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Office of Water &
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WATER

Proposed Sediment Quality Criteria for the Protection of Benthic Organisms:

ACENAPHTHENE

CONTENTS

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). 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 value (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 stable at equilibrium; (2) the concentration in either phase can be predicted using appropriate partition coefficients and the measured concentration in another 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; and (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: (a) pore water is difficult to adequately sample; and (b) 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 acenaphthene 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 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 acenaphthene. 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: ACENAPHTHENE:

Acenaphthene is a member of the polycyclic aromatic hydrocarbon (PAH) group of organic compounds. It occurs both naturally in coal tar, and as a by product of manufacturing processes such as petroleum refining, shale oil processing and coal tar distilling (Verschueren, 1983). Other man made sources of acenaphthene include its generation as a by product of the combustion of tobacco, and its presence in asphalt and in soots generated by the combustion of aromatic fuels amended with pyridine (Verschueren, 1983). Acenaphthene is used in

manufacturing processes to produce dyes, plastics, insecticides and fungicides (Windholtz et al., 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 be expected over the next several decades (Eadie et al., 1982).

Acenaphthene has a two ring bridged structure (Figure 1-1). It has a solubility in water at 25°C of 3.94 mg/l (Miller et al., 1985), and is a solid at room temperature (melting point of 116°C). Two significant processes which can influence the fate of acenaphthene in sediment are sorption and biodegradation (U.S. EPA, 1980). Sorption of acenaphthene onto solids in the water column and subsequent settling, as well as partitioning onto organics in the sediment, can significantly affect acenaphthene transport. Bioaccumulation is a short-term process in which PAHs with 4 rings or less are metabolized and 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 acenaphthene in the sediment are oxidation, hydrolysis and volatilization (U.S. EPA, 1980).

The acute toxicity of acenaphthene from individual toxicity tests ranges from 120.0 to 2,045 μg/L for freshwater and 160 to 16,440 μg/L for saltwater organisms (Appendix A). Differences between concentrations of acenaphthene causing acute lethality and chronic toxicity are small; acute-chronic ratios range from 1.5 to 6.7 (Table 3-3). Although acenaphthene 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 acenaphthene, and the technical basis for setting the SQC for acenaphthene. Section 2 reviews a variety of methods and data useful in deriving partition coefficients for acenaphthene and
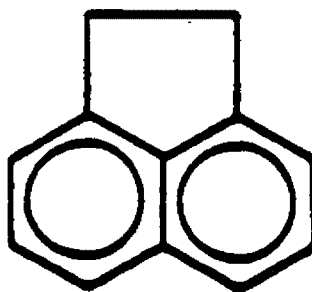
MOLECULAR FORMULA	$C_{12}H_{10}$
MOLECULAR WEIGHT	154.21
DENSITY	1.069 g/cc @ 20°C
MELTING POINT	90-95°C
PHYSICAL FORM	Orthorhombic
	bipyramidal needles
VAPOR PRESSURE	0.0026 mPa (25°C)

CAS NUMBER:	83-32-9
CHEMICAL NAME:	1,2-Dihydroacenaphthylene;
	periethylenenaphthalene;
	1,8-ethylenenaphthalene

Figure 1-1.   Chemical structure and physical-chemical properties of acenaphthene.

includes the K_{oc} recommended for use in the derivation of the acenaphthene SQC. Section 3 reviews aquatic toxicity data contained in the acenaphthene 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 acenaphthene in the derivation of the SQC. Section 4 reviews data on the toxicity of acenaphthene in sediments, the need for organic carbon normalization of acenaphthene 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 acenaphthene and its uncertainty. The SQC for acenaphthene is then compared to STORET (U.S. EPA, 1989b) and National Status and Trends (NOAA, 1991) data on acenaphthene's environmental occurrence in sediments. Section 6 concludes with the criteria statement for acenaphthene. 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

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quantify the exposure concentration for an organism. Thus, knowledge of the partitioning of 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 acenaphthene 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:

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

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 acenaphthene, 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:

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

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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 ACENAPHTHENE:

Several approaches have been used to determine K_{ow} for 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}'s. The measurement methods were shake-centrifugation and generator column, and the estimation methods were SPARC and CLOGP (Appendix B). Data were also extracted from the literature (Appendix B). 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.

Only one primary reference for acenaphthene was found, with a measured $\log_{10}K_{ow}$ value of 3.92 (Banerjee et al., 1980). Preliminary experience with the SPARC program suggests that the program can compute values for partition coefficients for high log P chemical 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 acenaphthene is 3.88. The CLOGP program estimate of the $\log_{10}K_{ow}$ value for acenaphthene using structure activity relationships is 4.07.

The two measurement methods provide additional data from which to define K_{ow} for acenaphthene (Table 2-1; Appendix B). The shake-centrifugation method yielded $\log_{10}K_{ow}$ = 3.84 $\pm$ 0.022 (n=4) and the generator column method yielded $\log_{10}K_{ow}$ = 4.17 $\pm$ 0.007 (n=4). There is no clear-cut best value from the data that has been developed. Considering the agreement among the one measured value in the literature, the SPARC estimated value, and

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the average for the values measured by the shake-centrifugation method under carefully controlled conditions in the ERL,A Laboratory, 3.84 is the recommended $\log_{10}K_{ow}$ value for deriving the sediment quality criterion. The range of of the four $\log_{10}K_{ow}$ value from the shake-centrifugation measurements is 3.82 to 3.88.

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

Measurement Technique	Number of Analyses	$\log_{10}K_{ow}$	
		Mean	SD
Shake-Centrifugation	4	3.84	0.022
Generator Column	4	4.17	0.007
SPARC	-	3.88	-
CLOGP	-	4.07	-

2.3 DERIVATION OF K_{oc} FROM ADSORPTION STUDIES:

Several types of experimental measurements 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 acenaphthene and pore water acenaphthene concentrations were 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 effect. This effect suppresses the partition coefficient relative to that observed for undisturbed

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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:

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

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:

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

Figure 2-1 compares observed partition coefficient data for the reversible component with calculated values estimated with the particle interaction model (Equation 2-4 and Equation 2-5) for a wide range of compounds (Di Toro, 1985). The observed partition coefficient for acenaphthene using adsorption data (Mihelcic and Luthy, 1988) is highlighted on this plot. The measured value reflects significant particle interaction effects (the partition coefficient about a factor of four lower than the value expected in the absence of particle effects.)

In the absence of particle effects, K_{oc} is related to K_{ow} via Equation 2-5, shown above. For log $K_{ow} = 3.84$ (ERL,A mean measured value), this expression results in an estimate of log $K_{oc} = 3.78$.

2.3.2 K_{oc} FROM SEDIMENT TOXICITY TESTS:

Measurements of K_{oc} are available from sediment toxicity tests using acenaphthene (Swartz, 1991). These tests were with different saltwater sediments having a range of organic

Partition Coefficient

Reversible Component
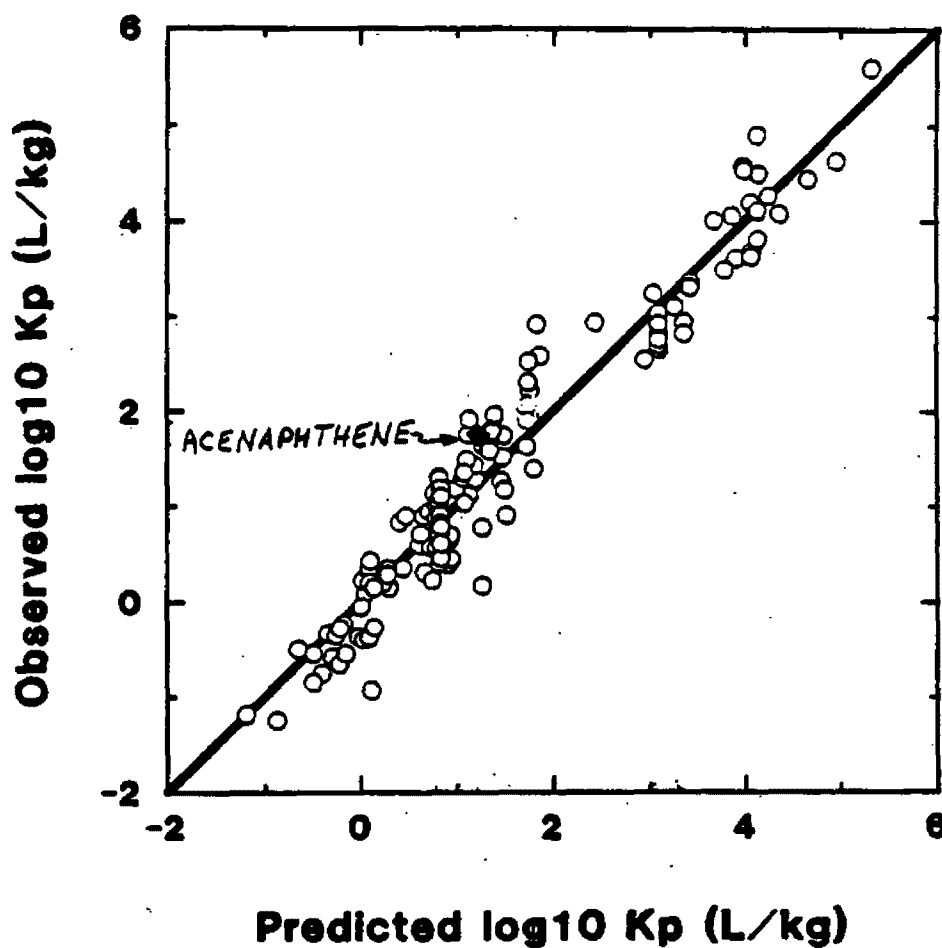
Figure 2-1. Observed versus calculated (equation 2-4) partition coefficients for non-ionic organic chemicals (acenaphthene datum is highlighted).

carbon contents of 1.02 to 4.37 percent (Table 4-1; Appendix C). Acenaphtene concentrations were measured in sediments and pore waters providing the data necessary to calculate the partition coefficient for an undisturbed sediment. The pore water measurements did not increase at values greater than 1,000 μg/L suggesting that the limit of aqueous solubility was being approached. These tests were run at 15°C, but a literature search for acenaphthene revealed no solubility data at this temperature. Solubility for acenaphthene is reported as 3.94 mg/L at 25°C (Miller et al., 1985), supporting the idea of saturation limitation. As a result, computations for the partition coefficient did not include treatments where pore water concentrations were greater than 1,000 μg/L.

