

Impacts of Low Levels of Residual Oils on Toxicity Assessment of Oil Spills

A Final Report Submitted to
The Coastal Response Research Center

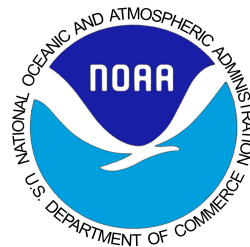
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Abstract

A method is presented for developing scientifically defensible numeric guidelines for oil-related constituents, specifically monoaromatic hydrocarbons (MAH) and polycyclic aromatic hydrocarbons (PAHs), in the water column and in the sediment. The guidelines are equivalent to a HC5, a hazard concentration value that protects 95 percent of the test species. The model of toxicity used in this evaluation is the target lipid model (TLM) that was developed for assessing the toxicity of Type I narcotic chemicals (Di Toro et al. 2000). Structurally the aromatic components of oil should exert a narcotic mode of action. This research focused on validating the TLM for its appropriateness in assessing the toxicity of these oil components, both on an acute and chronic basis. The methodology was determined to be effective at predicting the toxicity of MAHs and PAHs. The resulting HC5 guidelines were found to be protective of sublethal effects commonly associated with blue sac diseases resulting from early life stage exposure to PAHs. The use of toxic units as the metric for expressing the toxicity of mixtures of oil-related components, or mixtures of hydrocarbons in general, is demonstrated to be an effective means of normalizing toxicity data across different sources and different species. The toxicity of the mixture depends on which hydrocarbons are present because the toxicity of the individual components in the mixture varies. A concentration of 1 TU from the components in the mixture implies toxicity. A concentration of 1 $\mu\text{g/L}$ of total measured compounds in a mixture may or may not be toxic and depends on which components are present and the concentration of those components. The use of toxic units eliminates this confusion and normalizes the data across sources. The methodology presented can be used by the oil spill community, which includes the regulators and the regulated industries, to compare residual concentrations of MAHs and PAHs against defensible numeric guidelines to assess potential ecological impacts.

Keywords: Polycyclic Aromatic Hydrocarbons, Target Lipid Model, Model Validation, Oil Toxicity, Guidelines

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1.0 Introduction

This research project is directed at evaluating the impacts of low levels of residual oils based on assessment of the toxicity of oil-related constituents and their exposure risks. The primary compounds of interest in this research are the monoaromatic and polycyclic aromatic hydrocarbons (MAHs and PAHs). Structurally, these compounds are Type I narcotic chemicals and their toxic mode of action is narcosis. The toxicity of such compounds is additive and therefore a methodology is needed that accounts for exposure to a mixture of hydrocarbons. The target lipid model (TLM) and the concept of toxic units are used to assess the toxicity of oil-related chemicals. The TLM is a method of computing water criteria for Type I narcotic chemicals (Di Toro et al. 2000). Equivalent sediment criteria were derived using the equilibrium partitioning (EqP) model (Di Toro and McGrath, 2000). Aqueous and sediment criteria were derived using methodology based on narcotic chemicals in general, rather than MAHs and PAHs specifically. The United States Environmental Protection Agency (U.S. EPA) developed sediment benchmarks (water-only benchmarks were not presented) for PAH mixtures based on the TLM (U.S. EPA, 2003). These benchmarks were derived with the objective of protecting sediment organisms from long-term effects of mortality, growth and reproduction. Recent literature suggests that exposure to PAHs during an organism's early life stage results in various sublethal effects similar to those of blue-sac disease (Carls et. 1999; Heintz et al. 1999; Incardona et al. 2004). These sub-lethal effects were not addressed in the EPA's sediment benchmarks for PAH mixtures and therefore they may not be protective of these types of effects.

For this research, the appropriateness of the TLM for predicting the toxicity of MAHs and PAHs as single chemical exposures and in mixtures is investigated. The TLM is validated for predicting the toxicity of these chemicals in water-column and sediment exposures, both on an acute and chronic basis. Additionally, the TLM is evaluated to determine if computed endpoints are protective of sublethal endpoints such as yolk sac edema, hemorrhaging, larvae abnormalities, etc. Once it has been demonstrated that the TLM methodology can be used to assess whether or not effects are expected at a certain concentration of a chemical or from a mixture of chemicals, the methodology is used to derive defensible chemical-specific guidelines. HC5 values, concentrations that protect 95% of species, are presented on an aqueous basis and a sediment basis.

The beneficiaries of this research include regulators and the regulated communities because they will have an innovative scientifically defensible method to estimate toxicity of oil components in water and sediment.

2.0 Objectives

The overall objective of this project is to evaluate the impacts of low levels of residual oils based on the toxicity assessment of oil-related constituents and their exposure risks. Generally, the toxicity of petroleum is attributed to the water-soluble MAHs (i.e., benzene, toluene, ethylbenzene and xylene, commonly referred to as BTEX) and PAHs. BTEX are fairly volatile compounds and are not expected to persist in the environment. PAHs are less volatile and the heavier PAHs (those with 4 or 5 rings) are known to persist and they can potentially have a long-term impact on the aquatic environment. Specific objectives and how they were met are :

- Identify key components of residual oil that contribute to toxicity – The literature was reviewed for toxicity data resulting from exposure to single chemicals and mixtures of chemicals expected to be present in oils (i.e., MAHs and PAHs) both in the water column and in the sediment. Toxicity endpoints reflected both short-term (acute) and long-term (chronic) effects.
- Validate that the TLM of toxicity can predict the aqueous toxicity of oil related compounds – Toxicity predictions based on the TLM methodology were performed on the data sets identified in the literature review. Predictions were made for single chemical exposures for both acute and chronic effects. The predicted toxicity was compared to the observed toxicity.
- Establish that the toxic unit (TU) can be used as a universal endpoint for expressing the toxicity from mixtures of compounds such as those that result resulting from different oil sources – The toxicity of different mixtures of compounds that result from various oil sources were normalized to TU and compared to mass based (i.e., mg/L) endpoints.
- Demonstrate that EqP theory is appropriate for converting the TLM-predicted aqueous effect concentrations for oil-related compounds to equivalent sediment effect concentrations – Sediment toxicity predictions based on the TLM and EqP methodologies were performed on the data sets identified in the literature. Predictions were made for single chemical exposures and mixtures of chemicals for both acute and chronic effects. Sediment toxicity predictions were compared to observed effect data.
- The TLM in conjunction with EqP theory were used to derive guidelines for oil-related compounds that are protective of aquatic and benthic species from long-term sub-lethal effects.

These project objectives are directly related to the work of the oil spill community. A scientifically defensible methodology for computing guidelines to judge what levels of oil-related compounds should not have an adverse impact on the aquatic community. The methodology is simple to use, only the log (K_{ow}) values of the chemicals in the mixture are needed. The method is versatile in that it allows the user to compute protective guidelines for a particular species or guidelines that protect 95% of all species considered in the method development.

In addition, the use of the TU as the toxicity metric for mixtures normalizes differences in toxicity between chemicals. This is of critical importance to the oil spill community because it allows data from one location/test to be directly comparable to data for another location/test. Historically, the measured concentrations of chemicals in the water phase have been summed to assess the aqueous toxicity of crude oils. Water-soluble fractions (WSFs) are prepared from different sources of oil and although the compositions of the WSFs are different and different compounds are measured, the interpretation of the toxicity used these summed concentrations. The effects are often expressed as total petroleum hydrocarbons on a mass basis (i.e., mg TPH/L) (Anderson et al. 1974; Rossi and Anderson, 1976; Moles et al. 1979; Brodersen, 1987) or total

PAH concentrations (i.e., mg TPAH/L) (Anderson, 1977; Neff and Stubblefield, 1995; Carl et al. 1999; Heintz et al. 1999). The fundamental problem with reporting toxicities of hydrocarbon mixtures on a total concentration basis is that it assumes all of the compounds have equal toxicities, which is not true. The toxicity of hydrocarbons varies widely over orders of magnitude and has been related to the K_{OW} (Konemann, 1981; Veith et al. 1983). The toxicity of individual chemicals in a mixture is normalized by expressing the toxicity of each chemical in terms of toxic units (Hermens, 1989; Peterson, 1994) and comparisons of different oils can be made.

This research effort for determining impacts of low-levels of residual oil components focused on meeting the objectives described above. It is impractical and probably impossible to develop guidelines that address every possible situation that may occur in the environment. The following is a listing of conditions that can impact the toxicity of oil-related components, which were *NOT* addressed in this research but are important to consider when determining the effects from oil.

- Effects of photoactivation of PAHs – Some PAHs exert photoenhanced toxicity after accumulation in the tissues of organisms and exposure to ultraviolet radiation. Photoinduced toxicity can be orders of magnitude greater than baseline toxicity (i.e., narcosis).
- Other water-soluble components of oil – This research focused on MAHs and PAHs, the most commonly measured oil components, as being the causative agents of oil toxicity. There may be other water-soluble components that exert toxicity. Note that this methodology can be applied to any chemical, but the toxicity computed will be the chemical's baseline or minimum toxicity.
- Time-variable concentrations – This methodology assumes that the exposure concentrations are constant with time or equilibrium conditions have been achieved, particular for sediment exposures. Time-variable concentrations are not addressed and it is difficult to assign observed effects to a concentration if the concentration is varying with time.
- Non-standard conditions – The physical chemical properties used in this research were determined at 25 deg C. These parameters vary with temperature. For example, organic compounds are usually less soluble in colder temperatures. Therefore, the computed guidelines would be conservative for temperature conditions less than 25 deg C.
- Other sediment partitioning phases – Equilibrium partitioning theory assumes organic carbon is the only partitioning phase, described by K_{OC} , for non-polar organic contaminants. Some field data sets indicate that other partitioning phases may be present and include soot carbon or coal. PAHs seem to have a higher affinity for these other carbon phases than for organic carbon as described by K_{OC} . Therefore, the PAHs will be less bioavailable than predicted using K_{OC} as the sole partitioning coefficient. Ignoring

other possible partitioning phases is conservative since the maximum toxicity will be predicted.

3.0 Methods

3.1 Aqueous Acute Toxicity Prediction - Target Lipid Model

Based on chemical structure, the MAHs and PAHs should exhibit a narcotic mode of action (Verhaar et al. 1992). The TLM has been extensively validated using a large database to predict the aquatic toxicity of classic Type I narcotic chemicals (Di Toro et al. 2000; Di Toro and McGrath, 2000). The TLM is a quantitative structure activity relationship based on the inverse relationship between the aqueous toxicity in water-only exposures and the K_{ow} , octanol-water partition coefficient. The TLM equation that predicts the critical aqueous concentration is

$$\log(C_w^*) = m \log(K_{ow}) + \log(C_L^*) + \Delta c \quad (1)$$

where C_w^* is the critical aqueous concentration (mmol/L) (i.e., LC50 for a mortality endpoint), m is the universal slope, K_{ow} is the octanol-water partition coefficient, and C_L^* is the critical target lipid body burden, CTLBB ($\mu\text{mol/g}$ octanol = $\mu\text{mol/g}$ lipid). There is also a correction Δc for chemical classes, e.g. MAHs and PAHs, which exhibit additional toxicity when compared to baseline narcotics, e.g. alkanes and alcohols. In the model development it is shown that C_L^* is dependent on the species and Δc and K_{ow} are dependent on the chemical. Therefore, C_w^* is dependent on both organism and chemical. The slope m is a universal constant, independent of both organism identity and chemical classes.

Equation 1 is used to compute the critical aqueous concentration for a particular species from the K_{ow} of the chemical and the CTLBB of the species. CTLBB for 33 aquatic species (Di Toro et al. 2000) and 5 algae (McGrath et al. 2004) were computed with the TLM using the K_{ow} values determined from a 1997 version of SPARC, a computer program that was available as a DOS executable program (Karickhoff et al. 1991). SPARC estimates numerous physical-chemical properties for chemicals based on chemical structure. SPARC is now available to use as an on-line program and has undergone enhancements in its programming. Therefore, K_{ow} values computed using the 1997 version may be different than the K_{ow} values computed using the enhanced on-line version. To take advantage of the enhancements to SPARC, new K_{ow} values were determined for all chemicals in the narcosis toxicity database and revised coefficients for the TLM were computed. These results are presented in Appendix A.

For this work, CTLBBs for eight additional species not included in the model development were computed if acute toxicity data were available. A total of 46 CTLBBs are available and provided in Appendix A. If the acute toxicity data for a particular species included more than four data points, corresponding standard errors were computed. If less than four data points were available, the associated standard errors were not calculated.

3.2 Aqueous Chronic Toxicity Prediction

The critical aqueous concentrations computed from Equation 1 are acute concentrations, the concentrations that produce an effect in a short-term test (i.e., 96-h LC50). To convert the acute critical concentration to a chronic effect concentration, the TLM adopts the acute-to-chronic ratio (ACR) methodology used by the U.S. EPA in deriving water quality criteria (Stephan et al. 1985). The ACR is computed from paired acute and chronic toxicity data for a particular chemical to a specific organism as follows

$$ACR = \frac{\text{Acute Effect Concentration}}{\text{Chronic Effect Concentration}} \quad (2)$$

where the effect concentrations are in the same units. The chronic effect concentrations are those that caused an adverse effect on the organism's ability to survive, grow or reproduce on a long-term basis. The ACR is a means of comparing the acute and chronic toxicities. It does not assume that the toxic mode of action is the same for acute and chronic toxicity.

In the TLM development (Di Toro et al. 2000; McGrath et al. 2004) ACRs were provided for 64 paired data sets from 14 different species and several narcotic chemicals. The ACRs ranged from 1.1 to 96.4 with a geometric mean value of 4.47.

3.3 Sediment Toxicity Prediction

The equilibrium partitioning (EqP) model (Di Toro et al. 1991) is used to convert the critical aqueous concentration computed from Equation 1 to the equivalent critical sediment concentration. EqP theory is based on two concepts. The first is that nonionic chemicals in sediments will partition between sediment organic carbon, pore water and benthic organisms. The second is the observation by Adams et al. (1985) that the sediment toxicity can be predicted by comparing the pore water concentration to the critical concentration determined in a water-only exposure. EqP rationalizes that for both of these concepts to be true, the pore water and the organic carbon phase of the sediment must be in equilibrium. At equilibrium, if the concentration in any one phase is known, then the concentrations in the other phases can be predicted. Assuming that the critical aqueous concentration computed using the TLM (Equation 1) is equivalent to the critical pore water concentration, the equivalent critical sediment concentrations producing the same effect on the same organism is

$$C_s^* = K_{oc} C_w^* \quad (3)$$

where C_s^* is the organic carbon normalized critical sediment concentration ($\mu\text{mol/g OC}$) and K_{oc} is the organic carbon partitioning coefficient (L/kg OC). The organic carbon partition coefficient K_{oc} can be estimated using (Di Toro et al. 1991)

$$\log(K_{oc}) = 0.00028 + 0.983 \log(K_{ow}) \quad (4)$$

Equations 1, 3 and 4 can be combined to yield

$$\log(C_s^*) = 0.00028 + 0.047 \log(K_{ow}) + \log(C_L^*) + \Delta c \quad (5)$$

which is the equation to predict the critical sediment concentration for acute effects based on the TLM.

3.4 Uncertainty in Toxicity Predictions – Uncertainty in Target Lipid Model

The species-specific acute critical water effect concentrations computed from Equation 1 are dependent on the regression coefficients, the universal narcosis slope and the C_L^* . Each of these coefficients has an uncertainty associated with it and therefore, there is some inherent uncertainty in the predicted effect concentrations. McGrath et al. (2004) presented statistical extrapolation methodology to compute the fifth percentile concentration (HC₅, mmol/L) that considers the variance in the universal narcosis slope and C_L^* . The resulting concentration is the acute HC₅, which is the hazard concentration effecting 5% of the test population on an acute basis. When the ACR and its uncertainty are considered, the resulting effect concentration is the chronic HC₅. The final equation was presented as

$$\log(\text{HC}_5) = \log(K_{ow})E\{m\} + E\{\log(C_L^*)\} - E\{\log(\text{ACR})\} - k_Z \sqrt{(\log(K_{ow}))^2 V\{m\} + V\{\log C_L^*\} + V\{\log(\text{ACR})\}} \quad (6)$$

where the E and V terms represent respectively the mean and variance of the slope, C_L^* , and ACR, and k_Z is the 95% confidence sample size-dependent extrapolation factor. By using the fifth percentile C_L^* , Equation 8 can be used to compute the aqueous concentration that protects 95% of the species from chronic effects, as was presented by McGrath et al. (2004). This idea of using the methodology to derive protective guidelines is addressed in Section 5.0. However, if a specific-specific C_L^* and the variance associated with it are used, Equation 8 can be used to compute the predicted critical aqueous concentration that effects 5% of a particular species. Note that the k_Z value varies for each species due to sample size and these values are provided in Appendix A. To compute the ninety-fifth percentile concentration, HC₉₅, the variance term in Equation 8 is added to yield

$$\log(\text{HC}_{95}) = \log(K_{ow})E\{m\} + E\{\log(C_L^*)\} - E\{\log(\text{ACR})\} + k_Z \sqrt{(\log(K_{ow}))^2 V\{m\} + V\{\log C_L^*\} + V\{\log(\text{ACR})\}} \quad (7)$$

The HC₅ and HC₉₅ values represent the lower and upper confidence intervals, respectively. The mean slope of the equation does not change, since it is universal across species. The ACR terms are only considered when computing chronic effect concentrations.

3.5 Application to Mixtures

Type I narcotic chemicals are non-ionic organic chemicals that have a similar mode of action namely, narcosis (Bradbury et al. 1989; Verhaar et al. 1992). Hermens (1989) summarized the

data that demonstrate that the toxicity of narcotic chemicals is additive if their concentrations are expressed as toxic units (TU) (Sprague and Ramsay, 1965). Based on chemical structure, MAHs and PAHs are classified as Type I narcotic chemicals. PAHs are typically found as mixtures, rather than as single chemicals. It is therefore appropriate to express the toxicity of mixtures of PAHs using toxic units.

The TLM incorporated the use of toxic units in assessing the toxicity of PAH mixtures in water, tissue and sediments (Di Toro and McGrath, 2000). The TLM and TU concept were validated for predicting the toxicity of gasoline, a complex mixture of hydrocarbons (McGrath et al. 2005). This discussion is limited to the water phase only, but applies to other phases such as sediments and tissue of an organism. In water, a TU is defined as

$$TU_{w,i} = C_{w,i} / C_{w,i}^* \quad (8)$$

where $C_{w,i}$ is the measured concentration of chemical i in the water (mmol/L) and $C_{w,i}^*$ is the critical effect concentration for chemical i computed from Equation 1. The molar concentrations are used in computing TUs to normalize molecular weight differences between compounds in the mixture. For each chemical in the mixture, the individual TUs are computed using Equation 8. The individual TUs are then summed to compute the toxicity of the mixture

$$TU = \sum_i TU_{w,i} \quad (9)$$

If the total TUs of the mixture are greater than or equal to 1, the mixture is predicted to be toxic. Using the LC50 as an example, death would be predicted for 50% of the test organisms.

Toxicity data from aqueous or sediments tests using mixtures of chemicals, are presented graphically as percent observed effect (usually mortality) as a function of the predicted total toxic units. The observed effects are graphed on an arithmetic scale and the predicted total toxic units are graphed on a base ten logarithmic scale. An example of this type of graph is shown in Figure 1. Low effect levels are expected at low total toxic units with high effect levels occurring at high total toxic units. Ideally 50% effects will be observed at a total toxic unit of 1.0 as computed from Equations 8 and 9. These indices will be shown as solid lines and are shown for illustrative purposes only. However, the indices of 50% effect and a total toxic unit of 1.0 are not absolute. The HC5 and HC95 values represent the uncertain bounds for when effects are expected and are a function of the uncertainty associated with the species specific CTLBB and ACR. These indices will be shown as dashed lines (Figure 1) and will vary for each species. Effects are expected to be low (less than 50%) for predicted total toxic units to the left of the HC5 bound. Effects are expected to be high (greater than 50%) for predicted total toxic units to the right of the HC95 bound. The area of uncertainty lies between the HC5 and HC95 bounds. Within this area of uncertainty effects may or may not occur. The larger the uncertainty associated with the CTLBB, the larger the area of uncertainty. In addition, the area of uncertainty will be larger for chronic predictions due to the uncertainty associated with the ACR.

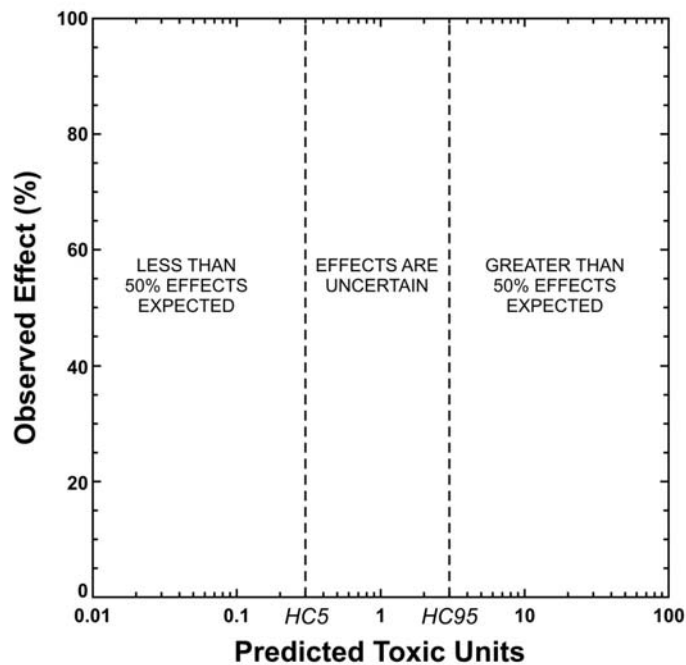


Figure 1. Diagram of how toxicity data from aqueous and sediment tests using mixtures of chemicals will be displayed. Percent effect as a function of predicted total toxic units. Solid lines present 50% effect and total toxic unit of 1.0. Dashed lines represent HC5 and HC95 values.

To estimate the toxicity from exposure to MAH and PAH mixtures, such as those in WSFs prepared from oil or those that result from an oil spill, ideally measurements for all of the components in the mixture, whether in the water column or sediment, are needed. These measurements are then used in Equations 8 and 9 to estimate the total toxicity, expressed as TU, from the mixture. If measurements are not provided for all components, the total TU of the mixture can be underestimated. Even chemicals with high $\log(K_{OW})$ values will contribute TUs, with the maximum TU at their water solubility (Di Toro et al. 2006). Given the complex nature of oils, it is impractical to measure for the presence of every chemical that may be sufficiently water soluble to find its way into the environment. Since MAHs and PAHs are assumed to be the causative agents in oils, sufficient characterization of the MAHs and PAHs is desirable. A reasonable question to pose is: What characterization data are needed to compute a total TU? The U.S. EPA addresses this issue for sediments (see Section 3.6), but does not address it for water column exposures. In this research, for water column exposures, at a minimum measurement for sufficient parent PAHs and the alkylated homologs of naphthalenes and phenanthrenes is required. Alkylated homologs are the parent PAHs substituted with carbon groups (i.e., methyl, ethyl, propyl, etc.). For example, C1-naphthalene represents parent naphthalene with one carbon (a methyl) substitution and C2-naphthalene represents parent naphthalene with two carbon (two methyls or one ethyl) substitutions. C1-naphthalene has two structural isomers, 1-methylnaphthalene and 2-methylnaphthalene. C2-naphthalene has twelve structural isomers. The number of structural isomers increases with the degree of alkylation. This pragmatic approach for water column measurements is necessary to capture some of the

alkylated PAHs that are prevalent in petrogenic PAH sources and to eliminate data sets that have too few measurements where the toxicity can be severely underestimated

3.6 Computing Total PAH Toxic Units in Sediment

The U.S. EPA defined total PAH in sediments to be the sum of the toxic units from a minimum of 34 PAHs (18 parent PAHs and 16 alkylated PAHs) (EPA, 2003). These 34 PAHs were selected because they represented the maximum number of PAHs that were being routinely measured in the U.S. EPA EMAP sediment monitoring program. The EPA recognized that different sediment monitoring programs require varying PAH characterization. Among the available sediment data sets, there were 13 and 23 common subsets of PAHs. Rather than requiring measurements for the 34 PAHs, adjustment factors were computed from the EMAP data sets to convert the commonly measured 13 or 23 to be equivalent to the 34 PAHs from a toxicity perspective. The mean adjustment factors for the 13 and 23 PAHs were 2.75 and 1.64, respectively. For sediments that had measurements for 13 PAH, the sum TU_{PAH13} from the 13 PAHs would be computed and then multiplied by 2.75 to convert the TU_{PAH13} to TU_{PAH34} , which is equivalent to TU_{PAHTOT} . A listing of the PAHs that comprise the 13 PAHs and 23 PAHs subsets as well as the 34 PAHs is provided in Table 1. The application of adjustment factors puts all of the sediment data on the same footings and reduces the uncertainty associated with the unmeasured PAHs. However, the EPA encourages the measurement of the 34 PAHs, particularly for situations where important decisions are being made.

