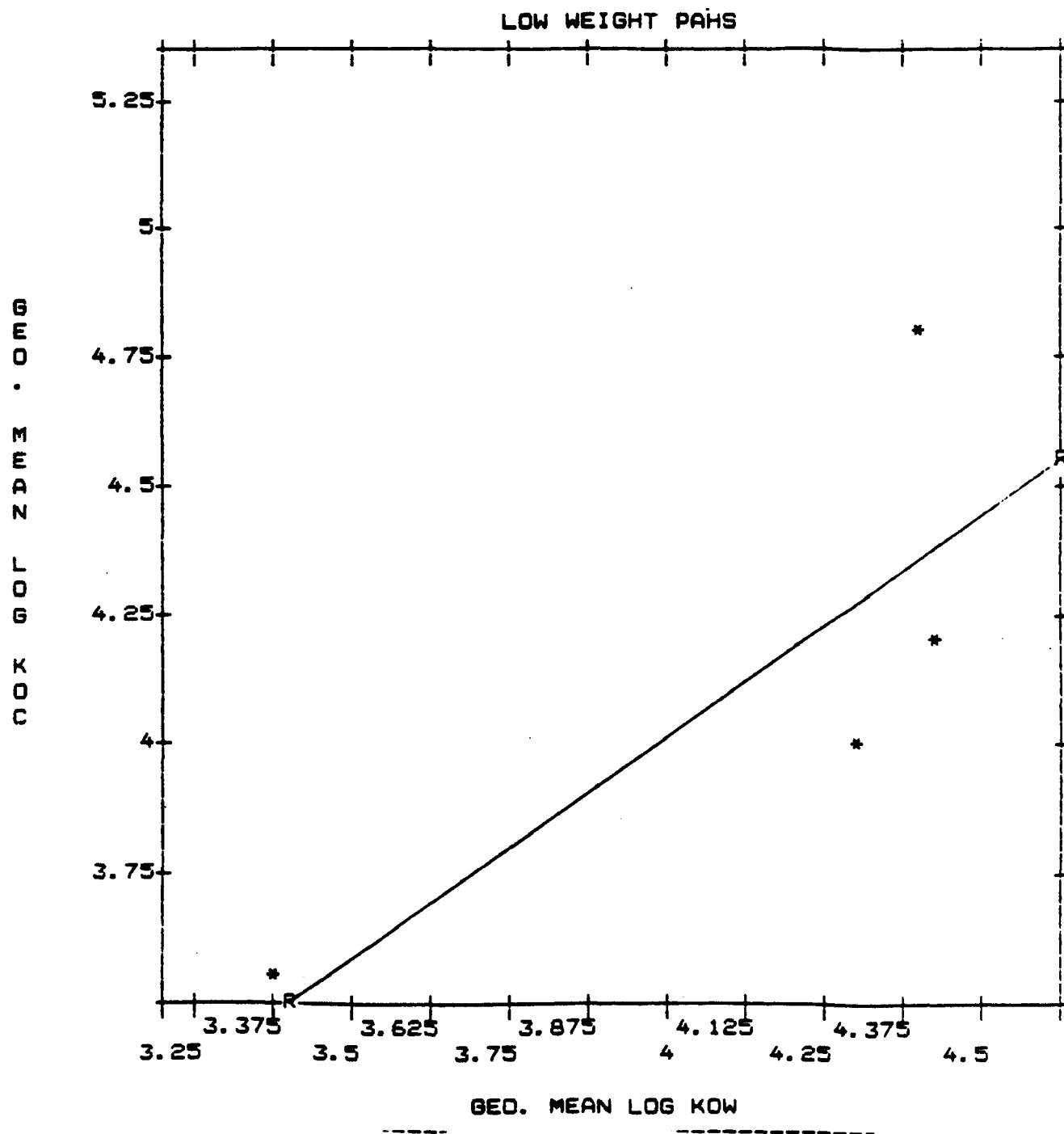
21 cases plotted. Regression statistics of GKOC on GKOW:  
 Correlation .87403 R Squared .76393 S.E. of Est .68913 Sig. .00  
 Intercept(S.E.) .41891( .56402) Slope(S.E.) .88086( .11234