Figure 2-2 is a plot of the organic carbon-normalized sorption isotherm for acenaphthene where the sediment acenaphthene concentration (μg/g_{oc}) is plotted versus pore water concentration (μg/L). The data used to make this plot are included in Appendix C. Data from treatments where pore water concentrations were greater than 1,000 μg/L were not included on the plot. The line of unity slope corresponding to the $\log_{10}K_{oc} = 3.78$ is compared to the data.

A probability plot of the observed experimental $\log_{10}K_{oc}$ values is shown in Figure 2-2. The $\log_{10}K_{oc}$ values are approximately normally distributed with a mean of $\log_{10}K_{oc} = 3.58$ and a standard error of the mean of 0.012. This value is statistically indistinguishable from $\log_{10}K_{oc} = 3.78$, which was computed from the experimentally determined acenaphthene $\log_{10}K_{ow}$ of 3.84 (Equation 2-5). Complexation with pore water DOC has not been accounted for in the experimentally based estimate of $\log_{10}K_{oc} = 3.58$. 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 the SQC, the SQC concentration would tend to be environmentally conservative.

2.4 SUMMARY OF DERIVATION OF K_{oc} FOR ACENAPHTHENE:

The K_{oc} selected to calculate the sediment quality criteria for acenaphthene is based on

the regression of $\log_{10} K_{OC}$ from $\log_{10} K_{OW}$ (Equation 2-5), using the acenaphthene $\log_{10} K_{OW}$ of 3.84 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 a $\log_{10} K_{OC} = 3.78$. This value is in very good agreement with the $\log_{10} K_{OC}$ of 3.58 measured in the sediment toxicity tests.
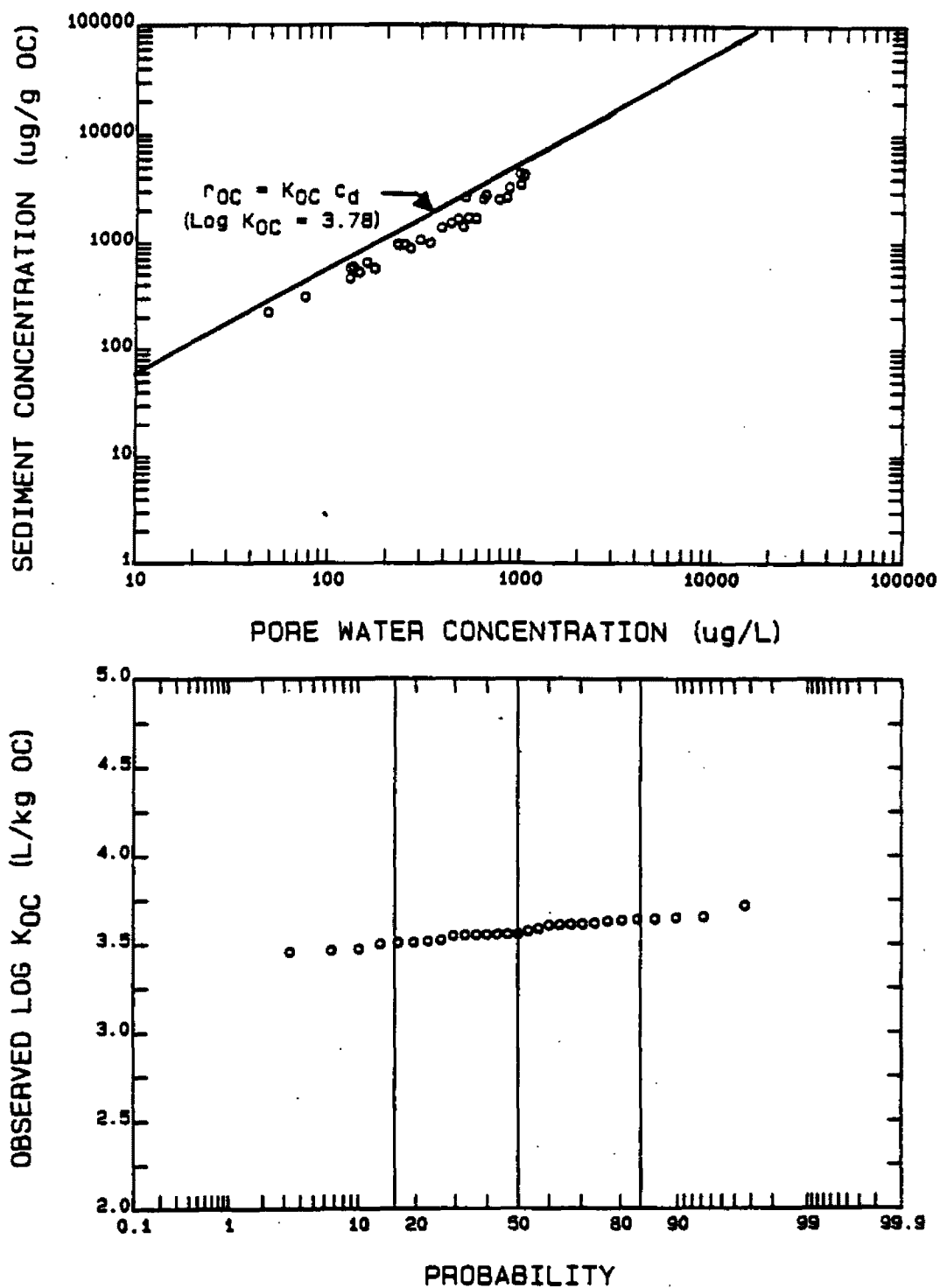
Figure 2-2.   Organic carbon-normalized sorption isotherm for acenaphthene (top) and probability plot of K_{oc} (bottom) from sediment toxicity tests conducted by Swartz (1991).

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SECTION 3

TOXICITY OF ACENAPHTHENE: WATER EXPOSURES

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

The equilibrium partitioning method for derivation of sediment quality criteria uses the acenaphthene water quality criteria 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 on the sediment surface (epibenthic) and obtain their food from either the sediment or water column (U.S.EPA, 1989c). In this section (1) the FCV from the acenaphthene WQC document (U.S. EPA, 1980) is revised using new aquatic toxicity test data, and (2) the use of this FCV is justified as the effects concentration for SQC derivation.

3.2 ACUTE TOXICITY-WATER EXPOSURES:

Twenty standard acute toxicity tests with acenaphthene have been conducted on 10 freshwater species from 10 genera (Appendix A). Overall genus mean acute values (GMAVs) range from 120 to 2,045 $\mu g/L$. Three invertebrates and two fishes were among the most sensitive species; overall GMAVs for these taxa range from 120 to 670 $\mu g/L$. Tests on the benthic life-stages of 5 species from 5 genera are contained in this database (Table 3-1; Appendix A). Benthic organisms were among both the most sensistive, and most resistant, freshwater genera to acenaphthene. Three epibenthic species, stoneflies, a snail and channel catfish, were tested; GMAVs range from 240 and >2,040 $\mu g/L$. Two infaunal species were tested, including the amphipod, Gammarus minus (LC50 = 460 $\mu g/L$), and the midge, Paratanytarsus sp. (LC50 = 2,045 $\mu g/L$). The Final Acute Value derived from the overall GMAVs (Stephan et al., 1985) for freshwater organisms is 80.01 (Table 3-3).

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TABLE 3-1. - ACUTE SENSITIVITY OF FRESHWATER AND SALTWATER BENTHIC SPECIES TO ACENAPHTHENE.

RANK[1] HMAV GENUS	COMMON/SCI. NAME	LIFE[2] STAGE	HAB-[3] ITAT	HMAV SPECIES[4]	HMAV GENUS[5]
				µg/L	µg/L
	FRESHWATER SPECIES				
2	Stonefly, Peltoperla maria	X	E	240	240
3	Amphipod, Gammarus minus	X	I	460	460
8	Channel catfish, Ictalurus punctatus	J	E	1,720	1,720
9	Snail, Aplexa hypnorum	A	E	>2,040	>2,040
10	Midge, Paratanytarsus sp.	X	I	2,045	2,045
	SALTWATER SPECIES				
1	Sand shrimp, Crangon septemspinosus	X	E	245.0	245.0
2	Mysid, Mysidopsis bahia	J	E	317.7	317.7
3	Amphipod, Leptocheirus plumulosus	A	I	589.4	589.4
5	Amphipod, Ampelisca abdita	J	I	1,125	1,125
6	Sheepshead minnow, Cyprinodon variegatus	J	E,W	3,100	3,100
9	Annelid worm, Neanthes arenaceodentata	J	I	7,693	7,693

TABLE 3-1. (Cont'd)

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

[b]Life stage: A = adult, J = juvenile, L = larvae, E = embryo, U = life stage and habitat unknownm, X = life stage unknown but habitat known.

