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WATER

Proposed Sediment Quality Criteria for the Protection of Benthic Organisms:

PHENANTHRENE

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FOREWORD

Under the Clean Water Act (CWA) the U.S. Environmental Protection Agency (U.S. EPA) is responsible for protecting the chemical, physical, and biological integrity of the nation's waters. Section 104 of the CWA authorizes the Administrator to conduct and promote research into the causes, effects, extent, prevention, reduction, and elimination of pollution, and to publish relevant information. Section 104(n)(1) in particular provides for study of the effects of pollution, including sedimentation, in estuaries on aquatic life. Section 304(a)(1) directs the Administrator to develop and publish "criteria" reflecting the latest scientific knowledge on the kind and extent of effects on plankton, fish, shellfish, and wildlife which may be expected from the presence of pollutants in any body of water, including ground water, the concentration and dispersal of pollutants, or their byproducts, through biological, physical and chemical processes; and the effects of pollutants on biological community diversity, productivity, and stability. Section 304(a)(2) directs the administrator to develop and publish information on the factors necessary for the protection and propagation of shellfish, fish, and wildlife for classes and categories of receiving waters.

To meet this objective, in 1980 EPA published ambient water quality criteria (WQC) for 64 of the 65 toxic pollutants or pollutant categories designated as toxic under Section 307(a)(1) of the CWA. Additional water quality documents that update criteria for selected consent decree chemicals and new criteria have also been published since 1980. In addition to the development of water quality criteria and to continue to comply with the mandate of the CWA, EPA has conducted efforts to develop and publish sediment quality criteria for some of the 65 toxic pollutants or toxic pollutant categories.

Toxic contaminants in bottom sediments of the nations's lakes, rivers, wetlands, and coastal waters create the potential for continued environmental degradation even where water column contaminant levels comply with established water quality criteria. In addition, contaminated sediments can lead to water quality degradation, even when pollutant sources are stopped. It is intended that sediment quality criteria be used to assess the extent of sediment contamination, to aid in implementing measures to limit or prevent additional contamination and to identify and implement appropriate remediation activities when needed.

The criteria presented in this document are the U.S. Environmental Protection Agency's best recommendation of the concentrations of a substance in sediment that will not unacceptably affect benthic organisms. These criteria are applicable to a variety of freshwater and marine sediments because they are based on the biologically available concentration of the substance in sediments. These criteria do not protect against additive, synergistic or antagonistic effects of contaminants or bioaccumulative effects to aquatic life or human health.

The criteria and derivation methods outlined in this document are proposed to provide protection of benthic organisms from biological impacts from chemicals associated with sediments. Recommendations on the use of these criteria will follow completion of the public response process. In the interim, until final Sediment Quality Criteria are promulgated, these criteria should only be used to support site specific assessments for sediments that are consistent with assumptions of equilibrium partitioning theory on which these Sediment Quality Criteria are developed.

Guidelines and guidance have been developed by EPA to assist in the application of criteria presented in this document, in the development of sediment quality standards, and in other water-related programs of this Agency.

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SECTION 1

INTRODUCTION

1.1 GENERAL INFORMATION:

Under the Clean Water Act (CWA) the U.S. Environmental Protection Agency (U.S. EPA) is responsible for protecting the chemical, physical and biological integrity of the nation's waters. In keeping with this responsibility, U.S. EPA published ambient water quality criteria (WQC) in 1980 for 64 of the 65 toxic pollutants or pollutant categories designated as toxic in the CWA. Additional water quality documents that update criteria for selected consent decree chemicals and new criteria have been published since 1980. These water quality criteria are numerical concentration limits that are the U.S. EPA's best estimate of concentrations protective of human health and the presence and uses of aquatic life. While these water quality criteria play an important role in assuring a healthy aquatic environment, they alone are not sufficient to ensure the protection of environmental or human health.

Toxic pollutants in bottom sediments of the nation's lakes, rivers, wetlands, estuaries and marine coastal waters create the potential for continued environmental degradation even where water-column concentrations comply with established water quality criteria. In addition, contaminated sediments can be a significant pollutant source that may cause water quality degradation to persist, even when other pollutant sources are stopped. The absence of defensible sediment quality criteria (SQC) makes it difficult to accurately assess the extent of the ecological risks of contaminated sediments and to identify, prioritize and implement appropriate clean up activities and source controls. As a result of the need for a procedure to assist regulatory agencies in making decisions concerning contaminated sediment problems, a U.S. EPA Office of Science and Technology, Health and Ecological Criteria Division (OST/HEC) research team was established to review alternative approaches (Chapman, 1987).

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All of the approaches reviewed had both strengths and weaknesses and no single approach was found to be applicable for SQC derivation in all situations (U.S. EPA, 1989a). The equilibrium partitioning (EqP) approach was selected for non-ionic organic chemicals because it presented the greatest promise for generating defensible national numerical chemical-specific sediment quality criteria applicable across a broad range of sediment types. The three principal observations that underlie the EqP method of establishing sediment quality criteria are:

1. The concentrations of non-ionic organic chemicals in sediments, expressed on an organic carbon basis, and in pore waters correlate to observed biological effects on sediment dwelling organisms across a range of sediments.

2. Partitioning models can relate sediment concentrations for non-ionic organic chemicals on an organic carbon basis to pore water concentrations.

3. The distribution of sensitivities of benthic and water column organisms to chemicals are similar; thus, the currently established water quality criteria final chronic values (FCV) can be used to define the acceptable effects concentration of a chemical freely-dissolved in pore water.

The EqP approach, therefore, assumes that: (1) the partitioning of the chemical between sediment organic carbon and interstitial water is at equilibrium; (2) the concentration in either phase can be predicted using appropriate partition coefficients and the measured concentration in the other phase; (3) organisms receive equivalent exposure from water-only exposures or from any equilibrated phase: either from pore water via respiration, from sediment via ingestion or from a mixture of both exposure routes; (4) for non-ionic chemicals, effect concentrations in sediments on an organic carbon basis can be predicted using the organic carbon partition coefficient (K_{oc}) and effects concentrations in water; (5) the FCV concentration is an appropriate effects concentration for freely-dissolved chemical in interstitial water; and (6) the SQC ($\mu g/g_{oc}$) derived as the product of the K_{oc} and FCV is protective of benthic organisms. Sediment quality criteria concentrations presented in this document are expressed as μg

chemical/g sediment organic carbon and not on an interstitial water basis because: (1) pore water is difficult to adequately sample; and (2) significant amounts of the dissolved chemical may be associated with dissolved organic carbon; thus, interstitial concentrations may overestimate exposure.

The data that support the equilibrium partitioning approach for deriving SQC for non-ionic organic chemicals are reviewed by Di Toro et al. (1991) and in the sediment quality criteria guidelines (U.S. EPA, 1992a). Data supporting these observations for phenanthrene are presented in this document.

Sediment quality criteria generated using the equilibrium partitioning method are suitable for use in providing guidance to regulatory agencies because they are:

1. numerical values;

2. chemical specific;

3. applicable to most sediments;

4. predictive of biological effects; and

5. protective of benthic organisms.

As is the case with water quality criteria, the sediment quality criteria reflect the use of available scientific data to: (1) assess the likelihood of significant environmental effects to benthic organisms from chemicals in sediments; and (2) to derive regulatory requirements which will protect against these effects.

It should be emphasized that these criteria are intended to protect benthic organisms from the effects of chemicals associated with sediments. SQC are intended to apply to sediments permanently inundated with water, intertidal sediment and to sediments inundated periodically for durations sufficient to permit development of benthic assemblages. They do not apply to occassionally inundated soils containing terrestrial organisms. In spills, where chemical equilibrium between water and sediments has not yet been reached, sediment chemical concentrations in excess of SQC indicate benthic organisms may be at risk. This is because for

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spills, disequilibrium concentrations in interstitial and overlying water may be proportionally higher relative to sediment concentrations. In spills, sediments having concentrations less than SQC may also pose risks to benthic organisms. These criteria do not address the question of possible contamination of upper trophic level organisms or the synergistic, additive or antagonistic effects of multiple chemicals. SQC addressing these issues may result in values lower or higher than those presented in this document. The SQC presented in this document represent the U.S. Environmental Protection Agency's best recommendation at this time of the concentration of a chemical in sediment that will not unacceptably affect benthic organisms. SQC values may be adjusted to account for future data or site specific considerations.

This document presents the theoretical basis and the supporting data relevant to the derivation of the sediment quality criterion for phenanthrene. An understanding of the "Guidelines for Deriving Numerical National Water Quality Criteria for the Protection of Aquatic Organisms and Their Uses" (Stephan et al., 1985), response to public comment (U.S. EPA, 1985) and "Guidelines for Deriving Numerical National Sediment Quality Criteria for Non-ionic Organic Chemicals for the Protection of Benthic Organisms" (U.S. EPA, 1992a) is necessary in order to understand the following text, tables and calculations. Guidance into the acceptable use of SQC values is contained in U.S. EPA, 1992b.

1.2 GENERAL INFORMATION: PHENANTHRENE

Phenanthrene is a member of the polycyclic aromatic hydrocarbon (PAH) group of organic compounds. Phenanthrene is produced by fractional distillation of high-boiling coal-tar oil and the subsequent purification of the crystalline solid (Hawley, 1981). Some uses of phenanthrene are in the manufacturing of dyestuffs and explosives, in the synthesis of drugs and in biochemical research (Verschueren, 1983). Some PAHs are of environmental concern because they are known to be carcinogens and/or mutagens (Brookes, 1977). With an increase in fossil fuel consumption in the United States an increase in emissions of PAHs to the environment can

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be expected over the next several decades (Eadie et al., 1982).

Phenanthrene has a three ring structure and exists as colorless leaflets (Figure 1-1). It has a solubility in water at 25°C of 1.18 mg/L and is a solid at room temperature (melting point of 100.85°C) (Miller et al., 1985). Phenanthrene has a reported vapor pressure of 69.3 - 110.6 mPa at 25°C (Bidleman, 1984). Two significant processes which can influence the fate of phenanthrene in the sediment are sorption and biodegradation (U.S. EPA, 1980). Sorption of phenathrene onto solids in the water column and subsequent settling, as well as partitioning onto organics in the sediment, can significantly affect phenanthrene transport. Bioaccumulated PAHs with 4 rings or less are rapidly metabolized. Therefore, long-term partitioning into biota is not considered a significant fate process (U.S. EPA, 1980). Other processes found to have little or no effect on the fate of phenanthrene in the sediment are oxidation, hydrolysis and volatilization (U.S. EPA, 1980).

The acute toxicity of phenanthrene ranges from 96 to > 1150 ug/L for freshwater and 21.9 to 600 μg/L for saltwater organisms (Appendix A). Differences between phenanthrene concentrations causing acute lethality and chronic toxicity in invertebrates are small; acute-chronic ratios range from 1.2 to 3.3 for two species. The only available acute-chronic ratio for rainbow trout is 59 (Table 3-3). Although phenanthrene bioaccumulates in aquatic biota, the associated health or ecological risks are unknown.

1.3 OVERVIEW OF DOCUMENT:

The goal of this document is to provide a brief review of the equilibrium partitioning methodology, a summary of the physical-chemical properties and aquatic toxicity of phenanthrene, and the technical basis for setting the SQC for phenanthrene. Section 2 reviews a variety of methods and data useful in deriving partition coefficients for phenanthrene and includes the K_{oc} recommended for use in the derivation of the phenanthrene SQC. Section 3
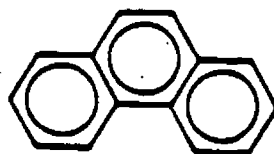
MOLECULAR FORMULA	C14H10
MOLECULAR WEIGHT	178.22
DENSITY	1.179 g/cc @25 C
MELTING POINT	100.85 C
PHYSICAL FORM	colorless leaflets
VAPOR PRESSURE	5.2x10-4 to 8.3x10-4 mm Hg at 25 C
CAS NUMBER	85-0108
CHEMICAL NAME	Phenanthrene

FIGURE 1-1. Chemical structure and physical-chemical properties of phenanthrene

reviews aquatic toxicity data contained in the phenanthrene WQC document (U.S. EPA, 1980) and new data that were used to derive the Final Chronic Value (FCV) used in this document to derive the SQC concentration. In addition, the comparative sensitivity of benthic and water column species is examined as the justification for the use of the FCV for phenanthrene in the derivation of the SQC. Section 4 reviews data on the toxicity of phenanthrene in sediments, the need for organic carbon normalization of phenanthrene sediment concentrations and the accuracy of the EqP prediction of sediment toxicity using K_{oc} and an effect concentration in water. Data from Sections 2, 3 and 4 are used in Section 5 as the basis for the derivation of the SQC for phenanthrene and its uncertainty. The SQC for phenanthrene is then compared to STORET (U.S. EPA, 1989b) and National Status and Trends (NOAA, 1991) data on phenanthrene's environmental occurrence in sediments. Section 6 concludes with the criteria statement for phenanthrene. The references used in this document are listed in Section 7.

SECTION 2

PARTITIONING

2.1 DESCRIPTION OF THE EQUILIBRIUM PARTITIONING METHODOLOGY:

Sediment quality criteria are the numerical concentrations of individual chemicals which are intended to be predictive of biological effects, protective of the presence of benthic organisms and applicable to the range of natural sediments from lakes, streams, estuaries and near coastal marine waters. As a consequence, they can be used in much the same way as water quality criteria; ie., the concentration of a chemical which is protective of the intended use such as aquatic life protection. For non-ionic organic chemicals, SQC are expressed as μg chemical/g organic carbon and apply to sediments having $\geq$ 0.2% organic carbon by dry weight. A brief overview follows of the concepts which underlie the equilibrium partitioning methodology for deriving sediment quality criteria. The methodology is discussed in detail in the "Guidelines for Deriving Numerical National Sediment Quality Criteria for Non-ionic Organic Chemicals for Protection of Benthic Organisms" (U.S. EPA, 1992a), hereafter referred to as the SQC Guidelines.

Bioavailability of a chemical at a particular sediment concentration often differs from one sediment type to another. Therefore, a method is necessary for determining a sediment quality criterion based on the bioavailable chemical fraction in a sediment. For non-ionic organic chemicals, the concentration-response relationship for the biological effect of concern can most often be correlated with the interstitial water (i.e., pore water) concentration (μg chemical/liter pore water) and not to the sediment chemical concentration (μg chemical/g sediment) (Di Toro et al., 1991). From a purely practical point of view, this correlation suggests that if it were possible to measure the pore water chemical concentration, or predict it from the total sediment concentration and the relevant sediment properties, then that concentration could be used to quantify the exposure concentration for an organism. Thus, knowledge of the partitioning of

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chemicals between the solid and liquid phases in a sediment is a necessary component for establishing sediment quality criteria. It is for this reason that the methodology described below is called the equilibrium partitioning (EqP) method.