3.7 Literature Review

The literature was reviewed for water column and sediment effect data resulting from exposure to MAHs or PAHs, both as single compounds and as mixtures. For data to be accepted and used in the analysis, the following criteria had to be met

- A CTLBB must be available for the test organism.
- For water column exposures, the concentration of the chemical(s) must be below its water solubility. If a chemical is tested at a concentration above its water solubility, then the chemical is present as a pure-phase which may exert a different toxic mode of action. For single chemical exposures, the solid solubility of the chemical is used. For mixtures of chemicals that are liquids, such as those in oils, the sub-cooled liquid solubility – the solubility of the component if it were a liquid at the temperature of interest – is used.
- For single-chemical spiked sediment exposures, the EqP based chemical concentration in the pore-water (computed using Equation 3 where the organic normalized measured sediment concentration is used instead of C_s^* , the critical concentration) must be below the spiked-chemical's water solubility. The reason is as stated above. For single chemical exposures, the solid solubility of the chemical is used. For mixtures of individual spiked chemicals, the appropriate solubility is the sub-cooled liquid solubility.
- The exposure concentrations must be constant with time, particularly for long-term exposures where chronic effects are being observed. Laboratory studies that show

diminishing or varying concentrations over time are impossible to interpret. One cannot assign a specific concentration to the observed effect.

- For exposures to mixtures of chemicals, such as water-soluble fractions prepared from oils or fuels or sediment contamination from an oil spill, the concentrations of the individual chemicals must be measured. Ideally, to determine the toxicity from a chemical mixture, the concentration of all components in the mixture should be measured because each component could potentially contribute toxicity. For sediments, the toxicity from unmeasured PAHs can be estimated from the concentration of select PAHs following guidelines established by the U.S. EPA (see Section 3.6). Using this methodology, the toxicity of total PAH can be estimated. A similar normalization to total PAH toxicity is not available for water column exposures. Therefore, for water exposures, the majority of expected water-soluble constituents must be measured. For a fresh petroleum source (i.e., non-weathered), the majority includes the BTEX, naphthalenes, phenanthrenes and their alkylated homologs at a minimum. For weathered petroleum source, the concentration of the heavier PAHs (i.e., chrysenes and fluoranthenes) must also be measured.
- For sediment exposures, the total organic carbon content in the exposure sediment must be reported.

3.8 Physical Chemical Properties

A listing of chemicals that appeared in data sets is provided in Table 1. Types of chemicals include, aliphatic alkanes, cyclic alkanes, MAHs and PAHs. In some data sets, concentrations of alkylated homologs were reported for MAHs and PAHs. These are represented with a 'C#' where the C represents a carbon and the number represents the number of carbon substitutions. For example, C3 represents three carbon substitutions (3 methyls, 1 methyl plus 1 ethyl, 1 propyl). Section 3.6 contains a more detailed discussion. The chemical properties include molecular weight, $\log(K_{OW})$, solid solubility and sub-cooled liquid solubility. SPARC was used to compute the molecular weight and $\log(K_{OW})$. Recommended solid solubility and sub-cooled solubility values were taken from the MacKay et al. (1992a, 1992b, 1993 and 1995) handbooks. Relationships between $\log(\text{solubility})$ and $\log(K_{OW})$ were used to compute solid solubility and sub-cooled liquid solubility for chemicals that were not listed in the handbook. These relationships are provided in Table 1.

4.0 Results

4.1 Literature Review

The literature was reviewed for data sets where the effects on aquatic organisms exposed to oil-related chemicals were observed. For water column exposures, 141 references were reviewed of which 80 contained data used in this research. For sediment exposures, 64 reference were reviewed of which 21 contained data used in this research. In total, 205 references were reviewed of which 101 (approximately 49%) contained data deemed acceptable. A summary of the references reviewed and brief explanations for not accepting data are provided in Appendix B.

4.2 TLM Validation - Water Column

In this section, toxicity predictions using the TLM and toxic unit methodologies are presented and compared to observed values. For large data sets, graphical summaries are presented. Data for these large data sets are provided in Appendix C.

4.2.1 Acute Effects (lethality) - Single Compound Exposures

In this section, the TLM is applied to predict the acute lethal effects from exposure to single compounds. Acute toxicity data were considered if a CTLBB was available for the test organism. In addition to BTEX, other monoaromatic hydrocarbons are included in the comparison. Most of these additional MAHs have a higher degree of alkylation (i.e., three methyl group substitutions) and include compounds such as trimethylbenzenes and propylbenzenes. Based on structure, the toxic mode of action for these compounds should be similar to BTEX. For MAHs, there are a total of 164 data points from 28 different species (Appendix C, Table C1). For PAHs, there are a total of 139 data points from 20 different species. Toxicity data are summarized in Table 2, which also provides information relevant to the exposure condition, such as test type, organism life-stage, etc. Note that Table 2 also contains data from eight tests where the observed LC50s were greater than the aqueous solubility of the test chemical. These data were not included in any analysis and are only shown for completeness. The predicted LC50 values for each exposure are also presented in Table 2. Example calculations are provided in Appendix E. The observed and predicted LC50s are compared in the top panel of Figure 2. The solid line represents the 1:1 relationship. The dashed line represent the 90% confidence interval. The confidence limits were computed as the 5th and 95th percentiles of the residuals where the residuals were the difference in the observed and predicted effect concentrations. The confidence limits are not symmetrical indicating that the distribution is not exactly log normal. The model tends to slightly underestimate the toxicity. Based on this data analysis, the TLM is able to predict acute toxicity to within a factor of approximately 7.

4.2.2 Acute Effects (lethality) – Mixtures

In this section, the TLM is applied to predict the acute effects, meaning lethality, from exposure to a mixture of oil-related compounds. Data sets were considered if the CTLBB of the test organism was available, sufficient characterization of the components in the mixture was provided, the concentrations of individual components in the mixture were provided and the concentrations of the chemicals were relatively constant over time. Three data sets were available that met the selection criteria. Two data sets were laboratory investigations of the toxicity of WSFs prepared from oils. The other data set was a laboratory experiment using a prepared PAH mixture. All MAHs and PAHs measured in the mixture were included in the analysis.

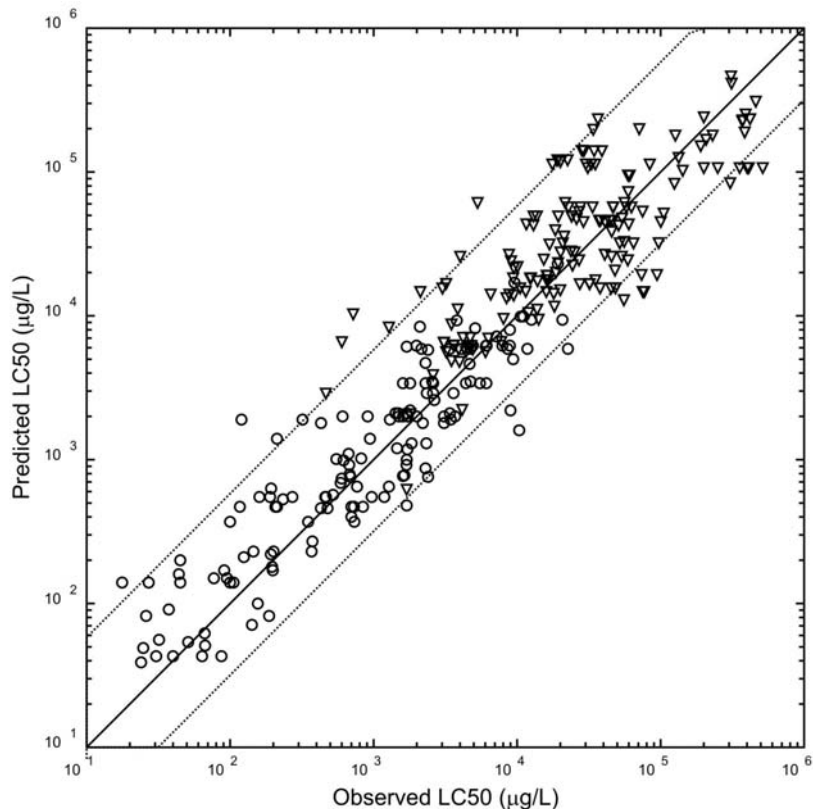


Figure 2. Acute Exposures- Single Compounds - TLM predicted acute LC50 versus observed LC50 for monoaromatic hydrocarbons (▽) and PAHs (○). Solid line represents 1:1 relationship. Dashed lines represent 90% confidence interval

The toxicity of WSFs prepared from neat (unweathered) and naturally weathered Exxon Valdez Alaska North Slope crude oil (EVCO) was measured (ENSR, 2001). Neat oil was collected from the Exxon Valdez oil tanker 7 days after the tanker ran aground in the Prince William Sound, Alaska. Naturally weathered oil was collected approximately five months after the tanker grounded. WSFs were prepared from 10:1 (water:oil) solutions for the neat and weathered oils. Each WSF was analyzed for BTEX, biphenyl, 19 parent PAHs and 21 alkylated homologs of parent PAHs. These concentrations are provided in Appendix C Table C2. Six dilutions of the WSFs were used in toxicity testing. The 48-hour mortality to fathead minnows (*Pimephales promelas*) was determined. The TLM total toxic units for the 100% WSF from neat and weathered oil were 0.62 and 0.28, respectively. The TLM computed toxic units associated with each chemical are provided in the Appendix C Table C2. For the neat oil, the BTEX contribute significantly to the toxic units, accounting for approximately 60% of the computed toxic units. This is not the case for weathered oil, where the BTEX account for less than 10% of the toxic unit. This analysis suggests that BTEX are important contributors to the toxicity of neat oil compared to their toxic contribution in weathered oil. For a discussion of the effect of weathering on the toxicity of oils, the reader is referred to Di Toro et al. (2006). The observed mortality as a function of the total measured concentration (mg TMC/L) in each treatment is shown in Figure 3A. The open and closed symbols represent the neat and weathered oil treatments, respectively. Greater than 50 percent mortality was only observed in the highest

WSF exposure (100% WSF) using neat oil, indicating that the neat oil was more toxic than the weathered oil. All other dilutions resulted in less than 30 percent mortality. For each dilution, the observed mortality normalized to total toxic units is presented in Figure 3B. Solid lines at a TU of 1.0 and 50% mortality are shown for guidance. The dashed lines represent the 5 and 95% uncertainties in the TLM predictions for *P. promelas* and are computed using Equations 6 and 7. For this data set the dose-response pattern was as expected. The one data point where greater than 50% mortality occurred falls within the uncertainty limits of the TLM. All of the other data points that have low observed mortality and corresponding low total TU fall to the left of the lower uncertainty bound where low mortality is expected.

States et al. (1982) also investigated the acute toxicity of PAH mixtures. In this study, WSFs were prepared from No. 6 fuel oil, No. 2 fuel oil and a solvent refined coal liquid. Acute toxicity to *Daphnia magna* (48 hour immobilization) was determined under static conditions. The major chemical constituents were provided for No. 2 fuel oil and the coal liquid only. No chemical analysis was provided for No. 6 fuel oil; therefore, the TU computation could not be performed and the TLM could not be applied to predict effects from the No. 6 fuel oil. Measurements were provided for aromatic hydrocarbons, which included, indan, tetralin, naphthalene and alkylated

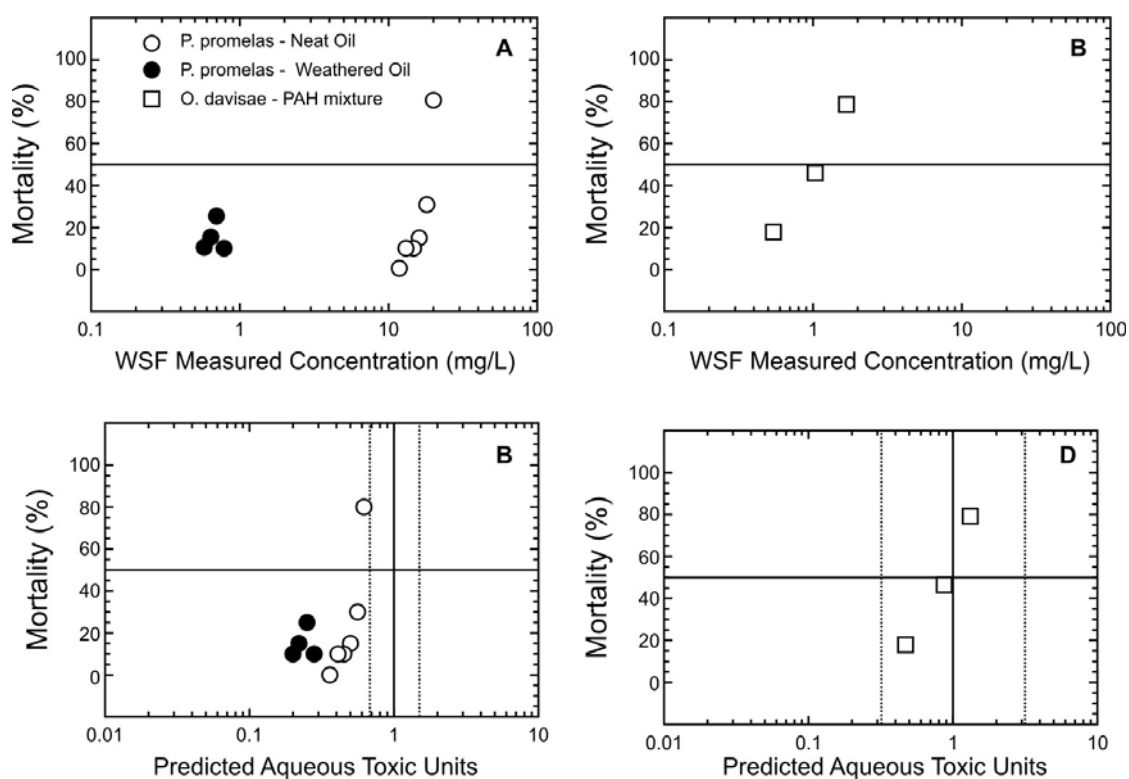


Figure 3. Acute Exposures- Mixtures - Percent mortality as a function of total measured concentration (mg/L) (top panels) and predicted aqueous toxic units (bottom panels). Data on the right is for *Pimephales promelas* exposure to WSFs prepared from neat and weathered Exxon Valdez crude oil (ENSR, 2000). Data on the left is for *Oithona davisae* exposure to WSF prepared from a mixture of 9 PAHs (Barata et al. 2005). Solid lines represent 50% mortality and 1 toxic unit. Dashed lines represent HC5 and HC95 for each species.

homologs of benzene and naphthalene. The chemical concentrations and computed toxic units are provided in Appendix C Table C3. The total computed TUs in the 100% WSF for No. 2 fuel oil were 0.36, suggesting that no toxic effects are expected. This result was in agreement with the no observed effects for the 100% WSF. The total TUs computed for the 100% WSF from the coal liquid were 8.4 indicating that the 100% WSF would be predicted to be toxic. Observed data indicated that 0.25% WSF from the coal liquid was toxic. The equivalent TU at this dilution is 0.021 and at this level no toxicity would be predicted from the aromatic hydrocarbons. In this case, the TLM predictions were not in agreement with the observed effects (low TU, high effect levels). However, States et al. (1982) attributed the toxicity of the coal liquid to phenolic compounds, which are not type I narcotic chemicals and are not included in the TLM analysis. The phenolic compounds were present at significantly higher levels on the coal liquid WSF (1360 mg/L) compared to the No. 2 fuel oil WSF (1.7 mg/L). If the phenolic compounds are the main contributors to the toxicity, it is not surprising that the TLM did not predict the effects correctly because they are not included in the TLM and TU calculation.

Barata et al. (2005) tested the acute toxicity of a mixture of 9 PAHs. The PAHs included naphthalene, 1-methylnaphthalene, 1,2-dimethylnaphthalene, phenanthrene, pyrene, fluorene, 1-methylphenanthrene, dibenzothiophene and fluoranthene. The mixture was tested at six dose levels (0.25x, 0.5x, 1x, 1.5x, 2x, 2.5x); however, chemical measurements were only provided for three exposures (0.5x, 1x, 1.5x). Mortality of the adult copepod, *Oithona davisae*, was measured after 48 hours of exposure. The measured chemical concentrations and computed toxic units are provided in Appendix C, Table 4C. The observed mortality as a function of the total measured concentration (mg TMC/L) and normalized to total toxic units is shown in Figures 3C and 3D, respectively. The dashed lines are the 5th and 95th % uncertainties for *O. davisae* based on variation in species-specific CTLBB. For *O. davisae*, the dose-response is as expected and 50% mortality occurs around 1.0 TU.

The data analysis presented above demonstrated that the TLM and TU concept (i.e., theory of additivity) correctly predicted the acute effects from exposure to a mixture of oil-related compounds. The benefit of normalizing the concentration data to TU can also be realized through the above data analysis. If the toxicity of the PAH mixture is expressed on a mass of total measured concentration, then 50% observed mortality resulted from exposure of approximately 1 mgTMC/L of a mixture of 9 PAH (Figure 3C) and 10 mgTMC /L of water soluble compounds in neat EVCO (Figure 3A). There is an order of magnitude difference in the concentration that resulted in similar effects. A comparison based on mass concentrations does not consider chemical differences in the mixtures or differences in organism sensitivity. Once normalized to toxic units, 50% mortality occurs in the range of 0.6 to 1.0 toxic units (within a factor of 2). Normalizing to toxic units reduces the uncertainty because the methodology considers differences in chemical composition and organism sensitivity. This illustrates that the total measured hydrocarbon concentration should not be used to assess toxicity, while the TU concept can be applied across different sources and organisms to express toxicity.

4.2.3 Chronic Effects (Growth, Reproduction and Mortality)- Single Compound Exposures

The analysis presented previously suggests that the TLM, which was developed for chemicals that have a narcotic mode of toxic action, can be used to predict the acute toxicity of BTEX (and

other MAHs) and PAHs. To convert the acute TLM endpoint to a chronic endpoint, an acute-to-chronic ratio (ACR) is applied (Equation 2). Di Toro et al. (2000) demonstrated that the ACR is independent of chemical and species and can therefore be applied to any chemical and any species in their analysis. A mean ACR of 5.09 was computed from a database that included BTEX and PAHs as well as other chemicals, such as chlorinated alkanes and MAHs (i.e., 1,2-dichloroethane, 1,2,4-trichlorobenzene). More than half of the acute and chronic paired data sets were chlorinated compounds. Since petroleum products do not contained halogenated components, an analysis of the ACRs from non-halogenated compounds is more appropriate. In this section, the distribution of ACRs for aliphatic hydrocarbons, MAHs and PAHs were compared. A total of 29 paired data sets were available (Table 3), of which 17 were PAHs, 6 were MAHs and 6 were aliphatic hydrocarbons. The distributions for each chemical class are shown in Figures 4A-C. The distributions are similar expanding an ACR range of approximately 1 to 11. Since the distributions were similar, the data sets were combined (Figure 4D). The geometric mean ACR from the combined data sets is 3.83. Although this research focuses on MAHs and PAHs, aliphatic hydrocarbons were included in the ACR computation because (1) based on structure aliphatic hydrocarbons are not expected to have a different mode of action and (2) the ACRs for aliphatic hydrocarbons fell on the high on of the distribution and including them in the computation resulted in a higher average ACR and is therefore the more conservative approach for computing a chronic endpoint.

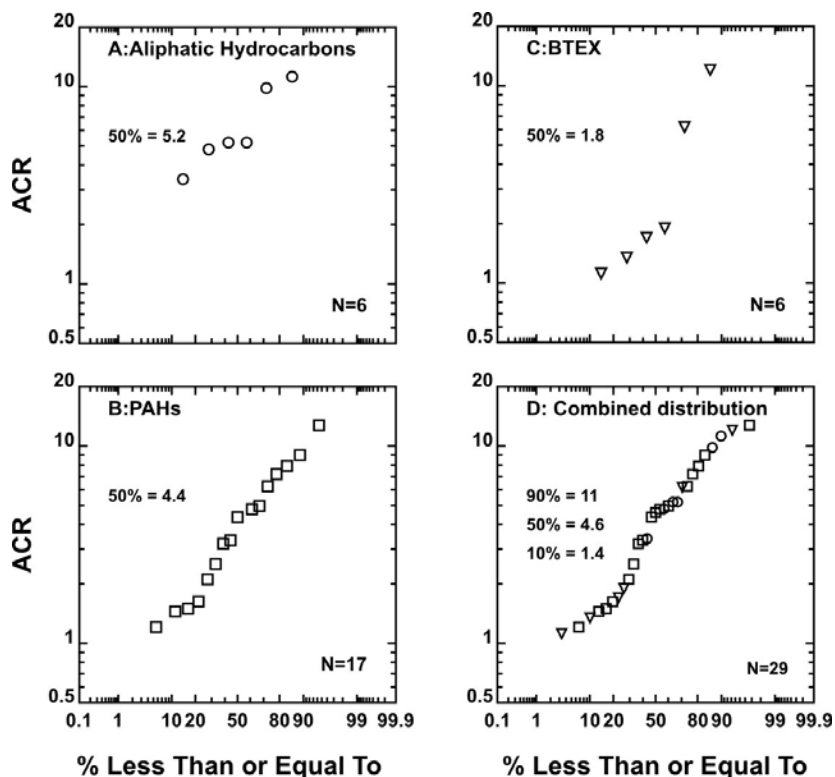


Figure 4. Chronic Effects – Single Compounds - Distribution of acute to chronic ratios (ACRs) for aliphatic hydrocarbons (A), PAHs (B), BTEX (C) and the combined data set (D).

The use of an ACR to convert an acute endpoint to a chronic endpoint does not mean that the toxic mode of actions for acute toxicity and chronic toxicity are the same. Rather, an ACR is a means of relating the acute toxicity of a chemical to its chronic toxicity. In addition, the toxic modes of action are not necessarily the same for different chemical classes that have similar ACRs. The ACRs for PAH, MAH and aliphatic hydrocarbons were similar; however, this does not mean that the toxic modes of action for these different chemical classes are similar. The fact that the distributions are similar supports the application of an average ACR. If the ACRs were orders of magnitude different, then perhaps the use of an average ACR would not be appropriate.