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

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

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

Twenty-one acute toxicity tests have been conducted on 10 saltwater species from 10 genera (Appendix A). Overall GMAVs range from 245.0 to 8,163 μg/L. Crustaceans were most sensitive; GMAVs range from 245.0 to 1,125 μg/L. Benthic life-stages from 6 species from 6 genera have been tested (Table 3-1; Appendix A). They are among both the most sensitive, and most resistant, saltwater genera to acenaphthene. The most sensitive benthic species is the sand shrimp, Crangon septemspinosus, with a 96-hour LC50 of 245.0 μg/L based on unmeasured concentrations. The mysid, Mysidopsis bahia, has a similar sensitivity with an average, flow-through 96-hour LC50 of 317.7 μg/L based on measured concentrations. Other benthic species for which there are data appear less sensitive; GMAVs range from 589.4 to 7,693 μg/L. The Final Acute Value for saltwater species derived from the overall GMAVs (Stephan et al., 1985) is 140.8 μg/L (Table 3-3).

3.3 CHRONIC TOXICITY - WATER EXPOSURES:

Life cycle toxicity tests have been conducted with the freshwater midge (Paratanytarsus sp.) and the saltwater mysid (M. bahia) and early life stage tests have been conducted with the fathead minnow (Pimephales promelas) and sheepshead minnow (Cyprinodon variegatus) (Table 3-2; 3-3). For each of these species, except for fathead minnows, one or more benthic life stages were exposed to acenaphthene. Other chronic toxicity tests have been conducted with these two freshwater species (Lemke, 1984; Lemke et al.,1983; Lemke and Anderson, 1984) but insufficient documentation is available to permit use of these results (Thursby, 1991a).

Two acceptable life cycle toxicity tests have been conducted with midges (Northwestern Aquatic Sciences, 1981). In the first test there was a 59% reduction in growth and an 85% reduction in reproduction in 575 μg/L relative to control animals (Table 3-2). Eggs produced by animals in this first test failed to hatch at 575 μg/L. There was no significant effect on parents or egg hatchability in acenaphthene concentrations from 32 to 295 μg/L. In the second test with midges, there was a 21% reduction in survival in 315 μg/L relative to control animals;

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

Common Name, Scientific Name	Test[a]	Habitat[b] (Life stage)	NOEC(s)[c] µg/L	Parental LOEC[c] µg/L	Parental Effect[d]	Progeny LOEC µg/L	Progeny Effect[d]	References
				FRESHWATER SPECIES				
Midge, Paratanytarsus sp.	LC	E	32 - 295	575	59% G 85% M	575	100% M	Northwestern Aquatic Sciences, 1982
Midge, Paratanytarsus sp.	LC	E	27 - 164	315 676	21% M 64% M	>676	-	Northwestern Aquatic Sciences, 1981; Thursby, 1991a
Fathead minnow, Pimephales promelas	ELS	W	50	109 410 630	5% G 26% G;45% M 100% M	-	-	Academy of Natural Sciences, 1981; Thursby, 1991a
Fathead minnow, Pimephales promelas	ELS	W	50, 109	410 630	20% G;66% M 100% M	-	-	1991a Academy of Natural Sciences, 1981
Fathead minnow, Pimephales promelas	ELS	W	67-332	495	54% G	-	-	Cairns and Nebeker, 1982
Fathead minnow, Pimephales promelas	ELS	W	197, 345	509 682 1,153	30% G 52% G;45% M 87% G;97% M	-	-	Cairns and Nebeker, 1982

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TABLE 3-2. (Cont'd)

Common Name, Scientific Name	Test[a]	Habitat[b] (Life stage)	NOEC(s)[c] µg/L	Parental OEC[c] µg/L	Parental Effect[d]	Progeny OEC µg/L	Progeny Effect[d]	References
Fathead minnow, Pimephales promelas	ELS	W	64	98 149 271 441	24% M 65% M 75% M 80% M	-	-	ERCO, 1981
Fathead minnow, Pimephales promelas	ELS	W	50, 91	139 290 426	20% M 50% M 52% M	-	-	ERCO, 1981
SALTWATER SPECIES								
Mysid, Mysidopsis bahia	LC	E (J,A)	100-240	340 510	93% R 100% M	>340	-	Horne et al., 1983
Mysid, Mysidopsis bahia	LC	E (J,A)	0.394[e]- 44.6	91.8 168 354	91% R 100% R;34% G 100% R;96% M	-	-	Thursby et al., 1989
Sheepshead minnow, Cyprinodon variegatus	ELS	E (E) E, W (J,A)	240-520	970 2,000 2,800	70% M 100% M 100% M	-	-	Ward et al., 1981

[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.

[e]Carrier control

3-6

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 ACENAPHTHENE.

Common Name, Scientific Name	Acute Value(µg/L)	Chronic Value(µg/L)	Acute-Chronic Ratio	Species Mean Acute-Chronic Ratio
FRESHWATER SPECIES				
Fathead minnow, Pimephales promelas	608	405.4	1.500	--
Fathead minnow, Pimephales promelas	608	419.1	1.451	1.475
Fathead minnow, Pimephales promelas	--	73.82	--	--
Fathead minnow, Pimephales promelas	--	211.4	--	--
Fathead minnow, Pimephales promelas	--	79.20	--	--
Fathead minnow, Pimephales promelas	--	112.5	--	--
Midge, Paratanytarsus sp.	2,045[a]	411.9	4.965	--
Midge, Paratanytarsus sp.	2,045[a]	227.3	8.997	6.683
SALTWATER SPECIES				
Mysid, Mysidopsis bahia	466.1	285.7	1.631	--
Mysid, Mysidopsis bahia	460	63.99	7.189	3.424

TABLE 3-3. (Cont'd)

Common Name, Scientific Name	Acute Value(µg/L)	Chronic Value(µg/L)	Acute-Chronic Ratio	Species Mean Acute-Chronic Ratio
Sheepshead minnow, Cyprinodon variegatus	3,100	710.2	4.365	4.365

ªGeometric mean of two flow-through measured tests from the same laboratory.

Freshwater:

Final Acute Value = 80.01 µg/L
Final Acute-chronic Ratio = 3.484
Final Chronic Value = 22.96 µg/L

Saltwater:

Final Acute Value = 140.8 µg/L
Final Acute-chronic Ratio = 3.484
Final Chronic Value = 40.41 µg/L

egg hatchability was not affected at the highest concentration tested (676 μg/L); although survival of hatched midge larvae was reduced 64% in this concentration.

A total of six early life-stage toxicity tests have been conducted with the fathead minnow as part of a round-robin test series ; two each from three laboratories (Table 3-2). The effect concentrations across laboraotories and tests ranged from 98 to 509 μg/L, a factor of 5.2. Growth (dry weight), survival or both growth and survival were reduced. Only one of these test pairs had a suitable measured acute value, allowing calculation of an acute-chronic ratio (Cairns and Nebeker, 1982). The concentration-response relationships were similar for these two tests. Parental fish were unaffected in the first test at acenaphthene concentrations ranging from 67 to 332 μg/L, while fish exposed to 495 μg/L had a 54% reduction in growth relative to control fish. Cairns and Nebeker (1982) observed a 30% reduction in growth in parental fish in 509 μg/L while there was no effect on fish exposed to 197 to 345 μg/L.

Data from three saltwater chronic toxicity tests are available, two with mysids and one with sheepshead minnows. Mysid reproduction was affected by acenaphthene in two tests from two different laboratories. In the first test (Horne et al., 1983) there was a 93% decrease in reproduction in 340 μg/L relative to control mysids; all mysids in 510 μg/L died. No effects were observed at 100 or 240 μg/L in the parental generation, and juveniles released in $\geq$ 340 μg/L were not affected. In the second test (Thursby et al., 1989b) there was a 41% decrease in growth in 168 μg/L and 96% increase in mortality at 354 μg/L. There was a 91% decrease in reproduction in mysids exposed to 91.8 μg/L and mysids exposed to 168 and 354 μg/L did not reproduce. Mysids exposed to $\leq$ 44.6 μg/L were not affected.

Sheepshead minnows exposed to acenaphthene in an early life stage test (Ward et al., 1981) were affected at acenaphthene concentrations of $\geq$970 μg/L (Table 3-2). There was a 70% reduction in survival of fish hatched in 970 μg/L. Fewer than 10% of the embryos at $\geq$ 2,000 μg/L hatched and all fish that hatched died. There was no effect on either survival or growth in fish exposed to 240 or 520 μg/L.

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The difference between acute and chronic toxicity of acenaphthene is small (Table 3-3). Species mean acute-chronic ratios are 1.475 for fathead minnows, 3.424 for mysids, 4.365 for sheepshead minnows and 6.683 for midges. The Final Acute-Chronic Ratio, the geometric mean of these four values, is 3.484.

The Final Chronic Values (Table 3-3) are used as the effect concentrations for calculating the sediment quality criteria for protection of benthic species. The Final Chronic Value for freshwater organisms of 22.96 μg/L is the quotient of the Final Acute Value of 80.01 μg/L and the Final Acute Chronic Ratio of 3.484. Similarly, the Final Chronic Value for saltwater organisms of 40.41 μg/L is the quotient of the Final Acute Value of 140.8 μg/L and the Final Acute-Chronic Ratio of 3.484.

3.4 APPLICABILITY OF THE WATER QUALITY CRITERION AS THE EFFECTS CONCENTRATION FOR DERIVATION OF THE ACENAPHTHENE 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 acenaphthene-specific comparisons in sensitivity of benthic and water-column species conducted. The following paragraph examines the data for acenaphthene.

An initial test of the difference between the probability distributions of freshwater and saltwater acenaphthene LC50s for all species (water column and benthic) is presented in Figure

3-10

3-1. The top panel is a log probability plot of the two LC50 distributions on a log scale versus 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 (0.500), and the probability (0.948) 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 the samples came from the same distribution is accepted at a 95% confidence level. Therefore for acenaphthene, comparisons of LC50s for benthic and water column species are conducted for combined freshwater and saltwater LC50 values.