It is shown in the SQC Guidelines (U.S. EPA, 1992a), that benthic and water column species from freshwater and saltwater environments exhibit similar sensitivities to a wide range of chemicals. The data for phenanthrene are presented in Section 3. Thus, a sediment quality criteria can be established using the final chronic value (FCV) derived using the Water Quality Criteria Guidelines (Stephan et al., 1985) as the effect concentration, and the partition coefficient can be used to relate the pore water concentration (FCV) to the sediment quality criteria via the partitioning equation.

The calculation is as follows: Let FCV (μg/L) be the no effect concentration in water for the chemical of interest; then the sediment quality criteria, SQC (μg/kg sediment), is computed using the partition coefficient, K_p (L/kg sediment), between sediment and water:

$$SQC = K_p \text{ FCV} \tag{2-1}$$

This is the fundamental equation used to generate the sediment quality criterion. Its utility depends upon the existence of a methodology for quantifying the partition coefficient, K_p.

For phenanthrene, and other hydrophobic non-ionic organic chemicals, the chemical property of importance is the octanol-water partition coefficient, K_{ow}. It is empirically related to the partition coefficient via K_{oc} (Equation 2-5), the organic carbon partition coefficient, and f_{oc}, the weight fraction of organic carbon in the sediment (g_{oc}/g sediment). Organic carbon appears to be the predominant sorption phase for non-ionic organic chemicals in naturally occurring sediments. The relationship is as follows:

$$K_p = f_{oc} K_{oc} \tag{2-2}$$

It follows that:

$$SQC_{oc} = K_{oc} \text{ FCV} \tag{2-3}$$

where SQC_{oc} is the sediment quality criterion on a sediment organic carbon basis.

The next section reviews the available information for K_{ow}.

2.2 DETERMINATION OF K_{ow} FOR PHENANTHRENE:

Several approaches have been used to determine K_{ow} for the derivation of a SQC, as discussed in the SQC Guidelines. At the U.S. EPA, Environmental Research Laboratory at Athens, GA (ERL,A) two methods were selected for measurement and two for estimation of K_{ow}. The measurement methods were shake-centrifugation (SC), generator column (GCol) and the estimation methods were SPARC and CLOGP (Appendix B). Data were also extracted from the literature. The shake-centrifugation method is a standard procedure in the Organization for Economic Cooperation and Development (OECD) guidelines for testing chemicals, therefore it has regulatory precedence.

Examination of the literature reveals that the $log_{10}K_{ow}$ values for phenanthrene range from 4.28 to 4.64.

Preliminary experience with the SPARC program suggests that the program can compute values for partition coefficients for high logP chemicals which may be more reliable and accurate than laboratory measurements which may suffer from errors inherent in many methodologies. However, the program needs more validation by comparison with laboratory-measured data for a wide range of chemical structures before it is recommended as a basis for computing partition coefficients for regulatory purposes. The SPARC estimated $log_{10}K_{ow}$ value for phenanthrene is 4.58. The CLOGP program estimate of the $log_{10}K_{ow}$ value for phenanthrene using structure activity relationships is 4.49.

Two measurement methods provide additional data from which to define K_{ow} for phenanthrene (Table 2-1; Appendix B). The shake-centrifugation method yielded $log_{10}K_{ow}$ = 4.30, and the generator column method yielded $log_{10}K_{ow}$ = 4.40. There is no clear-cut best value from the data that has been developed. Considering the agreement among the SPARC

estimated value and the measured values using shake-centrifugation and generator column methods, the recommended vaue for $\log_{10}K_{ow}$ is 4.36. This is the $\log_{10}K_{ow}$ of the average of shake-centrifugation and generator column measurements made under carefully controlled conditions in the ERL, Athens Laboratory. The four shake-centrifugation measurements range from 4.25 to 4.33 and the four generator column measurements range from 4.24 to 4.47.

TABLE 2-1. SUMMARY OF MEASURED AND ESTIMATED K_{ow} VALUES FOR PHENANTHRENE BY THE U.S. EPA, ENVIRONMENTAL RESEARCH LABORATORY, ATHENS, GA.

Measurement Technique	Number of Analyses	$\log_{10}K_{ow}$	
		Mean	CV
Shake-Centrifugation	4	4.30	0.075
Generator Column	4	4.40	0.190
SPARC	-	4.58	-
CLOGP	-	4.49	-

2.3 DERIVATION OF K_{oc} FROM ADSORPTION STUDIES:

Several types of experimental measurement of the organic carbon partition coefficient are available. The first type involves experiments which were designed to measure the partition coefficient in particle suspensions. The second type of measurement is from sediment toxicity tests in which sediment phenanthrene and pore water phenanthrene concentrations are used to compute K_{oc}.

2.3.1 K_{oc} FROM PARTICLE SUSPENSION STUDIES:

Laboratory studies to characterize adsorption are generally conducted using particle suspensions. The high concentrations of solids and turbulent conditions necessary to keep the mixture in suspension make data interpretation difficult as a result of a particle interaction

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effect. This effect suppresses the partition coefficient relative to that observed for undisturbed sediments (Di Toro, 1985; Mackay and Powers, 1987).

Based on analysis of an extensive body of experimental data for a wide range of compound types and experimental conditions, the particle interaction model (Di Toro, 1985) yields the following relationship for estimating K_p:

$$K_p = \frac{f_{oc} K_{oc}}{1 + mf_{oc} K_{oc} / \nu_x} \qquad (2-4)$$

where:

m = particle concentration in the suspension (kg/L)

ν_x = 1.4, an empirical constant (unitless).

The other quantities are defined previously. In this expression, the organic carbon partition coefficient is given by:

$$\log_{10}K_{oc} = 0.00028 + 0.983 \log_{10}K_{ow} \qquad (2-5)$$

A sorption isotherm experiment that demonstrates the effect of particle suspensions was found in a comprehensive literature search for partitioning information for phenanthrene (Table 2-2) (Magee et al., 1991). The experiment showed an observed K_p of 12.9 L/kg for a phenanthrene solution and sand with 0.11% organic carbon content. Calculated K_p using K_{oc} (Equation 2-5) and f_{oc} is 21 L/kg. The difference between the observed and calculated K_p can be explained by particle interaction effects. Particle interaction results in a lower observed partition coefficient. The particle interaction model (Equation 2-4) predicts K_p of 8.29 L/kg, which is in agreement with the observed K_p. $\log_{10}K_{oc}$ computed from observed K_p and f_{oc} is 4.07. This value is lower than K_{oc} from laboratory measurements due to particle interaction effects. This data is presented as an example of particle interaction effects only, as 100 percent reversibility is assumed in the absence of a desorption study and an actual K_{oc} can not be computed.

TABLE 2-2. SUMMARY OF K_{oc} VALUES FOR PHENANTHRENE
DERIVED FROM LITERATURE SORPTION ISOTHERM DATA.

Observed $Log_{10}K_{oc}$	n	Solids (g/L)	References
4.07	1	100	Magee et al., 1991

In the absence of particle effects, K_{oc} is related to K_{ow} via Equation 2-5, shown above. For $log_{10}K_{ow}$ = 4.36 (ERL,A, mean measured value), this expression results in an estimate of $log_{10}K_{oc}$ = 4.29.

2.3.2 K_{oc} FROM SEDIMENT TOXICITY TESTS:

Measurements of K_{oc} are available from sediment toxicity tests using phenanthrene (Swartz, 1991). These tests represent freshwater sediments having a range of organic carbon contents of 0.82 to 3.6 percent (Table 4-1; Appendix C). Phenanthrene concentrations were measured in the sediment and pore waters providing the data necessary to calculate the partition coefficient for an undisturbed sediment.

Figure 2-1 is a plot of the organic carbon-normalized sorption isotherm for phenanthrene, where the sediment phenanthrene concentration ($\mu g/g_{oc}$) is plotted versus pore water concentration ($\mu g/L$). The data used to make this plot are included in Appendix C. The line of unity slope corresponding to the $log_{10}K_{oc}$ = 4.29 is compared to the data. The intercept at a pore water concentration of 1 $\mu g/L$ is equivalent to $log_{10}K_{oc}$.

A probability plot of the observed experimental $log_{10}K_{oc}$ values is shown in Figure 2-1. The $log_{10}K_{oc}$ values are approximately normally distributed with a mean of $log_{10}K_{oc}$ = 4.33 and a standard error of the mean of 0.016. This value is statistically indistinguishable from $log_{10}K_{oc}$ = 4.29, which was computed from the experimentally determined phenanthrene $log_{10}K_{ow}$ of 4.36 (Equation 2-5). Complexation with pore water DOC has not been accounted

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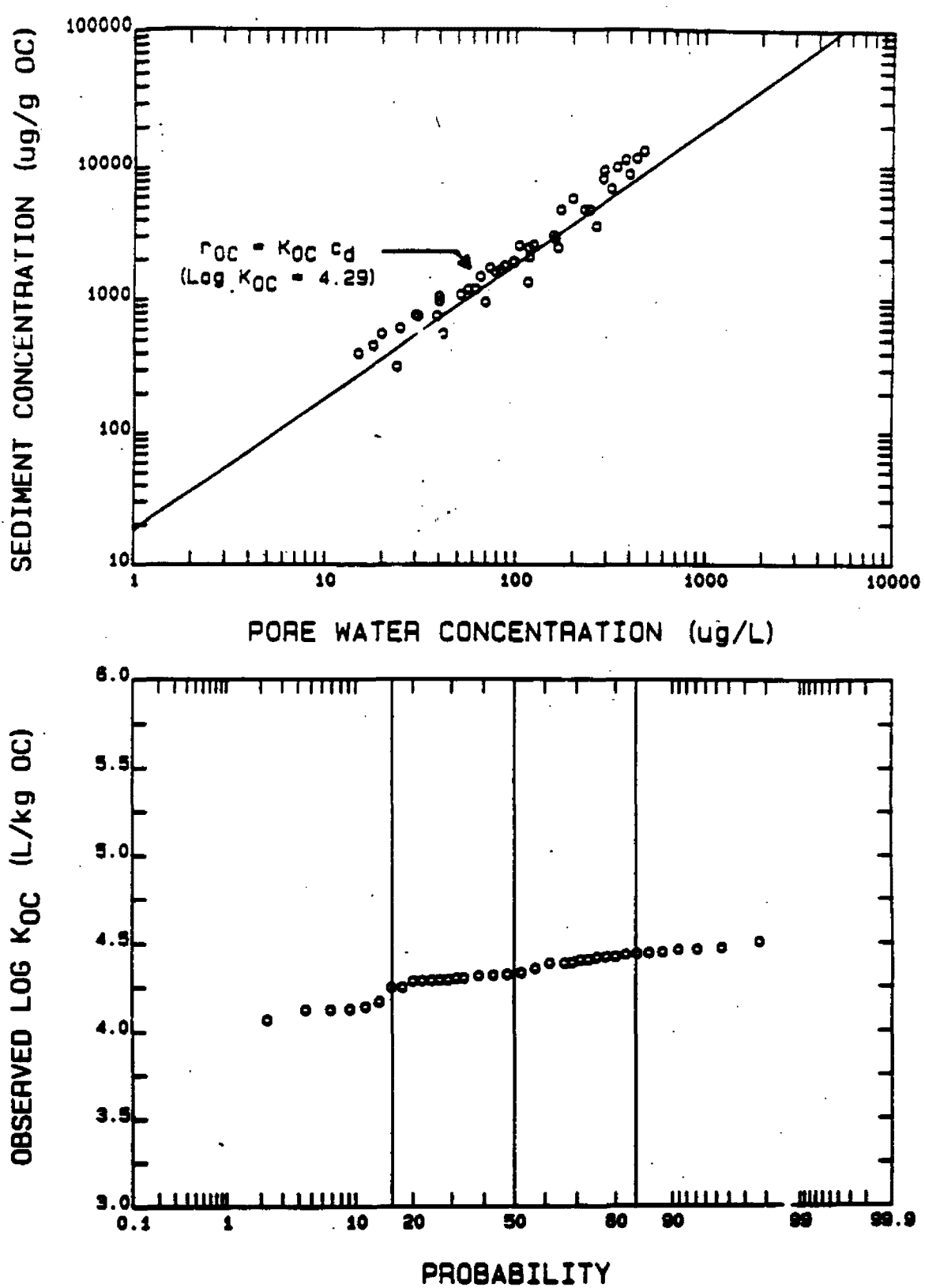
Figure 2-1. Organic carbon-normalized sorption isotherm for phenanthrene (top) and probability plot of K_{oc} (bottom) from sediment toxicity tests conducted by Swartz (1991).

for in the experimentally based estimate of $\log_{10}K_{OC} = 4.33$. Though it is not expected to be a major factor, consideration of DOC effect would increase the estimate of $\log_{10}K_{OC}$ relative to the value based on total pore water concentrations. If this uncorrected value was used to set SQC, the SQC concentration would tend to be environmentally conservative.

2.4 SUMMARY OF DERIVATION OF K_{OC} FOR PHENANTHRENE:

The K_{OC} selected to calculate the sediment quality criteria for phenanthrene is based on the regression of $\log_{10}K_{OC}$ to $\log_{10}K_{OW}$ (Equation 2-5), using the phenanthrene $\log_{10}K_{OW}$ of 4.36 recently measured by ERL,A. This approach was adopted because the regression equation is based on the most robust data set available that spans a broad range of chemicals and particle types, thus encompassing a wide range of K_{OW} and f_{OC}. The regression equation yields $\log_{10}K_{OC}$ = 4.29. This value is in agreement with the $\log_{10}K_{OC}$ of 4.33 measured in the sediment toxicity tests.

SECTION 3

TOXICITY OF PHENANTHRENE: WATER EXPOSURES

3.1 TOXICITY OF PHENANTHRENE IN WATER: DERIVATION OF PHENANTHRENE WATER QUALITY CRITERIA:

The equilibrium partitioning method for derivation of sediment quality criteria uses the phenanthrene water quality criterion Final Chronic Value (FCV) and partition coefficients (K_{oc}) to estimate the maximum concentrations of non-ionic organic chemicals in sediments, expressed on an organic carbon basis, that will not cause adverse effects to benthic organisms. For this document, life stages of species classed as benthic are either species that live in the sediment (infauna) or primarily on the sediment surface (epibenthic) and obtain their food from either the sediment or water column (U.S. EPA, 1989c). The toxicological basis for derivation of the final chronic value and the justification for use of this value as the effects concentration or sediment quality criteria derivation are discussed in this section.

3.2 ACUTE TOXICITY - WATER EXPOSURES:

Fourteen standard toxicity tests with phenanthrene have been conducted on 9 freshwater species from 8 genera (Appendix A). Overall genus mean acute values (GMAVs) range from 96 to > 1,150 μg/L. The acute values for all species tested, except for fathead minnows, differed by only a factor of 5; 96 to 490 μg/L. Three tests on three benthic species from three genera are contained in this database (Table 3-1; Appendix A). Benthic organisms were similar to water column species in sensitivity to phenanthrene; GMAVs range from 126 to 490 μg/L. One epibenthic species was tested, the amphipod, Gammarus pseudolimnaeus (LC50 = 126 μg/L). Infaunal species tested included the annelid, L. variegatus (LC50 = >419 μg/L) and the midge, Chironomus tentans (LC50 = 490 μg/L). The Final Acute Value derived from the overall GMAVs (Stephan et al., 1985) for freshwater organisms is 59.63 μg/L (Table 3-3).