4.2.4 Chronic Effects (Growth, Reproduction and Mortality)- Mixtures

One study that satisfied all of the criteria investigated the chronic effects from exposure to No. 2 fuel oil. Anderson et al. (1977) investigated the hatching success of three marine species, *Cyprinodon variegates*, *Fundulus heteroclitus* and *Fundulus similis*. A CTLBB is only available for *C. variegates* and therefore only the effects on this organism can be evaluated. Embryos were exposed to various dilutions of a WSF prepared for No. 2 fuel oil. The WSF was renewed daily. Concentrations of 31 hydrocarbons (11 alkanes, 8 monoaromatic hydrocarbons, 12 PAHs) in the WSF were provided in Anderson et al. (1974a). With the exception of the lowest dilution, 100% mortality was observed in all exposures. The observed mortality as a function of total concentration in the WSF (mg/L) (top panel) and predicted aqueous toxic units (bottom panel) is shown in Figure 5. For this data set, the TLM correctly predicted the observed effects, 100% mortality occurred at greater than 1 TU and low effects occurring at less than 1 TU.

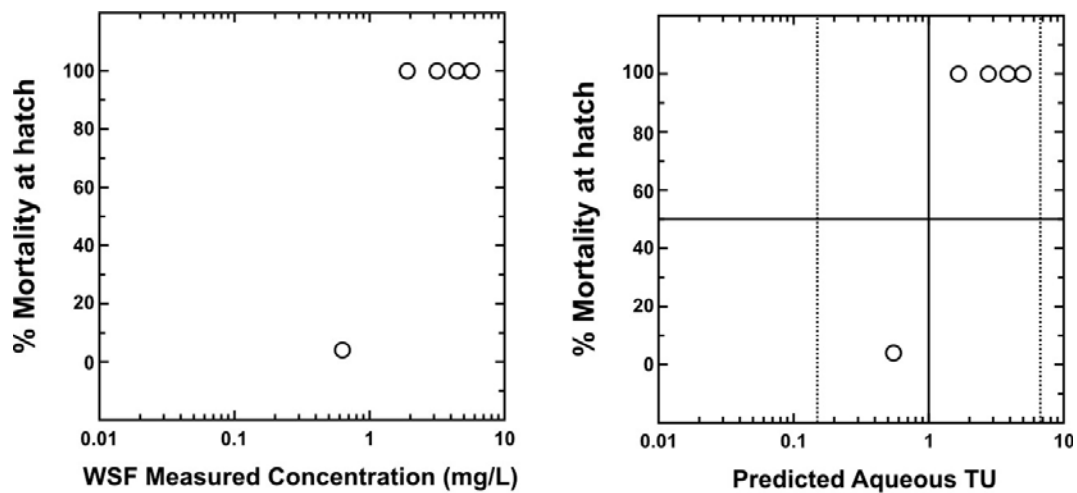


Figure 5. Chronic Effects – Mixtures – Observed mortality as a function of total measured concentration in WSF (mg/L) (left panel) and predicted aqueous toxic units (right panel). Data are for *Cyprinodon variegates* embryos exposed to WSF prepared from No. 2 fuel oil (Anderson et al. 1977). Dashed lines represent 5th and 95th percentiles based on variations in CTLBB and ACR.

Moles (1998) compared the sensitivity of ten aquatic species to long-term exposure to crude oil. In this study, WSFs were prepared from Cook Inlet crude oil. Organisms were exposed to various dilutions of the WSFs for 4 and 28 days. Although the concentrations of individual components in the WSFs were not measured, the 4-d and 28-d LC50 were reported and used to compute ACRs. The computed ACRs ranged from 1 to 2.5 (data for which 4-d LC50 could not be computed were omitted from analysis). These ACRs for crude oil are similar to the ACRs computed for individual chemicals that comprise oil and further support the use of a mean ACR of 3.8 for oil-related components.

4.2.5 Sub-lethal Effects

There is a significant amount of recent literature that suggests exposure to PAH during a fish's early life-stage can result in a variety of sub-lethal effects, such as yolk sac edema, pericardial edema, hemorrhaging, craniofacial and spinal deformities, lesions, defects in cardiac function and reduced growth (Carls et. 1999; Heintz et al. 1999; Brinkworth et al 1993; Incardona et al. 2004; Rhodes et al. 2005). Many of these symptoms are similar to those of blue-sac disease, which is related to exposure to planar, halogenated aromatic compounds such as TCDD (Hornung et al. 1999). These sub-lethal effects were not included in the development of the ACRs and so, the ACRs may not be protective of these types of effects. This section presents the application of the TLM and ACR methodology to determine if it is protective of these types of effects. This means that the methodology predicts chronic endpoints that are lower than concentrations observed to cause these effects.

4.2.5.1 Single Compound Exposures

The literature was reviewed to identify data sets where early life-stage organisms were exposed to single compounds (BTEX and PAHs) and sub-lethal effects were observed. These data sets were then screened to meet the four main criteria of (1) constant exposure (i.e., flow-through vs. static test conditions), (2) exposure concentrations below compound solubility, (3) measured concentrations, and (4) available CTLBB. Fifteen data sets were identified for analysis; however, all 15 datasets did not satisfy all four criteria. In all data sets, the chemical exposure concentrations were below the chemical's water solubility and species-specific CTLBBs were available for all test organisms. The concerns are that for some of the exposures, the reported test concentrations are nominal values rather than measured values and that the exposure conditions were static (not constant exposure concentrations) rather than flow-through (constant exposure concentrations). In following the U.S. EPA water quality criteria guidelines (Stephan et al. 1985) credence is given to measured data generated under flow-through or static renewal conditions. Due to the scarcity of data, all data were analyzed. However, to put some perspective to the conditions under which the data were generated, the data are given a ranking number determine as follows

- 1 = Nominal concentration
- 2 = Static test conditions, measured concentrations
- 3 = Static renewal conditions, measured concentrations
- 4 = Flow-through conditions, measured concentrations

Data that have a ranking number of 3 or higher are more credible since the effect concentrations were based on measured concentrations and the test concentrations were relatively stable throughout the test duration. Six data sets were given a ranking number of 3 or higher (see Table 4)

A summary of the data sets is provided in Table 4. For each exposure, the organism, chemical, relevant test conditions, observed effects and reported effect concentration are listed. The TLM chronic endpoint and HC5 and HC95 values are also provided for comparison. The TLM chronic endpoint is computed from Equations 1 and 2 using the average ACR of 3.83. The HC5 and HC95 are the 5th and 95th percentiles and include variability in ACR and CTLBB. Example calculations are provided in Appendix E. Data were available for five fish species, Japanese medaka (*Oryzias latipes*), fathead minnow (*Pimephales promelas*), rainbow trout (*Oncorhynchus mykiss*), Inland silverside (*Menidia beryllina*) and zebra danio (*Brachydanio rerio*). The compounds tested included toluene, naphthalene, phenanthrene, dibenzothiophene, retene, benzo(a)pyrene, benzo(a)anthracene, 4,6-dimethyldibenzothiophene, 7,12-dimethylbenzo(a)anthracene and benzo(k)fluoranthene. The reported concentrations included lowest observed effect concentrations (LOEC), no observed effect concentrations (NOEC) and observed effect concentrations (OEC). Ideally the TLM chronic endpoint should fall between the reported LOEC and NOEC. In two exposures no effects were reported at concentrations tested below the chemicals water solubility (Table 4 - benzo(a)anthracene and 4,6-dimethyldibenzothiophene exposure to Japanese medaka). Based on the TLM, effects should have been observed at the concentrations tested. The fact that no effects were observed at levels predicted by the TLM suggests that the TLM is protective and conservative. For eight data points, the average TLM chronic endpoint was above the LOEC. However, it is more appropriate to compare the HC5 value to the observed effect concentration when determining if a criterion is protective. For the majority (13 out of 15) of the early life stage exposures, the TLM methodology was protective of sub-lethal effects. There were two data points for which the TLM chronic endpoints fell above the observed effect concentrations (i.e., not protective). In one test, the reported 27-d LC50 for mortality (grossly deformed larvae counted as dead) for rainbow trout exposed to naphthalene was 120 µg/L (Black et al. 1983) compared to the TLM HC5 of 170 µg/L. The reported 36-d LOEC for abnormalities to rainbow trout exposed to phenanthrene was 0.21 µg/L (Hannah et al 1982; Hose et al 1984) compared to the TLM HC5 of 0.36 µg/L. Both of these exposures had a ranking number of 3 or 4, indicating that the test conditions were optimum and that the data should be of high quality. A graphical presentation comparing the early life stage data to the TLM predictions is shown in Figure 6. The lower and upper bars around the TLM chronic endpoint represent the HC5 and HC95, respectively.

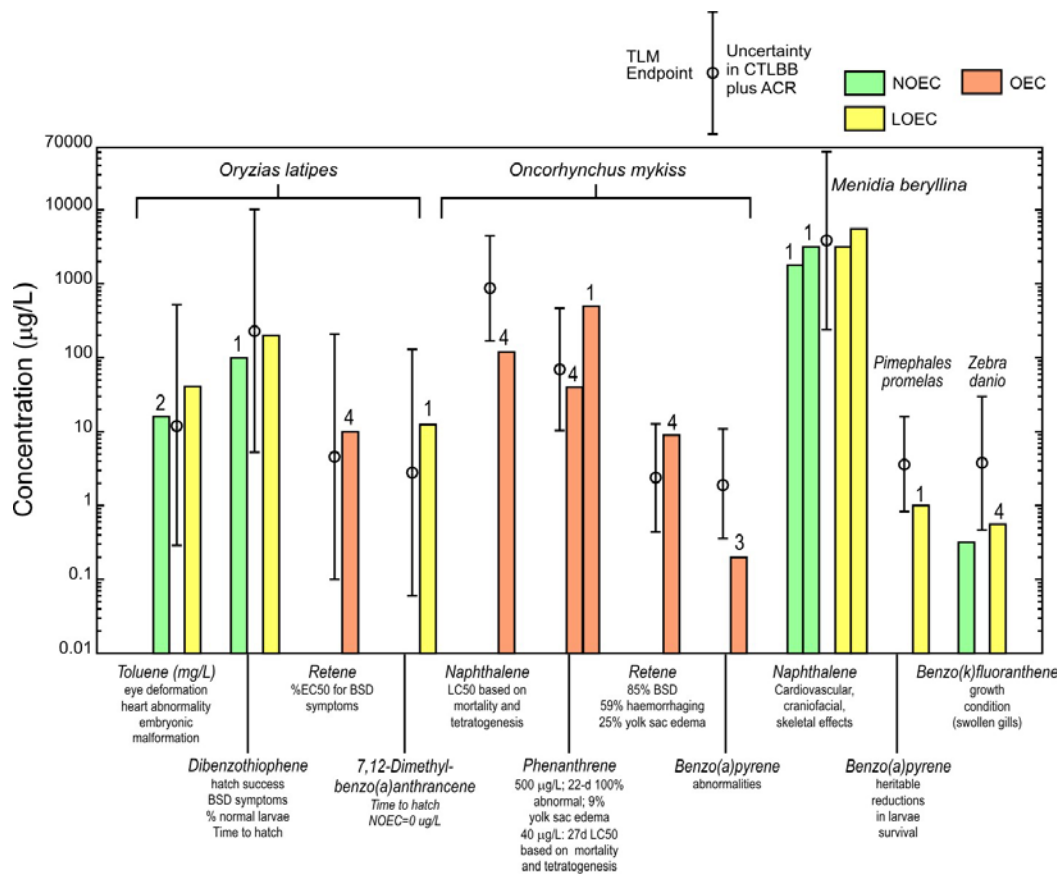


Figure 6. Sublethal effects – Single Compounds – Comparison of OEC/LOEC/NOEC observed from early life stage fish exposures to single compounds to TLM chronic effect concentrations. The effects are those associated with sublethal endpoints such as abnormal larvae development and blue sac disease-like symptoms. The symbols represent the TLM chronic endpoint. The lines represent the 5th and 95th percentiles based on variations in CTLBB and ACR. The number located above the reported effect concentration is the assigned ranking number.

4.2.5.2 PAH Mixtures

Several laboratory studies demonstrated that long-term exposure to oil results in various sublethal effects in early life stage pink salmon (*Oncorhynchus gorbuscha*) and pacific herring (*Clupea pallasii*) (Marty et al. 1997; Carls et al. 1999; Heintz et al. 1999). Data from these studies could not be analyzed because CTLBBs were not available for the test organisms (and acute toxicity data are not available to compute CTLBBs) and the chemical exposure concentrations were not constant and drastically decreased during the exposure period. Due to the variable exposure concentrations, linking the observed effects to the exposure concentrations was not possible.

Rhodes et al. (2005) determined the effects of PAH mixtures on embryonic development. In this study, early-life stage *O. latipes* was exposed for 18-day to three different mixtures of PAHs. One mixture contained three parent PAHs, phenanthrene, dibenzothiophene and benzo(a)anthracene. Another mixture contained three dimethylated PAHs, 3,6-

dimethylphenanthrene, 4,6-dimethyldibenzothiophene and 7,12-dimethylbenzo(a)anthracene. The last mixture was an oil sands extract. The exposure system was static renewal. Nominal concentrations were reported for the two mixtures prepared from three PAHs. For the extract, the concentrations of 16 U.S.EPA priority pollutant PAHs and their alkylated homologs were measured. The endpoints evaluated were prevalence of BSD symptoms, % hatch, time to hatch and % normal larvae. For each mixture, the NOEC and LOEC were reported when effects were observed. For the parent PAH mixture, the NOEC and LOEC values for % hatch and % normal larvae were 100 and 200 $\mu\text{g TPAH/L}$, respectively. The TLM chronic endpoint for the parent mixture was 80 $\mu\text{g TPAH/L}$. The only observed effect from the dimethylated PAH mixture was % hatch, where the NOEC and LOEC values were 25 and 50 $\mu\text{g TPAH/L}$, respectively. The TLM chronic endpoint for the dimethylated parent mixture was 15 $\mu\text{g TPAH/L}$. The oil sands extract was the only mixture that induced BSD symptoms. The NOEC and LOEC values for BSD and % normal larvae were 8.8 and 22 $\mu\text{g TPAH/L}$, respectively. Hatch length was effected at lower concentrations of the oil sands extract with NOEC and LOEC values of 0 and 2.2 $\mu\text{g TPAH/L}$, respectively. The TLM chronic endpoint for the oil sands mixture was 10 $\mu\text{g/L}$. A comparison of the observed and predicted effect concentrations for the three mixtures is shown in Figure 7. All data are provided in Appendix C Tables C6 and C7. For the TLM predicted concentrations, the symbol represents the predicted concentration. The bars represent the 5th and 95th percentiles and are based on variation in CTLBB for a species and variation in ACR. For all three mixtures, the TLM chronic endpoint was below the LOEC and in some cases below the reported NOEC, indicating that the method is protective. The one exception was for the oil sands extract where the LOEC for hatch length was 2.2 $\mu\text{g/L}$, which was below the average TLM endpoint of 10 $\mu\text{g/L}$. However, the HC5 of 0.2 $\mu\text{g/L}$, is below the LOEC. This is another dataset that supports the use of the HC5 as the criterion value. It should be noted that the large uncertainty in predictions for Japanese medaka (i.e., wide range in HC5 and HC95) is due to the large k_z value of 4.47. The dataset used to compute the CTLBB only consisted of 5 data points. With such a high k_z value, it is almost certain that the HC5 will be lower than the observed effect concentration. Medaka is a commonly used test organism and additional acute toxicity data are needed to better quantify the statistics of the CTLBB.

4.3 TLM Validation- Sediment

In this section, the TLM and equilibrium partitioning theory are coupled to predict the effects of organisms exposed to oil-related contaminants in sediments. Graphical comparisons of the toxicity predictions and observed values are presented.

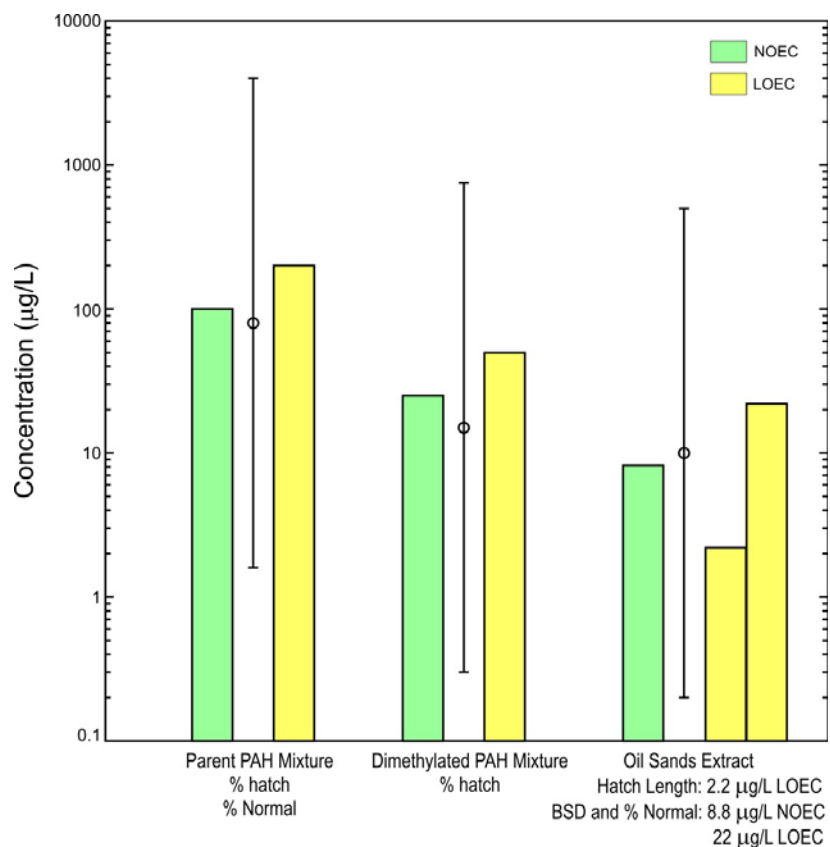


Figure 7. Sublethal effects – Mixtures – Comparison of 18-d NOEC and LOEC from early life stage toxicity tests exposing *Oryzias latipes* to three prepared mixtures of PAHs to TLM chronic endpoints. The symbols represent the TLM effect concentration. The bars represent the 5th and 95% percentiles based on variations in CTLBB and ACR.

4.3.1 Acute Effects – Single Compound Exposures

For sediment toxicity, 40 data points were found for acute exposures to single PAH compounds. Interestingly, sediment toxicity data for BTEX were not available. Since BTEX are fairly volatile compounds, most likely they are not expected to partition to the sediment. As a result, investigations of their sediment toxicity are not commonly done. Data were available for six different species, *Rhepoxynius abronius*, *Eohaustorius estuaries*, *Leptocheirus plumulosus*, *Hyalella azteca*, *Schizopera knabeni* and *Coullana sp.*, and ten different PAHs. The measured data and the corresponding TLM acute predictions are presented in Table 5. The observed and TLM predicted LC50 values are compared in Figure 8. Dashed lines represent the 90% confidence intervals (see Section 4.2.1). The two data points that fall way to the right were considered outliers and not used in the computation of the 90% confidence limits. The majority of the data fall within a factor a three. Based on this analysis, the TLM methodology coupled with EqP theory can be used to predict the toxicity of sediment-associated PAHs.

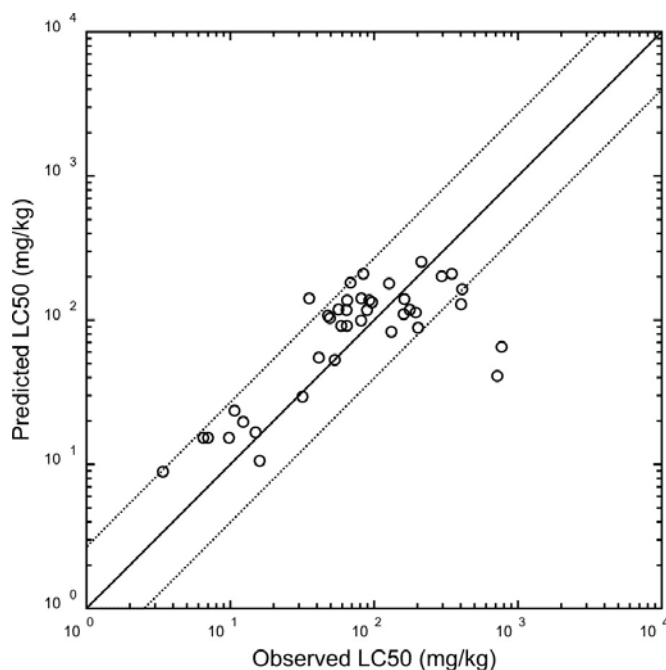


Figure 8. Acute Sediment Exposures – Single Compound - Comparison of observed and TLM predicted sediment effect concentrations (see Table 5 for data). Solid line is 1:1 relationship. The dashed lines are 90% confidence intervals.

4.3.2 Acute Effects – PAH Mixtures

There were twelve data sets available that had acute toxicity for PAH mixtures (Table 6). Three data sets were for laboratory prepared exposures where the contaminants were spiked into the sediment. Two of the laboratory tests were with various mixtures of PAHs. The other laboratory exposure involved spiking diesel fuel into sediment. Nine data sets were various field sediments where PAHs were expected to be the major contaminants of concern. Toxicity data were available for five sediment dwelling organisms, with *Rhepoxinus abronius* being the most commonly used sediment bioassay organism. For each of these data sets, the concentrations of PAH in the mixtures and the corresponding TOC concentrations were provided. An inconsistency among the field data sets is in how many PAHs were measured. Some data sets have measurements only for the 13 PAHs the EPA defined as priority pollutants (see Table 1). Other data sets have measurements for all parent PAHs and their alkylated homologs (greater than 30 PAHs). For PAH contamination from petrogenic sources the alkylated component is known to be large and if the toxicity from those alkylated PAHs is not accounted for, the toxicity from PAHs can be underestimated. For data sets that only have 13 PAHs measured, the TU from 13 PAH was normalized to total PAHs TU via adjustment factors provided in the U.S. EPA Equilibrium Partitioning Sediment Benchmarks for PAH mixtures (U.S. EPA, 2003) (see Section 3.6). The measured concentrations of PAHs, TOC, sample ID, effect data and TLM toxic units are provided in Appendix D, Tables D1 through D12.

The 10-d mortality data for *R. abronius* are presented in Figure 9. The top panel presents the percent mortality as a function of measured PAH, mg/kg dry weight basis. In the bottom panel,

the sediment concentration data are normalized to total PAH toxic units. On a mg/kg basis, relatively low mortality occurs below a measured PAH concentration of 3 mg/kg and 100 % mortality occurs above 500 mg/kg. The area of uncertainty – the area where low and high effects occur at similar levels - is 3 to 500 mg/kg. At this concentration range, effects may or may not be observed. Normalizing to total PAH TU slightly reduces that uncertainty. On a total PAH TU basis, low mortality occurs below a TU of 0.1 and 100% mortality occurs at a TU of greater than 5.0. This comparison indicates that dry weight normalization works almost as well as PAH TU. This is not unexpected and was explained in Di Toro and McGrath (2000). The TLM predicted species-specific sediment LC50s for PAHs are similar on an organic carbon basis. For *R. abronius*, the LC50s range from 19.7 $\mu\text{mol/g}_{\text{oc}}$ for naphthalene to 27.8 $\mu\text{mol/g}_{\text{oc}}$ for benzo(a)pyrene (see Table D4). Since the sediment effect concentrations are similar, a comparison of measured total PAH concentration on an organic carbon basis to the average sediment LC50 on an organic carbon basis is equivalent to the TU analysis (see Di Toro and McGrath, 2000 for equations). If the organic carbon concentration is similar for different sediments, then the dry weight normalization will work as well as the organic carbon normalization and the TU analysis. The advantages of the organic carbon normalization and TU approach are that bioavailability is considered and the data are normalized to a total PAH basis.