FIGURE 1 PLOT OF GEOMETRIC MEAN LOG  $K_{ow}$  VS. GEOMETRIC MEAN LOG  $K_{oc}$  FOR ALL COMPOUNDS



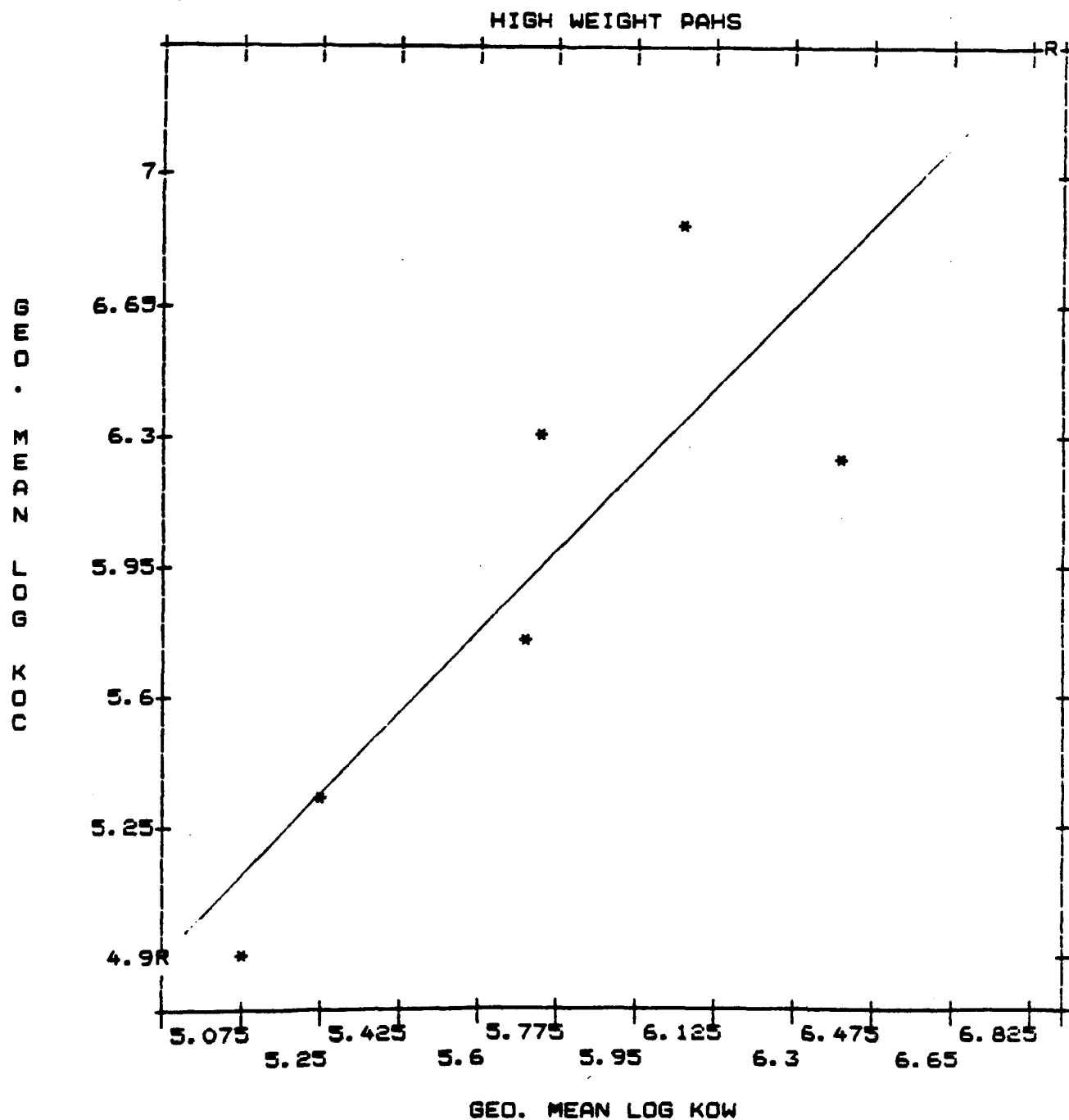
10 cases plotted. Regression statistics of GKOC on GKOW:  
 Correlation .94519 R Squared .89339 S.E. of Est .37906 Sig. .0000  
 Intercept (S.E.) -.37610 ( .69030) Slope (S.E.) 1.09591 ( .13385)