The probability distributions of combined freshwater and saltwater acenaphthene 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 (0.300), and the probability (0.759) that a value of this magnitude or less cannot occur given that these two samples came from the same distribution. This analysis of the relative sensitivities of benthic and water column organisms that have been tested indicates they are from the same probability distribution of LC50's. Therefore they have similar acute sensitivities. This suggests that the final chronic value (FCV) for acenaphthene is an appropriate effects concentrations for both benthic and water column organisms.
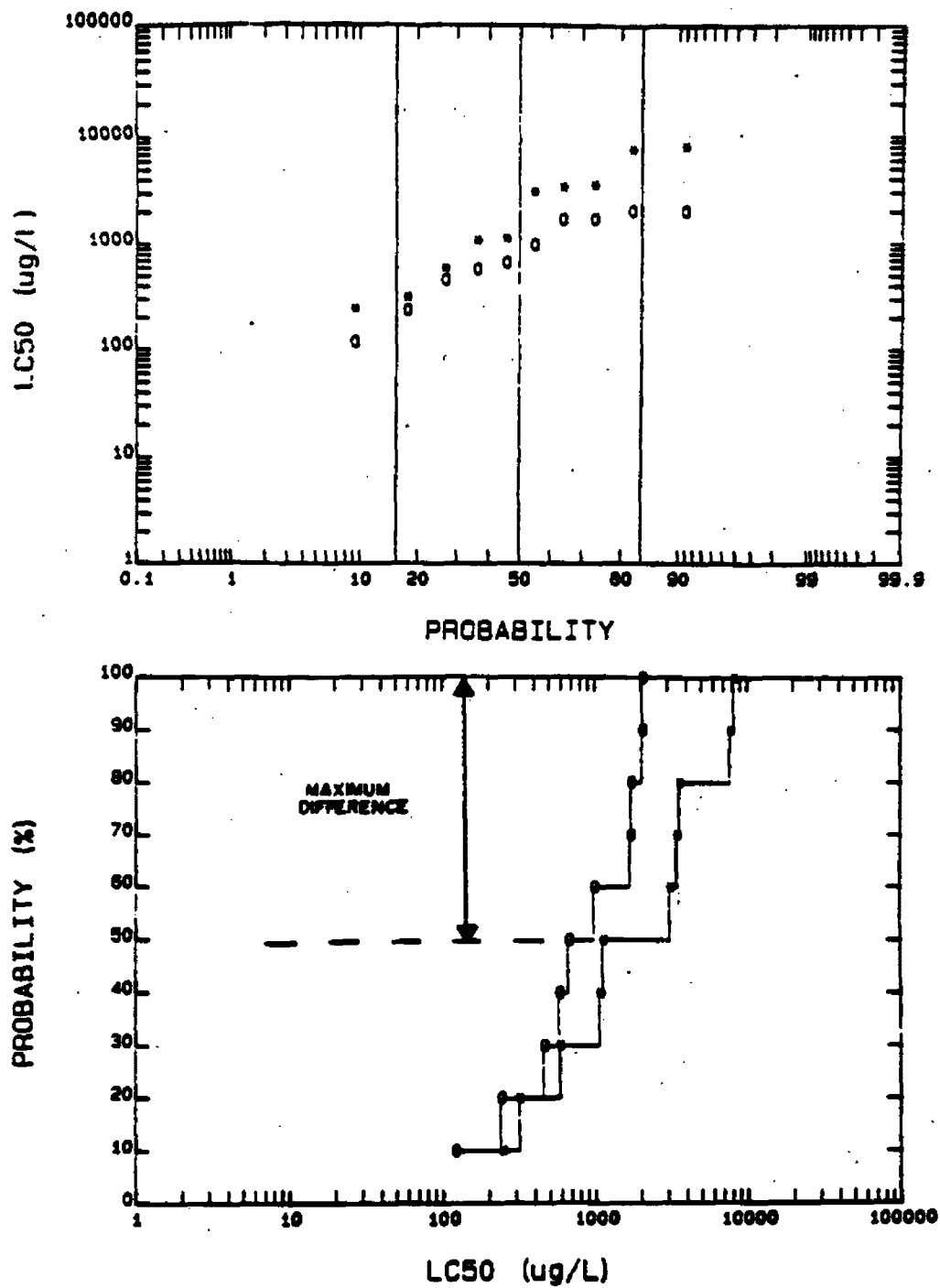
Figure 3-1.   Comparison of acenaphthene water only LC50 probability distributions for freshwater (O) and saltwater (*) species (top panel).   Cumulative distribution functions for calculating the K-S statistic (bottom panel).

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

Compar-ison	Habitat or Water Type[a]		K-S Statistic[b]	Probability[c]
Fresh vs Salt	Fresh (10)	Salt (10)	0.500	0.948
Benthic vs Water Column (Freshwater and saltwater)	Benthic (10)	Water (10) Column	0.300	0.759

[a]Value in parentheses is 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.
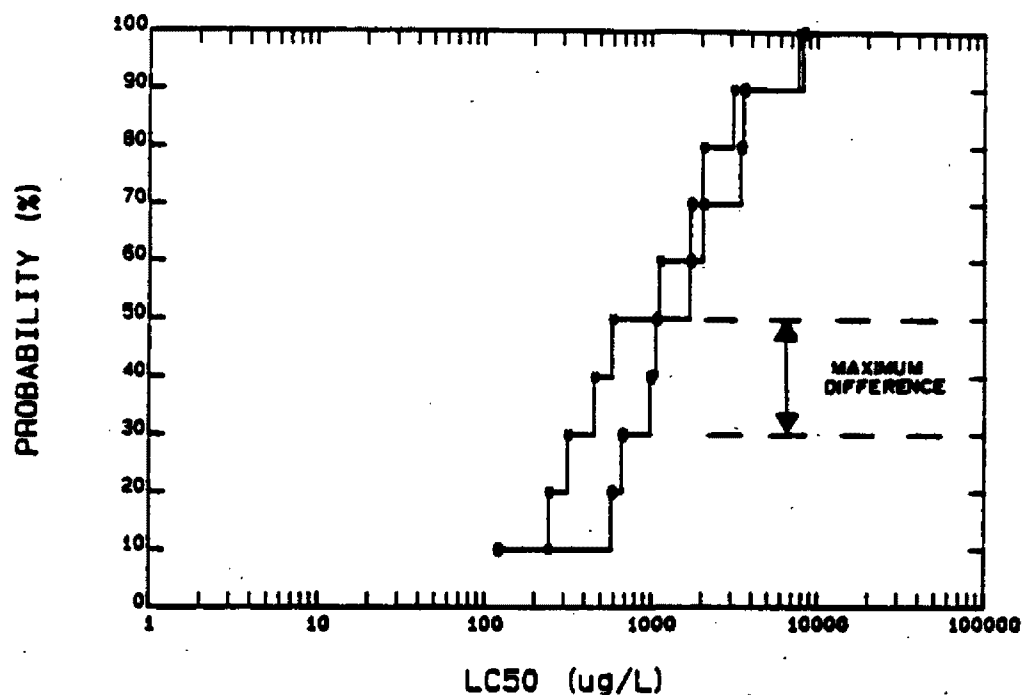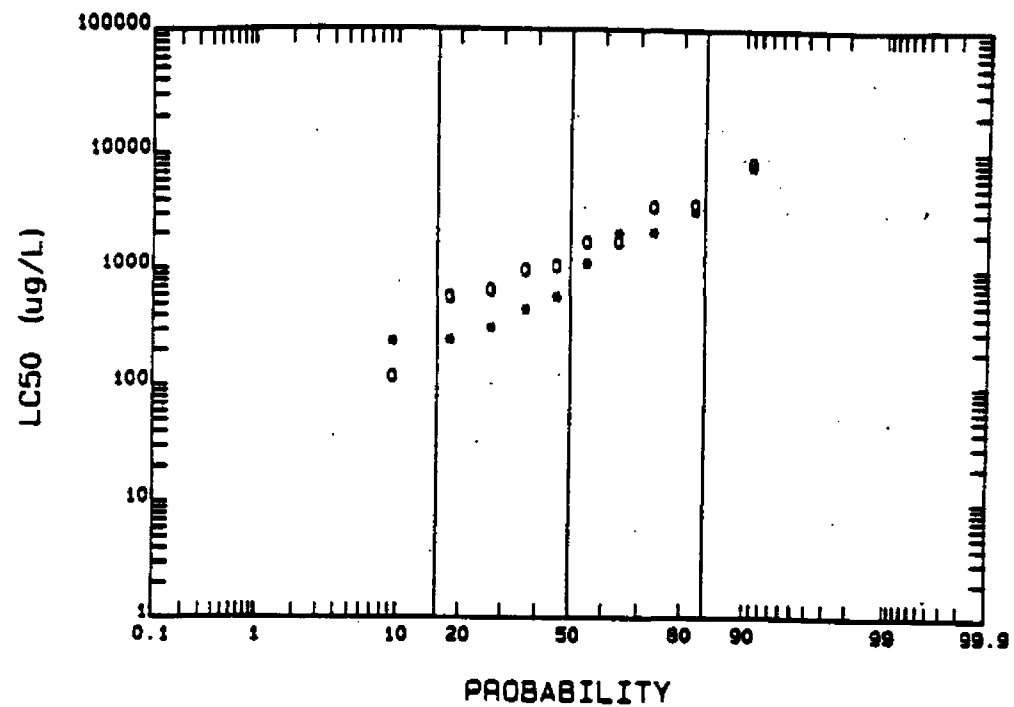
Figure 3-2. Comparison of acenaphthene water only LC50 probability distributions for water column (0) and benthic (*) freshwater and saltwater species (top panel). Cumulative distribution functions for calculating the K-S statistic (bottom panel).