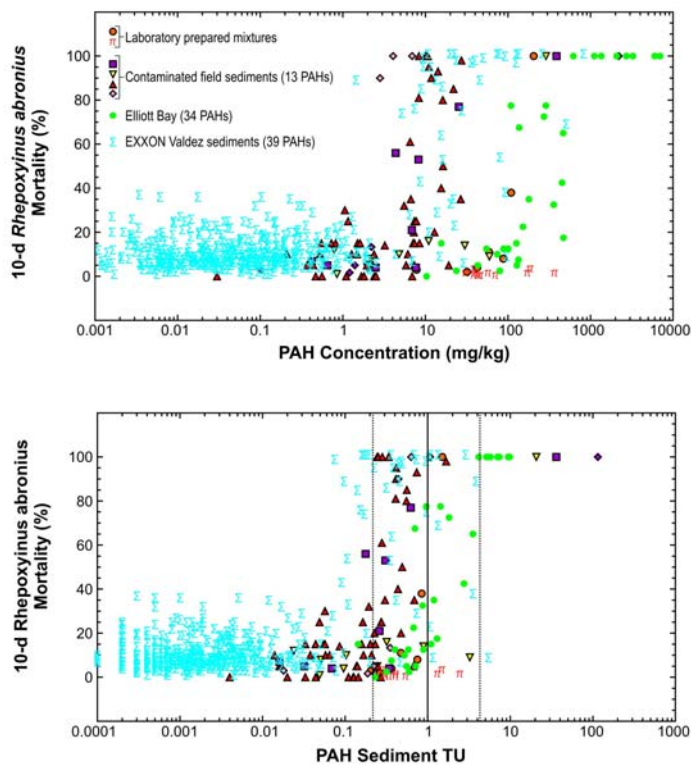


Figure 9. Acute Sediment Exposures – Mixtures – Percent mortality of *Rhepoxyinus abronius* as a function of PAH concentration (mg/kg) (top panel) and normalized to total PAH sediment toxic units (bottom panel). All data are 10-d exposures. See Table 6 for references. Solid lines at a toxic unit of 1.0 and 50 % mortality are shown for guidance. Dashed lines represent 5th and 95th percentiles based on variation in CTLBB.

On a TU basis the area of uncertainty ranges from 0.1 to 5, which is slightly lower than the uncertainty range determined on a mass concentration basis, suggesting that TUs are the better metric for relating concentration to effects. This uncertainty is slightly larger than the range bracketed by the HC5 and HC95 (0.23 to 4.3 TU) and could be attributed to the high degree of scatter commonly observed in field-collected data, compared to laboratory data. In addition, this analysis assumes that PAHs are the primary causative agent, which may not be the case for all field data sets. If other constituents are present in the sediments and contributing to the toxicity, higher than expected mortality would occur at low toxic units.

There are four data sets that have acute mortality data for species other than *R. abronius*. Comparisons of percent mortality as a function of measured PAH (mg/kg) and total PAH TU are shown in Figure 11. DeWitt et al. (1992b) determined the mortality to two species (*E. estuaries* and *L. plumulosus*). Since the CTLBB for these species are very similar (41.4 and 43.1 $\mu\text{mol/g}$ octanol), the computed total PAH TU are almost identical. Therefore, the observed mortality for the two species is shown as a range as a function of the sediment concentration (Figure 10, panels E and F). Due to limited data available to compute CTLBB for sediment organisms, HC5 and HC95 values could not be computed for *E. estuaries*, *Chironomus riparius*, *Schizopera knabeni* and *Ampelisca abdita*. For all four data sets, the dose-response is as expected with low total PAH TU corresponding to low mortality and around 1 TU corresponding to about 50 percent mortality.

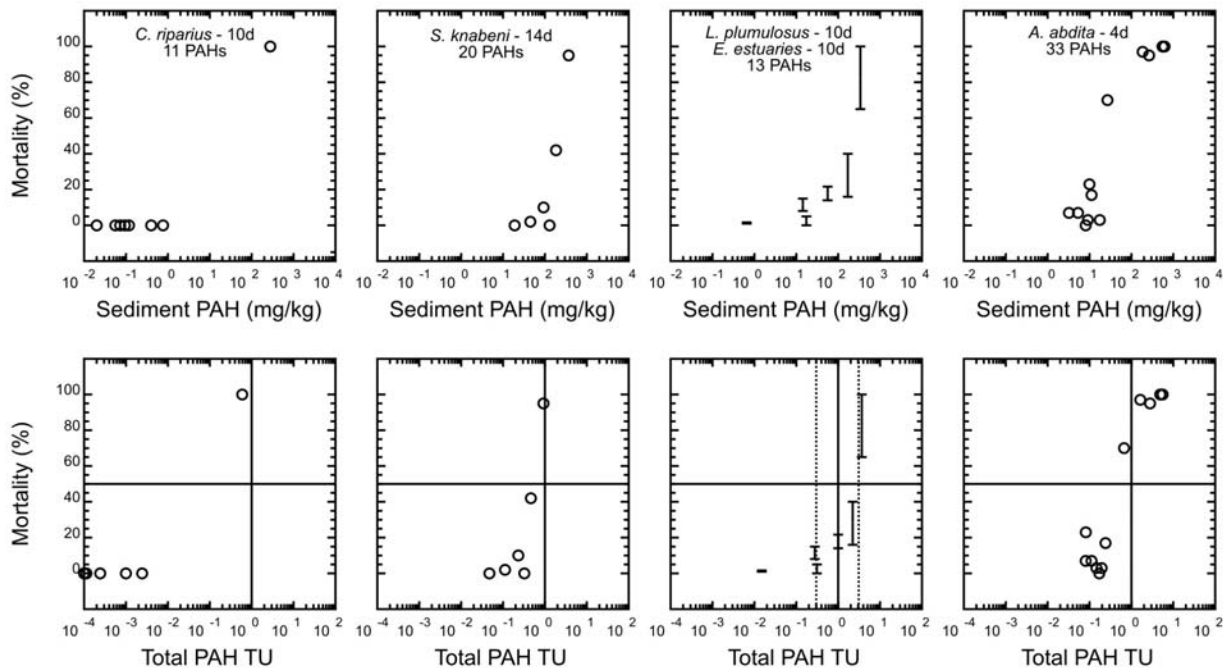


Figure 10. Acute Sediment Exposures – Mixtures – Percent mortality as a function of PAH concentration (mg/kg) (top panel) and normalized to total PAH sediment toxic units (bottom panel). See Table 6 for exposure information. Solid lines at a toxic unit of 1.0 and 50 % mortality are shown for guidance.

It should be noted that the measured concentrations in the field datasets represent a different number of PAHs measured, which ranged from 13 to 40. For example, a value of 10 mg/kg in the Exxon Valdez sediment that was computed as the sum of 40 PAHs is not necessarily equivalent to a value of 10 mg/kg in the sediments collected in Eagle Harbor that was computed as the sum of 13 PAHs. In addition, the bioavailability of the sediment-associated PAHs is a function of the organic carbon concentration of the sediment (Di Toro et al. 1999). Two sediment samples that have 10 mg/kg of the same 40 PAHs, may have different toxicities if the organic carbon concentrations are different. Therefore, comparing concentrations of measured PAH in different sources and assigning effects based on mass based concentrations should not be done. Normalizing to total sediment PAH TU considers the toxicity from unmeasured PAHs and considers the difference in organic carbon concentration and therefore reduces the uncertainty associated with PAHs measurements across different sources.

The importance of applying the adjustment factor to account for unmeasured PAHs is demonstrated using the San Diego Bay sediment dataset (Swartz et al. unpublished). In this data set, 13 PAHs were measured in 54 sediment samples. The test organism was *R. abronius* and the endpoint was 10-d mortality. Table 7 presents a comparison of the TU computed from the measured 13 PAH and the TU from Total PAH as they relate to the observed mortality. A correction prediction was one where the observed mortality was greater than or equal to 50% and the computed TU was greater than or equal to 0.4 (based on the ratio of the HC5 and the TLM endpoint for *R. abronius*) or where the observed mortality was less than 50% and the computed TU was less than 0.4. When the TUs are computed from the 13 PAH only, there were 42 correct predictions. When the adjustment for unmeasured PAHs is considered the number of correct predictions increases to 45. In addition to the number of correct predictions, one can compare the number of times that the criterion was protective, meaning high mortality was observed and correctly predicted. The observed mortality was $\geq 50\%$ in thirteen samples. Based on TU from 13 PAHs, one sample would have been predicted to be toxic (station STA28 100% with TU of 0.608 from 13 PAH). In comparison, the TUs from Total PAHs were greater than 0.4 in 8 of the samples with high mortality. This analysis demonstrates the importance of adjusting for the toxicity from unmeasured PAHs. The overall number of correct predictions (toxic and non-toxic) increased. Furthermore, the number of correct toxic predictions increased from 1 to 8 with the incorporation of the adjustment factor.

4.3.3 Chronic Effects – Single Compound Exposures

There are several data sets available that report chronic effects from exposure to sediment spiked with single PAHs. The chronic effects are growth and reproduction endpoints. The tests species are *Coullana sp.* and *S. knabeni* (Figure 11). The CTLBBs for these species were measured on a lipid basis (Lotufo, 1998). For *Coullana sp.* the effect of fluoranthene on grazing and reproduction was reported (Lotufo, 1998). The 10-d LOECs ranged from 3133 to 8800 $\mu\text{g}/\text{g}_{\text{oc}}$ for grazing and reproduction, respectively. The 10-d NOECs ranged from 1200 to 3111 $\mu\text{g}/\text{g}_{\text{oc}}$. The TLM predicted chronic effect concentration is 1410 $\mu\text{g}/\text{g}_{\text{oc}}$, which is below the observed LOECs indicating that the TLM correctly predicted the effects. For *S. knabeni*, the chronic effects of phenanthrene and fluoranthene on grazing and reproduction were determined (Lotufo, 1997; Fleeger and Lotufo, 1999). Phenanthrene had a reported 14-d IC25 (concentration causing 25% reduction of measured endpoint in relation to control) of 1730 $\mu\text{g}/\text{g}_{\text{oc}}$ for reproduction

effects. The reported 10-d NOEC and LOEC were 1470 and 3000 $\mu\text{g}/\text{g}_{\text{oc}}$ for hatching success, respectively. The TLM predicted chronic effect concentration is 3560 $\mu\text{g}/\text{g}_{\text{oc}}$, which is slightly higher than the reported OEC/LOEC. Fluoranthene had reported 10-d LOECs of 1200 and 3133 $\mu\text{g}/\text{g}_{\text{oc}}$ for grazing and reproduction, respectively (Lotufo, 1998). The TLM predicted chronic effect concentration is 4130 $\mu\text{g}/\text{g}_{\text{oc}}$, which is slightly higher than the reported LOEC. These data are summarized in Table 8 and Figure 11.

The CTLBBs for *S. knabeni* and *Coullana* are measured values based on a single compound (flouranthene) and the uncertainty associated with them could not be determined. In addition, Lotufo (1998) states that the lipid content was based on an initial value, which could have changed during the exposure time. The variability in the reported CTLBB for these species is unknown. Therefore, these data are presented just for informational purposes and the results of the analysis should not be used to assess the performance of the TLM.

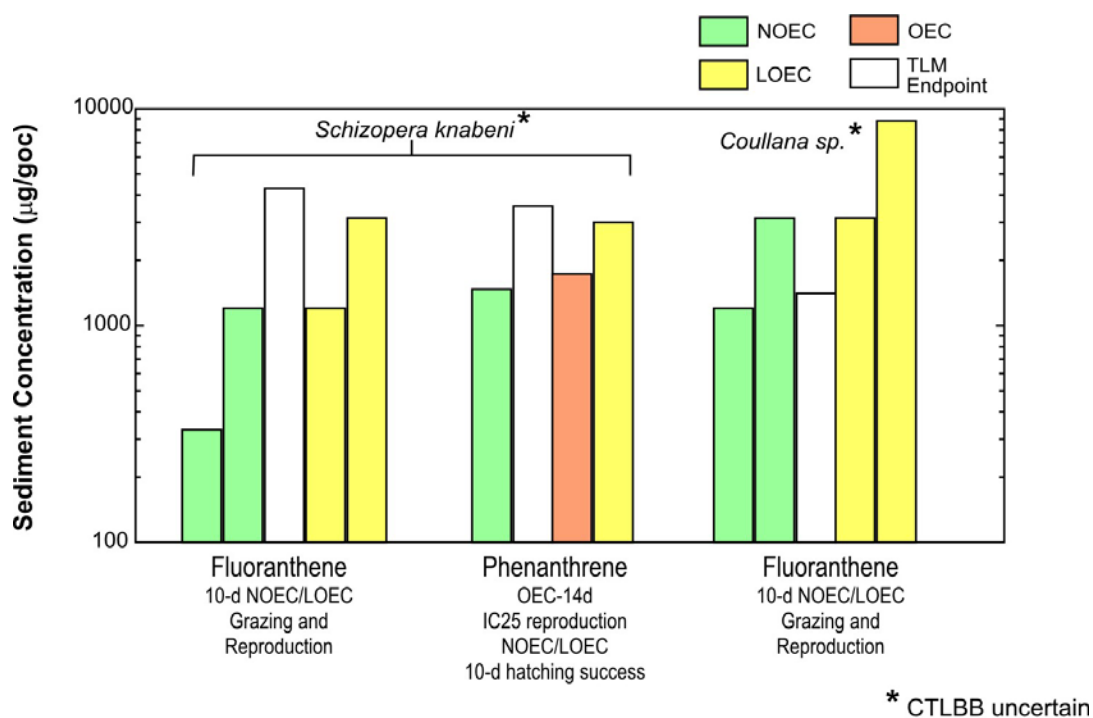


Figure 11. Chronic Sediment Exposures – Single Compounds - Comparison of reported OEC/LOEC/NOEC and TLM effect concentrations from long-term exposures of fluoranthene and phenanthrene to marine copepods *Coullana sp.* and *Schizopera knabeni*. See Table 8 for references.

4.3.4 Chronic Effects – PAH Mixtures

Fleeger and Lotufo (1999) investigated the chronic effects on *S. knabeni* from exposure to a sediment spiked with diesel fuel. They measured the concentrations of 20 PAHs and TOC in the sediment. The sediment was spiked with the diesel fuel and dilutions were prepared for use in the bioassay. The total PAH concentrations in the sediment were 19, 45, 93, 130, 185 and 370 mg/kg. The LOEC for reproduction effects was 93 mg/kg. The NOEC was 45 mg/kg. The equivalent TLM total PAH TU for the LOEC and NOEC were 1.7 and 0.8, respectively (Table

10D). Based on these equivalent TUs, effects should have been observed at 45 mg/kg. For this data set the TLM was over protective because effects were predicted at concentrations where no effects were observed. However, due to the uncertainty in the CTLBB discussed in section 4.3.3, these data should not be used to assess the performance of the TLM.

5.0 Discussion and Importance to Oil Spill Response/Restoration

This research focused on developing a methodology that can be used to assess the toxicity of low levels of residual oil, focusing on the MAH and PAH components. The methodology has to be able to predict the toxicity of these components in the aqueous phase and in the sediment, both on an acute basis and a chronic basis. The methodology had to include the derivation a metric that enabled the toxicity from one location to be comparable to the toxicity at another location.

It has been demonstrated that the TLM can be used to assess the acute and chronic toxicity of oil-related components on an acute basis in the water column and sediments. It has been shown that the use of an ACR to relate the acute toxicity to an equivalent chronic toxicity is appropriate without consideration of the toxicity mechanism. Within the uncertainty of the model, the TLM has been shown to be protective of sublethal effects that result from exposure to low levels of PAHs during an organism's early life stage. The TLM coupled with the theory of additivity via the concept of toxic units can be used to predict the toxicity of mixtures of chemicals present in oils. Toxic units are a means of normalizing the toxicity of different chemicals. A total toxic unit of 1.0, implies toxicity. A total concentration of 1 µg/L is not necessarily toxic and is dependent on the chemical(s) and the sensitivity of the test organism.

For sediment assessment, the TLM aqueous effect concentrations are converted to sediment effect concentrations via EqP methodology. Normalizing the chemical concentration to the organic carbon concentration of the sediment is a means of relating the chemical concentration in the sediment to the bioavailability of the sediment. The toxic unit metric allows for the consideration of the toxicity from unmeasured PAHs by incorporating the U.S.EPA adjustment factors, which cannot be done on a mass basis (i.e., mg/kg). Organic carbon normalization and toxic unit conversion allow for the generation of a toxicity metric that is applicable across a broad range of sediment types and representative of toxicity from total PAH.

In addition to being used a tool that can assess whether or not effects are expected at a certain concentration of a chemical or from a mixture of chemicals, the methodology can be used to derive defensible chemical-specific guideline values. When the statistics (geometric mean and variance) of the CTLBB of all test species are used in Equation 6, the computed HC5 is the aqueous concentration that protects 95% of the species. These HC5s can be used as decision-making values to determine the concentration of a particular chemical that most likely will not have an adverse impact on the aquatic community. The geometric mean CTLBB of all tests species for baseline chemicals (i.e. aliphatic hydrocarbons, alcohols, see Appendix A) is 123 µmol/g octanol. The geometric mean CTLBB for specific chemical classes is computed as

$$C_L^* (\text{geometricmean, Chemicalclass}_i) = C_L^* (\text{geometricmean, baseline}) \times \Delta C_i \quad (10)$$

where Δ_c is the chemical class correction factor for chemical class i (see Appendix A). The CTLBBs for the various chemical class are provided in Table 9.

The final equation to compute the chronic HC5 values for PAHs is

$$\log(HC_5) = (-0.936) \log(K_{ow}) + \log(54.5) - \log(3.83) - 2.3 \sqrt{[0.000225(\log(K_{ow}))^2] + 0.105 + 0.104} \quad (11)$$

The final equation to compute the chronic HC5 values for MAHs is

$$\log(HC_5) = (-0.936) \log(K_{ow}) + \log(95.3) - \log(3.83) - 2.3 \sqrt{[0.000225(\log(K_{ow}))^2] + 0.105 + 0.104} \quad (12)$$

The 95% confidence sample size-dependent extrapolation factor ($k_z = 2.3$) was based on the number of ACRs (29) rather than the number of CTLBB (46) to ensure that the calculations are conservative. A summary of chronic HC5 values for MAHs and PAHs is provided in Table 10. EqP theory was used to convert the aquatic HC5s to sediment HC5 values (Equation 3). The values are presented on a molar basis (i.e., $\mu\text{mol/L}$, mmol/Kg_{OC}) and a mass basis (i.e., $\mu\text{g/L}$, mg/Kg_{OC}). Details of the calculations are provided in Appendix E.

To assess the management implications of adopting chronic HC5s derived via the TLM for decision-making, a comparison was made of the aqueous HC5 values to NOECs values for PAHs. The NOECs values used in this analysis are presented in Table 11 and Figure 12. A total of 27 NOECs were compiled for 7 different PAHs. Two NOECs fell below the HC5 line (Figure 12). Both of these NOECs were for phenanthrene and ranged from 5 to 5.5 $\mu\text{g/L}$, which were considerably lower than NOECs for other compounds. The excursion of two data points below the HC5 is consistent with the 95% protection level goal, i.e., 92.6% (25/27). The HC5 derived from the TLM is very close to the expected level of protection. Therefore, these values are appropriate for use as numeric chemical-specific benchmarks and can be used to assess the ecological risk of contaminated sediments and/or establish safe levels for cleanup activities.

6.0 Technology Transfer

The results of this research effort on the application of the target lipid model to predict acute and chronic effects on oil-related compounds and the derivation of HC5 will be submitted to *Environmental Chemistry and Toxicology*. An abstract has been submitted focusing on the application of TLM to be protective of sublethal effects from exposure to PAHs has been submitted to the Society of Environmental Chemistry and Toxicology (SETAC) for presentation at the 2006 North America meeting. Intermediate results of this research effort were presented at a March 2005 workshop entitled “Emerging Research in Oil Spill Response and Restoration” sponsored by CRRC and at the 2005 SETAC North America meeting.

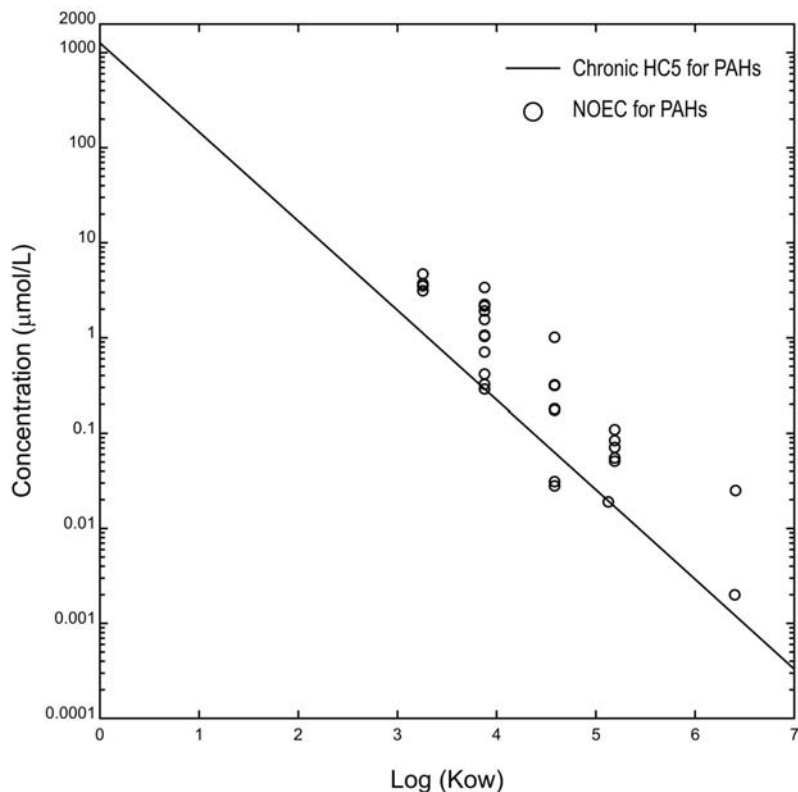


Figure 12. Chronic HC5 concentration for PAHs versus log (K_{ow}). The HC5 concentration is based on the 5th percentile CTLBB for all species in database. The observed NOECs for PAH are denoted with a ○ (Table 10).

7.0 Achievement and Dissemination

Workshops and Conferences

Workshop on Emerging Research in Oil Spill Response and Restoration. 2005. Office of Response and Restoration of NOAA. Silver Spring, Maryland. March 2005. Number of participants unknown.

26th Annual SETAC North America Meeting. 2005. Baltimore, Maryland. November 2005.