Fourteen acute tests have been conducted on 11 saltwater species from 11 genera

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RANK[a] HMAV GENUS	COMMON/SCI. NAME	LIFE[b] STAGE	HAB-[c] ITAT	HMAV SPECIES[d]	GENUS[e]
				μg/L	μg/L
FRESHWATER SPECIES					
3	Amphipod, Gammarus pseudolimnaeus	X	E	126	126
6	Annelid, Lumbriculus variegatus	X	I	>419	>419
7	Midge, Chironomus tentans	X	I	490	490
SALTWATER SPECIES					
1	Mysid, Mysidopsis bahia	J	E	21.9	21.9
3	Grass shrimp, Palaemonetes pugio	A	E,W	145	145
4	Hermit crab, Pagurus longicarpus	A	E	164	164
5	Archiannelid, Dinophilus gyrociliatus	J	I	185	185
6	Amphipod, Leptocheirus plumulosus	J	I	198	198
8	Mud snail, Nassarius obsoletus	A	I,E	>245	>245
8	Blue mussel, Mytilus edulis	A	E,W	>245	>245
8	Soft-shell clam, Mya arenaria	A	I	>245	>245
10	Sheepshead minnow, Cyprinodon variegatus	J	E,W	429	429

[a]Rank of HMAVs by genus are from Appendix A which included benthic and water column species.

[b]Lifestage: A = adult, J = juvenile, L = larvae, E = embryo, U = lifestage and habitat unknown, X = lifestage unknown but habitat known.

[c]Habitat: I = infauna, E = epibenthic, W = water column.

[HMAV species: Geometric mean of acute values for benthic (habitat) lifestages of each] species. (See Appendix A).

[e]HMAV genus: Geometric mean of HMAV for species within a genus.

(Appendix A). Overall genus mean acute values (GMAVs) range from 21.9 to 600 μg/L, similar to the range for freshwater genera. Fish and crustaceans were the most sensitive. Within this database there are results from nine tests on benthic life-stages of nine species from nine genera (Table 3-1; Appendix A). Benthic organisms were among both the most sensitive, and most resistant, saltwater genera to phenanthrene. The most sensitive benthic species is the mysid, Mysidopsis bahia, with an average flow-through 96 hour LC50 of 21.9 μg/L based on two tests with measured concentrations. Other benthic species for which there are data appear less sensitive; GMAVs range from 145 to 429 μg/L. The Final Acute Value derived from the overall GMAVs (Stephan et al., 1985) for saltwater organisms is 16.61 μg/L (Table 3-3).

3.3 CHRONIC TOXICITY - WATER EXPOSURES:

Chronic toxicity tests have been conducted with phenanthrene using a freshwater cladoceran (Daphnia magna) and rainbow trout (Oncorhynchus mykiss) and a saltwater mysid (Mysidopsis bahia). The cladoceran and mysid were tested in life-cycle exposures. Rainbow trout embryos, sac fry and swim-up benthic (intergravel) stages were tested in an early life-stage toxicity test.

Call et al. (1986) conducted both freshwater tests. Daphnia magna exposed 21 days to a mean phenanthrene concentration of 163 μg/L experienced 98% reduction in reproduction and 83% reduction in survival relative to controls (Table 3-2). There was no statistically significant effect on survival or reproduction of daphnids in phenanthrene concentrations from 46 to 57 μg/L. Rainbow trout exposed to phenanthrene for 90 days in an early life-stage toxicity test were not affected in 5 μg/L. Duration of incubation and hatching success were not affected in any treatment. However, the percentage of abnormal and dead fry at hatch was significantly increased at the highest exposure (66 μg/L). Sac fry were underdeveloped from hatching until test termination and swim-up delayed in $\geq$ 14 μg/L. At test termination, wet weights and standard lengths were reduced in $\geq$ 32 μg/L. Survival was reduced in $\geq$ 8 μg/L.

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TABLE 3-2. - CHRONIC SENSITIVITY OF FRESHWATER AND SALTWATER ORGANISMS TO PHENANTHRENE. TEST SPECIFIC DATA.

Common Name, Scientific Name	Test[a]	Habitat[b] (Life stage)	NOEC(s)[c]	Parental LOEC[c]	Parental Effect[d]	Progeny LOEC	Progeny Effect[d]	References
			µg/L	µg/L		µg/L		
FRESHWATER SPECIES								
Cladoceran, Daphnia magna	LC	W(J,A)	46,57	163	98% R 83% M	-	-	Call et al., 1986
Rainbow trout, Oncorhynchus mykiss	ELS	I(E,L)	5	8	33% G 41% M	-	-	Call et al., 1986
SALTWATER SPECIES								
Mysid, Mysidopsis bahia	LC	B(J,A)	1.50-5.55	11.9	100% R 100% M	-	-	Kuhn and Lussier, 1987

[a]TEST: LC = lifecycle, PLC = partial lifecycle, ELS = early lifestage

[b]HABITAT: I = infauna, E = epibenthic, W = water column
LIFESTAGE: E = embryo, L = larval, J = Juvenile, A = Adult

[c]NOEC = No observed effect concentration; LOEC = lowest observed effect concentration.

[d]EFFECT: Percentage decrease relative to controls. M = mortality, G = growth, R = reproduction.

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Saltwater mysids exposed to phenanthrene in a life-cycle toxicity test (Kuhn and Lussier, 1987) were affected at phenanthrene concentrations similar to those affecting the the rainbow trout (Table 3-2). Survival, growth and reproduction were not affected in $\leq$ 5.5 μg/L. At the highest concentration of phenanthrene (11.9 μg/L) all mysids died.

Derivation of the Final Chronic Value (FCV) for phenanthrene is complicated because Acute-Chronic Ratios (ACR) differ in the three species tested by a factor of almost 50 (Table 3-3). The final ACR, therefore, can not be the mean of these three values (Stephan et al., 1985). The difference between concentrations of phenanthrene acutely and chronically toxic to invertebrates is small. ACR are 1.214 for the freshwater cladoceran (Daphnia magna) and 3.333 for the saltwater mysid (Mysidopsis bahia); mean ratio 2.012. The ACR of 59.29 for rainbow trout (Call et al., 1986) probably should not be used to derive the final ACR or chronic values for untested fishes because (1) it is over 10 x the ratio for tested invertebrates, (2) the trout 96 hr LC50 of 375 μg/L would be 50 μg/L if based on immobilization (Call et al., 1986), thus the ACR would be 7.905 and (3) the chronic value may be conservative based on tests with other fish species. In non-standard chronic exposures, sensitivities of early life-stages of largemouth bass (Micropterus salmoides) and rainbow trout (Black et al., 1983; Milleman et al., 1984) were less than observed by Call et al. (1986). These chronic exposures lasted from fertilization to four days after hatching, about 7 days for bass and 27 days for trout. Hatching and survival of trout were reduced in 38 μg/L but not in 31 μg/L; in contrast to the effect concentration of 8 μg/L was observed by Call et al. (1986). The LC50 for these tests was 40 μg/L for trout and 180 μg/L for bass (Black et al., 1983; Milleman et al., 1984). Because the most acutely sensitive species to phenanthrene were invertebrates, the Final Acute Value (FAV), 59.63 μg/L for freshwater and 16.61 μg/L for saltwater, was divided by the invertebrate mean ACR of 2.012 to derive an initial estimate of the FCV. These initial FCVs were 29.64 μg/L for freshwater and 8.255 μg/L for saltwater aquatic life. The initial freshwater FCV was lowered to 6.325 μg/L the chronic value from the rainbow trout early life-stage test for this

TABLE 3-3. – SUMMARY OF ACUTE AND CHRONIC VALUES, ACUTE-CHRONIC RATIOS AND FRESHWATER AND SALTWATER FINAL ACUTE VALUES, FINAL ACUTE-CHRONIC RATIOS, AND FINAL CHRONIC VALUES FOR PHENANTHRENE.

Common Name, Scientific Name	Acute Value(μg/L)	Chronic Value(μg/L)	Acute-Chronic Ratio
		FRESHWATER SPECIES	
Cladoceran, Daphnia magna	117	96.39	1.214
Rainbow trout, Oncorhynchus mykiss	375	6.325	59.29
		SALTWATER SPECIES	
Mysid, Mysidopsis bahia	27.10	8.129	3.333

Freshwater:

Final Acute Value = 59.63 μg/L
Invertebrate Acute-Chronic Ratio = 2.012
Initial Final Chronic Value = 29.64 μg/L
Chronic Value for rainbow trout = 6.325 μg/L
Final Chronic Value = 6.325 μg/L

Saltwater:

Final Acute Value = 16.61 μg/L
Invertebrate Acute-Chronic Ratio = 2.012
Final Chronic Value = 8.255 μg/L

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important species. The initial saltwater FCV of 8.255 μg/L was not lowered because the chronic sensitivitie of saltwater fishes is not known and should not be estimated using the ACR for trout which is probably not appropriate for other fish species. The initial FCV for saltwater aquatic life is used as the FCV because it is 13 to 52 times lower than acute values for tested saltwater fishes and approximately equal to the chronic value of 8.129 μg/L for the mysid. Although this procedure to derive the FCV is complicated and does not follow exactly the WQC Guidelines (Stephan et al.,1985) for idealized databases, the procedure is consistent with the guidelines requirement that the criterion be consistent with sound scientific evidence.

3.4 APPLICABILITY OF THE WATER QUALITY CRITERION AS THE EFFECTS CONCENTRATION FOR DERIVATION OF THE PHENANTHRENE SEDIMENT QUALITY CRITERION:

The use of the Final Chronic Value (the chronic effects-based water quality criteria concentration) as the effects concentration for calculation of the equilibrium partitioning-based sediment quality criterion assumes similar sensitivities of benthic (infauna and epibenthic) species and species tested to derive the water quality criteria concentration. Data supporting the reasonableness of this assumption over all chemicals for which there are published or draft water quality criteria documents are presented in Di Toro et al. (1991) and U.S. EPA (1989c, 1992a). The conclusion of similarity of sensitivity is supported by comparisons between acute values: (1) for the most sensitive benthic and water column species for all chemicals; (2) all species across all chemicals after standardizing the LC50 values; and (3) individual chemical comparisons for benthic and water column species. Only in this last comparison are phenanthrene-specific comparisons in sensitivity of benthic and water-column species conducted. The following paragraphs examine the data for phenanthrene.

An initial test of the difference between the probability distributions of freshwater and saltwater phenanthrene LC50s for all species (water column and benthic) is presented in Figure 3-1. The top panel is a log probability plot of the two LC50 distributions on a log scale versus

3-8
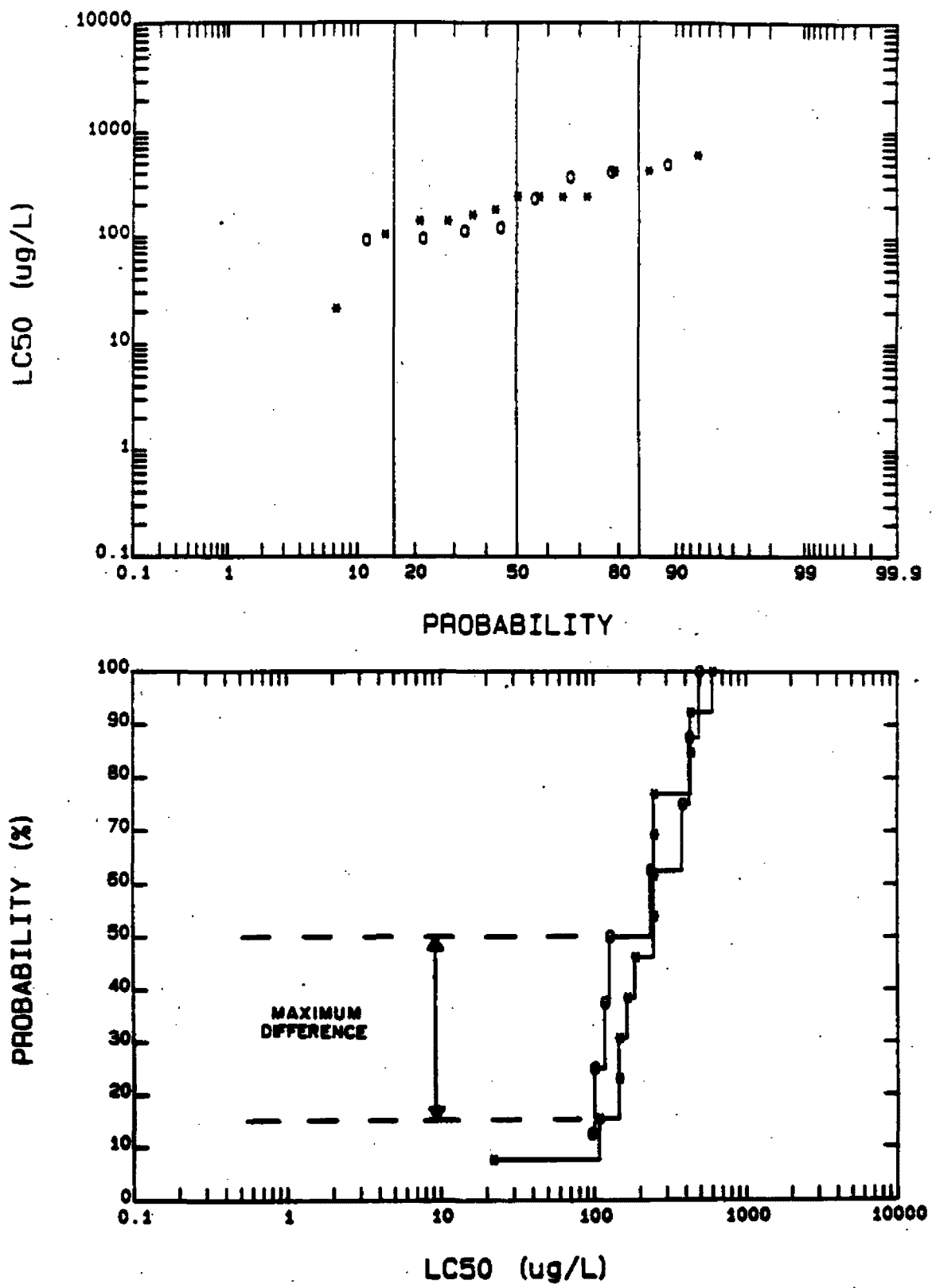
Figure 3-1. Comparison of phenanthrene water only LC50 probability distributions for freshwater (0) and saltwater (*) species (top panel). Cumulative distribution functions for calculating the K-S statistic (bottom panel).