SECTION 4

TOXICITY OF ACENAPHTHENE (ACTUAL AND PREDICTED): SEDIMENT EXPOSURES

4.1 TOXICITY OF ACENAPHTHENE IN SEDIMENTS:

The toxicity of acenaphthene spiked into sediments has been tested with two saltwater amphipod species. Freshwater benthic species have not been tested in acenaphthene-spiked sediments. All concentrations of acenaphthene in sediments or interstial 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 acenaphthene 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 acenaphthene. Data from these studies have not been included here because it is not possible to determine the contribution of acenaphthene to toxicity observed.

Swartz (1991) exposed the amphipods Eohaustorius estuarius and Leptocheirus plumulosus to three acenaphthene-spiked sediments with total organic carbon content (TOC) of 1.0%, 2.6%, and 4.4%. Sediments were rolled (1) for four hours in acenaphthene-coated bottles, (2) stored at 4°C for either 72 hours (experiments with E. estuarius) or overnight (experiments with L. plumolosus), (3) rolled for an additional four hours, and (4) then stored for 7 days at 4°C. The 10-day LC50's for both species increased slightly with increasing organic carbon concentration when the acenaphthene concentration was expressed on a dry

4-1

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

Common/Sci. Name	Sediment Source, Description	TOC (%)	Method[b]/ Duration (Days)	Response	Sediment Acenaphthene LC50, μg/g Dry wt.	Org. Car.	Pore Water LC50, μg/L	References
				FRESHWATER SPECIES				
Amphipod, Eohaustorius estuarius	South Beach, OR	1.23 0.82[a]	S,M/10	LC50	44.4	4,330	800	Swartz, 1991
Amphipod, Eohaustorius estuarius	McKinney Slough, OR	2.49	S,M/10	LC50	47.8	1,920	609	Swartz, 1991
Amphipod, Eohaustorius estuarius	Eckman Slough, OR	4.21	S,M/10	LC50	68.4	1,630	542	Swartz, 1991
Amphipod, Leptocheirus plumulosus	South Beach, OR	1.62 0.82[a]	S,M/10	LC50	>193	>23,500	>1,720	Swartz, 1991
Amphipod, Leptocheirus plumulosus	McKinney Slough, OR	2.52	S,M/10	LC50	193	7,730	1,410	Swartz, 1991
Amphipod, Leptocheirus plumulosus	Eckman Slough, OR	3.66 2.97[a]	S,M/10	LC50	382	11,200	1,490	Swartz, 1991

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

[b] S = Static; M = Measured.

weight basis, but decreased for E. estuarius and no pattern was apparent for L. plumulosus when concentration was expressed on an organic carbon basis. LC50's normalized to dry weight differed by less than a factor of 1.6 (43.3 to 68.4 $\mu g/g$) for E. estuarius and less than a factor of 1.9 for L. plumulosus over a 4.3-fold range of TOC. The organic carbon normalized LC50's for E. estuarius differed by a factor of 2.6 (1,600 to 4,180 $\mu g/g_{oc}$) while for L. plumulosus they differed by a factor of > 2.2 (10,890 to > 23,500 $\mu g/g_{oc}$).

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 acenaphthene is somewhat 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 acenaphthene and other non-ionic organic chemicals on an organic carbon basis for a range of sediments. Evidence supporting this prediction for acenaphthene and all SQC chemicals follows in Section 4.3.

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 1.4 (623 to 851 $\mu g/L$) for E. estuarius and by a factor of > 1.2 (1,400 to > 1,720 $\mu g/L$) for L. plumulosus. This variability is somewhat less than that shown when either dry weight (factors of 1.6 and 1.9) or organic carbon (factors of 2.6 and 2.2) normalization are used to determine LC50s based on acenaphthene concentration in sediments.

A more detailed evaluation of the degree to which the response of benthic organisms can

4-3

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

Common/Sci. Name	Method[a] Duration(days)	Water Only LC50	Pore Water LC50	Sediment Acenaphthene LC50			Predicted[c] LC50	Ratio: Actual LC50	Reference
				TOC (%)	μg/g Dry Wt.	μg/g OC	μg/g OC	Predicted	
		$\mu g/L$	$\mu g/L$						
Amphipod, Eohaustorius estuarius	FT,M/10	374	800	1.23 / 0.82[b]	44.4	4,330	2,250	1.92	Swartz, 1991
Amphipod, Eohaustorius estuarius	FT,M/10	374	609	2.49	47.8	1,920	2,250	0.85	Swartz, 1991
Amphipod, Eohaustorius estuarius	FT,M/10	374	542	4.21	68.4	1,630	2,250	0.72	Swartz, 1991
Amphipod, Leptocheirus plumulosus	FT,M/10	678	>1,720	1.62 / 0.82[b]	>193	>23,500	4,080	>5.76	Swartz, 1991
Amphipod, Leptocheirus plumulosus	FT,M/10	678	1,410	2.52	193	7,730	4,080	1.89	Swartz, 1991
Amphipod, Leptocheirus plumulosus	FT,M/10	678	1,490	3.66 / 2.97[b]	382	11,200	4,080	2.74	Swartz, 1991

[a]FT = flow-through, M = measured concentration

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

[c]Predicted LC50 ($\mu g/g_{OC}$) = water-only LC50 ($\mu g/L$) x K_{oc} (L/Kg_{OC}) x 1 $Kg_{OC}/1000g_{OC}$; Where $K_{oc} = 10^{3.78}$

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 acenaphthene 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 ($\mu g/L$) divided by the water only LC50 ($\mu g/L$). 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 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

PORE WATER TOXIC UNITS

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 and phenanthrene SQC documents, and original references for raw data.)

concentrations across sediment types. Data are available to test the normalization for acenaphthene 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 acenaphthene-spiked sediment tests on a $\mu g/g_{oc}$ basis with E. estuarius and L. plumulosus were predicted (Table 4-2) using the value of K_{oc} ($10^{3.7}$) from Section 2 of this document and the 10-day water-only LC50 values in Swartz (1991). Ratios of predicted to actual LC50s for acenaphthene averaged 1.01 (range 0.64 to 1.64) for E. estuarius and 3.09 (range 1.83 to >5.09) for L. plumulosus. The overall mean for both species was 2.05.