Table 1. Chemicals and their properties (at 25°C) measured in various data sets

	Log K _{ow} ^a	Molecular Weight (g/mol)	Subcooled Liquid		Key PAHs ^e
			Solid Solubility (µg/L) ^b	Solubility (µg/L) ^{b,d}	
ethane	1.730	30.00	1350000	1350000	
benzene	1.943	78.11	1780000	1780000	
propane	2.370	44.09	248000	248000	
toluene	2.438	92.14	515000	515000	
butane	2.868	58.12	61400	61400	
isobutane	2.869	58.12	48900	48900	
o-xylene	2.946	106.17	220000	220000	
cyclopentane	2.991	70.00	156000	156000	
ethylbenzene	3.006	106.17	152000	152000	
m-xylene	3.032	106.17	160000	160000	
p-xylene	3.051	106.17	215000	215000	
9,10-Anthracenedione	3.080	208.22	116000	130000	
naphthalene	3.256	128.19	31000	110000	A,B,C
isopentane	3.335	72.15	13800	13800	
acenaphthylene	3.436	152.20	16100	75000	A,B,C
C3-benzenes ^c	3.455	120.00	19700	19700	
pentane	3.471	72.15	38500	38500	
9-fluorenone	3.510	180.20	25000	48000	
methylcyclopentane	3.571	84.00	42000	42000	
1-methylnaphthalene	3.781	142.20	28000	28000	B
C1-naphthalenes ^c	3.788	142.20	7900	22000	C
2-methylnaphthalene	3.789	142.20	25000	31100	B
acenaphthene	3.878	154.21	3800	19200	A,B,C
fluorene	3.930	166.20	1900	15100	A,B,C
biphenyl	3.936	154.21	7000	20000	
2-chloronaphthalene	3.940	162.64	5500	18000	
1-chloronaphthalene	3.950	162.64	5400	5400	
methylcyclohexane	3.963	98.19	14000	14000	
hexane	4.053	86.00	9500	9500	
C2-naphthalenes ^c	4.244	156.23	1970	9400	C
1,3-dimethylnaphthalene	4.257	156.23	8000	8000	
1-methylfluorene	4.370	180.25	1090	4270	
C1-fluorenes ^c	4.370	180.25	1510	8400	C
anthracene	4.546	178.20	45	3500	A,B,C
2,3,5-trimethylnaphthalene	4.570	170.20	580	5200	B
2,3,6-trimethylnaphthalene	4.570	170.20	740	5200	
phenanthrene	4.584	178.23	1100	6210	A,B,C
n-heptane	4.584	100.20	2930	2930	
dimethylbiphenyl ^c	4.692	182.00	530	4400	
C3-naphthalenes ^c	4.730	170.25	440	3800	C
C2-fluorenes ^c	4.819	194.27	380	3600	C
C1-Dibenzothiophene ^c	4.859	198.30	340	3400	
9-methylanthracene	4.996	192.26	261	945	

Table 1. Chemicals and their properties (at 25°C) measured in various data sets (Continued)

	Log K_{ow} ^a	Molecular Weight (g/mol)	Subcooled Liquid		Key PAHs ^e
			Solid Solubility ($\mu\text{g/L}$) ^b	Solubility ($\mu\text{g/L}$) ^{b,d}	
1-methylphenanthrene	5.036	192.26	270	2520	B
C1-phenanthrene/anthracene ^c	5.037	192.26	180	2300	C
2-methylphenanthrene	5.040	192.26	180	2300	
pyrene	5.126	202.26	132	2610	A,B,C
fluoranthene	5.190	202.26	260	1700	A,B,C
C4-naphthalenes ^c	5.220	184.28	97	1500	C
C1-fluoranthene/pyrene ^c	5.257	216.28	101	1600	C
C3-fluorenes ^c	5.318	208.30	80	1400	C
C2-Dibenzothiophene ^c	5.332	212.30	78	1400	
3,6-dimethylphenanthrene	5.340	206.29	73	1300	
4,6-dimethyldibenzothiophene	5.450	212.30	53	1100	
C2-phenanthrene/anthracene ^c	5.455	206.29	51	1000	C
C2-fluoranthene/pyrene ^c	5.557	230.31	40	950	
Triphenylene	5.630	228.30	43	2260	
benzo(a)anthracene	5.744	228.29	11	240	A,B,C
chrysene	5.782	228.29	2.0	376	A,B,C
C3-Dibenzothiophene ^c	5.810	226.30	17	560	
C4-phenanthrene/anthracene ^c	6.357	234.34	3.0	190	C
benzo(b)fluoranthene	6.341	252.32	1.5	38.9	A,B,C
C3-fluoranthene/pyrene ^c	6.384	244.34	2.9	190	
benzo(k)fluoranthene	6.400	252.32	0.80	63.6	A,B,C
benzo(a)pyrene	6.409	252.31	3.8	116	A,B,C
7,12-dimethylbenzo(a)anthracene	6.420	256.35	50.00	455	
Benzo(e)pyrene	6.447	252.30	4.0	130	B,C
perylene	6.447	252.31	0.40	124	B,C
C2-Chrysenes/benzo(a)anthracene ^c	6.593	256.34	1.5	130	C
C4-fluoranthene/pyrene ^c	6.687	258.35	1.1	110	
C5-phenanthrene/antracene ^c	6.700	248.37	1.1	99.5	
C1-benzofluoranthene ^c	6.743	266.11	1.0	97.6	
benzo(ghi)perylene	6.886	276.34	0.26	83.2	B,C
C3-Chrysenes/benzo(a)anthracene ^c	6.972	270.36	0.47	62	C
dibenz(a,h)anthracene	7.129	278.35	0.60	148	B,C
C2-benzofluoranthene ^c	7.200	280.13	0.23	40.5	
C4-Chrysenes/benzo(a)anthracene ^c	7.421	284.38	0.12	26	C

^a Log K_{ow} computed from SPARC

^b Solubility data from Mackay et al. 1992a, 1992b, 1993 and 1995 or computed from relationships below

Solid solubility computed from $\text{Log } S = (-1.4136)(\text{Log}K_{ow}) + 7.1022$ where solubility has units of $\mu\text{mol/L}$

Sub-cooled solubility computed from $\text{Log } S = (-0.8857)(\text{Log}K_{ow}) + 5.5367$ where solubility has units of $\mu\text{mol/L}$

^c Mixture of isomers

^d For compounds that are liquid at room temperature, the solid solubility and sub-cooled solubility are equal.

^e A = PAH is one of key 13 PAHs; B= PAH is one of key 23 PAHs; C = PAH is one of 34 PAHs

Table 2. Observed water-only acute LC50/EC50 values for PAHs and TLM predictions.

Species	PAH	Life Stage	Test Type ^b	Observed LC50 (µg/L)	Predicted LC50 (µg/L)	Reference
<i>Artemia salina</i>	naphthalene	larvae	S,U	10600	9000	Abernethy et al. 1986
	naphthalene	larvae	S,M	11070	9000	Maclean and Doe, 1989
	1-methylnaphthalene	larvae	S,U	2560	3500	Abernethy et al. 1986
	2-methylnaphthalene	larvae	S,U	4740	3500	Abernethy et al. 1986
	2-chloronaphthalene	larvae	S,U	2330	1300	Abernethy et al. 1986
	1-chloronaphthalene	larvae	S,U	1840	1300	Abernethy et al. 1986
	phenanthrene	larvae	S,U	680	790	Abernethy et al. 1986
<i>Chlamydomonas angulosa</i>	naphthalene	not applicable	S,U	9600	16000	Hutchinson et al. 1980
	1-methylnaphthalene	not applicable	S,U	1700	6100	Hutchinson et al. 1980
	2-methylnaphthalene	not applicable	S,U	4480	6000	Hutchinson et al. 1980
	phenanthrene	not applicable	S,U	945	1400	Hutchinson et al. 1980
<i>Chlorella vulgaris</i>	naphthalene	not applicable	S,U	19200	21000	Hutchinson et al. 1980
	1-methylnaphthalene	not applicable	S,U	5100	8200	Hutchinson et al. 1980
	2-methylnaphthalene	not applicable	S,U	8900	8000	Hutchinson et al. 1980
<i>Cyprinodon variegatus</i>	naphthalene	unknown	M	2400	5300	Anderson et al. 1974 ^a
	1-methylnaphthalene	unknown	M	3400	2100	Anderson et al. 1974a
	2-methylnaphthalene	unknown	M	2000	2000	Anderson et al. 1974a
	acenaphthene	juvenile	S,U	2200	1800	Heitmuller et al. 1981
	acenaphthene	adult	FT,M	3100	1800	Ward et al. 1981
	1-chloronaphthalene	juvenile	S,U	2400	760	Heitmuller et al. 1981
	1-chloronaphthalene	juvenile	F,M	690	760	Ward et al. 1981
	phenanthrene	juvenile	FT,M	429.4	460	Battelle Ocean Sciences, 1987
	phenanthrene	juvenile	R	478	460	Moreau et al. 1999
<i>Daphnia magna</i>	naphthalene	juvenile	S,U	4723	5400	Abernethy et al. 1986
	naphthalene	unknown	S,U	8600	5400	U.S. EPA, 1978
	naphthalene	neonate	S,M	11800	5400	Maclean and Doe, 1989
	naphthalene	unknown	S,U	3400	5400	Crider et al. 1982
	naphthalene	unknown	S,U	4100	5400	Crider et al. 1982
	naphthalene	unknown	S,U	22600	5400	Eastman et al. 1984
	naphthalene	unknown	S,M	2160	5400	Millemann et al. 1984
	1-methylnaphthalene	juvenile	S,U	1420	2100	Abernethy et al. 1986
	2-methylnaphthalene	juvenile	S,U	1491	2100	Abernethy et al. 1986
	acenaphthene	unknown	S,M	320	1900	EG&G Bionomics, 1982
	acenaphthene	unknown	S,M	1300	1900	EG&G Bionomics, 1982
	acenaphthene	unknown	FT,M	120	1900	EG&G Bionomics, 1982
	acenaphthene	unknown	S,U	3450	1900	Randall and Knopp, 198
	fluorene	unknown	S,U	430	1800	Finger et al. 1985
	2-chloronaphthalene	juvenile	S,U	1640	780	Abernethy et al. 1986
	1-chloronaphthalene	unknown	S,U	1600	770	LeBlanc, 1980
	phenanthrene	juvenile	S,U	207	470	Abernethy et al. 1986
	phenanthrene	unknown	S,U	843	470	Eastman et al. 1984

Table 2. Observed water-only acute LC50/EC50 values for PAHs and TLM predictions (Continued)

Species	PAH	Life Stage	Test Type ^b	Observed LC50 (µg/L)	Predicted LC50 (µg/L)	Reference
<i>Daphnia pulex</i>	phenanthrene	neonate	S,M	700	470	Millemann et al. 1984
	phenanthrene	unknown	FT,M	117	470	Call et al. 1986
	9-methylanthracene	juvenile	S,U	124.8	210	Abernethy et al. 1986
	pyrene	juvenile	S,U	90.9	170	Abernethy et al. 1986
	fluoranthene	juvenile	S,M	45	140	Oris et al. 1991
	fluoranthene	unknown	S,M	100	140	EG&G Bionomics, 1982
	fluoranthene	unknown	S,M	105.7	140	Suedel and Rogers, 1996
	benzo(a)pyrene	unknown	S	250 ^a	13	Atienzar et al. 1999
	naphthalene	unknown	S,U	4663	4210	Smith et al. 1988
	fluorene	unknown	S,U	212	1400	Smith et al. 1988
	1,3-dimethylnaphthalene	unknown	S,U	767	650	Smith et al. 1988
	1,3-dimethylnaphthalene	neonate	S,U	1280	650	Passino and Smith, 1987
	2,6-dimethylnaphthalene	unknown	S,U	193	630	Smith et al. 1988
	phenanthrene	neonate	S,U	734	370	Passino and Smith, 1987
	<i>Ictalurus punctatus</i>	phenanthrene	unknown	S,M	100	370
phenanthrene		unknown	S,U	350	370	Smith et al. 1988
acenaphthene		juvenile	FT,M	1720	1180	Holcombe et al. 1983
fluoranthene		juvenile	S,M	37.4	91	Gendusa, 1990
<i>Lepomis macrochirus</i>		acenaphthene	juvenile	S,U	1700	2100
	fluorene	unknown	S,U	910	2000	Finger et al. 1985
	1-chloronaphthalene	juvenile	S,U	2300	870	Buccafusco et al. 1981
	phenanthrene	juvenile	FT,M	234	540	Call et al. 1986
	fluoranthene	juvenile	FT,M	44	160	Spehar et al. 1999
<i>Leptoichirus plumulosus</i>	acenaphthene	adult	FT,M	589.4	690	Swartz, 1991
	phenanthrene	adult	FT,M	198.4	180	Swartz, 1991
	pyrene	juvenile	FT,M	66.49	62	Champlin and Poucher, 1992
	fluoranthene	unknown	R,M	51	54	Boese et al. 1997
	<i>Menidia beryllina</i>	acenaphthene	juvenile	R,U	5564 ^a	4700
acenaphthene		unknown	S,U	2300	4700	Horne et al. 1983
fluoranthene		unknown	R,U	616 ^a	360	Spehar et al. 1999
<i>Mysidopsis bahia</i>	acenaphthene	juvenile	R,U	1190	550	Thursby et al. 1989a
	acenaphthene	juvenile	S,U	970	550	Ward et al. 1981
	acenaphthene	juvenile	FT,M	460	550	Thursby et al. 1989b
	acenaphthene	juvenile	S,M	160	550	EG&G Bionomics, 1982
	acenaphthene	juvenile	FT,M	190	550	EG&G Bionomics, 1982
	acenaphthene	juvenile	FT,M	466.1	550	Horne et al. 1983; Thursby, 1991
	acenaphthene	juvenile	FT,M	271.9	550	Horne et al. 1983; Thursby, 1991
	1-chloronaphthalene	juvenile	S,U	370	230	U.S. EPA, 1978
	phenanthrene	juvenile	FT,M	17.7	140	Battelle Ocean Sciences, 1987
	phenanthrene	juvenile	FT,M	27.1	140	Kuhn and Lussier, 1987

Table 2. Observed water-only acute LC50/EC50 values for PAHs and TLM predictions (Continued)

Species	PAH	Life Stage	Test Type ^b	Observed LC50 (µg/L)	Predicted LC50 (µg/L)	Reference
<i>Neanthes arenaceodentata</i>	fluoranthene	juvenile	S,U	40	43	U.S. EPA, 1978
	fluoranthene	juvenile	FT,M	87	43	EG&G Bionomics, 1982
	naphthalene	immature young adult	S,U	3800	8500	Rossi and Neff, 1978
	acenaphthene	unknown	S,U	3600	2900	Horne et al. 1983
	phenanthrene	immature young adult	S,U	600	740	Rossi and Neff, 1978
<i>Oithona davisae</i>	fluoranthene	immature young adult	S,U	500 ^a	230	Rossi and Neff, 1978
	naphthalene	adult	S,M	7195	6600	Barata et al. 2005
	1-methylnaphthalene	adult	S,M	2652	2600	Barata et al. 2005
	fluorene	adult	S,M	1800	2200	Barata et al. 2005
	1,2-dimethylnaphthalene	adult	S,M	617	990	Barata et al. 2005
	dibenzothiophene	adult	S,M	551 ^a	1010	Barata et al. 2005
	phenanthrene	adult	S,M	522	580	Barata et al. 2005
	1-methylphenanthrene	adult	S,M	931 ^a	230	Barata et al. 2005
	pyrene	adult	S,M	154 ^a	200	Barata et al. 2005
	fluoranthene	adult	S,M	196	180	Barata et al. 2005
<i>Oncorhynchus mykiss</i>	naphthalene	juvenile	FT,M	1600	3100	DeGraeve et al. 1982
	naphthalene	unknown	FT,M	2300	3100	DeGraeve et al. 1980
	naphthalene	pre SU	S,U	1800	3100	Edsall, 1991
	naphthalene	pre SU	S,U	6100	3100	Edsall, 1991
	naphthalene	pre SU	S,U	2600	3100	Edsall, 1991
	naphthalene	pre SU	S,U	4400	3100	Edsall, 1991
	naphthalene	pre SU	S,U	5500	3100	Edsall, 1991
	2-methylnaphthalene	unknown	R	1456	1200	Kennedy, 1990
	acenaphthene	juvenile	FT,M	670	1100	Holcombe et al. 1983
	fluorene	juvenile	S,U	820	1020	Finger et al. 1985
	1,3-dimethylnaphthalene	pre SU	S,U	1700	480	Edsall, 1991
	phenanthrene	juvenile	FT,M	375	270	Call et al. 1986
	fluoranthene	unknown	S,M	187	82	Horne and Oblad, 1983
	fluoranthene	juvenile	FT,M	26	82	Spehar et al. 1999
<i>Palaemonetes pugio</i>	naphthalene	unknown	S,M	2350	2700	Tatum et al. 1978
	naphthalene	unknown	M	2600	2700	Anderson et al. 1974 ^a
	2-methylnaphthalene	unknown	M	1700	1000	Anderson et al. 1974a
	acenaphthene	larvae	R,U	1697	920	Thursby et al. 1989a
	acenaphthene	unknown	S,U	676	920	Horne et al. 1983; Thursby, 1991
	dimethylnaphthalene	unknown	M	700	400	Anderson et al. 1974a
	phenanthrene	adult	R,U	201	230	Battelle Ocean Sciences, 1987
	phenanthrene	adult	FT,M	145.4	230	Battelle Ocean Sciences, 1987
	fluoranthene	juvenile	S,U	142	71	Spehar et al. 1999
	naphthalene	juvenile	FT,M	6080	5700	Holcombe et al. 1984
<i>Pimephales promelas</i>	fluoranthene	juvenile	S,U	142	71	Spehar et al. 1999
	naphthalene	juvenile	FT,M	6080	5700	Holcombe et al. 1984

Table 2. Observed water-only acute LC50/EC50 values for PAHs and TLM predictions (Continued)

Species	PAH	Life Stage	Test Type ^b	Observed LC50 (µg/L)	Predicted LC50 (µg/L)	Reference
	naphthalene	juvenile	FT,M	7900	5700	DeGraeve et al. 1982
	naphthalene	unknown	FT,M	4900	5700	DeGraeve et al. 1980
	naphthalene	juvenile	FT,M	8900	5700	DeGraeve et al. 1980
	naphthalene	juvenile	S,M	1990	5700	Millemann et al. 1984
	1-methylnaphthalene	juvenile	S,U	9000	2200	Mattson et al. 1976
	acenaphthene	juvenile	FT,M	1600	2000	Holcombe et al. 1983
	acenaphthene	juvenile	FT,M	608	2000	Cairns and Nebeker, 1982
	acenaphthene	juvenile	S,M	1500	2000	EG&G Bionomics, 1982
	acenaphthene	adult	R,U	3700	2000	Academy of Natural Sciences, 1981
	acenaphthene	juvenile	S,M	3100	2000	Marine Bioassay Lab, 1981
	acenaphthene	juvenile	FT,M	1730	2000	Geiger et al. 1985
	fluoranthene	juvenile	S,M	95	150	Horne and Oblad, 1983
	fluoranthene	juvenile	S,M	77.1	150	Gendusa, 1990
<i>Tanytarsus dissimilis</i>	naphthalene	larvae	S,U	12600	8500	Darville and Wilhm, 1984
	naphthalene	larvae	S,U	20700	8500	Darville and Wilhm, 1984
<i>Tetrahymena ellioti</i>	1-methylnaphthalene	not applicable	S,M	9400	5000	Rogerson et al. 1983
<i>Xenopus laevis</i>	naphthalene	larvae	FT,M	2100	7600	Edmisten and Bantle, 1982
	benzo(a)pyrene	unknown	R	13400 ^a	18	Propst et al. 1997
<i>Rhepoxynius abronius</i>	2,3,5-trimethylnaphthalene	unknown	unknown	156	100	Ozretich et al. 1997
	fluoranthene	unknown	unknown	24	39	Ozretich et al. 1997
	naphthalene	unknown	unknown	10346	1400	Ozretich et al. 1997
	2,6-dimethylnaphthalene	unknown	unknown	192	220	Ozretich et al. 1997
	1-methylfluorene	unknown	unknown	45	200	Ozretich et al. 1997
	2-methylphenanthrene	unknown	unknown	67	51	Ozretich et al. 1997
	9-methylanthracene	unknown	unknown	32	56	Ozretich et al. 1997

^aObserved LC50 greater than solubility. These data were not used in the comparison.

^bS= static; R = renewal; FT= flow-through; U = unmeasured or nominal; M = measured

Table 3. Acute and chronic values used in the development of ACRs. Chronic endpoints are those effecting growth, reproduction or mortality of an organism.

Species	Chemical	Chemical Code	Acute LC50/EC50 (µg/L)	Chronic Endpoint	Chronic (µg/L)	ACR	Source
<i>Cyprinodon variegatus</i>	Acenaphthene	PAH	3,100	survival	710	4.36	Ward et al. 1981
<i>Daphnia magna</i>	Fluoranthene	PAH	117	growth	24.5	4.78	Spehar et al. 1999
	Phenanthrene	PAH	117	survival and reproduction	96.4	1.21	Call et al. 1986
	Biphenyl	MAH	362		322	1.12	Gersich et al. 1989
	Methyltertbutylether	ALI	472,000	not specified	42,000	11.2	Mancini et al. 2002
<i>Mysidopsis bahia</i>	Acenaphthene	PAH	466	reproduction	286	1.63	Horne et al. 1983
	Acenaphthene	PAH	460	reproduction	64.0	7.19	Thursby et al. 1989b
	Fluoranthene	PAH	30.5	survival and reproduction	14.4	2.11	Spehar et al. 1999
	Fluoranthene	PAH	40.0	survival and reproduction	15.9	2.52	U.S. EPA, 1978
	Phenanthrene	PAH	27.1	survival	8.13	3.33	Kuhn and Lussier, 1987
	Pyrene	PAH	28.3	reproduction	4.53	6.24	Champlin and Poucher, 1992a and b
	Methyltertbutylether	ALI	187,000	not specified	36,000	5.2	Mancini et al. 2002
<i>Onchorhynchus mykiss</i>	Phenanthrene	PAH	50.0	survival and growth	6.32	7.91	Call et al. 1986
<i>Paratanytarsus species</i>	Acenaphthene	PAH	2,040	survival, growth and reproduction	411	4.96	Northwestern Aquatic Sciences, 1982
	Acenaphthene	PAH	2,040	survival and growth	227	8.97	Northwestern Aquatic Sciences, 1982; Thursby, 1991
<i>Pimephales promelas</i>	Acenaphthene	PAH	608	growth	405	1.50	Cairns and Nebeker, 1982; Thursby 1991
	Acenaphthene	PAH	608	growth	419	1.45	Cairns and Nebeker, 1982
	Naphthalene	PAH	7,900	survival and growth	620	12.7	DeGraeve et al. 1982
	Fluoranthene	PAH	69.0	survival and growth	15.0	4.60	Spehar et al. 1999
	Methyltertbutylether	ALI	980,000	not specified	289,400	3.39	Mancini et al. 2002
<i>Brachionus calyciflorus</i>	Xylene	MAH	248,500		40,300	6.17	Snell and Moffat, 1992
<i>Ceriodaphnia dubia</i>	Toluene	MAH	3,750		2,780	1.35	Niederlehner et al. 1998
	Ethylbenzene	MAH	3,200		1,680	1.90	Niederlehner et al. 1998
<i>Selenastrum capricornutum</i>	Benzene	MAH	100,000	biomass growth	8,300	12	Mayer et al. 2001
	Cyclohexane	ALI	9,317	biomass growth	952	9.8	Exxon Biomedical Sciences, 1998
	Methyltertbutylether	ALI	491,000	biomass growth	103,000	4.8	European Commission, 2000
	Pentane	ALI	10,700	biomass growth	2,040	5.2	Exxon Biomedical Sciences, 1997
<i>Skeletonema costatum</i>	Ethylbenzene	MAH	7,700		4,500	1.7	Boeri, R. 1987
<i>Onchorhynchus gorbuscha</i>	Naphthalene	PAH	1,200	growth	380	3.2	Moles and Rice, 1983
Geometric mean						3.8	
MAH: Monoaromatic hydrocarbon							
PAH: Polycyclic aromatic hydrocarbon							
ALI: Aliphatic hydrocarbon							

Table 4. Comparison of target lipid model chronic endpoints to NOECs, LOECs, OECs (sub-lethal effects) from early life stage tests for single PAH exposures