3-9

the rank order on a probability scale. The natural way to judge the equality of these distributions is to compare the LC50s at a particular probability, for example a comparison of the medians at 50% probability. The Kolmogorov-Smirnov test compares another difference (Conover, 1980). This is illustrated on the bottom plot which presents the same data but in a slightly different way. The rank order, as a percent, is plotted versus the LC50s. The points are connected with straight lines to form the empirical cumulative distribution functions from the two data sets. The Kolmogorov-Smirnov test is based on the maximum difference in probability between these two distributions, as indicated on the figure. Note that this difference is the horizontal distance on the top plot in Figure 3-1 (if the probability scale were linear). Table 3-4 presents the number of LC50s in each distribution, the maximum difference (0.346), and the probability (0.568) that a value of this magnitude or less cannot occur given that these two samples came from the same distribution. The method of computation for this probability value is given in Massey (1951). Since the probability is less than 0.95, the hypothesis that freshwater and saltwater LC50 values came from the same distribution is accepted at a 95% confidence level. Therefore, for phenanthrene comparisons of LC50s for benthic and water column species are conducted using combined freshwater and saltwater LC50 values.

The probability distributions of combined freshwater and saltwater phenanthrene LC50s for the water column and benthic species are presented in Figure 3-2. Table 3-4 presents the number of LC50s in each distribution, the maximum difference, and the probability that a value of this magnitude or less cannot occur given that these two samples came from the same distribution. For combined freshwater and saltwater species the maximum difference and the probability that a value of this magnitude or less cannot occur given that these two samples came from the same distribution were 0.361 and 0.655 respectively. This analysis of the relative sensitivities of combined freshwater and saltwater benthic and water column organisms that have been tested indicates that they are from the same probability distributions of LC50's. Therefore, benthic and water column organisms have similar acute sensitivities. This suggests

3-10
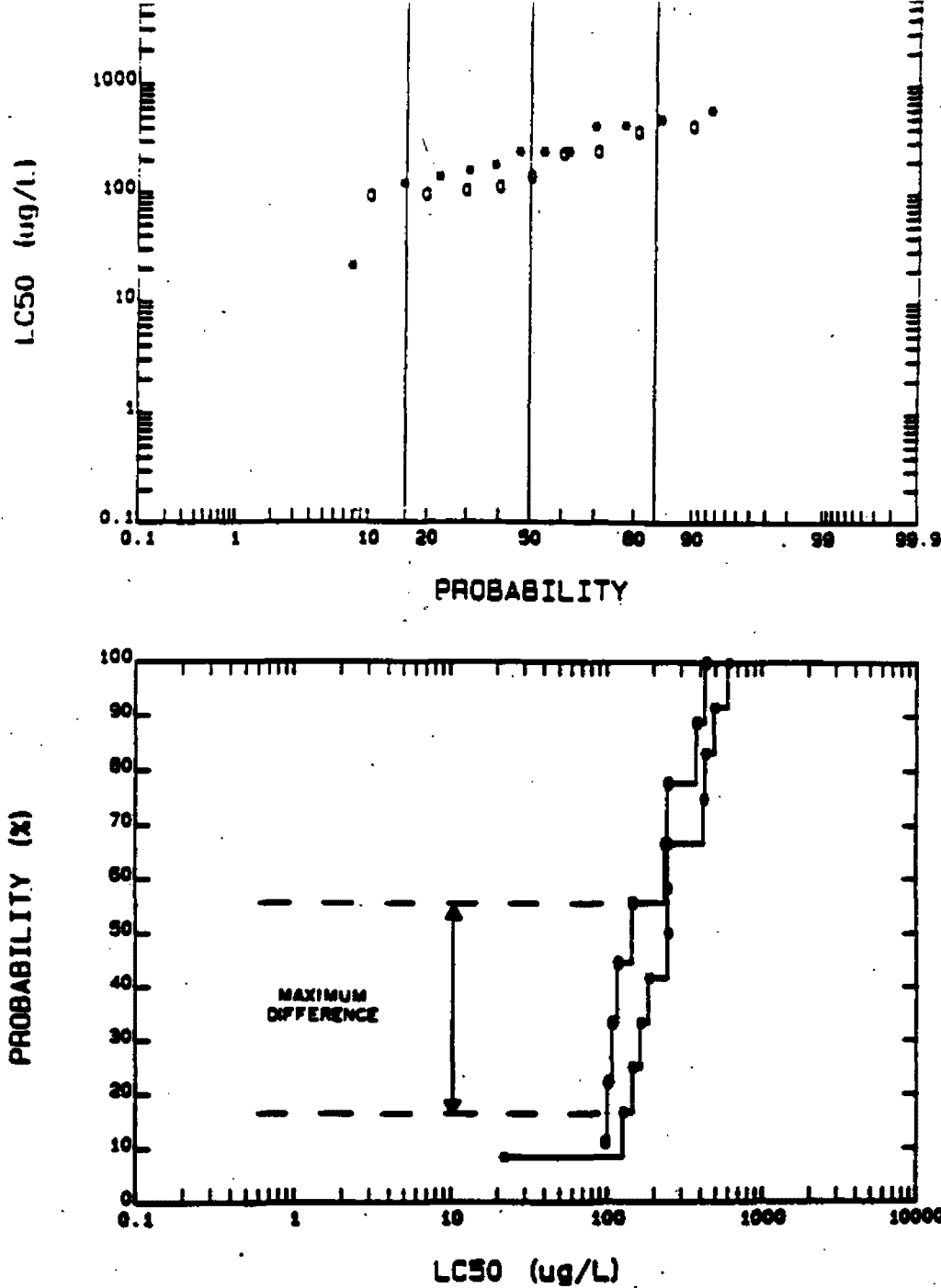
Figure 3-2. Comparison of phenanthrene water only LC50 probability distributions for water column (0) and benthic (*) freshwater and saltwater species (top panel). Cumulative distribution functions for calculating the K-S statistic (bottom panel).

that the final chronic value (FCV) for phenanthrene is an appropriate effects concentration for both benthic and water column organisms.

TABLE 3-4. KOLMOGOROV-SMIRNOV TEST FOR THE EQUALITY OF FRESHWATER AND SALTWATER LC50 DISTRIBUTIONS FOR PHENANTHRENE. KOLMOGOROV-SMIRNOV TEST FOR THE EQUALITY OF BENTHIC AND WATER COLUMN LC50 DISTRIBUTIONS.

Comparison	Habitat or Water Type[a]		K-S Statistic[b]	Probability[c]
Fresh vs Salt	Fresh (8)	Salt (13)	0.346	0.568
Benthic vs Water Column (Freshwater and saltwater)	Benthic (12)	Water (9) Column	0.361	0.655

[a]Values in parentheses are the number of LC50 values used in the comparison.
[b]K-S statistic = maximum difference between the cumulative distribution functions for benthic and water column species.

[c]Pr(K-S theoretical ≤ K-S observed) given that the samples came from the same population.

SECTION 4

TOXICITY OF PHENANTHRENE (ACTUAL AND PREDICTED): SEDIMENT EXPOSURES

4.1 TOXICITY OF PHENANTHRENE IN SEDIMENTS:

The toxicity of phenanthrene spiked into sediments has been tested with two saltwater amphipod species. Freshwater benthic species have not been tested in phenanthrene-spiked sediments. All concentrations of phenanthrene in sediments or interstitial water where effects were observed in benthic species (Table 4-1) are greater than SQC or FCV concentrations reported in this document. Details about exposure methodology are provided because, unlike aquatic toxicity tests, sediment testing methodologies have not been standardized. Generalizations across species or sediments are limited because of the limited number of experiments. Therefore, insights into relative sensitivities of aquatic species to phenanthrene can only be obtained from results of water-only tests (Section 3). Data are available from a number of experiments using both field and laboratory sediments contaminated with mixtures of PAHs and other compounds which include phenanthrene. Data from these studies have not been included here because it is not possible to determine the contribution of phenanthrene to toxicity observed.

Swartz (1991) exposed the amphipods Eohaustorius estuarius and Leptocheirus plumulosus to three phenanthrene-spiked sediments with total organic carbon content (TOC) of 1.0%, 2.6%, and 4.4%. Sediments were rolled (1) for two hours in phenanthrene-coated bottle; (2) stored at 4°C for 72 hours; (3) rolled for an additional two hours, and (4) then stored for 7 days at 4°C. In some of these experiments the concentration of phenanthrene was not sufficient to cause 50% mortality in any of the concentrations tested. In these cases additional experiments were performed with sediments from the same locations with similar

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TABLE 4-1: SUMMARY OF TESTS WITH PHENANTHRENE-SPIKED SEDIMENT.

Common/Sci. Name	Sediment Source; Description	TOC (%)	Method[a]/ Duration (Days)	Response	Sediment Phenanthrene LC50, µg/g Dry wt.	Org. Car.	Pore Water LC50, µg/L	References
				FRESHWATER SPECIES				
Amphipod, Eohaustorius estuarius	South Beach, OR	1.02, 0.82[b]	S,M/10	LC50	39.2	4,050	138	Swartz, 1991
Amphipod, Eohaustorius estuarius	McKinney Slough, OR	2.47	S,M/10	LC50	97.2	3,920	139	Swartz, 1991
Amphipod, Eohaustorius estuarius	Eckman Slough, OR	3.33, 2.97[b]	S,M/10	LC50	122	3,820	146	Swartz, 1991
Amphipod, Leptocheirus plumulosus	South Beach, OR	1.96, 0.82[b]	S,M/10	LC50	92.4	8,200	387	Swartz, 1991
Amphipod, Leptocheirus plumulosus	McKinney Slough, OR	2.50	S,M/10	LC50	162	6,490	306	Swartz, 1991
Amphipod, Leptocheirus plumulosus	Eckman Slough, OR	3.60, 2.97[b]	S,M/10	LC50	255	8,200	360	Swartz, 1991

[a] S = Static; M = Measured.

[b] TOC of sediment used in highest concentration(s).

TOC concentrations as were used in the original experiments, but with one or two treatments with higher phenanthrene concentrations and the appropriate controls (Tables 4-1, 4-2). When there was a difference between the control mortality in one of the original experiments and in the follow up experiment with the corresponding sediment and species, Abbott's correction was performed on the data for each treatment separately using the appropriate control mortality. Then the data for both experiments were pooled. The pooling of the data appears justified by the similarity of the dose-response relationships in the original and the follow up experiments (Appendix C). The 10-day LC50's for both species increased with increasing organic carbon concentration when the phenanthrene concentration was expressed on a dry weight basis, but decreased when concentration was expressed on an organic carbon basis. LC50's normalized to dry weight differed by a factor of 3.1 (39.2 to 122 $\mu g/g$) for E. estuarius over a 3.3-fold range of TOC and a factor of 2.8 (92.4 to 255 $\mu g/g$) for L. plumulosus over a 1.8-fold range of TOC. The organic carbon normalized LC50's for E. estuarius differed by a factor of 1.1 (3,820 to 4,050 $\mu g/g_{oc}$) while for L. plumulosus they differed by a factor of 1.3 (6,490 to 8,200 $\mu g/g_{oc}$).

Overall, the need for organic carbon normalization of the concentration of non-ionic organic chemicals in sediments is presented in the SQC Guidelines (U.S. EPA, 1992a). The need for organic carbon normalization for phenanthrene is also supported by the results of spiked-sediment toxicity tests described above. Although it is important to demonstrate that organic carbon normalization is necessary if SQC are to be derived using the EqP approach, it is fundamentally more important to demonstrate that K_{oc} and water only effects concentrations can be used to predict effects concentrations for phenanthrene and other non-ionic organic chemicals on an organic carbon basis for a range of sediments. Evidence supporting this prediction for phenanthrene and all SQC chemicals follows in Section 4.3.

TABLE 4-2: WATER-ONLY AND SEDIMENT LC50S USED TO TEST THE APPLICABILITY OF THE EQUILIBRIUM PARTITIONING THEORY FOR PHENANTHRENE.

Common/Sci. Name Method Duration(days)	Water Only LC50 µg/L	Pore Water LC50 µg/L	TOC (%)	Sediment Phenanthrene LC50 µg/g Dry Wt.	Sediment Phenanthrene LC50 µg/g OC	Predicted[a] LC50 µg/g OC	Ratio: Actual LC50 Predicted	Reference
Amphipod, Eohaustorius estuarius FT,M/10	131	138	1.02 0.82[b]	39.2	4,050	2,550	1.59	Swartz, 1991
Amphipod, Eohaustorius estuarius FT,M/10	131	139	2.47	97.2	3,920	2,550	1.54	Swartz, 1991
Amphipod, Eohaustorius estuarius FT,M/10	131	146	3.33 2.97[b]	122	3,820	2,550	1.50	Swartz, 1991
Amphipod, Leptocheirus plumulosus FT,M/10	185	387	1.96 0.82[b]	92.4	8,200	3,610	2.27	Swartz, 1991
Amphipod, Leptocheirus plumulosus FT,M/10	185	306	2.50	162	6,490	3,610	1.80	Swartz, 1991
Amphipod, Leptocheirus plumulosus FT,M/10	185	360	3.60 2.97[b]	255	8,200	3,610	2.27	Swartz, 1991

[a] Predicted LC50 ($\mu g/g_{OC}$) = water-only LC50 ($\mu g/L$) × K_{OC} (L/Kg_{OC}) × 1 $Kg_{OC}/1000g_{OC}$; where $K_{OC} = 10^{3.78}$.

[b] TOC of sediment used in highest concentration(s).

4.2 CORRELATION BETWEEN ORGANISM RESPONSE AND PORE WATER CONCENTRATION:

One corollary of the EqP theory is that pore-water LC50's for a given organism should be constant across sediments of varying organic carbon content (U.S. EPA, 1989a). Pore-water LC50 values are available for two species (Table 4-1; 4-2). Swartz (1991) found 10-day LC50 values based on pore-water concentrations varied by a factor of 1.1 (138 to 146 μg/L) for E. estuarius and by a factor of 1.3 (306 to 387 μg/L) for L. plumulosus. This variability is somewhat less than that shown when dry weight (factors of 3.1 and 2.8) normalization is used to determine LC50s based on phenanthrene concentration in sediments, but similar to that shown when organic carbon (factors of 1.1 and 1.3) normalization is used.