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 K_{ow} for kepone from ERL, Athens. Swartz (1991) exposed the saltwater amphipods E. estuarius 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 acenaphthene, dieldrin 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.
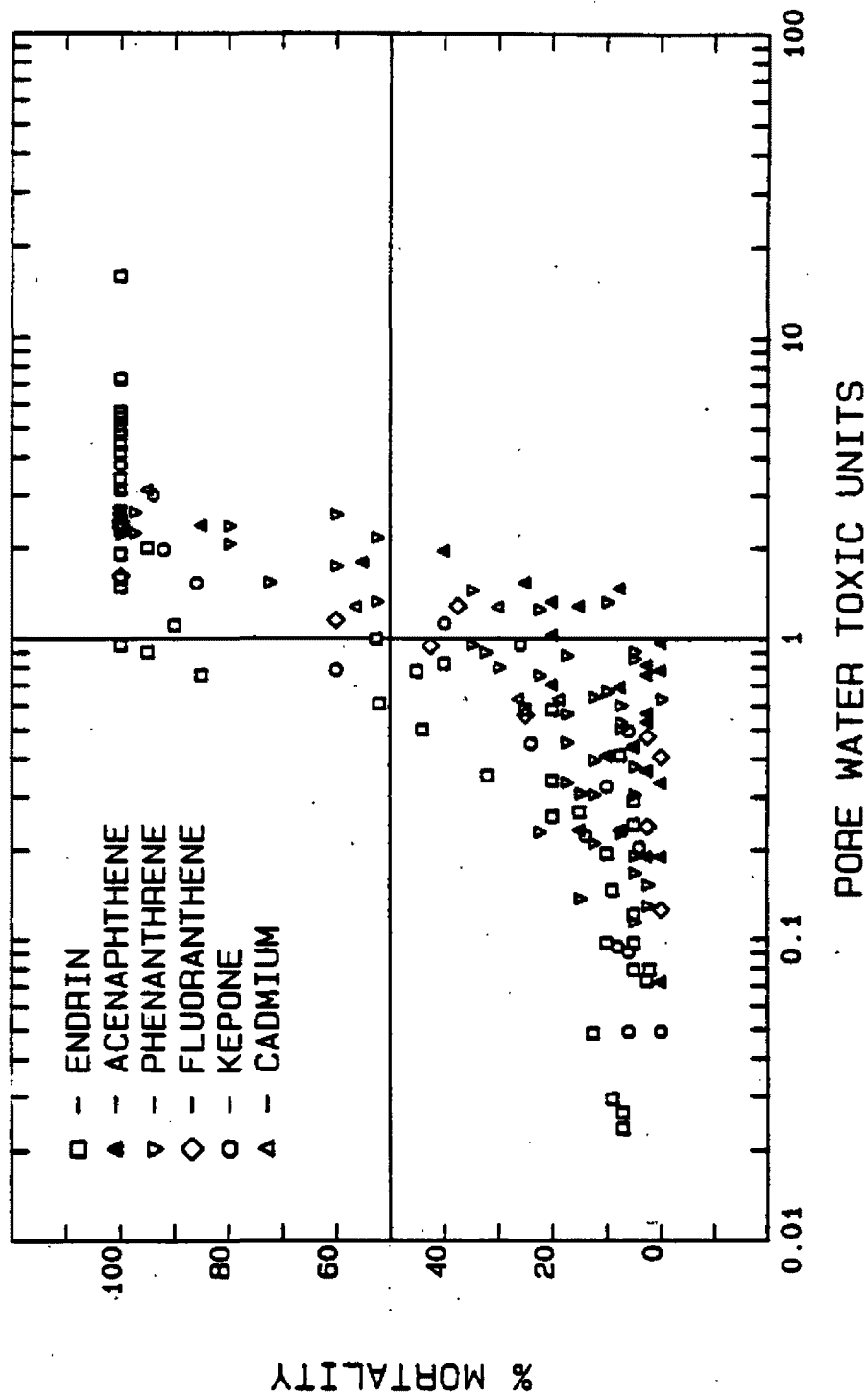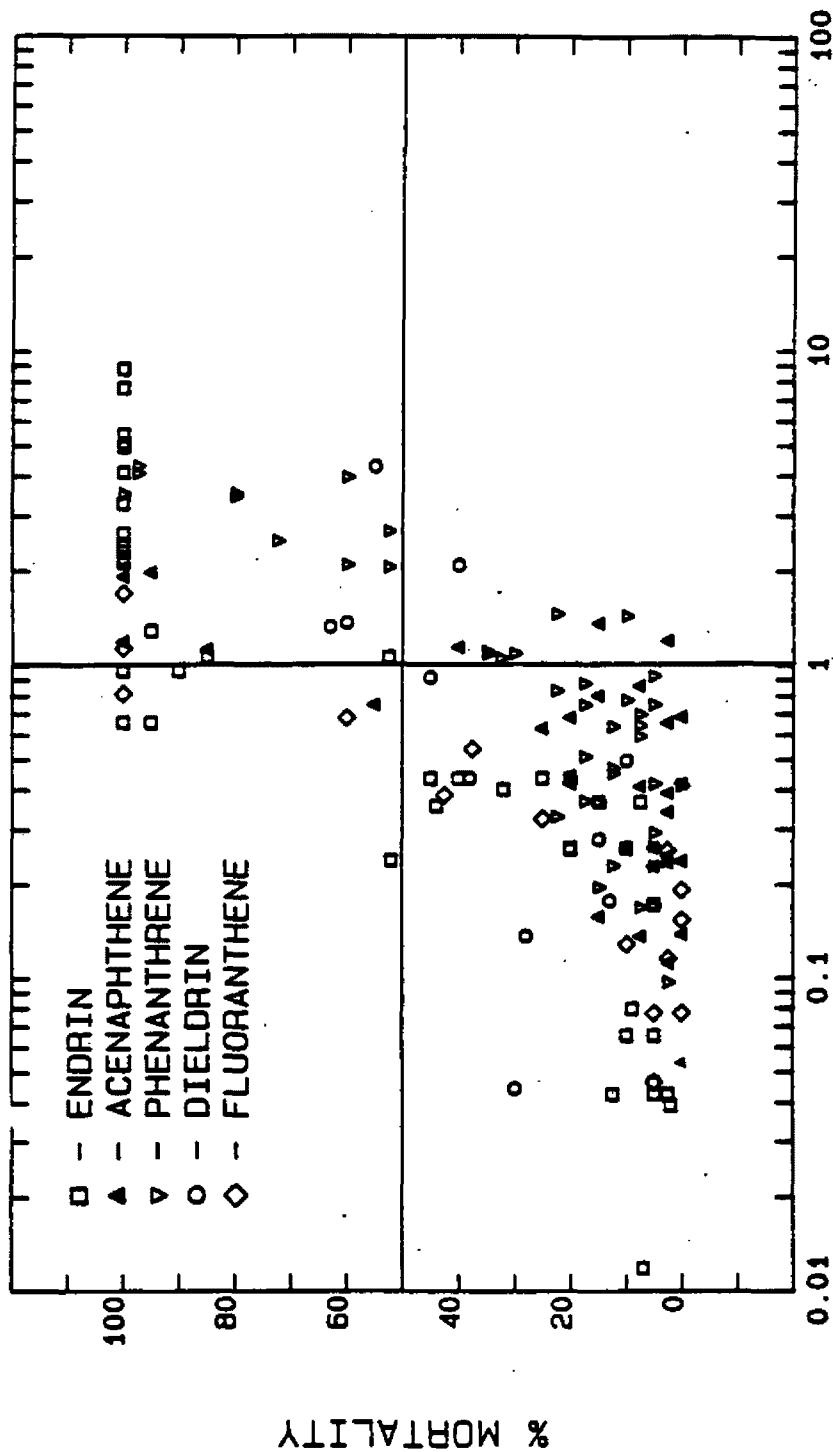
PREDICTED SEDIMENT TOXIC UNIT

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 phenanthrene SQC documents for raw data).

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SECTION 5

CRITERIA DERIVATION FOR ACENAPHTHENE

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:

$$SQC = K_p \, FCV \qquad (5\text{-}1)$$

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

$$SQC_{oc} = K_{oc} \, FCV \qquad (5\text{-}2)$$

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 acenaphthene sediment quality criteria.

TABLE 5-1. SEDIMENT QUALITY CRITERIA FOR ACENAPHTHENE.

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	3.84	3.78	23.0	138
Salt Water	3.84	3.78	40.4	243

^{a}SQC$_{oc}$ = $(10^{3.78}$ L/kg$_{oc})\bullet(10^{-3}$ kg$_{oc}$/g$_{oc})\bullet(23.0$ μg acenaphthene/L) = 138 μg acenaphthene/g$_{oc}$

^{b}SQC$_{oc}$ = $(10^{3.78}$ L/kg$_{oc})\bullet(10^{-3}$ kg$_{oc}$/g$_{oc})\bullet(40.4$ μg acenaphthene/L) = 243 μg acenaphthene/g$_{oc}$

5.2 UNCERTAINTY ANALYSIS:

Some of the uncertainty in the calculation of the acenaphthene sediment quality criteria can be estimated from the degree to which the equilibrium partitioning 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:

$$LC50_{s,oc} = K_{oc}LC50_w \qquad (5-3)$$

Therefore, K_{oc} can be used to define the equivalent sediment toxicity based on free

concentration in pore water:

$$LC50_{pw} = \frac{LC50_{s,oc}}{K_{oc}} \qquad (5\text{-}4)$$

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

$$LC50_{pw} = LC50_w \qquad (5\text{-}5)$$

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 ϵ represents the experimental error. Let $(\sigma_\alpha)^2$ and $(\sigma_\epsilon)^2$ 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 is:

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

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_1 and the variances of the model error, $(\sigma_a)^2$, 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 CRITERIA CONFIDENCE LIMITS FOR ACENAPHTHENE.

Source of Uncertainty	Parameter ($\mu g/g_{oc}$)	Value
Exposure media	σ_a	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 errors.

Hence:

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

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

The confidence limits are given in Table 5-3.

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

Type of Water Body	SQC_{oc} $\mu g/g_{oc}$	Sediment Quality Criteria 95% Confidence Limits ($\mu g/g_{oc}$)	
		Lower	Upper
Fresh Water	140	64	300
Salt Water	240	110	520

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 does not apply and the sediment quality criteria do not apply.

5.3 COMPARISON OF ACENAPHTHENE SQC TO STORET AND STATUS AND TRENDS DATA FOR SEDIMENT ACENAPHTHENE:

A STORET (U.S. EPA, 1989a) data retrieval was performed to obtain a preliminary assessment of the concentrations of acenaphthene in the sediments of the nation's water bodies. Log probability plots of acenaphthene concentrations on a dry weight basis in sediments since 1986 are shown in Figure 5-1. Acenaphthene is found at detectable concentrations in sediments from rivers, lakes and near coastal water bodies in the United States. Median concentrations are generally at about 0.1 $\mu g/g$ in each of these three types of water bodies. Acenaphthene concentrations in sediments range over seven orders of magnitude throughout the country.

The SQC for acenaphthene can be compared to existing concentrations of acenaphthene 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

5-5
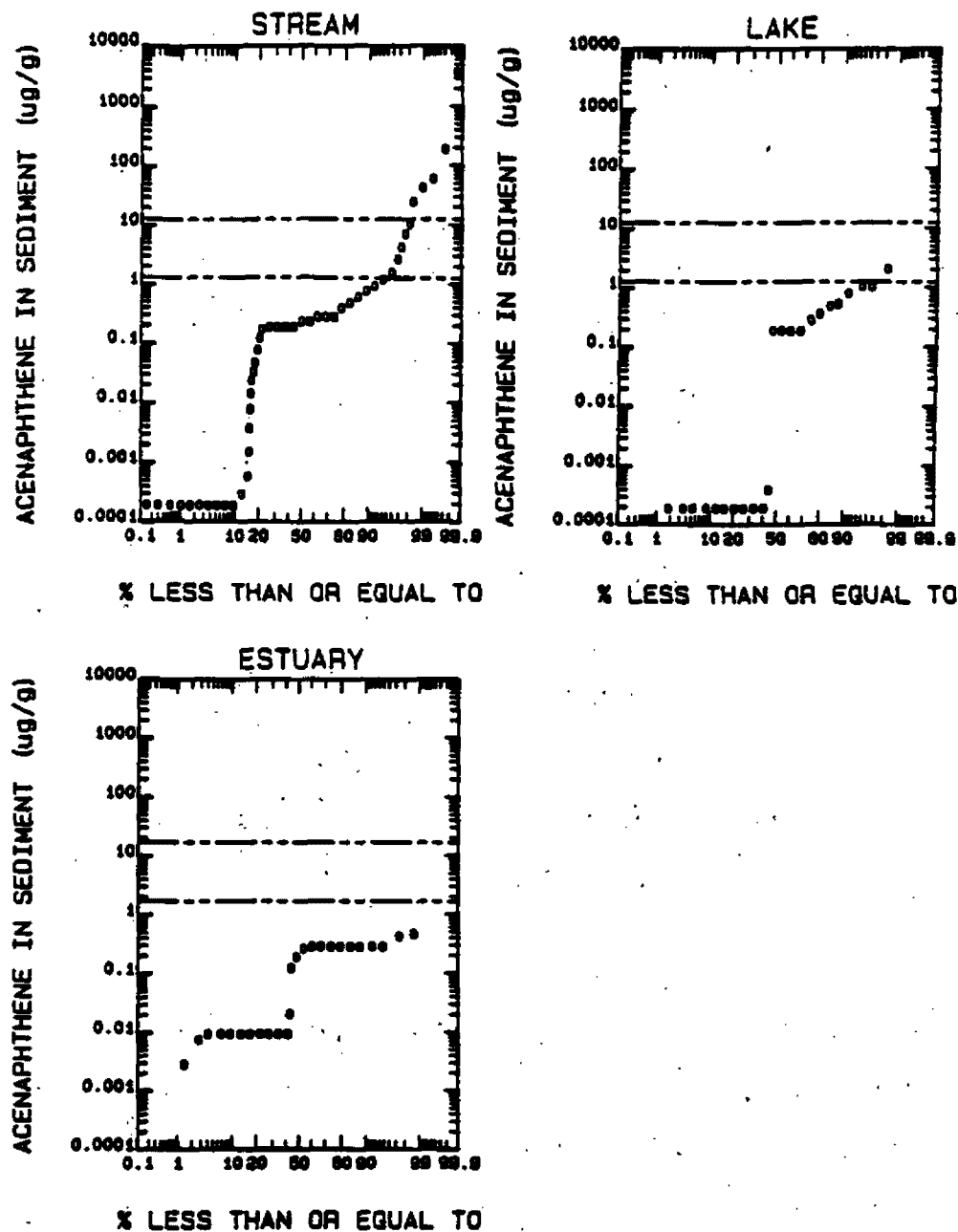
Figure 5-1. Probability distribution of concentrations of acenaphthene in sediments from streams (n=681), lakes (n=56) and estuaries (n=74) in the United States from 1986 to 1990 (0) from the STORET (U.S. EPA, 1989c) database compared to the acenaphthene SQC values of 14 $\mu g/g$ in freshwater sediments having TOC = 10% and 1.4 $\mu g/g$ in freshwater sediments having TOC = 1%; SQC values for saltwater sediments are 24 $\mu g/g$ when TOC =10% and 2.4 $\mu g/g$ 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%.