FIGURE 2 PLOT OF GEOMETRIC MEAN LOG K<sub>OW</sub> VS. GEOMETRIC MEAN LOG K<sub>OC</sub>  
 FOR ALL PAHS



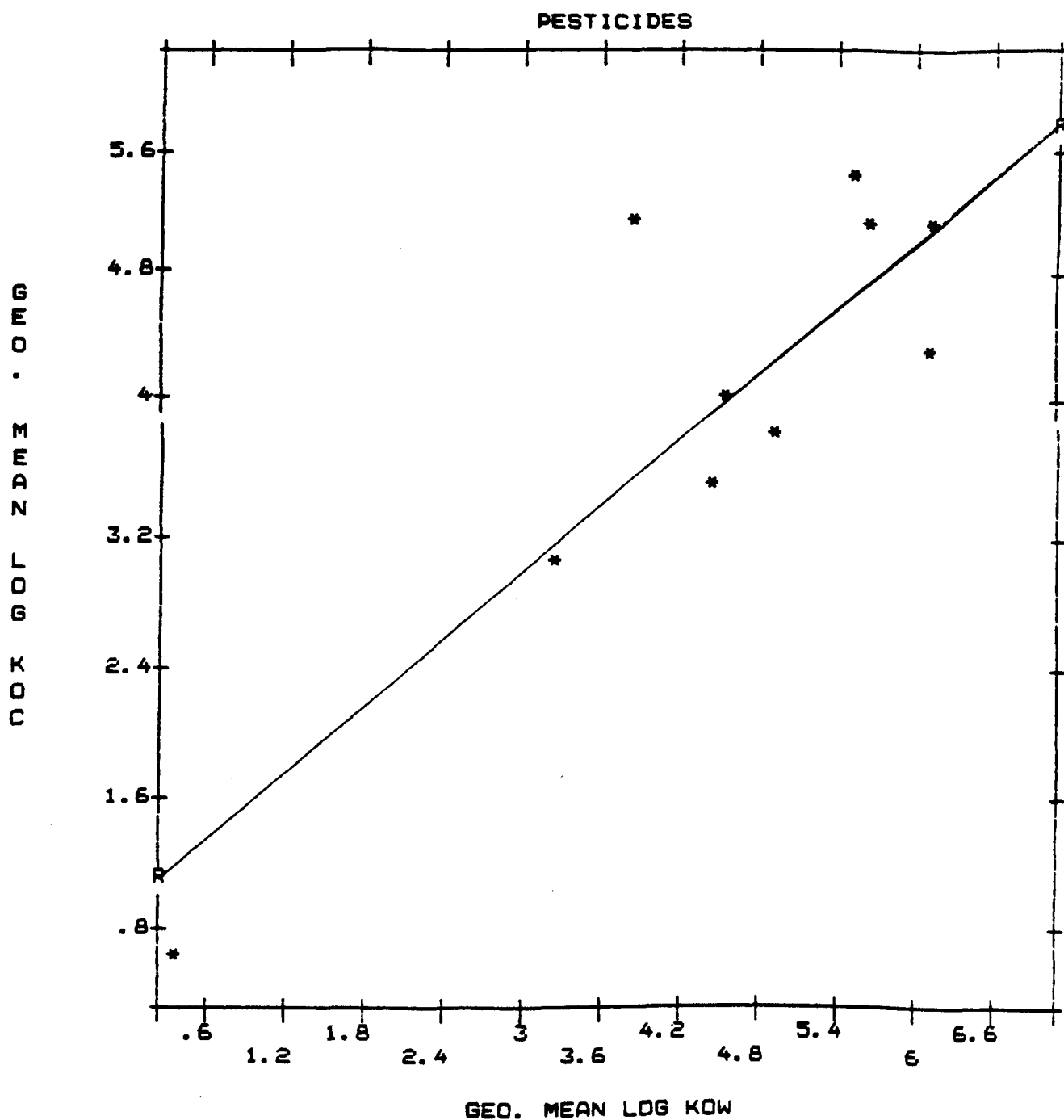
4 cases plotted. Regression statistics of GKOC on GKOW:  
 Correlation .80415 R Squared .64665 S.E. of Est .37146 Sig. .195  
 Intercept (S.E.) .76259 ( 1.77510) Slope (S.E.) .81827 ( .42771)