A more detailed evaluation of the degree to which the response of benthic organisms can be predicted from toxic units of substances in pore water can be made utilizing results from toxicity tests with sediments spiked with other substances, including acenanphthene and phenanthrene (Swartz, 1991), cadmium (Swartz et al., 1985), endrin (Nebeker et al., 1989; Schuytema et al., 1989), fluoranthene (Swartz et al., 1990), or kepone (Adams et al., 1985) (Figure 4-1; Appendix C). Tests with acenaphthene and phenanthrene used two saltwater amphipods (L. plumulosus and E. estuarius) and marine sediments. Tests with cadmium and fluoranthene used the saltwater amphipod (Rhepoxynius abronius) and marine sediments. Freshwater sediments spiked with endrin were tested using the amphipod Hyalella azteca; while the midge, Chironomous tentans, was tested using kepone-spiked sediments. Figure 4-1 presents the percentage mortalities of the benthic species tested in individual treatments for each chemical versus "pore water toxic units" for all sediments tested. Pore water toxic units are the concentration of the chemical in pore water (μg/L) divided by the water only LC50 (μg/L). In this normalization, 50% mortality should occur at one interstitial water toxic unit. In general, this comparison supports the concept that interstitial water concentrations can be used to predict the response of an organism to a chemical that is not sediment-specific. This pore water normalization was not used to derive sediment quality criteria in this document because

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Figure 4-1. Percent mortality of amphipods in sediments spiked with acenaphthene or phenanthrene (Swartz, 1991), cadmium (Swartz et al., 1985), endrin (Nebeker et al., 1989; Schuytema et al., 1989), or fluoranthene (Swartz et al., 1990), and midge in kepone-spiked sediments (Adams et al., 1985) relative to pore water toxic units. Pore water toxic units are ratios of concentrations of chemicals measured in individual treatments divided by the water-only LC50 value from water-only tests. (See Appendix C in this SQC document, Appendix C in the endrin, dieldrin, fluoranthene and acenaphthene SQC documents, and original references for raw data.)

of the complexation of non-ionic organic chemicals with pore water DOC (Section 2) and the difficulties of adequately sampling pore waters. Data from the dieldrin experiments (Hoke and Ankley, 1991) are not included because more knowledge of the pore water DOC will be required because dieldrin has a high K_{oc} value.

4.3 TESTS OF THE EQUILIBRIUM PARTITIONING PREDICTION OF SEDIMENT TOXICITY:

Sediment Quality Criteria derived using the equilibrium partitioning approach utilize partition coefficients and final chronic values from water quality criteria documents to derive the sediment quality criteria concentration for protection of benthic organisms. The partition coefficient (K_{oc}) is used to normalize sediment concentrations and predict biologically available concentrations across sediment types. Data are available to test the normalization for phenanthrene in sediments. Testing of this component of SQC derivation requires three elements: (1) a water-only effect concentration, such as a 10-day LC50 value in $\mu g/L$, (2) an identical sediment effect concentration on an organic carbon basis, such as a 10-day LC50 value in $\mu g/g_{oc}$, and (3) a partition coefficient for the chemical, K_{oc} in L/kg_{oc}. This section presents evidence that the observed effect concentration in sediments (2) can be predicted utilizing the water effect concentration (1) and the partition coefficient (3).

The observed 10-day LC50 values from phenanthrene-spiked sediment tests on a $\mu g \cdot g_{oc}$ basis with E. estuarius and L. plumulosus were predicted (Table 4-2) using the value of K_{oc} ($10^{4.29}$) from Section 2 of this document and the 10-day water-only LC50 values in Swartz (1991). Ratios of predicted to actual LC50s for phenanthrene averaged 1.54 (range 1.50 to 1.59) for E. estuarius and 2.10 (range 1.80 to 2.27) for L. plumulosus. The overall mean for both species was 1.80.

A more detailed evaluation of the accuracy and precision of the EqP prediction of the response of benthic organisms can be made using the results of toxicity tests with amphipods exposed to sediments spiked with acenaphthene, phenanthrene, dieldrin , endrin, or fluoranthene. Data from the kepone experiments are not included because we do not have a
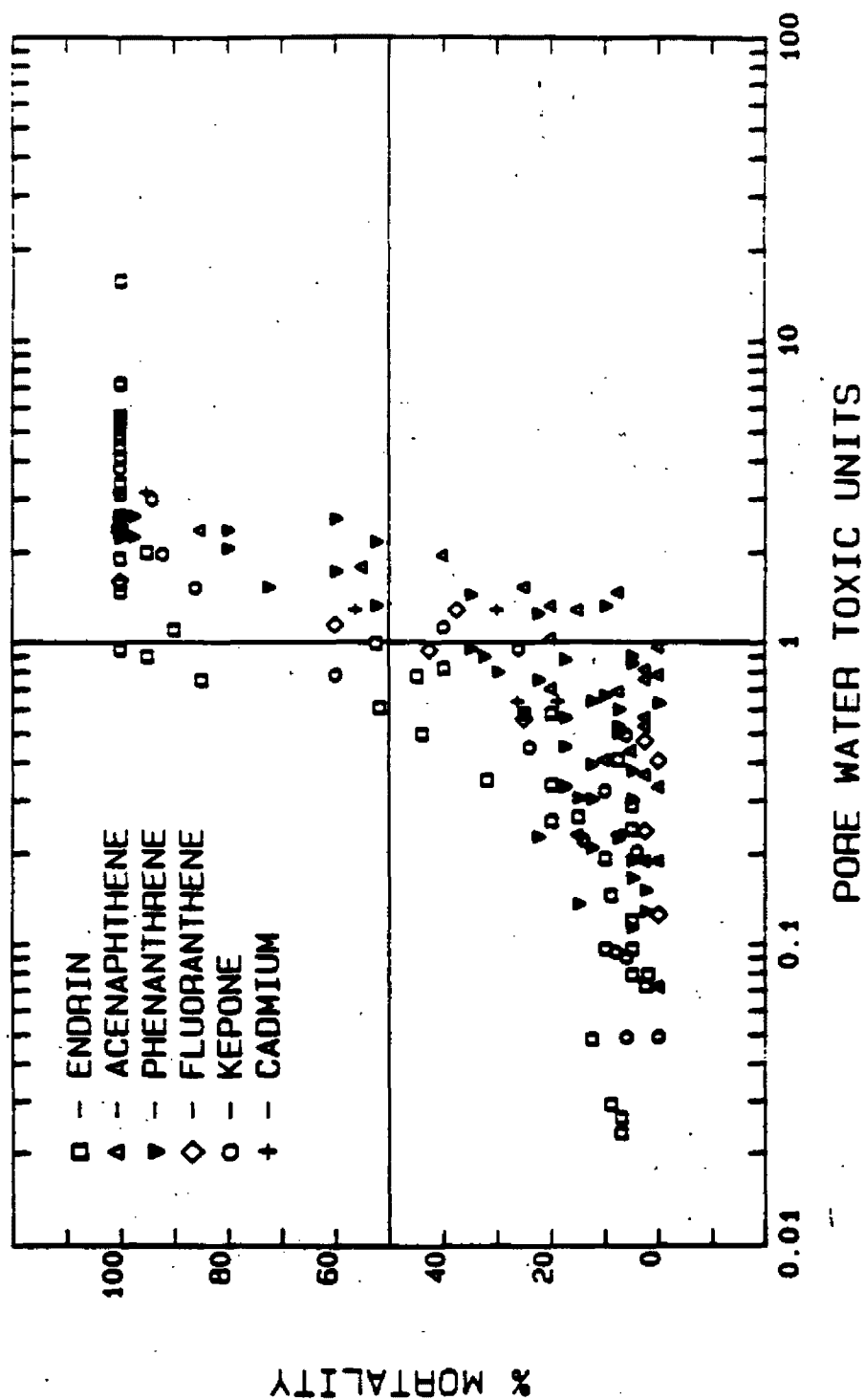
4-7
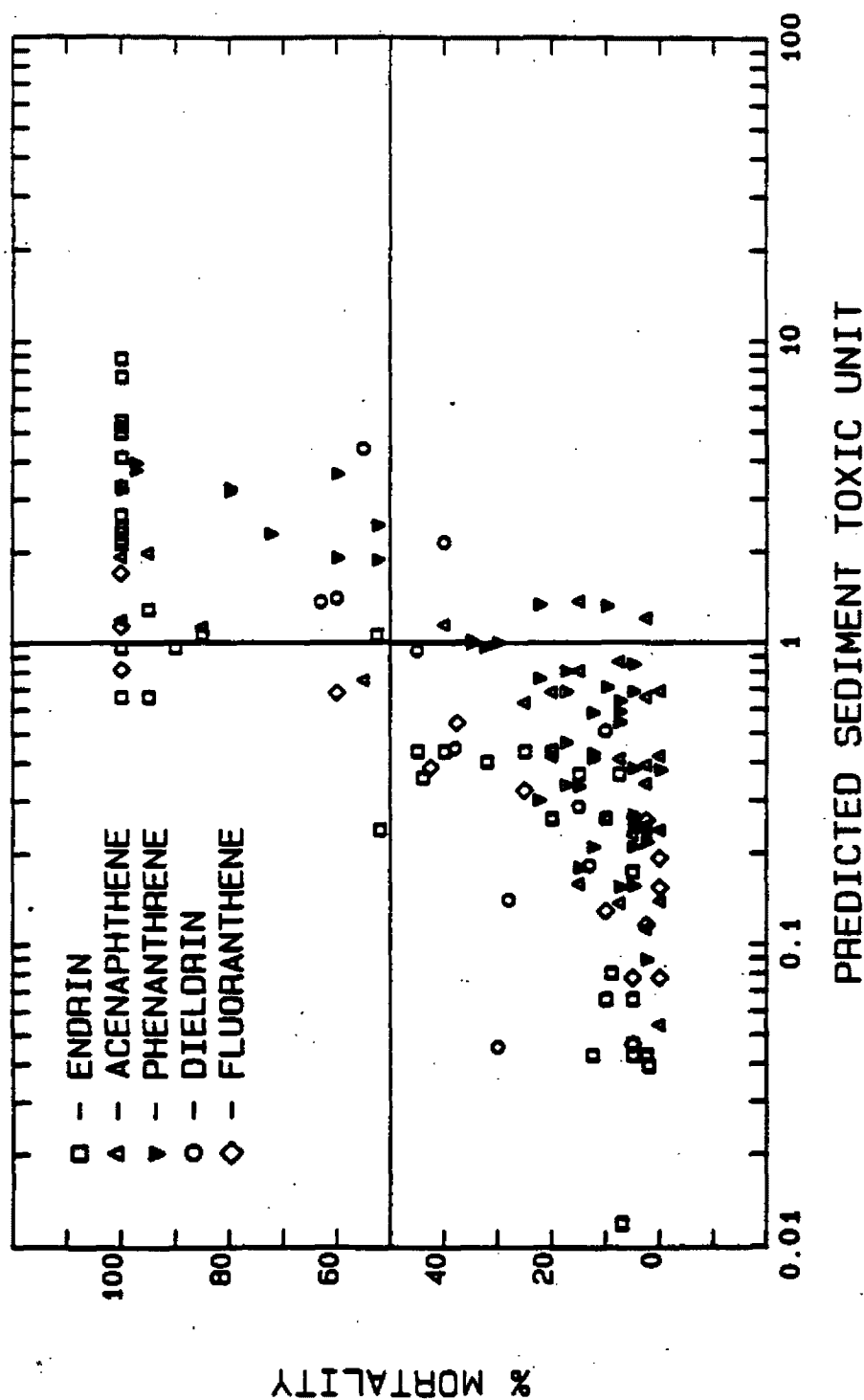
Figure 4-2. Percent mortality of amphipods in sediments spiked with acenaphthene or phenanthrene (Swartz, 1991), dieldrin (Hoke and Ankley, 1991), endrin (Nebeker et al., 1989; Schuytema et al., 1989) or fluoranthene (Swartz et al., 1990) relative to "predicted sediment toxic units." Predicted sediment toxic units are the ratios of measured treatment concentrations for each chemical in sediments ($\mu g/g_{OC}$) divided by the predicted LC50 ($\mu g/g_{OC}$) in sediments (K_{OC} x Water-only LC50, $\mu g/L$). (See Appendix C in this document and Appendix C in the dieldrin, endrin, fluoranthene, and acenaphthene SQC documents for raw data).

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K_{ow} for kepone from ERL, Athens. Swartz (1991) exposed the saltwater amphipods E. restuarius and L. plumulosus to acenaphthene and phenanthrene in three marine sediments having 1.02, 2.61 and 4.37% organic carbon. Swartz et al. (1990) exposed the saltwater amphipod R. abronius to fluoranthene in three marine sediments having 0.18, 0.31 and 0.48% organic carbon. Hoke and Ankley (1991) exposed the amphipod Hyalella azteca to three dieldrin-spiked freshwater sediments having 1.7, 3.0 and 8.5% organic carbon. Nebeker et al. (1989) and Schuytema et al. (1989) exposed H. azteca to three endrin-spiked sediments having 3.0, 6.1 and 11.2% organic carbon. Figure 4-2 presents the percentage mortalities of amphipods in individual treatments of each chemical versus "predicted sediment toxic units" for each sediment treatment. Predicted sediment toxic units are the concentration of the chemical in sediments ($\mu g/g_{oc}$) divided by the predicted LC50 ($\mu g/g_{oc}$) in sediments (the product of K_{oc} and the 10-day water-only LC50). In this normalization, 50% mortality should occur at one predicted sediment toxic unit. Endrin and fluoranthene data indicate a slight under prediction, and dieldrin, acenaphthene and phenanthrene a slight over prediction, of the observed mortality. In general, however, this comparison illustrates that the EqP method can account for the effects of different sediment properties and properly predict the effects concentration in sediments using the effects concentration from water only exposures. These are two fundamental propositions that underlie the EqP method for deriving sediment quality criteria.

SECTION 5

CRITERIA DERIVATION FOR PHENANTHRENE

5.1 CRITERIA DERIVATION:

The equilibrium partitioning method for calculating sediment quality criteria is based on the following procedure. If FCV (μg/L) is the Final Chronic Value which is the chronic effects concentration from the water quality criteria for the chemical of interest, then the sediment quality criteria, SQC (μg/g sediment), is computed using the partition coefficient, K_p (L/g sediment), between sediment and pore water:

$$SQC = K_p \, FCV \tag{5-1}$$

On a sediment organic carbon basis, the sediment quality criteria, SQC_{oc} (μg/g_{oc}), is:

$$SQC_{oc} = K_{oc} \, FCV \tag{5-2}$$

where K_{oc} is the organic carbon partition coefficient for the chemical. Since this quantity is presumably independent of sediment type for non-ionic organic chemicals, so also is SQC_{oc}. Table 5-1 contains the calculation of the phenanthrene sediment quality criteria.