carbon levels of 1 to 10 percent are compared to acenaphthene's distribution in sediments as examples only. For fresh water sediments, SQC values are 1.4 $\mu g/g$ in sediments having 1% organic carbon and 14 $\mu g/g$ dry wt. in sediments having 10% organic carbon; for marine sediments SQC are 2.4 $\mu g/g$ and 24 $\mu g/g$, respectively. Figure 5-1 presents the comparisons of these SQC to probability distributions of observed sediment acenaphthene levels for streams and lakes (fresh water systems, shown on the upper panels) and estuaries (marine systems, lower panel). For both streams (n = 681) and lakes (n = 56), the SQC of 1.4 $\mu g/g$ for 1 % organic carbon sediments is exceeded by about 4 % of the data; the 14 $\mu g/g$ criteria for 10% organic carbon freshwater sediments is exceeded in about 2 % of the samples and none of the lake samples. In estuaries, the data (n = 74) indicate that neither of the criteria of 2.4 $\mu g/g$ dry weight for sediments having 1 % organic carbon or 24 $\mu g/g$ dry weight for sediments having 10 % organic carbon are exceeded, although the STORET database for marine sediments is not as extensive as the database for freshwater sediments.

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 acenaphthene (240 $\mu g/g_{oc}$) on Figure 5-2. Data presented are from sediments with 0.20 to 31.9% organic carbon. None of these samples (n=288) exceeded the criteria. Hence, these results are consistent with the preceding comparison of the marine SQC to STORET data.

Regional differences in acenaphthene 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 acenaphthene sediment

concentrations and the extent to which they may exceed the sediment quality criteria.
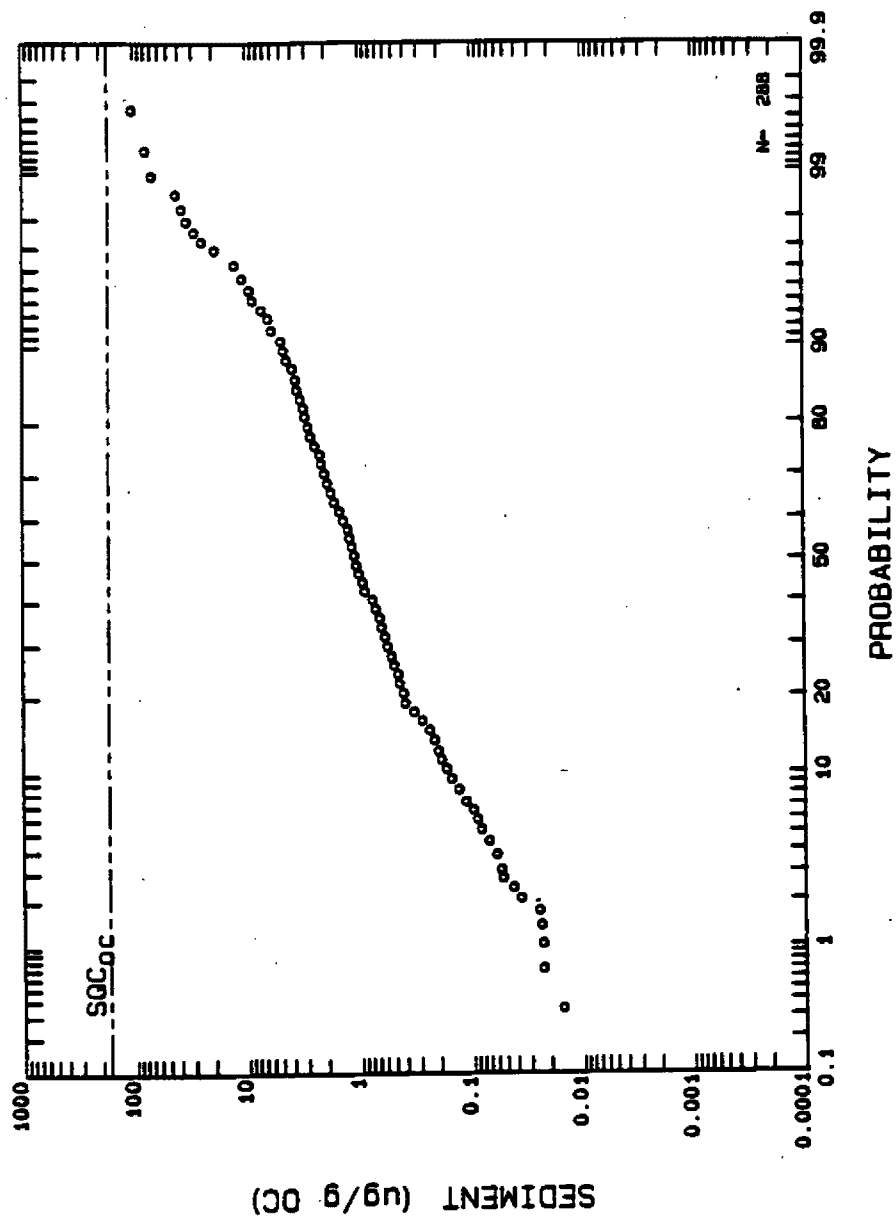
Figure 5-2. Probability distribution of concentrations of acenaphthene in sediments from coastal and estuarine sites from 1984 to 1989 as measured by the National Status and Trends Program (NOAA, 1991). The horizontal line is the SQC value of 240 $\mu g/g_{OC}$.

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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 $\leq$ 140 μg acenaphthene/g organic carbon and saltwater sediments containing $\leq$ 240 μg acenaphthene/g organic carbon.

These concentrations are the U.S. EPA's best scientific judgement at this time of the acceptable concentration of acenaphthene in sediments. Confidence limits of 64 to 300 μg/g_{oc} for freshwater sediments and 110 to 520 μg/g_{oc} for saltwater sediments are provided as an estimate of the uncertainty associated with the degree to which the observed concentration in sediment (μg/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 acenaphthene, 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.

SECTION 7

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Appendix A. - Acenaphthene: 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] BC50	HMAV SPECIES[f]	HMAV GENUS[g]	GMAV	OVERALL[h] GMAV	REFERENCES[1]
					μg/L	μg/L	μg/L	μg/L	μg/L	
FRESHWATER SPECIES										
Snail, Aplexa hypnorum	X	W	F	M	> 2,040	>2,040	>2,040	>2,040	>2,040	Holcombe et al., 1983
Cladoceran, Daphnia magna	X	W	S	M	320	-	-	-	-	EG&G, Bionomics, 1982
Cladoceran, Daphnia magna	X	W	S	M	1,300	-	-	-	-	EG&G, Bionomics, 1982
Cladoceran, Daphnia magna	X	W	F	M	120	-	-	-	-	EG&G, Bionomics, 1982
Cladoceran, Daphnia magna	X	W	S	U	41,000	-	-	-	-	LeBlanc, 1980
Cladoceran, Daphnia magna	X	W	S	U	3,450	120	120	120	120	Randall and Knopp, 1980
Amphipod, Gammarus minus	X	B	S	U	460	460	460	460	460	Horne et al., 1983
Stonefly, Peltoperla maria	X	B	S	U	240	240	240	240	240	Horne et al., 1983
Midge, Paratanytarsus sp.	X	B	S	M	2,000	-	-	-	-	Northwestern Aquatic Science, Inc., 1982
Midge, Paratanytarsus sp.	X	B	S	M	2,090	2,045	2,045	2,045	2,045	Northwestern Aquatic Science, Inc., 1982