Species	Chemical	Experiment Type	Measurement Type	Effects	Observed Concentration	TLM Chronic Endpoint (µg/L)	HC5 (µg/L)	HC95 (µg/L)	Ranking ¹	Reference
<i>Oryzias Latipes</i> (Japanese medaka)	Toluene	Static	Measured	8 d - deformation of eyes embryonic malformation heart abnormality	LOEC = 41 mg/L; NOEC = 16 mg/L	12 mg/L	0.29 mg/L	530 mg/L	2	Stoss and Haines, 1979
	dibenzothiophene	Static renewal	Nominal	18-d-Hatching success; time to hatch; BSD symptoms; % normal	LOEC = 200 µg/L; NOEC = 100 µg/L	240	5.3	10300	1	Rhodes et al. 2005
	4,6- dimethyldibenzothiophene	Static renewal	Nominal	No effects observed at water solubility of 53 µg/L		32	0.71	1440	1	Rhodes et al. 2005
	benzo(a)anthracene	Static renewal	Nominal	No effects observed at water solubility of 11 µg/L		14	0.31	650	1	Rhodes et al. 2005
	Retene	PCD (partition controlled delivery)- constant	Measured	17 day EC50 for BSD	10 µg/L	4.6	0.10	210	4	Kiparissis et al. 2003
	7,12- dimethylbenz(a)anthracene	Static renewal	Nominal	18 d - time to hatch	LOEC = 12.5 µg/L; NOEC = 0 µg/L	2.8	0.06	130	1	Rhodes et al. 2005
<i>Oncorhynchus mykiss</i> (Rainbow trout)	Naphthalene	Flow-through	Measured	27 day LC50; note that grossly deformed larvae counted as dead	120 µg/L	880	170	4500	4	Black et al. 1983
	Phenanthrene	Flow-through	Measured	27 day LC50; (based on mortality and tetragonogenesis)	40 µg/L	70	10.4	470	4	Black et al. 1983
	Phenanthrene	Not specified	Nominal	hatch (12 d)- 44% mortality and 100% abnormal; swim up (22 d) - 100% craniofacial abnormalities; 9% yolk sac edema; 100% abnormal	500 µg/L	70	10.4	470	1	Hawkins et al. 2002
	Retene	Flow through,	Measured	PREVALENCE (49 days) 85% BSD; 59% haemorrhaging; 25% yolk sac edema; < 5% mortality	9 µg/L	2.4	0.44	13	4	Brinkworth et al. 2003 (fig. 3a)

Table 4. Comparison of target lipid model chronic endpoints to NOECs, LOECs, OECs (sub-lethal effects) from early life stage tests for single PAH exposures (Continued)

Species	Chemical	Experiment Type	Measurement Type	Effects	Observed Concentration	TLM Chronic Endpoint (µg/L)	HC5 (µg/L)	HC95 (µg/L)	Ranking ¹	Reference
	Benzo(a)pyrene	Static renewal	Measured	36d - hatching duration; abnormalities	LOEC = 0.37 µg/L (hatch); LOEC = 0.21 µg/L	1.9	0.36	11	3	Hannah et al. 1982; Hose et al. 1984
<i>Menidia beryllina</i> (Inland silverside)	Naphthalene	Static	Nominal	2 to 4 cell stage - cardiovascular effects	LOEC = 3200 µg/L; NOEC = 1800 µg/L	3900	240	62000	1	Middaugh et al. 1988
				2 to 4 cell stage - LOEC for craniofacial and skeletal effects	LOEC = 5600 µg/L; NOEC = 3200 µg/L					
<i>Pimephales promelas</i> (fathead minnow)	Benzo(a)pyrene	Static renewal	Nominal	heritable reductions in larvae survival- LOEC	1 µg/L	3.6	0.83	16	1	White et al. 1999
<i>Brachydanio rerio</i> (Zebra danio)	Benzo(k)fluoranthene	Flow through	Measured	42 days - growth	LOEC = 0.56 µg/L; NOEC = 0.23 µg/L	3.8	0.47	30	4	Hoofman and Ruiter, 1992a
				42 days - deformities and haemorrhages	LOEC = 1.0 µg/L					

¹ The higher the ranking, the more criteria the data set met

- 1= Nominal values
- 2= Static test, measured values
- 3= Static renewal, measured values
- 4= Flow-through, measured values

Table 5. Observed sediment acute LC50 values for PAHs and TLM predictions

Species	Habitat	Chemical	Method ^a	Duration (days)	Observed LC50 (mg/kg dry)	TOC (mg/kg)	Observed LC50 (mg/g _{DOC})	TLM Predicted LC50 (mg/g _{DOC})	TLM Predicted LC50 (mg/kg)	Reference
<i>Rhepoxynius abronius</i>	saltwater	fluoranthene	S,M	10	3.4	1800	1890	4920	8.9	Swartz et al. 1990
		fluoranthene	S,M	10	6.5	3100	2100	4920	15.3	Swartz et al. 1990
		fluoranthene	S,M	10	10.7	4800	2230	4920	23.6	Swartz et al. 1990
		fluoranthene	S,M	10	65.0	28000	2320	4920	137.8	Swartz et al. 1997
		fluoranthene	S,M	10	92.7	28000	3310	4920	137.8	Swartz et al. 1997
		fluoranthene	S,M	10	15.0	3400	4410	4920	16.7	DeWitt et al. 1992
		fluoranthene	S,M	10	12.3	4000	3080	4920	19.7	DeWitt et al. 1992
		fluoranthene	S,M	10	9.8	3100	3150	4920	15.3	DeWitt et al. 1992
		fluoranthene	S,M	10	7.0	3100	2260	4920	15.3	DeWitt et al. 1992
		fluoranthene	S,M	13	16.0	2150	7400	4920	10.6	Cole et al. 2000
		fluoranthene	S,M	13	31.8	6000	5300	4920	29.5	Cole et al. 2000
		acenaphthene	S,M	10	59.1	28000	2110	3260	91.3	Swartz et al. 1997
		acenaphthene	S,M	10	64.7	28000	2310	3260	91.3	Swartz et al. 1997
		phenanthrene	S,M	10	89.3	29000	3080	4060	117.7	Swartz et al. 1997
		phenanthrene	S,M	10	64.4	29000	2220	4060	117.7	Swartz et al. 1997
		pyrene	S,M	10	35.4	29000	1220	4890	141.8	Swartz et al. 1997
		pyrene	S,M	10	81.5	29000	2810	4890	141.8	Swartz et al. 1997
		2,6-dimethylnaphthalene	S,M	10	202.3	25800	7840	3440	88.8	Boese et al. 1998
		2,3,6-trimethylnaphthalene	S,M	10	81.3	25800	3150	3870	99.8	Boese et al. 1998
		1-methylfluorene	S,M	10	49.3	25800	1910	4010	103.5	Boese et al. 1998
2-methylphenanthrene	S,M	10	56.5	25800	2190	4600	118.7	Boese et al. 1998		
9-methylanthracene	S,M	10	177.0	25800	6860	4580	118.2	Boese et al. 1998		
naphthalene	S,M	10	771.4	25800	29,900	2530	65.3	Boese et al. 1998		
<i>Eohaustorius estuarius</i>	saltwater	acenaphthene	FT,M	10	53.3	12300	4330	4320	53.1	Swartz, 1991
		acenaphthene	FT,M	10	47.8	24900	1920	4320	107.6	Swartz, 1991
		acenaphthene	FT,M	10	68.6	42100	1630	4320	181.9	Swartz, 1991
		phenanthrene	FT,M	10	41.3	10200	4050	5390	55.0	Swartz, 1991
		phenanthrene	FT,M	10	96.8	24,700	3920	5390	133.1	Swartz, 1991
		phenanthrene	FT,M	10	127.2	33,300	3820	5390	179.5	Swartz, 1991
<i>Leptocheirus plumulosus</i>	saltwater	acenaphthene	FT,M	10	194.8	25200	7730	4490	113.1	Swartz, 1991
		acenaphthene	FT,M	10	409.9	36,600	11200	4490	164.3	Swartz, 1991
		phenanthrene	FT,M	10	160.7	19,600	8200	5610	110.0	Swartz, 1991
		phenanthrene	FT,M	10	162.3	25,000	6490	5610	140.3	Swartz, 1991
		phenanthrene	FT,M	10	295.2	36,000	8200	5610	202.0	Swartz, 1991
		fluoranthene	FT,M	10	> 403	19000	>21200	6790	129.0	Kane Driscoll et al. 1998
<i>Hyalella azteca</i>	freshwater	fluoranthene	SR,M	16	718.0	8000	58900	5140	41.1	Kane Driscoll and Landrum, 1997
<i>Schizopera knabeni</i>	saltwater	fluoranthene	S,M	10	213.0	15000	14200	16950	254.3	Lotufo, 1998
<i>Schizopera knabeni (nauplii)</i>	saltwater	phenanthrene	S,M	10	84.0	15000	5600	13980	209.7	Fleeger and Lotufo, 1999; Lotufo, 1997
<i>Schizopera knabeni (adult)</i>	saltwater	phenanthrene	S,M	10	347.0	15000	23100	13980	209.7	Fleeger and Lotufo, 1999; Lotufo, 1997
<i>Coullana sp.</i>	saltwater	fluoranthene	S,M	10	132.0	15000	8700	5540	83.1	Lotufo, 1998

^aS= static; R = renewal; FT= flow-through; M = measured

Table 6. Summary of sediment data sets for acute toxicity from PAH mixtures

Contaminant Source	PAH Measurement	Number of Samples	Species	Endpoint	Reference
Laboratory prepared mixtures	4 Parent	7	<i>Rhepoxynius abronius</i>	10 day mortality	Swartz et al. 1997
PAH contaminated sediment (Halifax Harbor, Nova Scotia)	13 Parent PAHs	11	<i>Rhepoxynius abronius</i>	10 day mortality	Tay et al. 1992
PAH contaminated sediment (Curtis Creek, Virginia)	13 Parent PAHs	6	<i>Leptocheirus plumulosus</i> <i>Eohaustorius estuarius</i>	10 day mortality	DeWitt et al. 1992
PAH contaminated sediment (Eagle Harbor, Washington)	13 Parent PAHs	10	<i>Rhepoxynius abronius</i>	10 day mortality	Tetrattech, 1986
PAH contaminated sediment (San Diego Bay, California)	13 Parent PAHs	54	<i>Rhepoxynius abronius</i>	10 day mortality	Swartz et al. unpublished data
PAH contaminated sediment (Eagle Harbor, Washington)	13 Parent PAHs	8	<i>Rhepoxynius abronius</i>	10 day mortality	Swartz et al. 1989
PAH contaminated sediment (Elliott Bay, Washington)	40 PAHs (parent and alkylated)	30	<i>Rhepoxynius abronius</i> <i>Leptocheirus plumulosus</i>	10 day mortality	Ozretich et al. 2000
Laboratory prepared mixtures	2 to 6 PAHs	12	<i>Rhepoxynius abronius</i>	10 day mortality	Boese et al. 1999
PAH contaminated sediment (Asphalt) (Estonia)	11 Parent PAHs	8	<i>Chironomus riparius</i>	10 day mortality and growth	Huuskonen et al. 1998
Dilutions of Spiked Diesel fuel	20 PAHs (parent and alkylated)	4	<i>Schizopera knabeni</i>	4 day mortality	Fleeger and Lotufo, 1999
PAH contaminated sediment (Exxon Valdez Crude Oil Spill)	39 PAHs (parent and alkylated)	470	<i>Rhepoxynius abronius</i>	10 day mortality	Page et al. 2002
PAH contaminated sediment (North Cape Oil Spill)	33 PAHs (parent and alkylated)	12	<i>Ampelisca abdita</i>	4 day mortality	Ho et al. 1999

Table 7. Example demonstrating benefit of using adjustment factor to convert TU from 13PAH to Total PAH TU. Data are from Swartz et al. unpublished (Table D5).

STATIONS	Mortality (%)	No Adjustment factor for unmeasured PAHs				Total PAH TU	Toxic based on Total PAH TU	Correct prediction? ¹	Was Criterion Protective? ²
		13 PAH TU	Toxic based on 13 PAH TU	Correct prediction? ¹	Was Criterion Protective? ²				
STA 15-1	15.0	0.058	no	yes	0.159	no	yes		
STA 15-2	25.0	0.060	no	yes	0.164	no	yes		
STA 15-3	15.0	0.074	no	yes	0.202	no	yes		
STA 15-4	5.0	0.050	no	yes	0.137	no	yes		
STA 27-1	40.0	0.159	no	yes	0.437	yes	no		
STA 27-2	85.0	0.203	no	no	0.559	yes	yes	yes	
STA 27-3	80.0	0.201	no	no	0.553	yes	yes	yes	
STA 27-4	35.0	0.250	no	yes	0.689	yes	no		
STA 27-5	50.0	0.179	no	no	0.491	yes	yes	yes	
STA 28-1	100.0	0.103	no	no	0.283	no	no	no	
STA 28-2	95.0	0.151	no	no	0.417	yes	yes	yes	
STA 28-3	100.0	0.089	no	no	0.244	no	no	no	
STA 28-4	100.0	0.123	no	no	0.337	no	no	no	
STA 28-5	100.0	0.092	no	no	0.253	no	no	no	
STA 28-6	90.0	0.150	no	no	0.414	yes	yes	yes	
STA 28X-1	15.0	0.084	no	yes	0.232	no	yes		
STA 28X-2	20.0	0.083	no	yes	0.227	no	yes		
STA 28X-3	35.0	0.111	no	yes	0.304	no	yes		
STA 28X-4	25.0	0.099	no	yes	0.273	no	yes		
STA 28X-5	25.0	0.100	no	yes	0.276	no	yes		
STA 33-1	0.0	0.007	no	yes	0.020	no	yes		
STA 33-2	5.0	0.006	no	yes	0.017	no	yes		
STA 33-3	10.0	0.005	no	yes	0.014	no	yes		
STA 33-4	5.0	0.006	no	yes	0.016	no	yes		
STA 33-5	30.0	0.021	no	yes	0.057	no	yes		
STA 40-1	10.0	0.014	no	yes	0.038	no	yes		
STA 40-2	0.0	0.012	no	yes	0.033	no	yes		
STA 40-3	15.0	0.016	no	yes	0.044	no	yes		
STA 40-4	15.0	0.012	no	yes	0.033	no	yes		
STA 40-5	15.0	0.016	no	yes	0.044	no	yes		
STA 13-1	10.0	0.076	no	yes	0.209	no	yes		
STA 13-2	20.0	0.173	no	yes	0.476	yes	no		
STA 13-4	0.0	0.098	no	yes	0.270	no	yes		
STA 13-5	5.0	0.090	no	yes	0.247	no	yes		
STA 13-6	5.0	0.244	no	yes	0.672	yes	no		
STA 11-1	10.0	0.023	no	yes	0.065	no	yes		
STA 11-2	10.0	0.021	no	yes	0.058	no	yes		
STA 11-3	15.0	0.020	no	yes	0.055	no	yes		
STA 11-4	0.0	0.016	no	yes	0.044	no	yes		
STA 11-5	25.0	0.018	no	yes	0.049	no	yes		

Table 7. Example demonstrating benefit of using adjustment factor to convert TU from 13PAH to Total PAH TU. Data are from Swartz et al. unpublished (Table D5) (Continued)

STATIONS	Observed Mortality	No Adjustment factor for unmeasured PAHs				Total PAH TU	Toxic based on Total PAH TU	Correct prediction? ¹	Was Criterion Protective? ²
		13 PAH TU	Toxic based on 13 PAH TU	Correct prediction? ¹	Was Criterion Protective? ²				
STA 11-6	15.0	0.021	no	yes	0.057	no	yes		
STA 44-1	0.0	0.053	no	yes	0.145	no	yes		
STA 44-2	0.0	0.046	no	yes	0.128	no	yes		
STA 44-3	10.0	0.061	no	yes	0.167	no	yes		
STA 44-4	0.0	0.040	no	yes	0.110	no	yes		
STA 44-5	0.0	0.045	no	yes	0.125	no	yes		
STA 44-6	5.0	0.051	no	yes	0.141	no	yes		
YAQ BAY	0.0	0.001	no	yes	0.004	no	yes		
STA28 0%	14.0	0.031	no	yes	0.086	no	yes		
STA28 13%	32.0	0.070	no	yes	0.194	no	yes		
STA28 22%	61.0	0.101	no	no	0.279	no	no	no	
STA28 36%	81.0	0.149	no	no	0.410	yes	yes	yes	
STA28 60%	93.0	0.268	no	no	0.738	yes	yes	yes	
STA28 100%	98.0	0.608	yes	yes	1.672	yes	yes	yes	
Number of overall correction predictions:				42			45		
Number of incidences criterion was not protective					1			8	

¹ A correction prediction is where the observed mortality was greater than 50% and the computed TU was greater than 0.4.

² yes = greater than 50% mortality observed and greater than 0.4 TU computed
no = greater than 50% mortality observed and less than 0.4 TU computed

Table 8. Chronic effects from single PAH sediment exposures

Species	Chemical	Method ^a	Effect	Observed Effect (mg/goc)	TLM Predicted chronic (mg/g oc)	Reference
<i>Schizopera knabeni</i>	fluoranthene	S,M	10-d LOEC (grazing)	1200	4310	Lotufo, 1998
			10-d NOEC (grazing)	330		
			10-d LOEC (offspring prod.)	3133		
			10-d NOEC (offspring prod.)	1200		
<i>Schizopera knabeni</i>	fluoranthene	S,M	14-d IC25 realized reproduction	1230	3560	Fleeger and Lotufo, 1999; Lotufo, 1997
	phenanthrene	S,M	14-d IC25 realized reproduction	1730		
	phenanthrene	S,M	10-d LOEC (hatching success)	3000		
	phenanthrene	S,M	10-d NOEC (hatching success)	1470		
<i>Coullana sp.</i>	fluoranthene	S,M	10-d LOEC (grazing)	3133	1410	Lotufo, 1998
			10-d NOEC (grazing)	1200		
			10-d LOEC (offspring prod.)	8800		
			10-d NOEC (offspring prod.)	3133		

^a S = static; M = measured

Table 9. Summary of CTLBBs for different chemical classes

Class of Compounds	Chemical class correction		(C _L [*]) (μmol/goctanol)
	Δc_{ℓ}^a	$10^{\Delta c_{\ell}}$	
Baseline	0		123
Halogenated	-0.339	0.458	56.1
Monoaromatic hydrocarbon (MAH)	-0.109	0.778	95.3
Halogenated MAH	-0.448	0.356	43.7
Polycyclic aromatic hydrocarbon (PAH)	-0.352	0.445	54.5
Halogenated PAH	-0.701	0.199	24.4

^asee Appendix A

Table 10. Chronic HC5 values for MAHs and PAHs for aqueous and sediment toxicity

Chemical	log K _{ow}	Aqueous		Sediment	
		HC5 (µmol/L)	HC5 (µg/L)	HC5 (mmol/kgoc)	HC5 (mg/kgoc)
benzene	1.943	33.399	2609	2.72	212
toluene	2.438	11.460	1056	2.86	263
o-xylene	2.946	3.821	406	3.01	319
ethylbenzene	3.006	3.356	356	3.03	321
m-xylene	3.032	3.172	337	3.03	322
p-xylene	3.051	3.045	323	3.04	323
naphthalene	3.256	1.117	143	1.77	227
acenaphthylene	3.436	0.756	115	1.81	275
C3-benzenes	3.455	1.270	152	3.17	380
1-methylnaphthalene	3.781	0.358	51.0	1.87	266
C1-naphthalenes	3.788	0.353	50.2	1.87	266
2-methylnaphthalene	3.789	0.352	50.1	1.87	266
acenaphthene	3.878	0.291	44.8	1.89	291
fluorene	3.93	0.260	43.1	1.90	315
biphenyl	3.936	0.448	69.2	3.32	512
2-chloronaphthalene	3.94	0.116	18.9	0.87	141
1-chloronaphthalene	3.95	0.114	18.5	0.87	142
C2-naphthalenes	4.244	0.132	20.5	1.95	305
1,3-dimethylnaphthalene	4.257	0.128	20.0	1.96	306
methylbiphenyl	4.259	0.223	37.5	3.43	576
2,6-dimethylnaphthalene	4.27	0.124	19.4	1.96	306
1,2-dimethylnaphthalene	4.27	0.124	19.4	1.96	306
dibenzothiophene	4.34	0.107	19.7	1.97	364
1-methylfluorene	4.37	0.100	18.0	1.98	357
C1-fluorenes	4.37	0.100	18.0	1.98	357
anthracene	4.546	0.068	12.2	2.01	359
2,3,5-trimethylnaphthalene	4.57	0.065	11.0	2.02	343
2,3,6-trimethylnaphthalene	4.57	0.065	11.0	2.02	343
phenanthrene	4.584	0.063	11.2	2.02	360
dimethylbiphenyl	4.692	0.087	15.9	3.57	650
C3-naphthalenes	4.73	0.046	7.81	2.05	349
C2-fluorenes	4.819	0.038	7.35	2.07	401
C1-Dibenzothiophene	4.859	0.035	6.88	2.07	411
9-methylanthracene	4.996	0.026	4.96	2.10	404
1-methylphenanthrene	5.036	0.024	4.54	2.11	406
C1-phenanthrene/anthracene	5.037	0.024	4.53	2.11	406
2-methylphenanthrene	5.04	0.023	4.50	2.11	406

Table 10. Chronic HC5 values for MAHs and PAHs for aqueous and sediment toxicity (Continued)

Chemical	log K _{ow}	Aqueous		Sediment	
		HC5 (µmol/L)	HC5 (µg/L)	HC5 (mmol/kgoc)	HC5 (mg/kgoc)
pyrene	5.126	0.019	3.93	2.13	430
fluoranthene	5.19	0.017	3.42	2.14	433
C4-naphthalenes	5.22	0.016	2.92	2.15	396
C1-fluoranthene/pyrene	5.257	0.015	3.17	2.15	466
C3-fluorenes	5.318	0.013	2.67	2.17	451
C2-Dibenzothiophene	5.332	0.012	2.64	2.17	461
3,6-dimethylphenanthrene	5.34	0.012	2.52	2.17	448
4,6-dimethyldibenzothiophene	5.45	0.010	2.04	2.19	466
C2-phenanthrene/anthracene	5.455	0.010	1.97	2.20	453
C2-fluoranthene/pyrene	5.557	0.008	1.76	2.22	510
Triphenylene	5.63	0.007	1.49	2.23	509
benzo(a)anthracene	5.744	0.005	1.16	2.26	515
chrysene	5.782	0.005	1.07	2.26	517
C3-Dibenzothiophene	5.81	0.004	0.998	2.27	514
C3-phenanthrene/anthracene	5.907	0.004	0.787	2.29	505
Retene	6.12	0.002	0.527	2.34	547
indeno(1,2,3-cd)pyrene	6.158	0.002	0.573	2.34	648
C1-Chyrsenes/benzo(a)anthracene	6.19	0.002	0.468	2.35	570
C4-phenanthrene/anthracene	6.357	0.001	0.315	2.39	559
benzo(b)fluoranthene	6.341	0.001	0.351	2.38	602
C3-fluoranthene/pyrene	6.384	0.001	0.310	2.39	585
benzo(k)fluoranthene	6.4	0.001	0.309	2.40	605
benzo(a)pyrene	6.409	0.001	0.303	2.40	605
7,12-dimethylbenzo(a)anthracene	6.42	0.001	0.301	2.40	616
Benzo(e)pyrene	6.447	0.001	0.279	2.41	607
perylene	6.447	0.001	0.279	2.41	607
C2-Chyrsenes/benzo(a)anthracene	6.593	0.001	0.207	2.44	625
C4-fluoranthene/pyrene	6.687	0.001	0.170	2.46	636
C5-phenanthrene/antracene	6.7	0.001	0.159	2.46	612
C1-benzofluoranthene	6.743	0.001	0.155	2.47	658
benzo(ghi)perylene	6.886	0.000	0.118	2.51	692
C3-Chyrsenes/benzo(a)anthracene	6.972	0.000	0.096	2.53	683
dibenz(a,h)anthracene	7.129	0.000	0.0700	2.56	713
C2-benzofluoranthene	7.2	0.000	0.0604	2.58	722
C4-Chyrsenes/benzo(a)anthracene	7.421	0.000	0.0379	2.63	748

Table 11. PAH NOEC toxicity data for various species (measured data considered only)