TABLE 5-1. SEDIMENT QUALITY CRITERIA FOR PHENANTHRENE

Type of Water Body	$Log_{10}K_{ow}$ (L/kg)	$Log_{10}K_{oc}$ (L/kg)	FCV (μg/L)	SQC_{oc} (μg/g_{oc})
Fresh Water	4.36	4.29	6.32	123[a]
Salt Water	4.36	4.29	8.26	161[b]

[a] $SQC_{oc} = (10^{4.29} \text{ L/kg}_{oc}) \cdot (10^{3} \text{ kg}_{oc}/g_{oc}) \cdot (6.32 \, \mu g \text{ phenanthrene/L}) = 123 \, \mu g$ phenanthrene/g_{oc}

[b] $SQC_{oc} = (10^{4.29} \text{ L/kg}_{oc}) \cdot (10^{3} \text{ kg}_{oc}/g_{oc}) \cdot (8.26 \, \mu g \text{ phenanthrene/L}) = 161 \, \mu g$ phenanthrene/g_{oc}

5.2 UNCERTAINTY ANALYSIS:

Some of the uncertainty in the calculation of the phenanthrene sediment quality criteria can

be estimated from the degree to which the equilibrium partioning model, which is the basis for the criteria, can rationalize the available sediment toxicity data. The EqP model asserts that (1) the bioavailability of non-ionic organic chemicals from sediments is equal on an organic carbon basis, and (2) that the effects concentration in sediment ($\mu g/g_{oc}$) can be estimated from the product of the effects concentration from water only exposures ($\mu g/L$) and the partition coefficient K_{oc} (L/kg). The uncertainty associated with the sediment quality criteria can be obtained from a quantitative estimate of the degree to which the available data support these assertions.

The data used in the uncertainty analysis are the water-only and sediment toxicity tests that have been conducted in support of the sediment criteria development effort. These freshwater and saltwater tests span a range of chemicals and organisms; they include both water-only and sediment exposures and they are replicated within each chemical-organism-exposure media treatment. These data were analyzed using an analysis of variance (ANOVA) to estimate the uncertainty (i.e. the variance) associated with varying the exposure media and that associated with experimental error. If the EqP model were perfect, then there would be only experimental error. Therefore, the uncertainty associated with the use of EqP is the variance associated with varying exposure media.

The data used in the uncertainty analysis are the LC50s from the water-only and sediment exposures illustrated in Figure 4.2 in Section 4. The EqP model can be used to normalize the data in order to put it on a common basis. The LC50 for sediment on an organic carbon basis, $LC50_{s,oc}$, is related to the LC50 obtained from a water-only exposure, $LC50_{w}$ via the partitioning equation:

$$LC50_{s,oc} = K_{oc}LC50_{w} \qquad (5\text{-}3)$$

Therefore, K_{oc} can be used to define the equivalent sediment toxicity based on free concentration in pore water:

$$LC50_{pw} = \frac{LC50_{s,oc}}{K_{oc}} \tag{5-4}$$

The EqP model asserts that toxicity of sediments expressed as the free pore water concentration equals toxicity in water only tests.

$$LC50_{pw} = LC50_{w} \tag{5-5}$$

Therefore, either $LC50_{pw}$ or $LC50_{w}$ are estimates of the true LC50 for this chemical - organism pair. In this analysis, the uncertainty of K_{oc} is not treated separately. Any error associated with K_{oc} will be reflected in the uncertainty attributed to varying the exposure media.

In order to perform an analysis of variance, a model of the random variations is required. As discussed above, experiments that seek to validate equation 5-5 are subject to various sources of random variations. A number of chemicals and organisms have been tested. Each chemical - organism pair was tested in water-only exposures and in different sediments. Let α represent the random variation due to this source. Also, each experiment is replicated. Let $\in$ represent the random variation due to this source. If the model were perfect, there would be no random variations other than that due to experimental error which is reflected in the replications. Hence α represents the uncertainty due to the approximations inherent in the model and $\in$ represents the experimental error. Let $(\sigma_{\alpha})^2$ and $(\sigma_{\in})^2$ be the variances of these random variables. Let i index a specific chemical-organism pair. Let j index the exposure media, water-only, or the individual sediments. Let k index the replication of the experiment. Then the equation that describes this relationship:

$$\ln(LC50_{i,j,k}) = \mu_i + \alpha_{i,j} + \in_{i,j,k} \tag{5-6}$$

where $\ln(LC50)_{i,j,k}$ are either $\ln(LC50_{w})$ or $\ln(LC50_{s,oc})$ corresponding to a water-only or sediment exposure; μ_i are the population of $\ln(LC50)$ for chemical-organism pair i. The error structure is assumed to be lognormal which corresponds to assuming that the errors are proportional to the means, e.g. 20%, rather than absolute quantities, e.g. 1 mg/L. The statistical problem is: estimate μ_i and the variances of the model error, $(\sigma_{\alpha})^2$, and the

measurement error, $(\sigma_\epsilon)^2$. The maximum likelihood method is used to make these estimates (U.S. EPA, 1992a). The results are shown in Table 5-2.

Table 5-2: ANALYSIS OF VARIANCE FOR DERIVATION OF SEDIMENT QUALITY CRITERIA CONFIDENCE LIMITS FOR PHENANTHRENE.

Source of Uncertainty	Parameter	Value ($\mu g/g_{oc}$)
Exposure media	σ_α	0.39
Replication	σ_ϵ	0.21
Sediment Quality Criteria	σ_{SQC} *	0.39

$^*\sigma_{SQC} = \sigma_A$

The last line of Table 5-2 is the uncertainty associated with the sediment quality criteria; i.e., the variance associated with the exposure media variability.

The confidence limits for the sediment quality criteria are computed using this estimate of uncertainty for sediment quality criteria. For the 95% confidence interval limits, the significance level is 1.96 for normally distributed errrors.

Hence:

$$\ln(SQC_{oc})_{UPPER} = \ln(SQC_{oc}) + 1.96\sigma_{SQC} \qquad (5\text{-}7)$$

$$\ln(SQC_{oc})_{LOWER} = \ln(SQC_{oc}) - 1.96\sigma_{SQC} \qquad (5\text{-}8)$$

The confidence limits are given in Table 5-3.

The organic carbon normalized sediment quality criteria is applicable to sediments with an organic carbon fraction of $f_{oc} \geq 0.2\%$. For sediments with $f_{oc} < 0.2\%$, organic carbon normalization and sediment quality criteria do not apply.

TABLE 5-3. SEDIMENT QUALITY CRITERIA
CONFIDENCE LIMITS FOR PHENANTHRENE

Type of Water Body	SQC_{oc} $\mu g/g_{oc}$	Sediment Quality Criteria 95% Confidence Limits ($\mu g/g_{oc}$)	
		Lower	Upper
Fresh Water	120	56	260
Salt Water	160	74	340

5.3 COMPARISON OF PHENANTHRENE SQC TO STORET DATA FOR SEDIMENT PHENANTHRENE:

A STORET (U.S. EPA, 1989a) data retrieval was performed to obtain a preliminary assessment of the concentrations of phenanthrene in the sediments of the nation's water bodies. Log probability plots of phenanthrene concentrations on a dry weight basis in sediments are shown in Figure 5-1. Phenanthrene is found at varying concentrations in sediments from rivers, lakes and near coastal water bodies in the United States. Median concentrations are generally about 0.1 $\mu g/g$ in each of the three water bodies. There is significant variability with phenanthrene concentrations in sediments ranging over seven orders of magnitude within the country.

The SQC for phenanthrene can be compared to existing concentrations of phenanthrene in sediments of natural water systems in the United States as contained in the STORET database (U.S. EPA, 1989a). These data are generally reported on a dry weight basis, rather than an organic carbon normalized basis. Therefore, SQC values corresponding to sediment organic carbon levels of 1 to 10% are compared to phenanthrene's distribution in sediments as examples only. For fresh water sediments, SQC values are 1.2 $\mu g/g$ in sediments having 1% organic carbon and 12 $\mu g/g$ dry wt. in sediments having 10% organic carbon; for marine sediments SQC are 1.6 $\mu g/g$ and 16 $\mu g/g$, respectively. Figure 5-1 presents the comparisons of these SQC to probability distributions of observed sediment phenanthrene levels for streams
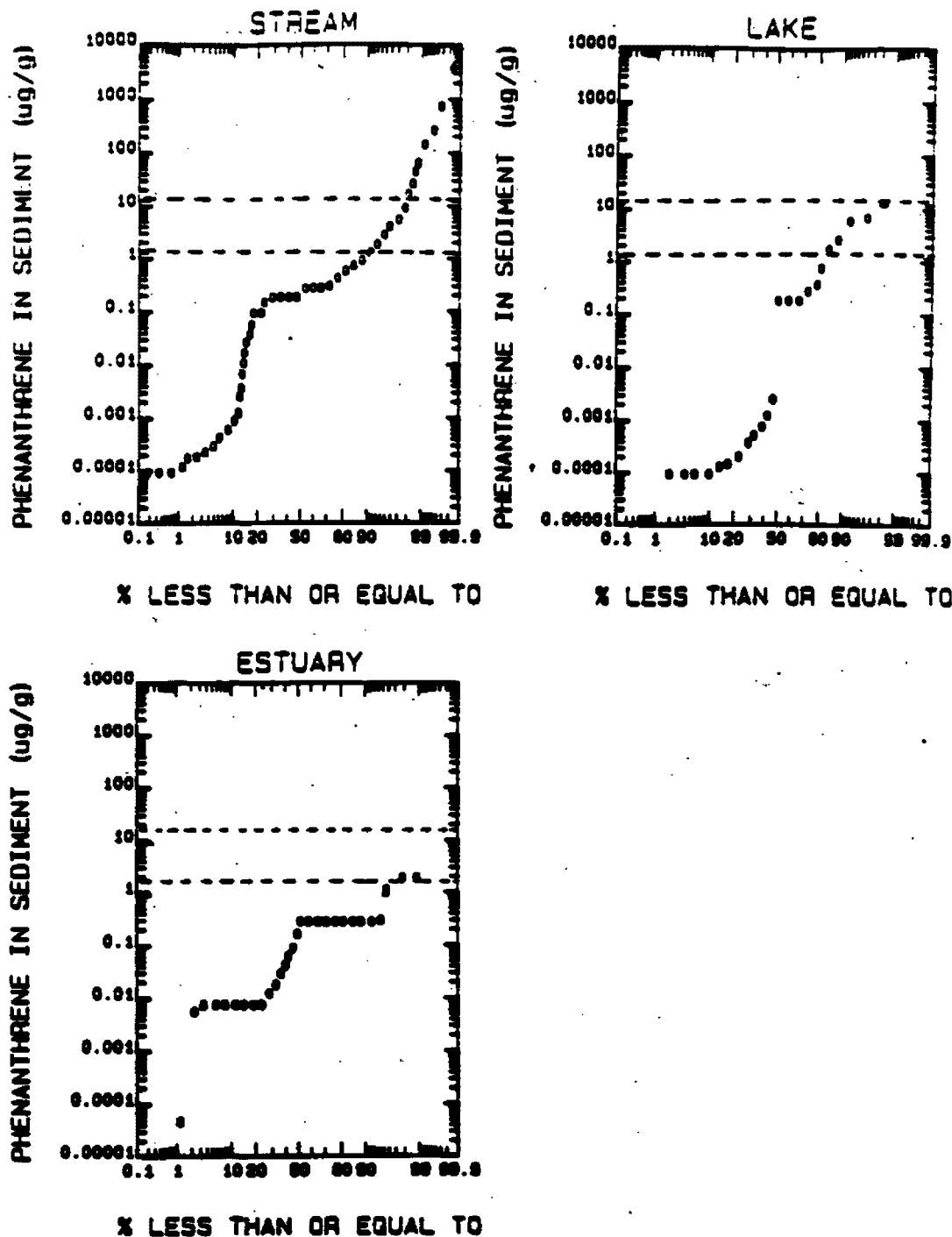
Figure 5-1.   Probability distribution of concentrations of phenanthrene in sediments from streams (n=584), lakes (n=50) and estuaries (n=87) in the United States from 1986 to 1990, from the STORET (U.S. EPA, 1989c) database, compared to the phenanthrene SQC values of 12 ug/g in freshwater sediments having TOC = 10% and 1.2 μg/g in freshwater sediments having TOC = 1%; SQC values for saltwater sediments are 16 μg/g when TOC =10% and 1.6 ug/g when TOC=1%. The upper dashed line on each figure represents the SQC value when TOC = 10%, the lower dashed line represents the SQC when TOC = 1%.

and lakes (fresh water systems, shown on the upper panels) and estuaries (marine systems, lower panel). For streams (n = 584) the SQC of 1.2 μg/g for 1% organic carbon sediments is exceeded for 10% of the data and the SQC of 12 μg/g for sediments having 10% TOC is exceeded by 2% of the data. For lakes (n = 50) the SQC for 1% organic carbon sediments is exceeded for almost 20% of the data and data for sediments with 10% organic carbon exceed the SQC 2% of the time. In estuaries, the data (n = 87) indicate that the criteria of 1.6 ug/g dry weight for sediments having 1% organic carbon is exceeded for about 5% of the data while the criteria of 16 μg/g dry weight for sediments having 10% organic carbon are not exceeded by the post 1986 samples.

A second database developed as part of the National Status and Trends Program (NOAA, 1991) is also available for assessing contaminant levels in marine sediments that are representative of areas away from sources of contamination. The probability distribution for these data, which can be directly expressed on an organic carbon basis, is compared to the saltwater SQC for phenanthrene (160 μg/g$_{oc}$) on Figure 5-2. Data presented are from sediments with 0.20 to 31.9 percent organic carbon. The median organic carbon normalized phenanthrene concentration (about 5.0 μg/g$_{oc}$) is a factor of 32 below the SQC of 160 μg/g$_{oc}$. About 2% of these samples (n = 900) exceeded the criteria. Hence, these results are consistent with the preceding comparison of the marine SQC to STORET data.