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COMMON/SCI. NAME	LIFE[a] STAGE	HAB.[b] ITAT	METHOD[c]	CONCEN-TRATION[d]	LC50/[e] EC50 µg/L	HMAV SPECIES[f] µg/L	HMAV GENUS[g] µg/L	OVERALL[h] GMAV µg/L	REFERENCES[i]
Rainbow trout, Oncorhynchus mykiss	J	W	F	M	670	670	670	670	Holcombe et al., 1983
Brown trout, Salmo trutta	J	W	F	M	580	580	580	580	Holcombe et al., 1983
Fathead minnow, Pimephales promelas	J	W	F	M	608	-	-	-	Cairns and Nebeker, 1982
Fathead minnow, Pimephales promelas	J	W	F	M	>1,400	-	-	-	EG&G, Bionomics, 1982
Fathead minnow, Pimephales promelas	J	W	S	M	1,500	-	-	-	EG&G, Bionomics, 1982
Fathead minnow, Pimephales promelas	J	W	F	M	1,600	-	-	-	Holcombe et al., 1983
Fathead minnow, Pimephales promelas	A	W	R	U	3,700	-	-	-	Academy of Natural Science, 1981
Fathead minnow, Pimephales promelas	J	W	S	M	3,100	986	986	986	Marine Bioassay Laboratories, 1981
Channel catfish, Ictalurus punctatus	J	W	F	M	1,720	1,720	1,720	1,720	Holcombe et al., 1983
Bluegill, Lepomis macrochirus	J	W	S	U	1,700	1,700	1,700	1,700	Buccafusco et al., 1981; Ward et al., 1981

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Appendix A. - Acenaphthene: (continued)

SALTWATER SPECIES

COMMON/SCI. NAME	LIFE STAGE [a]	HAB-ITAT [b]	METHOD [c]	CONCEN-TRATION [d]	LC50/EC50 [e] µg/L	SMAV SPECIES [f] µg/L	HMAV GENUS [g] µg/L	OVERALL [h] GMAV µg/L	REFERENCES [i]
Annelid worm, Neanthes arenaceodentata	J	I	R	U	16,440	-	-	-	Thursby et al., 1989a
Annelid worm, Neanthes arenaceodentata	X	I	S	U	3,600	7,693	7,693	7,693	Horne et al., 1983
Slipper limpet, Crepidula fornicata	L	W	R	U	3,436	3,436	3,436	3,436	Thursby et al., 1989a
Mysid, Mysidopsis bahia	J	E	R	U	1,190	-	-	-	Thursby et al., 1989a
Mysid, Mysidopsis bahia	J	E	S	U	970	-	-	-	U.S. EPA, 1978; Ward et al., 1981
Mysid, Mysidopsis bahia	J	E	F	M	460	-	-	-	Thursby et al., 1989b
Mysid, Mysidopsis bahia	J	E	S	M	160	-	-	-	EG&G, Bionomics, 1982
Mysid, Mysidopsis bahia	J	E	F	M	190	-	-	-	EG&G, Bionomics, 1982
Mysid, Mysidopsis bahia	J	E	F	M	466.1	-	-	-	Horne et al., 1983; Thursby, 1991b
Mysid, Mysidopsis bahia	J	E	F	M	250	317.7	317.7	317.7	Horne et al., 1983
Amphipod, Leptocheirus plumulosus	J	I	R	U	1,125	1,125	1,125	1,125	Thursby et al., 1989a

Appendix A. - Acenaphthene: (continued)

COMMON/SCI. NAME	STAGE[a]	HABITAT[b]	METHOD[c]	CONCEN-TRATION[d]	EC50/LC50[e] SPECIES[f] (µg/L)	GENUS[g] (µg/L)	GMAV (µg/L)	HMAV (µg/L)	OVERALL[h] REFERENCES[i]
Amphipod, Ampelisca abdita	A	I	F	M	589.4 589.4	589.5	589.4	589.4	Swartz et al., 1991
Grass shrimp, Palaemonetes pugio	L	W	R	U	1,697 -	-	-	-	Thursby et al., 1989a
Grass shrimp, Palaemonetes pugio	X	W	S	U	676.8 1,072	1,072	1,072	-	Horne et al., 1983; Thursby, 1991b
Sand shrimp, Crangon septemspinosus	X	E	S	U	245.0 245.0	245.0	245.0	-	Horne et al., 1983; Thursby, 1991b
Sea urchin, Arbacia punctulata	E	W	S	U	8,163 8,163	8,163	8,163	-	Thursby et al., 1989a
Sheepshead minnow, Cyprinodon variegatus	J	E,W	R	U	>50,000 -	-	-	-	Thursby et al., 1989a
Sheepshead minnow, Cyprinodon variegatus	A	E,W	F	M	3,100 -	-	-	-	Ward et al., 1981
Sheepshead minnow, Cyprinodon variegatus	J	E,W	S	U	2,200 3,100	3,100	3,100	-	Heitmuller et al., 1981
Inland silverside, Menidia beryllina	J	W	R	U	5,564 -	-	-	-	Thursby et al., 1989a
Inland silverside, Menidia beryllina	X	W	S	U	2,300 3,577	3,577	3,577	-	Horne et al., 1983

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Appendix A. Acenaphthene: (continued)

[a]Lifestage: A = adult, J = juvenile, L = larvae, E = embryo, 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.

[i]References: References listed can be found in the Acenaphthene Water Quality Criteria document (U.S. EPA, 1980) or in the references section of this Sediment Quality Criteria document.

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

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.2 LITERATURE DATA

An extensive literature search was performed for acenaphthene 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, independent experimental methods, [shake-centrifugation (SC), generator column (GCol),], were used to determine a K_{ow} value for acenaphthene 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
Acenaphthene	3.92	Banerjee, et al., 1980
Biphenyl	3.16	Rogers and Cammarata, 1969
	3.63	De Kock and Lord, 1969
	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
Acenaphthene	3.70	Yalkowsky et al., 1983
	3.92	Miller et al., 1985
	3.98	Mabey et al., 1982
	4.03	Yalkowsky et al., 1979
	4.15	Mackay et al., 1980
	4.22	Kamlet et al., 1988
	4.33	Callahan et al., 1979
	4.43	Arbuckle 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 acenaphthene and the SRCs, biphenyl and pyrene, measured at the Athens laboratory by the methods, SC, and GCol. The SRCs were not measured by the GCol or SSF method.

TABLE B-3. INDIVIDUAL $LOG_{10}K_{ow}$ VALUES MEASURED
BY SHAKE CENTRIFUGATION (SC), SLOW-STIR-FLASK
(SSF), AND GENERATOR COLUMN (GCOL).

Chemical	SC	GCol
Acenaphthene	3.84	4.17
Biphenyl	4.06	
Pyrene	5.17	

The log_{10} of the average of eight previous measurements 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 values are in good agreement with the SRC shake-centrifugation measurements made concurrently with the acenaphthene 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,A, and other scientists at the University of Georgia

(Karickhoff et al., 1989). The system has the capability of crossing chemical boundaries to 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.

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

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 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_j) 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.

$$Log_{10}K_{ow} = \sum_{i=1}^{n} (f_i + F_j) \qquad \text{(B-3)}$$

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.

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

Chemical	SPARC	CLOGP
Acenaphthene	3.88	4.07
Biphenyl	4.25	4.03
Pyrene	5.13	4.95

[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.

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

SEDIMENT SOURCE	MORTALITY (%)	SEDIMENT CONCENTRATION µg/g DRY WT.	ORG. CAR.	PORE WATER CONCENTRATION (ug/L)	TOC %	Log K_{oc}	REFERENCES
South Beach, OR. Rhaustorius estuarius	7.5	3.8	0.31	76	1.23	3.61	Swartz, 1991
	10	7.2	0.59	134	1.23	3.64	
	20	11.7	0.95	230	1.23	3.62	
	20	19.0	1.55	433	1.23	3.55	
	40	32.1	2.60	637	1.23	3.61	
	77.5	66.2	8.07	1060	0.82	3.88	
McKinney Slough, OR. Rhaustorius estuarius	5	13.0	0.52	144	2.49	3.56	Swartz, 1991
	2.5	22.1	0.89	266	2.49	3.52	
	25	35.7	1.43	500	2.49	3.46	
	85	63.6	2.55	773	2.49	3.52	
	95	111	4.48	986	2.49	3.66	
Eckman Slough Site 1, OR. Rhaustorius estuarius	2.5	23.5	0.56	173	4.21	3.51	Swartz, 1991
	20	41.9	1.00	337	4.21	3.47	
	55	71.6	1.70	583	4.21	3.46	
	100	113	2.69	859	4.21	3.50	
	100	183	4.35	1040	4.21	3.64	
South Beach, OR. plumulosus leptocheirus	0	3.6	0.22	49	1.62	3.65	Swartz, 1991
	2.5	7.5	0.46	129	1.62	3.55	
	0	45.8	2.83	659	1.62	3.63	
	7.5	57.5	3.55	1002	1.62	3.55	
	2.5	121	14.8	1470	0.82	4.00	
	20	193	23.5	1720	0.82	4.14	

APPENDIX C. Acenapthene (cont'd)

SEDIMENT SOURCE	MORTALITY (%)	SEDIMENT CONCENTRATION ug/g DRY WT.	ORG. CAR.	PORE WATER[a] CONCENTRATION (ug/L)	TOC %	Log K_{oc}	REFERENCES
McKinney Slough, OR. Leptocheirus plumulosus	0	14.3	0.57	129	2.52	3.65	Swartz, 1991
	2.5	24.3	0.97	249	2.52	3.69	
	7.5	42.2	1.69	470	2.52	3.56	
	2.5	67.5	2.70	516	2.52	3.72	
	2.5	124.1	4.96	1140	2.52	3.64	
	60	210	8.39	1470	2.52	3.76	
	75	422	17.9	1500	2.36	4.08	
Eckman Site 1, OR. Leptocheirus plumulosus	15	23.9	0.65	158	3.66	3.61	Swartz, 1991
	5	39.7	1.08	299	3.66	3.56	
	0	63.3	1.73	533	3.66	3.51	
	15	121	3.31	874	3.66	3.58	
	15	206	5.64	1210	3.66	3.67	
	45	356	9.73	1490	3.66	3.81	
	77.5	501	16.9	1580	2.97	4.03	