FIGURE 3 PLOT OF GEOMETRIC MEAN LOG  $K_{ow}$  VS. GEOMETRIC MEAN LOG  $K_{oc}$   
 LOW WEIGHT PAHS



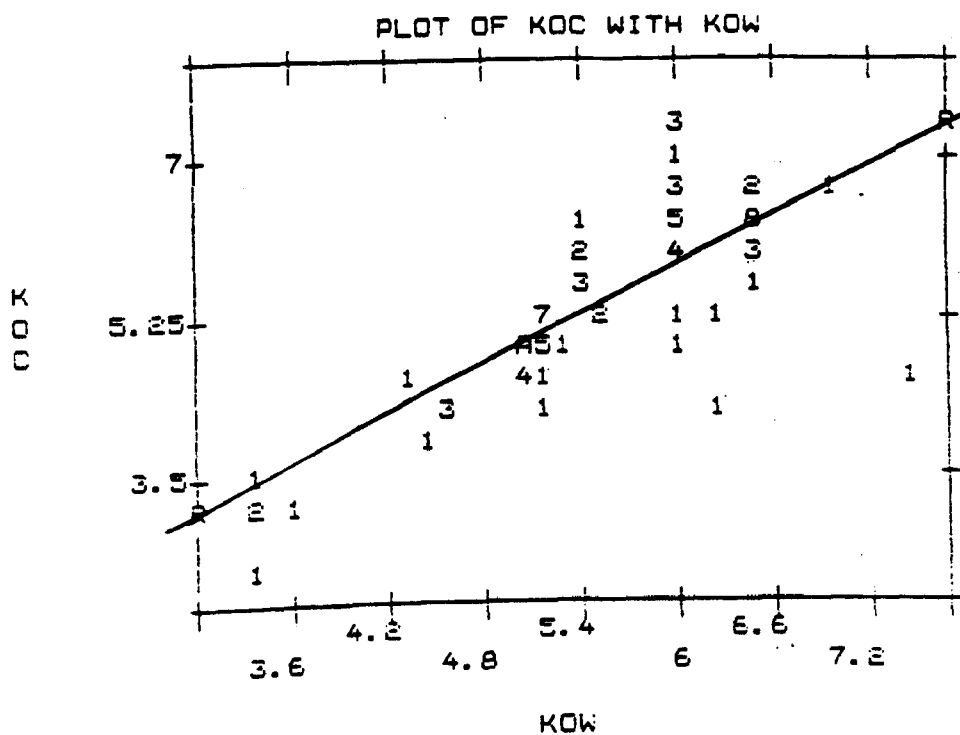
6 cases plotted. Regression statistics of GKOC on GKOW:  
 Correlation .83711 R Squared .70076 S.E. of Est .44535 Sig. .0376  
 Intercept(S.E.) -1.13018( 2.30094) Slope(S.E.) 1.22874( .40147)

FIGURE 4 PLOT OF GEOMETRIC MEAN LOG  $K_{ow}$  VS. GEOMETRIC MEAN LOG  $K_{oc}$  FOR HIGH WEIGHT PAHS.



10 cases plotted. Regression statistics of GKOC on GKOW;  
 Correlation .86868 R Squared .75461 S.E. of Est .74235 Sig. .0011  
 Intercept(S.E.) .80243( .68913) Slope(S.E.) .71715( .14459)

FIGURE 5 PLOT OF GEOMETRIC MEAN LOG  $K_{OW}$  VS. GEOMETRIC MEAN LOG  $K_{OC}$   
 FOR PESTICIDES



83 cases plotted. Regression statistics of KOC on KOW:  
 Correlation .81825 R Squared .66953 S.E. of Est .58262 Sig. .0000  
 Intercept(S.E.) -.08695( .43060) Slope(S.E.) .98818( .07714)