Regional differences in phenanthrene concentrations may affect the above conclusions concerning expected criteria exceedences. This analysis also does not consider other factors such as the type of samples collected (i.e., whether samples were from surficial grab samples or vertical core profiles), or the relative frequencies and intensities of sampling in different study areas. It is presented as an aid in assessing the range of reported phenanthrene sediment concentrations and the extent to which they may exceed the sediment quality criteria.
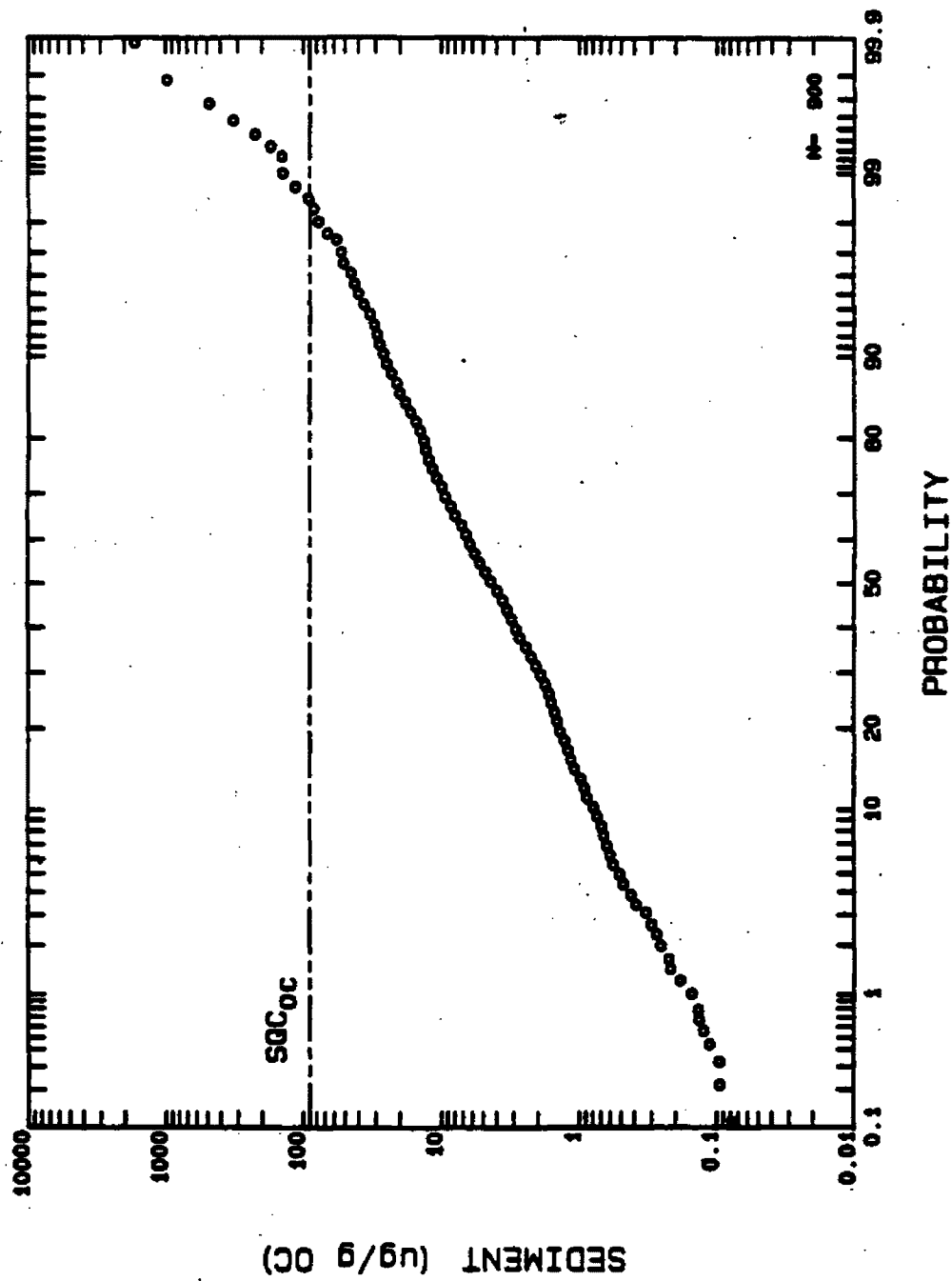
Figure 5-2. Probability distribution of concentrations of phenanthrene in sediments from coastal and estuarine sites from 1984 to 1989 as measured by the National Status and Trends Program (NOAA, 1991). The horizontal line is the SQC value of 160 $\mu g/g_{oc}$.

SECTION 6

CRITERIA STATEMENT

The procedures described in the "Guidelines for Deriving Numerical National Sediment Quality Criteria for Nonionic Organic Chemicals for the Protection of Benthic Organisms" (U.S. EPA, 1992a) indicate that, except possibly where a locally important species is very sensitive or sediment organic carbon is $< 0.2\%$, benthic organisms should be acceptably protected in freshwater sediments containing ≤ 120 μg phenanthrene/g organic carbon and saltwater sediments containing ≤ 160 μg phenanthrene/g organic carbon.

These concentrations are the U.S. EPA's best scientific judgement at this time of the acceptable concentration of phenanthrene in sediments. Confidence limits of 56 to 260 $\mu g/g_{oc}$ for freshwat

er sediments and 74 to 340 $\mu g/g_{oc}$ for saltwater sediments are provided as an estimate of the uncertainty associated with the degree to which the observed concentration in sediment ($\mu g/g_{oc}$), which may be toxic can be predicted using the K_{oc} and the water-only effects concentration. Confidence limits do not incorporate uncertainty associated with water quality criteria. An understanding of the theoretical basis of the equilibrium partitioning methodology, uncertainty, the partitioning and toxicity of phenanthrene, and sound judgement are required in the regulatory use of sediment quality criteria and their confidence limits. The upper confidence limit might be interpreted as a concentration above which impacts on benthic species would be highly likely. The lower confidence limit might be interpreted as a concentration below which impacts on benthic species would be unlikely.

6-1

SECTION 7

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Appendix A - Phenanthrene: Summary of acute values for freshwater and saltwater species.

COMMON/SCI. NAME	LIFE[a] STAGE	HAB-[b] ITAT	METHOD[c]	CONCEN-TRATION[d]	LC50/[e] EC50	HMAV SPECIES[f]	HMAV GENUS[g]	OVERALL[h] GMAV	REFERENCES[i]
					μg/L	μg/L	μg/L	μg/L	
FRESHWATER SPECIES									
Hydra, Hydra sp.	X	W	FT	M	96	96	96	96	Call et al., 1986
Annelid, Lumbriculus variegatus	X	I	FT	M	>419	>419	>419	>419	Call et al., 1986
Cladoceran, Daphnia magna	X	W	S	U	843	-	-	-	Eastmond et al., 1984
Cladoceran, Daphnia magna	1st instar	W	S	M	700	-	-	-	Millemann et al., 1984
Cladoceran, Daphnia magna	4-6 days	W	S	U	207	-	-	-	Abernethy et al., 1986
Cladoceran, Daphnia magna	X	W	FT	M	117	117	-	-	Call et al., 1986
Cladoceran, Daphnia pulex	<24 hr	W	S	U	734	-	-	-	Passino and Smith, 1987
Cladoceran, Daphnia pulex	X	W	S	U	>1150	-	-	-	Geiger and Buikema, 1981, 1982
Cladoceran, Daphnia pulex	X	W	S	M	100	100	108.2	108.2	Trucco et al., 1983
Amphipod, Gammarus pseudolimnaeus	X	E	FT	M	126	126	126	126	Call et al., 1986
Midge, Chironomus tentans	L	I	S	M	490	490	490	490	Millemann et al., 1984
Rainbow trout, Oncorhynchus mykiss	J	W	FT	M	375	375	375	375	Call et al., 1986

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Appendix A -- Phenanthrene: (continued)

COMMON/SCI. NAME	LIFE[a] STAGE	HAB-[b] ITAT	METHOD[c]	CONCEN-TRATION[d]	LC50/[e] EC50	SPECIES[f]	HMAV GENUS[g]	OVERALL[b] GMAV	REFERENCES[i]
					µg/L	µg/L	µg/L	µg/L	
Fathead minnow, Pimephales promelas	J	W	S	M	>1150	>1150	>1150	>1150	Millemann et al., 1986, EPA 1988
Bluegill, Lepomis macrochirus	J	W	FT	M	234	234	234	234	Call et al., 1986
SALTWATER SPECIES									
Archiannelid, Dinophilus gyrociliatus	J	I	R	U	185.4	185.4	185.4	185.4	Battelle Ocean Sciences, 1987
Polychaete worm, Neanthes arenaceodentata	A	I	S	U	600	600	600	600	Rossi and Neff, 1978
Mud snail, Nassarius obsoletus	A	I,E	R	M	>245	>245	>245	>245	Battelle Ocean Sciences, 1987
Blue mussel, Mytilus edulis	A	E,W	R	M	>245	>245	>245	>245	Battelle Ocean Sciences, 1987
Soft-shell clam, Mya arenaria	A	I	R	M	>245	>245	>245	>245	Battelle Ocean Sciences, 1987
Mysid, Mysidopsis bahia	J	E	FT	M	17.7	-	-	-	Battelle Ocean Sciences, 1987
Mysid, Mysidopsis bahia	J	E	FT	M	27.10	21.91	21.91	21.91	Kuhn and Lussier, 1987
Amphipod, Leptocheirus plumulosus	A	E	FT	M	198.4	198.4	198.4	198.4	Swartz, 1991
Grass shrimp, Palaemonetes pugio	A	E,W	R	U	200.8	-	-	-	Battelle Ocean Sciences, 1987
Grass shrimp, Palaemonetes pugio	A	E,W	FT	M	145.4	145.4	145.4	145.4	Battelle Ocean Sciences, 1

A-2

Appendix A - Phenanthrene: (continued)

COMMON/SCI. NAME	LIFE[a] STAGE	HAB-[b] ITAT	METHOD[c]	CONCEN-[d] TRATION	LC50/[e] EC50	HMAV[f] SPECIES	GENUS[g]	OVERALL[h] GMAV	REFERENCES[i]
					µg/L	µg/L	µg/L	µg/L	
Hermit crab, Pagurus longicarpus	A	E	FT	M	163.7	163.7	163.7	163.7	Battelle Ocean Sciences, 1987
Sheepshead minnow, Cyprinodon variegatus	J	E,W	R	U	>245	-	-	-	Battelle Ocean Sciences, 1987
Sheepshead minnow, Cyprinodon variegatus	J	E,W	FT	M	429.4	429.4	429.4	429.4	Battelle Ocean Sciences, 1987
Atlantic silverside, Menidia menidia	A	W	FT	M	108	108	108	108	Battelle Ocean Sciences, 1987

[a]Lifestage: A = adult, J = juvenile, L = larvae, E = embryo, U = lifestage, U = lifestage and habitat unknown, X = lifestage unknown but habitat known.

[b]Habitat: I = infauna, E = epibenthic, W = water column.

[c]Method: S = static, R = renewal, FT = flow-through.

[d]Concentration: U = unmeasured (nominal), M = chemical measured.

[e]Acute value: 96-hour LC50 or EC50, exceptions from Stephan et al. (1985).

[f]HMAV species: Habitat Mean Acute Value - Species is the geometric mean of acute values by species for benthic and water column lifestages.

[g]HMAV: genus: Geometric mean of HMAV for species within a genus.

[h]Overall GMAV: Geometric mean of acute values across species, habitats and lifestages within the genus.

A-3
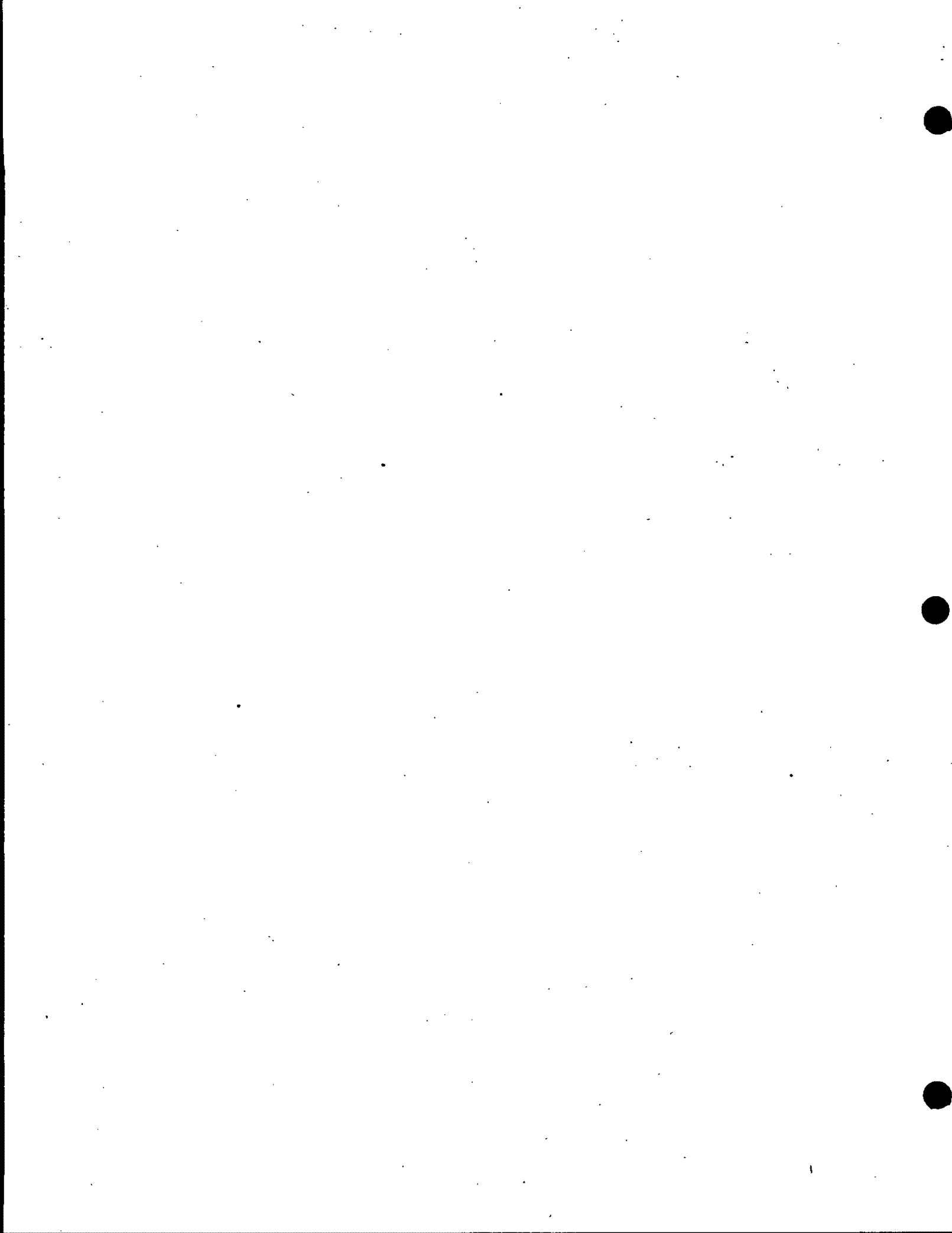
APPENDIX B: THE OCTANOL-WATER PARTITION COEFFICIENT, K_{ow} FOR PHENANTHRENE.

B.1 GENERAL INFORMATION:

Partitioning between water and natural soils, sediments, and aquifer materials is an important process affecting transformation rates, toxicity, and the ultimate disposition of organic chemicals in the environment. Extensive research, focusing on the partitioning of neutral organic compounds, has shown that adsorption of these compounds generally is controlled by hydrophobic interactions. As a result, the affinity that a natural sorbent has for neutral organic solutes, in most cases, can be reliably estimated from the hydrophobicity of the solute and the sorptive capacity of the sorbent. Organic carbon content has been used almost exclusively as a measure of the sorptive capacity of natural sedimentary material. (Organic matter or volatile solids content has also been used but not as widely.) To quantitatively characterize the hydrophobic nature of organic compounds, researchers have used various measurable parameters, including octanol/water partition coefficients (K_{ow}), water solubility (corrected for crystal energy), reverse phase HPLC retention, and topological parameters of the compounds such as calculated surface area. Generally, octanol/water partition coefficients have been used more extensively, not only for estimating the partitioning of organic compounds to sedimentary materials, but also for estimating bioaccumulation of organic compounds to aquatic organisms.