Chemical	Species	Endpoint	Endpoint (µg/L)	Reference
Naphthalene	<i>Daphnia magna</i>	21-d NOEC - Reproduction	600	European Commission, 2003
	<i>Oncorhynchus kisutch</i>	40-d NOEC - Larval growth	370	Moles et al. 1981
	<i>Pimephales promelas</i>	30-d NOEC - Larval growth	450	DeGraveve et al. 1982
Acenaphthene	<i>Paratanytarsus sp.</i>	26-d NOEC - Survival/Growth/Repro	295	Northwestern Aquatic Sciences, 1982
	<i>Paratanytarsus sp.</i>	26-d NOEC - Survival/Growth/Repro	164	Northwestern Aquatic Sciences, 1982
	<i>Pimephales promelas</i>	32-d NOEC - Growth	109	Academy of Natural Sciences, 1981
	<i>Pimephales promelas</i>	32-d NOEC - Growth	50	Academy of Natural Sciences, 1981
	<i>Pimephales promelas</i>	32-35-d - Growth	332	Cairns and Nebeker, 1982
	<i>Pimephales promelas</i>	32-35-d - Growth	345	Cairns and Nebeker, 1982
	<i>Pimephales promelas</i>	32-d NOEC - Survival	64	ERCO, 1981
	<i>Americamysis bahia</i>	35-d NOEC Survival	240	Horne et al. 1983
	<i>Americamysis bahia</i>	25-d NOEC Survival/Reproduction	44.6	Thursby et al. 1989
	<i>Cyprinodon variegatus</i>	28-d NOEC Survival	520	Ward et al. 1981
Phenanthrene	<i>Daphnia magna</i>	21-d NOEC - Reproduction	180	Hooftman and Evers-de Rooter, 1992b, c
	<i>Daphnia magna</i>	21-d NOEC - Survival	56	Hooftman and Evers-de Rooter, 1992b, c
	<i>Daphnia magna</i>	21-d NOEC - Growth	32	Hooftman and Evers-de Rooter, 1992b, c
	<i>Daphnia magna</i>	21-d NOEC - Reproduction	57	Call et al. 1986
	<i>Brachydanio rerio</i>	42-d NOEC - Growth	56	Hooftman and Evers-de Rooter, 1992b, c
	<i>Oncorhynchus mykiss</i>	90-d NOEC - Survival/Growth	5	Call et al. 1986
	<i>Americamysis bahia</i>	32-d NOEC Survival	5.5	Kuhn and Lussier, 1987
Fluoranthene	<i>Brachydanio rerio</i>	41-d NOEC - Growth	22	Hooftman and Evers-de Rooter, 1992d
	<i>Daphnia magna</i>	21-d NOEC - Growth	17	Spehar et al. 1999
	<i>Pimephales promelas</i>	32-d NOEC - Survival/Growth	10.4	Spehar et al. 1999
	<i>Americamysis bahia</i>	31-d NOEC - Survival/Reproduction	11.1	Spehar et al. 1999
Pyrene	<i>Americamysis bahia</i>	28-d NOEC Reproduction	3.82	Champlin and Poucher, 1992b
Benzo(k)fluoranthene	<i>Brachydanio rerio</i>	42-d NOEC - Growth	0.48	Hooftman and Evers-de Rooter, 1992a
Benzo(a)pyrene	<i>Brachydanio rerio</i>	42-d NOEC - Growth	6.3	Hooftman and Evers-de Rooter, 1992c

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Appendix A

Regression Coefficients for Target Lipid Model

Table A1. Revised Regression Coefficients for the Target Lipid Model

Species Scientific Name	Common Name	Environment	Habitat	N	k_e^a	$\log(C_L^*)$	SE ($\log(C_L^*)$)	(C_L^*)	SE (C_L^*) ^b
<i>Rhepoxyinus abronius</i>	Amphipod	Saltwater	Infauna	7	3.59	1.494	0.158	31.2	12.5
<i>Hyalella azteca</i>	Amphipod	Freshwater	Epibenthic	3	-	1.512		32.5	
<i>Mysidopsis bahia</i>	Mysid	Saltwater	Epibenthic	29	2.30	1.535	0.087	34.3	7.1
<i>Chlamydomonas reinhardtii</i>	Green algae	Many different	Variety	9	3.19	1.536	0.141	34.4	12.1
<i>Chironomus tentans</i>	Midge	Freshwater	Infauna	3	-	1.599		39.7	
<i>Eohaustorius estuarius</i>	Amphipod	Saltwater	Infauna	2	-	1.617		41.4	
<i>Leptocheirus plumulosus</i>	Amphipod	Saltwater	Epibenthic, Infauna	4	5.49	1.634	0.203	43.1	23.8
<i>Selenastrum capricornutum</i>	Green algae	Freshwater	Variety	24	2.41	1.687	0.091	48.6	10.5
<i>Portunus pelagicus</i>	Flower crab, sand crab	Saltwater	Epibenthic	4	5.49	1.727	0.203	53.3	29.4
<i>Ampelisca abdita</i>	Amphipod	Saltwater	Infauna	1	-	1.731		53.8	
<i>Palaemonetes pugio</i>	Grass shrimp	Saltwater	Epibenthic, Water column	10	3.06	1.758	0.127	57.3	17.9
<i>Oncorhynchus mykiss</i>	Rainbow trout	Freshwater	Infauna	47	2.13	1.820	0.067	66.1	10.4
<i>Jordanella floridae</i>	American flagfish	Saltwater	Water column	18	2.57	1.827	0.101	67.1	16.3
<i>Ictalurus punctatus</i>	Channel catfish	Freshwater	Epibenthic	7	3.59	1.864	0.149	73.1	27.4
<i>Daphnia pulex</i>	Cladoceran	Freshwater	Water column	26	2.36	1.957	0.089	90.6	19.2
<i>Cyprinodon variegatus</i>	Sheepshead minnow	Saltwater	Epibenthic, Water column	24	2.41	2.055	0.094	114	25.5
<i>Daphnia magna</i>	Cladoceran	Freshwater	Water column	117	1.93	2.062	0.050	115	13.4
<i>Pimephales promelas</i>	Fathead minnow	Freshwater	Water column	185	1.87	2.087	0.044	122	12.5
<i>Danio rerio</i>	Zebrafish	Freshwater	Water column	18	2.57	2.099	0.101	126	30.5
<i>Rana catesbian</i>	American bullfrog	Freshwater	Water column	5	4.47	2.101	0.174	126	57.1
<i>Oryzias latipes</i>	Japanese medaka	Freshwater	Water column	5	4.47	2.104	0.174	127	57.5
<i>Lepomis macrochirus</i>	Bluegill	Freshwater	Water column	70	2.04	2.117	0.059	131	18.1
<i>Orconectes immumis</i>	Crayfish	Freshwater	Epibenthic	6	3.93	2.137	0.160	137	56.0
<i>Oithona davisae</i>	Copepod	Saltwater	Epibenthic	9	3.19	2.151	0.142	142	50.2
<i>Carassius auratus</i>	Goldfish	Freshwater	Water column	43	2.16	2.180	0.067	151	23.8
<i>Leuciscus idus melanotus</i>	Golden orfe	Freshwater	Water column	27	2.34	2.183	0.078	152	28.1
<i>Xenopus laevis</i>	South african clawed frog	Freshwater	Water column	6	3.93	2.214	0.160	164	66.9
<i>Alburnus alburnus</i>	Bleak	Freshwater		7	3.59	2.234	0.147	171	63.3
<i>Nitocra spinipes</i>	Copepod	Freshwater		6	3.93	2.256	0.158	180	72.6
<i>Neanthes arenaceodentata</i>	Annelid worm	Saltwater	Infauna	4	5.49	2.260	0.202	182	99.8
<i>Tanytarsus dissimilis</i>	Midge	Freshwater	Infauna	10	3.06	2.264	0.132	184	59.9
<i>Artemia salina nauplii</i>	Brine shrimp	Saltwater		33	2.25	2.288	0.079	194	36.2
<i>Lymnaea stagnalis</i>	Snail	Freshwater		5	4.47	2.288	0.174	194	87.9
<i>Gambusia affinis</i>	Mosquito fish	Freshwater		8	3.37	2.310	0.147	204	75.4
<i>Hydra oligactis</i>	Brown hydra	Freshwater		5	4.47	2.329	0.174	213	96.6
<i>Culex pipiens</i>	House mosquito	not applicable		5	4.47	2.333	0.174	215	97.5
<i>Scenedesmus subspicatus</i>	Green algae	Freshwater		24	2.41	2.345	0.086	221	45.2
<i>Ambystoma mexicanum</i>	Mexican axolotl	Freshwater		5	4.47	2.388	0.174	244	111
<i>Daphnia cucullata</i>	Cladoceran	Freshwater	Water column	5	4.47	2.394	0.174	248	112
<i>Poecilia reticulata</i>	Guppy	Freshwater		14	2.74	2.402	0.108	252	65.8
<i>Aedes aegypti</i>	Yellow fever mosquito	not applicable		5	4.47	2.415	0.174	260	118
<i>Tetrahymena elliotii</i>	Ciliate	Freshwater		10	3.06	2.435	0.129	272	86.5
<i>Menidia beryllina</i>	Inland silverside	Saltwater	Water column	8	3.37	2.465	0.143	292	104
<i>Chlamydomonas angulosa</i>	Green algae	Freshwater		29	2.30	2.524	0.083	334	65.7
<i>Chlorella vulgaris</i>	Green algae	Freshwater		34	2.22	2.650	0.078	447	82.3
<i>Ankistrodesmus falcatus</i>	Green algae	Freshwater		9	3.19	2.699	0.139	500	173

Table A1. Revised Regression Coefficients for the Target Lipid Model (Continued)

Species Scientific Name	Common Name	Environment	Habitat	N	k_z^a	$\log(C_L^*)$	SE ($\log(C_L^*)$)	(C_L^*)	SE (C_L^*) ^b
Chemical Class corrections									
Aliphatic correction						0.000			
Alcohol correction						0.000			
Ketone correction						0.000			
Ether correction						0.000			
halogenated chemical correction						-0.339	0.032	0.458	0.034
PAHs correction						-0.352	0.053	0.445	0.055
Monoaromatic hydrocarbon correction						-0.109	0.034	0.778	0.061
slope						-0.936	0.015		

^a extrapolation constants for use in HC5/HC95 calculations (Aldenberg and Slob, 1993)

^b Standard errors are based on assumption that the estimation errors are gaussian. See Di Toro et al. 2000 for formulas.

Appendix B

Summary of Water Column and Sediment Literature Reviewed

Table B1. Summary of Water Column Literature reviewed

Reference	Acute Data	Chronic Data	Accepted	Not Accepted	Exposure Concentrations above Solubility	Exposure Concentrations Vary over Time	Exposure Concentrations report as something other than mass/vol
Abernethy et al. 1986	x		x				
Academy of Natural Sciences, 1981	x		x	x			
Al-Yakoob et al. 1996	x	x		x			
Anderson et al. 1974a	x		x ³	x			
Anderson et al. 1974b	x			x ²			
Anderson et al. 1977		x	x ¹				
Atienzar et al. 1999	x			x	x		
Barata et al. 2005	x		x				
Barron et al. 1999	x			x			
Basu et al. 2001		x					
Boxall and Maltby, 1997	x			x			x
Battelle Ocean Sciences, 1987	x ¹		x				
Brand et al. 2001		x		x			
Billiard et al. 1999		x		x	x		
Billiard et al. 2002		x		x			
Birge et al., 1982	x			x	x		
Birtwell et al. 1999		x		x			
Black et al. 1983		x	x				
Bobra et al. 1983	x			x			
Boeri, R. 1987	x	x	x				
Boese et al. 1997	x ¹		x				
Brinkworth et al. 2003		x	x				
Brodersen, 1987	x			x			
Brooke, 1994	x		x				
Buccafusco et al. 1981	x		x				
Cairns and Nebeker, 1982	x	x	x				
Caldwell et al. 1977	x	x		x			
Call et al. 1986	x ¹	x	x				
Carls et al. 1999		x	x			x	
Champlin and Poucher, 1992a	x ¹		x				
Champlin and Poucher, 1992b		x ¹	x				
Crider et al. 1982	x		x				
Darville and Wilhm, 1984	x		x				
DeGraeve et al. 1980	x		x				
DeGraeve et al. 1982	x	x	x				
Djomo et al. 2004	x	x		x ⁷	x		
Eastman et al. 1984	x		x				
Edmisten and Bantle, 1982	x		x				
Edsall, 1991	x		x				
EG&G Bionomics, 1982	x		x				
Emery and Dillon, 1996		x		x ⁸			
European Commission, 2000	x	x	x				

Table B1. Summary of Water Column Literature reviewed

Reference	Mixture Concentrations reported as Total PAHs/TPH/Total Oil or Incomplete Analysis	A Critical Target Lipid Body Burden (CTLBB) is not available	Toxicity reported as %WSF or %Effluent	Endpoint was CYP1A induction
Abernethy et al. 1986				
Academy of Natural Sciences, 1981				
Al-Yakoob et al. 1996	x			
Anderson et al. 1974a	x		x	
Anderson et al. 1974b			x	
Anderson et al. 1977				
Atienzar et al. 1999				
Barata et al. 2005				
Barron et al. 1999	x			
Basu et al. 2001				x
Boxall and Maltby, 1997				
Battelle Ocean Sciences, 1987				
Brand et al. 2001	x	x		
Billiard et al. 1999				
Billiard et al. 2002				x
Birge et al., 1982				
Birtwell et al. 1999	x	x		
Black et al. 1983				
Bobra et al. 1983	x		x	
Boeri, R. 1987				
Boese et al. 1997				
Brinkworth et al. 2003				
Brodersen, 1987	x	x		
Brooke, 1994				
Buccafusco et al. 1981				
Cairns and Nebeker, 1982				
Caldwell et al. 1977	x			
Call et al. 1986				
Carls et al. 1999				
Champlin and Poucher, 1992a				
Champlin and Poucher, 1992b				
Crider et al. 1982				
Darville and Wilhm, 1984				
DeGraeve et al. 1980				
DeGraeve et al. 1982				
Djomo et al. 2004				
Eastman et al. 1984				
Edmisten and Bantle, 1982				
Edsall, 1991				
EG&G Bionomics, 1982				
Emery and Dillon, 1996				
European Commission, 2000				

Table B1. Summary of Water Column Literature reviewed

Reference	Acute Data	Chronic Data	Accepted	Not Accepted	Exposure Concentrations above Solubility	Exposure Concentrations Vary over Time	Exposure Concentrations report as something other than mass/vol
Finger et al. 1985	x ¹		x				
Fink et al. 1995		x		x			
Fragoso et al. 1998		x		x			
Fragoso et al. 1999		x		x			
Geiger et al. 1985	x		x				
Gendusa, 1990	x		x				
Geiger and Buikema, 1981, 1982	x			x	x		
Goddard et al. 1987		x		x	x		
Hall and Oris, 1991		x		x ⁵			
Hannah et al. 1982		x	x				
Hargreaves et al. 1982	x			x			
Hawkins et al. 2002		x	x	x	PAH dependent		
Heintz et al. 1999		x	x			x	
Heitmuller et al. 1981	x		x				
Holcombe et al. 1983	x ¹		x				
Hooftman and Ruiter, 1992a,b,c,d		x	x				
Horne and Oblad, 1983	x ¹		x				
Horne et al. 1983	x ¹	x	x				
Hose et al. 1981		x		x	x		
Hose et al. 1982		x		x ⁴			
Hose et al. 1983		x		x			
Hose et al. 1984		x	x				
Hose and Puffer, 1984		x					
Hutchinson et al. 1980	x		x				
Incardona et al. 2004		x		x	x		
Incardona et al. 2005		x		x	x	x	
Ireland et al. 1996	x	x		x			
Kennedy, 1990	x		x				
Kiparissis et al. 2003		x	x				
Khan et al. 1994		x		x			x
Kocan et al. 1996	x	x		x			
Korn and Rice, 1981	x			x			
Korn et al. 1979	x ¹		x				
Kuhn and Lussier, 1987	x	x	x				
LeBlanc, 1980	x		x				
Lyons et al. 2002		x		x			
Maclean and Doe, 1989	x		x				
Marine Bioassay Lab, 1981	x		x				
Martinez-Jeronimo et al. 2005	x	x		x			
Marty et al. 1997		x		x		x	
Mattson et al. 1976	x		x				
Mayer et al. 2001	x	x	x				

Table B1. Summary of Water Column Literature reviewed

Reference	Mixture Concentrations reported as Total PAHs/TPH/Total Oil or Incomplete Analysis	A Critical Target Lipid Body Burden (CTLBB) is not available	Toxicity reported as %WSF or %Effluent	Endpoint was CYP1A induction
Finger et al. 1985				
Fink et al. 1995	x			
Fragoso et al. 1998				x
Fragoso et al. 1999				x
Geiger et al. 1985				
Gendusa, 1990				
Geiger and Buikema, 1981, 1982				
Goddard et al. 1987		x		
Hall and Oris, 1991				
Hannah et al. 1982				
Hargreaves et al. 1982		x		
Hawkins et al. 2002				
Heintz et al. 1999				
Heitmuller et al. 1981				
Holcombe et al. 1983				
Hooftman and Ruiter, 1992a,b,c,d				
Horne and Oblad, 1983				
Horne et al. 1983				
Hose et al. 1981		x		
Hose et al. 1982		x		
Hose et al. 1983		x		
Hose et al. 1984				
Hose and Puffer, 1984		x		
Hutchinson et al. 1980				
Incardona et al. 2004				
Incardona et al. 2005	x			
Ireland et al. 1996	x	x		
Kennedy, 1990				
Kiparissis et al. 2003				
Khan et al. 1994				x
Kocan et al. 1996		x		
Korn and Rice, 1981		x		
Korn et al. 1979	x			
Kuhn and Lussier, 1987				
LeBlanc, 1980				
Lyons et al. 2002		x		
Maclean and Doe, 1989				
Marine Bioassay Lab, 1981				
Martinez-Jeronimo et al. 2005	x		x	
Marty et al. 1997	x	x		
Mattson et al. 1976				
Mayer et al. 2001				

Table B1. Summary of Water Column Literature reviewed

Reference	Acute Data	Chronic Data	Accepted	Not Accepted	Exposure Concentrations above Solubility	Exposure Concentrations Vary over Time	Exposure Concentrations report as something other than mass/vol
Middaugh et al. 1988		x	x				
Middaugh et al. 2002		x		x			
Millemann et al. 1984	x		x				
Moles 1998		x	x				
Moles and Rice, 1983	x	x	x				
Moles et al. 1979	x			x			x
Moreau et al. 1999	x		x				
Neff et al. 2000	x			x			
Niederlehner et al. 1998	x	x	x				
Northwestern Aquatic Sciences, 1982	x ¹	x	x				
Oris et al. 1991	x		x				
Ort et al. 1995	x	x		x			x
Ostrander et al. 1988		x		x	x		
Ostrander et al. 1989		x		x	x		
Ostrander et al. 1990		x		x	x		
Ott et al. 1978	x			x			
Ozretich et al. 1997	x		x				
Passino and Smith, 1987	x		x				
Pelletier et al. 1997	x		x				
Pollino and Holdway, 2002				x			
Propst et al. 1997	x			x	x		
Randall and Knopp, 1980	x		x				
Riebell and Percy, 1989	x			x			
Rhodes et al. 2005		x	x				
Rice et al. 1975	x			x			
Rice and Thomas, 1989	x			x			
Rogerson et al. 1983	x		x				
Rossi and Anderson, 1976	x			x			
Rossi and Neff, 1978	x		x				
Rowe et al. 1983 ^a		x					
Rowe et al. 1983 ^b		x		x			
Sanborn and Malins, 1977	x			x			
Shelton et al. 1999	x			x			
Smith and Cameron, 1979		x		x			x
Smith et al. 1988	x		x				
Snell and Moffat, 1992	x	x	x				
Spehar et al. 1999	x ¹	x	x				
States et al. 1982	x ¹	x	x				
Steadman et al. 1991	x	x		x	x ⁶		
Stene and Lonning, 1984	x			x			
Stoss and Haines, 1979		x	x				
Struhsaker et al. 1974	x		x				
Suedel and Rogers, 1996	x		x				
Sved et al. 1997		x		x			
Swartz, 1991	x		x				

Table B1. Summary of Water Column Literature reviewed

Reference	Mixture Concentrations reported as Total PAHs/TPH/Total Oil or Incomplete Analysis	A Critical Target Lipid Body Burden (CTLBB) is not available	Toxicity reported as %WSF or %Effluent	Endpoint was CYP1A induction
Middaugh et al. 1988				
Middaugh et al. 2002	x			
Millemann et al. 1984				
Moles 1998				
Moles and Rice, 1983				
Moles et al. 1979	x	x		
Moreau et al. 1999				
Neff et al. 2000	x		x	
Niederlehner et al. 1998				
Northwestern Aquatic Sciences, 1982				
Oris et al. 1991				
Ort et al. 1995	x	x	x	
Ostrander et al. 1988		x		
Ostrander et al. 1989		x		
Ostrander et al. 1990				
Ott et al. 1978		x		
Ozretich et al. 1997				
Passino and Smith, 1987				
Pelletier et al. 1997				
Pollino and Holdway, 2002	x	x		
Propst et al. 1997				
Randall and Knopp, 1980				
Riebell and Percy, 1989	x	x		
Rhodes et al. 2005				
Rice et al. 1975	x			
Rice and Thomas, 1989		x		
Rogerson et al. 1983				
Rossi and Anderson, 1976	x			
Rossi and Neff, 1978				
Rowe et al. 1983 ^a	x		x	
Rowe et al. 1983 ^b	x		x	
Sanborn and Malins, 1977		x		
Shelton et al. 1999	x			
Smith and Cameron, 1979	x			
Smith et al. 1988				
Snell and Moffat, 1992				
Spehar et al. 1999				
States et al. 1982				
Steadman et al. 1991	x			
Stene and Lonning, 1984		x		
Stoss and Haines, 1979				
Struhsaker et al. 1974				
Suedel and Rogers, 1996				
Sved et al. 1997	x	x		
Swartz, 1991				

Table B1. Summary of Water Column Literature reviewed

Reference	Acute Data	Chronic Data	Accepted	Not Accepted	Exposure Concentrations above Solubility	Exposure Concentrations Vary over Time	Exposure Concentrations report as something other than mass/vol
Tatum et al. 1978	x		x				
Thursby et al. 1989a	x		x				
Thursby et al. 1989b	x	x	x				
Thursby, 1991	x	x	x				
Trucco et al. 1983	x		x				
U.S. EPA, 1978	x ¹	x	x				
Verrhiest et al. 2001	x		x				
Vines et al. 2000		x		x			
Ward et al. 1981	x	x	x				
White et al. 1999		x	x				
Winkler et al. 1983		x		x	x		
Woodward et al. 1981	x	x		x			

¹Not all reported data were accepted; some data were excluded due to exposure concentrations above solubility and/or lack of a CTLBB

²Concentrations of PAH in WSF determined via GC; toxicity of WSF determined based on Infared analysis ---> disagreement

³Only single exposures were accepted; mixture exposure reported as total hydrocarbons

⁴Toxic effects not observed for all organisms

⁵Observed reduced survivorship under no UV exposure conditions not significantly different than controls

⁶Exposure was to an oil-water dispersion, not a water soluble fraction. Oil droplets were present in exposure.

⁷May also be a phototoxicity issue.