FIGURE 6 PLOT OF GEOMETRIC MEAN LOG  $K_{ow}$  VS. GEOMETRIC MEAN LOG  $K_{oc}$   
 FOR ALL COMPOUNDS USING RAW DATA POINTS

Figure 7 Plot of Residuals For All Compounds Regression Equation

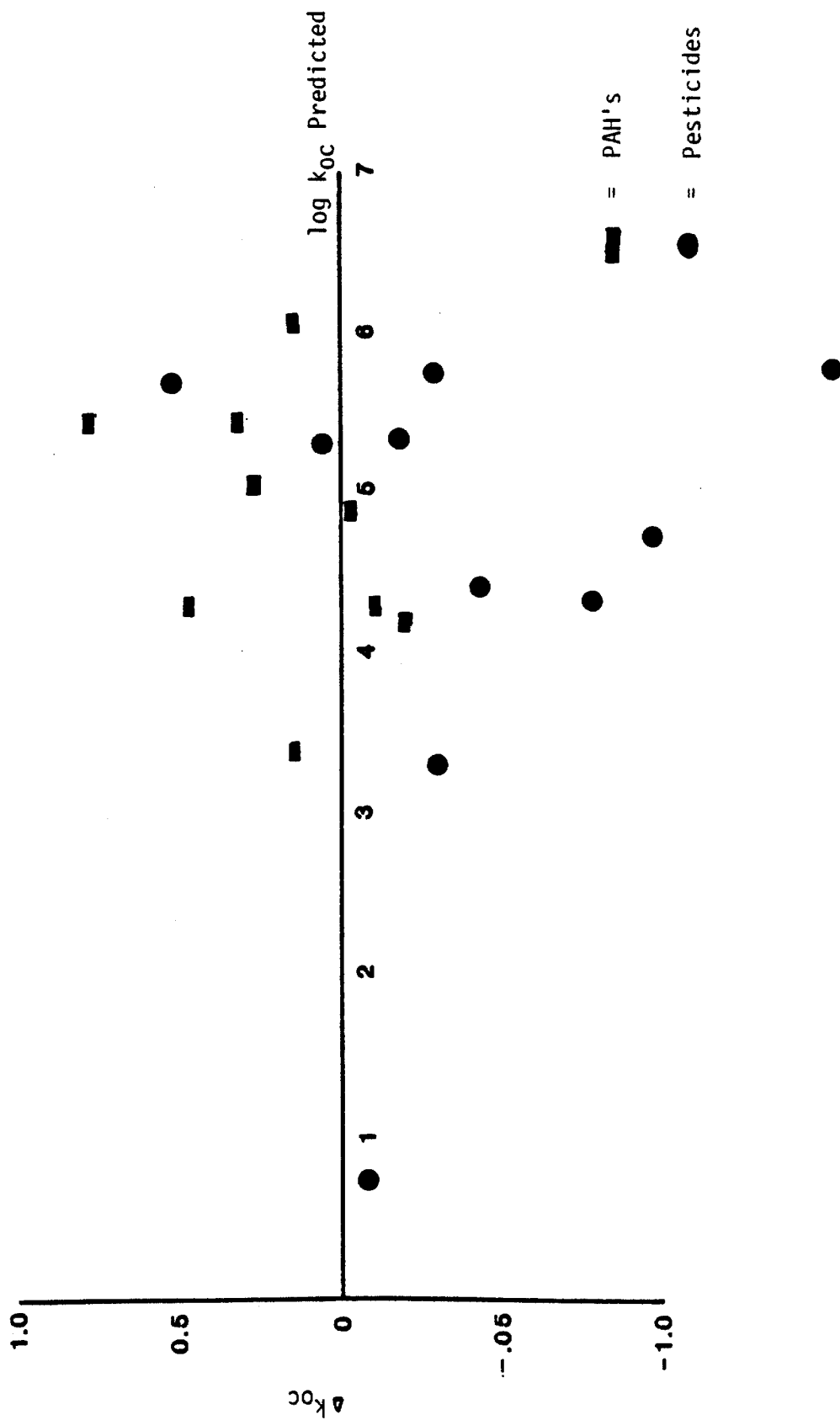




Figure 8 Plot of Residuals For All PAH's Regression Equation

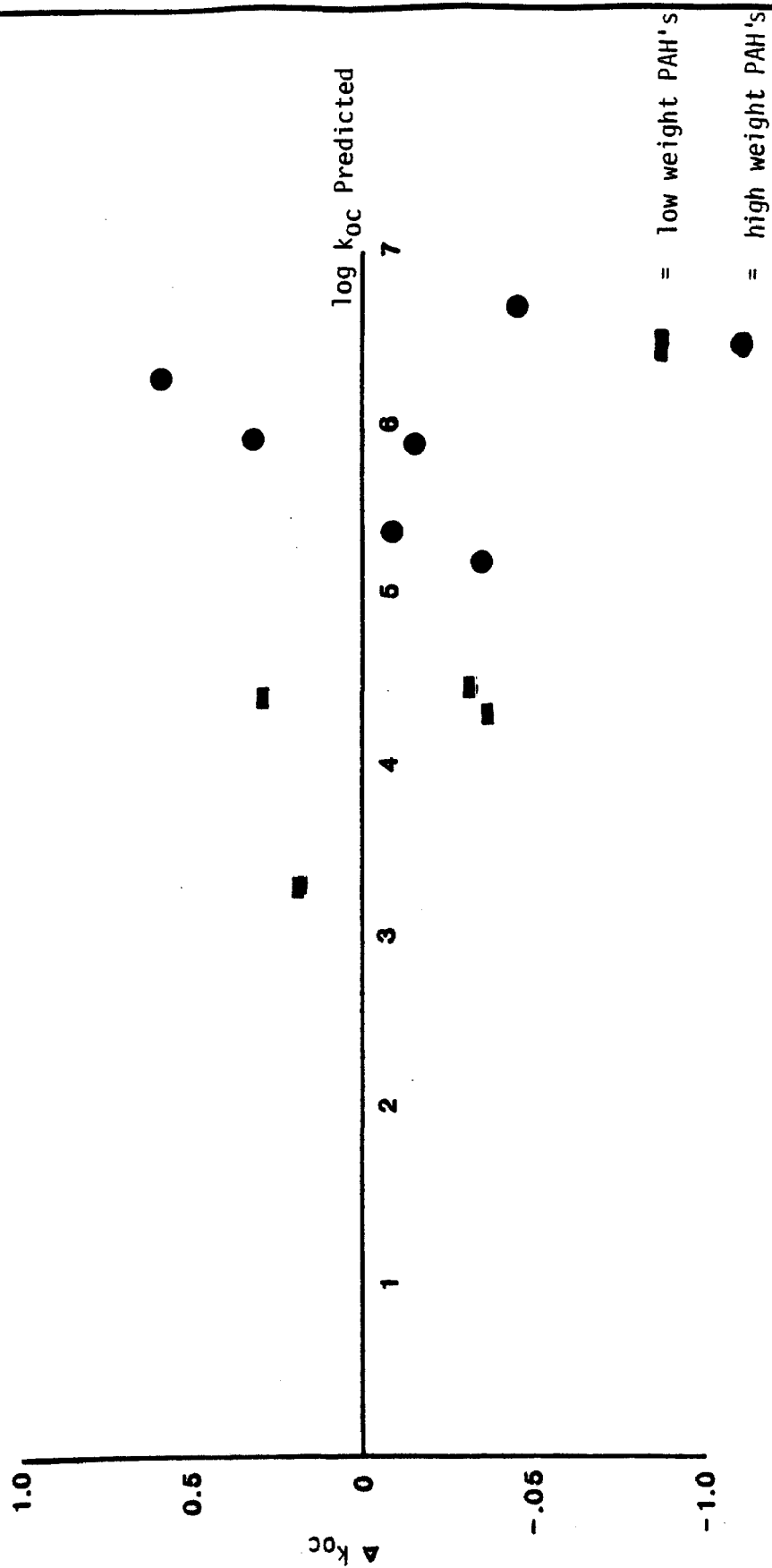


Figure 9 Plot of Residuals For Pesticide Regression Equation



## **APPENDIX III**

### **BIBLIOGRAPHY**

### APPENDIX III - BIBLIOGRAPHY

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**APPENDIX IV**

**NAMES AND ADDRESSES OF INDIVIDUALS  
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