The K_{ow} is defined as the ratio of the equilibrium concentration of a dissolved substance in a system consisting of n-octanol and water and is ideally dependent only on temperature and pressure:

$$K_{ow} = C_{oct}/C_w \qquad (B-1)$$

where C_{oct} is the concentration of the substance in n-octanol and C_w is the concentration of the substance in water. The K_{ow} is used in estimating the organic-carbon- normalized sediment-water partition coefficient (K_{oc}) and is frequently reported in the form of its logarithm to base ten as log P.

B-1

B.2 LITERATURE DATA:

An extensive literature search was performed for phenanthrene and two standard reference compounds, biphenyl and pyrene. Generally, problems encountered in compiling and reporting fate constants from published data and from databases during the last several years have ranged from retrieval of misquoted numbers to resolution of nested citations (Kollig, 1988). Some citations were three or more authors removed from the original work or contained data that were referenced as unpublished data or as personal communication. The same problems were experienced during this literature search. The largest difference in misquoting numbers was six orders of magnitude. For these reasons, ERL-Athens obtains data from the primary sources and releases values coming only from these primary sources. Unpublished data or data which originated through personal communication are rejected as well as data that are insufficiently documented to determine their credibility and applicability or reliability.

Tables B-1 and B-2 show the measured and estimated K_{ow} values, respectively, retrieved by this literature search. Each of the measured values was experimentally determined by the researcher using one of several laboratory methods. The individual experimental methods are not identified here. The estimated literature values were computed by the researchers by one of several published techniques. The individual computational techniques also are not identified here.

B.3 ERL-ATHENS MEASURED DATA:

To enhance confidence in the measured K_{ow} values, two independent experimental methods, [shake-centrifugation (SC), generator column (GCol)], were used to determine a K_{ow} value for phenanthrene at the U.S. EPA laboratory at Athens, Georgia. The SC method is routinely used to measure the partitioning of compounds with K_{ow} values on the order of 10^2 to 10^6. The method involves adding a layer of octanol containing the compound of interest onto the surface of water contained in a centrifuge tube. Both phases are mutually presaturated before beginning

the measurements. Equilibration is established by gentle agitation and any emulsions formed are broken by centrifugation. The concentration in each phase is determined usually by a chromatographic method and the K_{ow} value calculated using Equation B-1.

TABLE B-1. MEASURED $LOG_{10}K_{ow}$ VALUES FOUND IN THE LITERATURE

Chemical	$Log_{10}K_{ow}$ value	Reference
Phenanthrene	4.28	Haky and Young, 1984
	4.46	Hansch and Fujita, 1964
	4.562	De Bruijn et al., 1989
	4.57	Karickhoff et al., 1979
	4.63	Bruggeman et al., 1982
Biphenyl	3.16	Rogers and Cammarata, 1969
	3.63	De Kock and Lord, 1987
	3.75	Veith et al., 1979
	3.76	Miller et al., 1984
	3.79	Rapaport and Eisenreich, 1984
	3.89	Woodburn et al., 1984
	4.008	De Bruijn et al., 1989
	4.01	Eadsforth, 1986
	4.04	Banerjee et al., 1980
	4.09	Ellington and Stancil, 1988
	4.10	Bruggeman et al., 1982
Pyrene	4.96	Rapapaport and Eisenreich, 1984
	5.05	Ellington and Stancil, 1988
	5.09	Means et al., 1980
	5.18	Karickhoff et al., 1979
	5.22	Bruggeman et al., 1982
	5.52	Burkhard et al., 1985

The original GCol method, limited to compounds with K_{ow} values of less than 10^6 was modified (Woodburn et al., 1984) and used to determine K_{ow} values up to 10^8. Briefly, the method requires the packing of a 24-cm length of tubing with silanized Chromosorb W. Octanol, containing the chemical in a known concentration, is then pulled through the dry support by gentle suction until the octanol appears at the exit of the column. Water is then

pumped through the column at a rate of less than 2 ml per minute to allow equilibration of the chemical between the octanol and water. The first 100 ml are discarded followed by collection of an amount of water sufficient to determine the chemical concentration. The K_{ow} is calculated using Equation B-1.

TABLE B-2. ESTIMATED $LOG_{10}K_{ow}$ VALUES FOUND IN THE LITERATURE

Chemical	$Log_{10}K_{ow}$ value	Reference
Phenanthrene	4.44	Kamlet et al., 1988
	4.45	Mabey et al., 1982
	4.63	Mackay et al., 1980
	4.64	Yalkowsky et al., 1983
Biphenyl	3.79	Yalkowsky et al., 1983
	3.95	Miller et al., 1985
	3.98	Kamlet et al., 1988
	4.14	Mackay et al., 1980
	4.25	Arbuckle, 1983
	4.42	Doucette and Andren, 1987
Pyrene	4.50	D'Amboise and Hanai, 1982
	4.85	Kamlet et al., 1988
	4.88	Lyman et al., 1982
	4.90	Mabey et al., 1982
	5.12	Mackay et al., 1980
	5.22	Yalkowsky et al., 1983
	5.32	Callahan et al., 1979

When repetitive measurements are made in the Athens laboratory, a protocol is established to assure compatibility with future experiments. These protocols describe the entire experimental scheme including planning, sample requirements, experimental set up and chemical analysis, handling of data, and quality assurance. Only established analytical methods for solute concentration measurement are applied and the purity and identity of the chemical are determined by spectroscopic means. The name on the label of the chemical's container is not proof of the identity.

Standard reference compounds (SRCs) are tested with each experiment. SRCs are compounds that are used as quality assurance standards and as references in inter-laboratory

generation of data. The value of the process constant(s) has been established by repetitive measurements for an SRC and serves as baseline information for evaluating all experimental techniques and all aspects of quality assurance. Because the SRC is taken through the entire experimental scheme, its acceptable result will assure the experimenter that equipment and measurement methods are functioning satisfactorily. Table B-3 shows the K_{ow} values for phenanthrene and the SRCs, biphenyl and pyrene, measured at the Athens laboratory by the SC methods. The SRCs were not measured by the GCol method.

TABLE B-3. $LOG_{10}K_{ow}$ VALUES MEASURED BY SHAKE-CENTRIFUGATION (SC) AND GENERATOR COLUMN (GCOL). FOR PHENANTHRENE AND CONCURRENTLY ANALYZED STANDARD REFERENCE COMPOUNDS.

Chemical	SC	GCol
Phenanthrene	4.30	4.40
Biphenyl	4.06	
Pyrene	5.17	

The $\log_{10}$ of the average of eight previous measurments of K_{ow} by the shake-centrifugation method for biphenyl is 4.09. The $\log_{10}K_{ow}$ of the average of thirteen previous measurements by the shake-centrifugation method for pyrene is 5.05. These are in good agreement with the SQC shake-centrifugation measurements made concurrently with the phenanthrene measurements.

B.4 ESTIMATED DATA:

A promising new computational method for predicting chemical reactivity is the computer expert system SPARC (SPARC Performs Automated Reasoning in Chemistry) being developed by Samuel W. Karickhoff, at ERL-Athens, and other scientists at the University of Georgia (Karickhoff et al., 1989). The system has the capability of crossing chemical boundaries to

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cover all organic chemicals and uses algorithms based on fundamental chemical structural theory to estimate parameters. Organic chemists have in the past established the types of structural groups or atomic arrays that impart certain types of reactivity and have described, in "mechanistic" terms, the effects on reactivity of other structural constituents appended to the site of reaction. To encode this knowledge base, Karickhoff and his associates developed a classification scheme that defines the role of structural constituents in affecting or modifying reactivity. SPARC quantifies reactivity by classifying molecular structures and selecting appropriate "mechanistic" models. It uses an approach that combines principles of quantitative structure-activity relationships, linear free energy theory (LFET), and perturbed molecular orbital (PMO) or quantum chemistry theory. In general, SPARC utilizes LFET to compute thermal properties and PMO theory to describe quantum effects such as delocalization energies or polarizabilities of pi electrons.

SPARC computes K_{ow} values from activity coefficients in the octanol($\sim l_o$) and water ($\sim l_w$) phases using Equation B-2.

$$Log_{10}K_{ow} = log_{10} (\sim l_w / \sim l_o) + log_{10} (M_o/M_w) \qquad (B-2)$$

where M_o and M_w are solvent molecularities of octanol and water, respectively. SPARC computes activity coefficients for any solvent/solute pair for which the structure parser can process the structure codes. Ultimately, any solvent/solute combination can be addressed. New solvents can be added as easily as solutes by simply providing a Simplified Molecular Interactive Linear Entry System (SMILES) string (Anderson et al., 1987, Weininger, 1988). Activity coefficients for either solvent or solute are computed by solvation models that are built from structural constituents requiring no data besides the structures.

A goal for SPARC is to compute a value that is as accurate as a value obtained experimentally for a fraction of the cost required to measure it. Because SPARC does not depend on laboratory operations conducted on compounds with structures closely related to that of the solute of interest, it does not have the inherent problems of phase separation encountered

in measuring highly hydrophobic compounds ($\log_{10}K_{ow} > 5$). For these compounds, SPARC's computed value should, therefore, be more reliable than a measured one. Reliable experimental data with good documentation are still necessary, however, for further testing and validation of SPARC.

CLOGP (Chou and Jurs, 1979) is a computerized program that estimates the $\log_{10}K_{ow}$, based on Leo's Fragment Constant Method (Lyman et al., 1982). CLOGP provides an estimate of $\log_{10}K_{ow}$ using fragment constants (f_i) and structural factors (F_i) that have been empirically derived for many molecular groups. The estimated $\log_{10}K_{ow}$ is obtained from the sum of constants and factors for each of the molecular subgroups comprising the molecule using Equation B-3.

$$\text{Log}_{10}K_{ow} = \sum_{i=1}^{n} (f_i + F_i) \tag{B-3}$$

The method assumes that $\log_{10}K_{ow}$ is a linear additive function of the structure of the solute and its constituent parts and that the most important structural effects are described by available factors. The structure of the compound is specified using the SMILES notation. The CLOGP algorithm is included in the database QSAR[1] located at EPA's Environmental Research Laboratory at Duluth, Minnesota. All CLOGP values reported here were obtained through QSAR.

Table B-4 shows the estimated $\log_{10}K_{ow}$ values that were computed with SPARC and CLOGP.

[1]Quantitative Structure-Activity Relationships (QSAR) is an interactive chemical database and hazard assessment system designed to provide basic information for the evaluation of the fate and effects of chemicals in the environment. QSAR was developed jointly by the U.S. EPA Environmental Research Laboratory, Duluth, Minnesota, Montana State University Center for Data System and Analysis, and the Pomona College Medicinal Chemistry Project.

TABLE B-4. $LOG_{10}K_{OW}$ VALUES ESTIMATED BY SPARC AND CLOGP

Chemical	SPARC	CLOGP
Phenanthrene	4.58	4.49
Biphenyl	4.25	4.03
Pyrene	5.13	4.95

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APPENDIX C. - SUMMARY OF DATA FROM SEDIMENT SPIKING EXPERIMENTS WITH PHENANTHRENE THAT WERE USED TO CALCULATE K_{oc} VALUES (FIGURE 2-2) AND TO COMPARE MORTALITIES OF AMPHIPODS WITH INTERSTITIAL WATER TOXIC UNITS (FIGURE 4-1) AND PREDICTED SEDIMENT TOXIC UNITS (FIGURE 4-2).

SEDIMENT SOURCE	MORTALITY (%)	SEDIMENT CONCENTRATION ug/g DRY WT.	ORG. CAR.	PORE WATER CONCENTRATION (ug/L)	TOC (%)	Log K_{oc}	REFERENCES
South Beach, OR. Rhaustorius estuarius	5	0	0	0	0.82		Swartz, 1991
	5	0	0	0	1.02		
	5	4	400	15	1.02	4.43	
	5	6.3	620	25	1.02	4.39	
	12.5	10.8	1060	40	1.02	4.42	
	17.5	18	1760	74	1.02	4.38	
	30	26.3	2570	105	1.02	4.39	
	52.5	49.3	4830	174	1.02	4.44	
	97.5	82.5	10070	344	0.82	4.47	
McKinney Slough, OR. Rhaustorius estuarius	15	0	0	0	2.36		Swartz, 1991
	7.5	0	0	0	2.47		
	15	11.4	460	18	2.47	4.41	
	22.5	19	770	30	2.47	4.41	
	12.5	27.2	1100	52	2.47	4.33	
	22.5	48.4	1950	99	2.47	4.29	
	32.5	61.5	2480	118	2.47	4.32	
	72.5	145.5	5870	201	2.47	4.47	
	100	194	8220	291	2.36	4.45	
Eckman Slough Site 1, OR. Rhaustorius estuarius	25	0	0	0	2.97		Swartz, 1991
	5	0	0	0	3.33		
	2.5	18.6	560	20	3.33	4.45	
	5	32.7	980	40	3.33	4.39	
	7.5	50.2	1510	66	3.33	4.36	
	7.5	54.6	1640	79	3.33	4.32	
	10	60.6	1820	88	3.33	4.32	
	35	87	2610	125	3.33	4.32	
	97.5	282	9530	294	2.97	4.51	

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APPENDIX C. Phenanthrene (cont'd)

SEDIMENT SOURCE	MORTALITY (%)	SEDIMENT CONCENTRATION ug/g		PORE WATER CONCENTRATION (ug/L)	TOC (%)	Log K_{oc}	REFERENCES
		DRY WT.	ORG. CAR.				
South Beach, OR. Leptocheirus plumulosus	0	0	0	0	0.82		Swartz, 1991
	2.5	0	0	0	1.96		
	2.5	6.4	320	24	1.96	4.12	
	7.5	11	560	42	1.96	4.12	
	5	19.1	970	70	1.96	4.14	
	0	27	1370	117	1.96	4.07	
	5	48.8	2490	168	1.96	4.17	
	35	70.6	3600	268	1.96	4.13	
	60	107.7	13130	478	0.82	4.44	
McKinney Slough, OR. Leptocheirus plumulosus	0	0	0	0	2.36		Swartz, 1991
	2.5	0	0	0	2.5		
	5	19	760	31	2.5	4.39	
	15	30.3	1210	57	2.5	4.33	
	7.5	49.4	1970	98	2.5	4.30	
	5	77.1	3080	159	2.5	4.29	
	10	120	4800	246	2.5	4.29	
	60	173.2	6920	321	2.5	4.33	
	80	270	11440	382	2.36	4.48	
Eckman site 1, OR. Leptocheirus plumulosus	7.5	0	0	0	3.6		Swartz, 1991
	12.5	27.5	760	39	3.6	4.29	
	17.5	44.1	1220	62	3.6	4.29	
	17.5	61	1690	84	3.6	4.30	
	12.5	76.6	2120	119	3.6	4.25	
	17.5	105	2910	163	3.6	4.25	
	22.5	174.9	4850	232	3.6	4.32	
	52.5	263.4	8870	401	2.97	4.34	
	80	346.4	11660	438	2.97	4.43	

C-2