⁸Contaminant exposure via food slurry

Table B1. Summary of Water Column Literature reviewed

Reference	Mixture Concentrations reported as Total PAHs/TPH/Total Oil or Incomplete Analysis	A Critical Target Lipid Body Burden (CTLBB) is not available	Toxicity reported as %WSF or %Effluent	Endpoint was CYP1A induction
Tatum et al. 1978				
Thursby et al. 1989a				
Thursby et al. 1989b				
Thursby, 1991				
Trucco et al. 1983				
U.S. EPA, 1978				
Verrhiest et al. 2001				
Vines et al. 2000	x	x		
Ward et al. 1981				
White et al. 1999				
Winkler et al. 1983		x		
Woodward et al. 1981	x	x		

Table B2. Summary of Sediment Literature reviewed

Reference	Acute Data	Chronic Data	Accepted	Not Accepted	Did not conform to EPA Guidelines for performing				
					Feeding issue	Spiked sediments not at equilibrium	Spiked sediment stored too long (greater than 120 days)	No Organic Carbon measurement	Mixture Concentrations/ Endpoints reported as Total PAHs/TPH/Total Oil/%WSF
Anderson et al. 1978				x				x	
Anderson et al. 1979	x			x				x	x
Anderson et al. 1985		x		x				x	
Ankley et al. 1994	x			x					
Bhattacharyya et al. 2003	x	x		x				x	x
Blaise et al. 2004		x		x				x	x
Boese et al. 1998	x		x						
Boese et al. 1999	x		x						
Brils et al. 2002	x			x					x
Carman et al. 1996 ⁵									
Colavecchia et al. 2004		x		x				x	x
Cole et al. 2000	x		x						
DeWitt et al. 1989	x			x				x	
DeWitt et al. 1992a	x		x						
DeWitt et al. 1992b	x		x						
Duan et al. 2000	x			x					
Emery and Dillion, 1996		x	x						
Geffard et al. 2003		x		x					x
Guadalupe Meniconi et al. 2002	x			x				x	
Harkey et al. 1997	x			x	x				
Hatch and Burton, 1999	x			x					
Huuskonen et al. 1998		x	x ¹						
Hyotylainen and Oikari, 1999	x			x ²					
Kalke et al. 1982		x		x				x	
Kane Driscoll et al. 1997	x			x	x				
Kane Driscoll and Landrum 1997	x		x						
Kane Driscoll et al. 1998	x		x						
Kiparissis et al. 2004		x		x				x	x
Kocan et al. 1996	x	x		x				x	
Kosian et al. 1999	x			x					
Kravitz et al. 1999	x			x ³				x	
Kukkonen and Landrum, 1994	x			x					
Landrum et al. 1994	x			x		x			
Landrum et al. 2002	x			x					
Lotufo, 1998	x	x	x						
Lotufo, 1997	x	x	x						
Lotufo and Fleeger, 1996	x	x		x					
Lotufo and Fleeger, 1999	x	x	x	x ⁴					
Marvin et al. 1995		x		x				x	
McCain et al. 1978		x		x		x		x	
Monson et al. 1995	x			x					
Mueller et al. 1999	x			x				x	
Naes et al. 1999		x	x						
Olajire et al. 2005	x			x					x
Ozretich et al. 2000	x		x						
Page et al. 2002									

Table B2. Summary of Sediment Literature reviewed

Reference	A Critical Target Lipid Body Burden (CTLBB) is not available	Incomplete characterization of PAH in sediments	Test aimed at UV effects, but did not have non-UV conditions	Not Constant Exposure	Other endpoint
Anderson et al. 1978					species distribution
Anderson et al. 1979	x				
Anderson et al. 1985	x	x			
Ankley et al. 1994		x			
Bhattacharyya et al. 2003		x			
Blaise et al. 2004		x			
Boese et al. 1998					
Boese et al. 1999					
Brils et al. 2002	x	x			
Carman et al. 1996 ⁵					
Colavecchia et al. 2004					
Cole et al. 2000					
DeWitt et al. 1989					
DeWitt et al. 1992a					
DeWitt et al. 1992b					
Duan et al. 2000			x		
Emery and Dillion, 1996					
Geffard et al. 2003		x			
Guadalupe Meniconi et al. 2002	x				
Harkey et al. 1997					
Hatch and Burton, 1999			x		
Huuskonen et al. 1998					
Hytöyläinen and Oikari, 1999					
Kalke et al. 1982		x			colonization
Kane Driscoll et al. 1997					
Kane Driscoll and Landrum 1997					
Kane Driscoll et al. 1998					
Kiparissis et al. 2004		x			
Kocan et al. 1996	x				
Kosian et al. 1999	x				
Kravitz et al. 1999		x			
Kukkonen and Landrum, 1994	x				
Landrum et al. 1994	x				
Landrum et al. 2002	x				
Lotufo, 1998					
Lotufo, 1997					
Lotufo and Fleeger, 1996	x				
Lotufo and Fleeger, 1999					
Marvin et al. 1995	x				
McCain et al. 1978	x	x		x	
Monson et al. 1995	x	x			
Mueller et al. 1999	x				
Naes et al. 1999					
Olajire et al. 2005	x				
Ozretich et al. 2000					
Page et al. 2002					

Table B2. Summary of Sediment Literature reviewed

Reference	Acute Data	Chronic Data	Did not conform to EPA Guidelines for performing		Feeding issue	Spiked sediments not at equilibrium	Spiked sediment stored too long (greater than 120 days)	No Organic Carbon measurement	Mixture Concentrations/ Endpoints reported as Total PAHs/TPH/Total Oil/%WSF
			Accepted	Not Accepted					
Payne et al. 1988		x		x				x	
Payne et al. 1995		x		x				x	x
Roddie et al. 1994	x			x					x
Selck et al. 2003		x		x		x			
Selck et al. 2005	x			x		x			
Suedel et al. 1993	x			x		x			
Suedel et al. 1996	x			x		x			
Swartz unpublished	x		x						
Swartz et al. 1989	x		x						
Swartz et al. 1997	x		x						
Swartz et al. 1990	x		x						
Swartz, 1991	x		x						
Tay et al. 1992	x		x						
Tetra Tech. 1986	x		x						
Verrhiest et al. 2001	x			x		x			
Weinstein et al. 2003	x			x		x			
Wilcoxon et al. 2003	x			x			x		
Wirth et al. 1998	x	x		x		x		x	

¹Not reported date were accepted; some data were excluded due to exposure concentrations above solubility and/or lack of a CTLBB

²Reported concentrations of sediment PAHs, but toxicity was determined on sediment elutriates. PAHs concentration not reported in elutriates.

³Response was avoidance behavior over 2-3 day period, which is too short for a chronic exposure.

⁴Toxicity tests with diesel fuel were not accepted because of insufficient equilibrium time and predicted water concentrations based on EqP significantly exceeded

⁵Diesel fuel data provided to help with analysis of Fleeger and Lotufo, 1999.

Table B2. Summary of Sediment Literature reviewed

Reference	A Critical Target Lipid Body Burden (CTLBB) is not available	Incomplete characterization of PAH in sediments	Test aimed at UV effects, but did not have non-UV conditions	Not Constant Exposure	Other endpoint
Payne et al. 1988	x	x			
Payne et al. 1995	x	x			
Roddie et al. 1994	x				
Selck et al. 2003	x				
Selck et al. 2005	x				
Suedel et al. 1993					
Suedel et al. 1996					
Swartz unpublished					
Swartz et al. 1989					
Swartz et al. 1997					
Swartz et al. 1990					
Swartz, 1991					
Tay et al. 1992					
Tetra Tech. 1986					
Verrhiest et al. 2001					
Weinstein et al. 2003	x				
Wilcoxon et al. 2003					
Wirth et al. 1998					

Appendix C

Summary of Water Column Data

Table C1. Observed water-only acute LC50/EC50 values for Monoaromatic Hydrocarbons and TLM predictions.

Species	Chemical	Observed LC50 (mg/L)	Predicted LC50 (mg/L)	Reference
<i>Aedes aegypti</i>	benzene	200	240	Di Toro et al. 2000
<i>Ankistrodesmus falcatus</i>	benzene	310	461	McGrath et al. 2004
<i>Artemia salina nauplii</i>	benzene	127	179	Di Toro et al. 2000
	toluene	59	73	Di Toro et al. 2000
	ethylbenzene	15	25	Di Toro et al. 2000
	o-xylene	24	28	Di Toro et al. 2000
	m-xylene	19	23	Di Toro et al. 2000
	p-xylene	24	22	Di Toro et al. 2000
	cumene	14	11	Di Toro et al. 2000
	1,2,4-trimethylbenzene	12	10	Di Toro et al. 2000
	1,3,5-trimethylbenzene	14	9	Di Toro et al. 2000
	biphenyl	4.0	4.8	Di Toro et al. 2000
	<i>Lepomis macrochirus</i>	benzene	22	121
benzene		19	121	Di Toro et al. 2000
toluene		13	49	Di Toro et al. 2000
toluene		24	49	Di Toro et al. 2000
toluene		14	49	Di Toro et al. 2000
toluene		19	49	Di Toro et al. 2000
toluene		24	49	Di Toro et al. 2000
styrene		20	28	Di Toro et al. 2000
styrene		25	28	Di Toro et al. 2000
ethylbenzene		32	17	Di Toro et al. 2000
ethylbenzene		27	17	Di Toro et al. 2000
ethylbenzene		32	17	Di Toro et al. 2000
o-xylene		16	19	Di Toro et al. 2000
<i>Chlamydomonas angulosa</i>	benzene	461	308	McGrath et al. 2004
	toluene	134	125	McGrath et al. 2004
	ethylbenzene	51	42	McGrath et al. 2004
	p-xylene	46	38	McGrath et al. 2004
	isopropylbenzene	8.8	27	McGrath et al. 2004
	o-ethyltoluene	19	20	McGrath et al. 2004
	propylbenzene	18	14	McGrath et al. 2004
	biphenyl	1.3	8.3	McGrath et al. 2004
	isobutylbenzene	3.1	6.5	McGrath et al. 2004
	n-butylbenzene	3.5	4.8	McGrath et al. 2004
	<i>Chlorella vulgaris</i>	benzene	312	412
toluene		207	167	McGrath et al. 2004
ethylbenzene		63	57	McGrath et al. 2004
p-xylene		105	51	McGrath et al. 2004
isopropylbenzene		21	36	McGrath et al. 2004
o-ethyltoluene		41	27	McGrath et al. 2004
p-ethyltoluene		48	21	McGrath et al. 2004
propylbenzene		16	19	McGrath et al. 2004
biphenyl		3.9	11.1	McGrath et al. 2004
isobutylbenzene		3.5	8.7	McGrath et al. 2004
n-butylbenzene		3.1	6.5	McGrath et al. 2004
<i>Culex pipiens</i>	benzene	71	199	Di Toro et al. 2000
<i>Cyprinodon variegatus</i>	toluene	13.0	43	Di Toro et al. 2000
	styrene	9.1	24	Di Toro et al. 2000

Table C1. Observed water-only acute LC50/EC50 values for Monoaromatic Hydrocarbons and TLM predictions (Continued)

Species	Chemical	Observed	Predicted	Reference
		LC50 (mg/L)	LC50 (mg/L)	
<i>Danio rerio</i>	Methylbenzene	26.0	47	Sloff et al. 1979
	Xylene	20	15	Sloff et al. 1979
<i>Daphnia cucullata</i>	benzene	374	229	Di Toro et al. 2000
<i>Daphnia magna</i>	benzene	31	106	Di Toro et al. 2000
	benzene	200	106	Di Toro et al. 2000
	benzene	401	106	Di Toro et al. 2000
	benzene	356	106	Di Toro et al. 2000
	benzene	515	106	Di Toro et al. 2000
	benzene	412	106	Di Toro et al. 2000
	benzene	250	106	Di Toro et al. 2000
	toluene	12	43	Di Toro et al. 2000
	toluene	60	43	Di Toro et al. 2000
	styrene	59	24	Di Toro et al. 2000
	styrene	27	24	Di Toro et al. 2000
	ethylbenzene	2.1	15	Di Toro et al. 2000
	ethylbenzene	75	15	Di Toro et al. 2000
	ethylbenzene	77	15	Di Toro et al. 2000
	o-xylene	3.2	17	Di Toro et al. 2000
	m-xylene	9.5	14	Di Toro et al. 2000
	p-xylene	8.4	13	Di Toro et al. 2000
	cumene	0.60	6.6	Di Toro et al. 2000
	1,2,4-trimethylbenzene	3.6	6.2	Di Toro et al. 2000
	1,3,5-trimethylbenzene	6.0	5.6	Di Toro et al. 2000
1,2,4,5-tetramethylbenzene	0.5	2.9	Di Toro et al. 2000	
<i>Daphnia pulex</i>	benzene	305	84	Di Toro et al. 2000
<i>Tetrahymena ellioti</i>	benzene	391	251	Di Toro et al. 2000
	toluene	143	102	Di Toro et al. 2000
	o-xylene	18	39	Di Toro et al. 2000
	m-xylene	56	33	Di Toro et al. 2000
	p-xylene	17	31	Di Toro et al. 2000
	cumene	3.0	15.5	Di Toro et al. 2000
	1,2,4-trimethylbenzene	11	15	Di Toro et al. 2000
	n-propylbenzene	18	12	Di Toro et al. 2000
<i>Pimephales promelas</i>	benzene	17.6	113	Di Toro et al. 2000
	benzene	33.0	113	Di Toro et al. 2000
	benzene	84.1	113	Di Toro et al. 2000
	benzene	35.1	113	Di Toro et al. 2000
	benzene	30.2	113	Di Toro et al. 2000
	toluene	44	46	Di Toro et al. 2000
	toluene	38	46	Di Toro et al. 2000
	toluene	46	46	Di Toro et al. 2000
	toluene	37	46	Di Toro et al. 2000
	styrene	4.0	26	Di Toro et al. 2000
	styrene	54	26	Di Toro et al. 2000
	styrene	46	26	Di Toro et al. 2000
	ethylbenzene	11	16	Di Toro et al. 2000
	ethylbenzene	45	16	Di Toro et al. 2000
ethylbenzene	49	16	Di Toro et al. 2000	
ethylbenzene	38	16	Di Toro et al. 2000	

Table C1. Observed water-only acute LC50/EC50 values for Monoaromatic Hydrocarbons and TLM predictions (Continued)

Species	Chemical	Observed LC50 (mg/L)	Predicted LC50 (mg/L)	Reference
	o-xylene	16	18	Di Toro et al. 2000
	o-xylene	35	18	Di Toro et al. 2000
	o-xylene	16	18	Di Toro et al. 2000
	m-xylene	16	15	Di Toro et al. 2000
	p-xylene	6.5	14	Di Toro et al. 2000
	p-xylene	8.8	14	Di Toro et al. 2000
	cumene	6.3	6.9	Di Toro et al. 2000
	1,2,4-trimethylbenzene	7.8	6.6	Di Toro et al. 2000
	1,3-diethylbenzene	4.1	2.2	Di Toro et al. 2000
	amylbenzene	1.7	0.6	Di Toro et al. 2000
<i>Carassius auratus</i>	benzene	39	140	Di Toro et al. 2000
	benzene	29.2	140	Di Toro et al. 2000
	benzene	34.4	140	Di Toro et al. 2000
	toluene	47	57	Di Toro et al. 2000
	toluene	47	57	Di Toro et al. 2000
	toluene	34	57	Di Toro et al. 2000
	toluene	23	57	Di Toro et al. 2000
	toluene	58	57	Di Toro et al. 2000
	toluene	28	57	Di Toro et al. 2000
	styrene	21	32	Di Toro et al. 2000
	styrene	52	32	Di Toro et al. 2000
	styrene	65	32	Di Toro et al. 2000
	ethylbenzene	74	19	Di Toro et al. 2000
	ethylbenzene	94	19	Di Toro et al. 2000
	o-xylene	10	22	Di Toro et al. 2000
	m-xylene	12	18	Di Toro et al. 2000
	p-xylene	14	17	Di Toro et al. 2000
<i>Palaemonetes pugio</i>	benzene	27.0	53	Di Toro et al. 2000
	toluene	9.5	21	Di Toro et al. 2000
<i>Poecilia reticulata</i>	benzene	420	233	Di Toro et al. 2000
	benzene	37	233	Di Toro et al. 2000
	toluene	61	95	Di Toro et al. 2000
	toluene	59	95	Di Toro et al. 2000
	styrene	75	53	Di Toro et al. 2000
	ethylbenzene	97	32	Di Toro et al. 2000
<i>Hydra oligactis</i>	benzene	34	197	Di Toro et al. 2000
<i>Xenopus laevis</i>	benzene	190	151	Di Toro et al. 2000
<i>Lymnaea stagnalis</i>	benzene	231	179	Di Toro et al. 2000
<i>Ambystoma mexicanum</i>	benzene	370	225	Di Toro et al. 2000
<i>Gambusia affinis</i>	benzene	386	188	Di Toro et al. 2000
<i>Mysidopsis bahia</i>	toluene	56	13	Di Toro et al. 2000
<i>Leucisus idus melanotus</i>	benzene	28.3	141	Di Toro et al. 2000
<i>Oryzias latipes</i>	benzene	20.0	117	Di Toro et al. 2000
	toluene	54.0	48	Di Toro et al. 2000
<i>Scenedemus subspicatus</i>	toluene	125	83	McGrath et al. 2004
<i>Selenastrum capricornutum</i>	benzene	100	45	McGrath et al. 2004
	benzene	41.1	45	McGrath et al. 2004
	benzene	29.0	45	McGrath et al. 2004
	toluene	9.4	18	McGrath et al. 2004

Table C1. Observed water-only acute LC50/EC50 values for Monoaromatic Hydrocarbons and TLM predictions (Continued)

Species	Chemical	Observed LC50 (mg/L)	Predicted LC50 (mg/L)	Reference
	toluene	13	18	McGrath et al. 2004
	styrene	0.72	10	McGrath et al. 2004
	ethylbenzene	4.8	6.2	McGrath et al. 2004
	ethylbenzene	3.6	6.2	McGrath et al. 2004
	ethylbenzene	4.6	6.2	McGrath et al. 2004
	o-xylene	4.2	7.0	McGrath et al. 2004
	o-xylene	4.7	7.0	McGrath et al. 2004
	m-xylene	3.9	5.8	McGrath et al. 2004
	m-xylene	4.9	5.8	McGrath et al. 2004
	p-xylene	4.4	5.6	McGrath et al. 2004
	p-xylene	3.2	5.6	McGrath et al. 2004
	isopropylbenzene	2.6	3.9	McGrath et al. 2004
	n-propylbenzene	1.8	2.1	McGrath et al. 2004
<i>Oncorhynchus mykiss</i>	benzene	21.6	61	Di Toro et al. 2000
	benzene	5.3	61	Di Toro et al. 2000
	benzene	56	61	Di Toro et al. 2000
	o-xylene	8.1	10	Di Toro et al. 2000

Table C2. Measured concentrations and computed toxic units for 100% WSF of Neat and Weathered EVCO (ENSR, 2001)

<u>TLM Predictions and Uncertainties for <i>Pimephales promelas</i></u>									
PAH	96 Hr LC50 (µg/L)	Acute HC5 (µg/L)	Acute HC95 (µg/L)	Acute HC5/ 96 Hr LC50	Acute HC95/ 96 Hr LC50	Measured Neat	Measured Weathered	Toxic Units	Toxic Units
						Exxon Valdez Crude oil (µg/L)	Exxon Valdez Crude oil (µg/L)	Neat Exxon Valdez Crude Oil	Weathered Exxon Valdez Crude Oil
benzene	1.13E+05	8.97E+04	1.41E+05	0.797	1.26	11000	140	0.098	0.001
toluene	4.57E+04	3.57E+04	5.85E+04	0.782	1.28	6600	280	0.144	0.006
ethylbenzene	1.55E+04	1.18E+04	2.03E+04	0.762	1.31	320	31	0.021	0.002
m+p xylene	1.44E+04	1.10E+04	1.89E+04	0.761	1.31	1200	140	0.083	0.010
o-xylene	1.76E+04	1.35E+04	2.30E+04	0.765	1.31	440	73	0.025	0.004
biphenyl	3.03E+03	2.21E+03	4.16E+03	0.728	1.37	8.3	3.5	0.003	0.001
naphthalene	6.23E+03	4.69E+03	8.27E+03	0.753	1.33	110	20	0.018	0.003
C1-naphthalenes	2.20E+03	1.61E+03	2.99E+03	0.734	1.36	77	29	0.035	0.013
C2-naphthalenes	9.03E+02	6.47E+02	1.26E+03	0.717	1.40	32	25	0.035	0.028
C3-naphthalenes	3.45E+02	2.41E+02	4.95E+02	0.698	1.43	11	15	0.032	0.043
C4-naphthalenes	1.30E+02	8.83E+01	1.91E+02	0.679	1.47	4.200	6.100	0.032	0.047
acenaphthylene	5.02E+03	3.75E+03	6.72E+03	0.747	1.34	0.000	0.000	0.000	0.000
acenaphthene	1.96E+03	1.43E+03	2.69E+03	0.730	1.37	0.300	0.630	0.000	0.000
fluorene	1.89E+03	1.38E+03	2.59E+03	0.729	1.37	1.600	1.600	0.001	0.001
C1-fluorenes	7.94E+02	5.65E+02	1.12E+03	0.712	1.40	1.300	2.500	0.002	0.003
C2-fluorenes	3.25E+02	2.26E+02	4.68E+02	0.695	1.44	0.710	1.800	0.002	0.006
C3-fluorenes	1.19E+02	8.04E+01	1.76E+02	0.676	1.48	0.380	0.800	0.003	0.007
anthracene	5.37E+02	3.79E+02	7.62E+02	0.705	1.42	0.027	0.059	0.000	0.000
phenanthrene	4.95E+02	3.48E+02	7.04E+02	0.704	1.42	2.000	1.400	0.004	0.003
C1-phen/anthr	2.01E+02	1.38E+02	2.93E+02	0.686	1.46	1.400	1.600	0.007	0.008
C2-phen/anth	8.77E+01	5.88E+01	1.31E+02	0.670	1.49	0.660	1.000	0.008	0.011
C3-phen/anth	3.54E+01	2.31E+01	5.41E+01	0.653	1.53	0.250	0.400	0.007	0.011
C4-phen/anth	1.43E+01	9.07E+00	2.24E+01	0.636	1.57	0.150	0.250	0.011	0.018
Dibenzothiophene	8.64E+02	6.16E+02	1.21E+03	0.713	1.40	2.000	1.800	0.002	0.002
C1-Dibenzothiophene	3.05E+02	2.11E+02	4.39E+02	0.693	1.44	1.600	1.500	0.005	0.005
C2-Dibenzothiophene	1.18E+02	7.94E+01	1.74E+02	0.675	1.48	1.300	1.100	0.011	0.009
C3-Dibenzothiophene	4.48E+01	2.94E+01	6.81E+01	0.657	1.52	1.400	0.540	0.031	0.012
fluoranthene	1.52E+02	1.03E+02	2.23E+02	0.680	1.47	0.000	0.000	0.000	0.000
Pyrene	1.75E+02	1.19E+02	2.56E+02	0.683	1.46	0.019	0.054	0.000	0.000
C1-fluora/pyrene	1.41E+02	9.55E+01	2.08E+02	0.678	1.48	0.054	0.140	0.000	0.001
C2-fluora/pyrene	7.86E+01	5.24E+01	1.18E+02	0.666	1.50	0.037	0.180	0.000	0.002
C3-fluora/pyrene	1.40E+01	8.91E+00	2.21E+01	0.635	1.57	0.000	0.130	0.000	0.009
benzo(a)anthracene	4.45E+01	2.93E+01	6.74E+01	0.659	1.52	0.000	0.000	0.000	0.000
chrysene	4.80E+01	3.16E+01	7.29E+01	0.658	1.52	0.028	0.050	0.001	0.001
C1-Chrysenes	2.11E+01	1.36E+01	3.29E+01	0.642	1.56	0.017	0.043	0.001	0.002
C2-Chrysenes	9.38E+00	5.88E+00	1.49E+01	0.627	1.59	0.000	0.051	0.000	0.005
C3-Chrysenes	4.37E+00	2.68E+00	7.12E+00	0.614	1.63	0.000	0.000	0.000	0.000
C4-Chrysenes	1.75E+00	1.04E+00	2.92E+00	0.597	1.67	0.000	0.000	0.000	0.000
benzo(b)fluoranthene	8.43E+01	5.61E+01	1.27E+02	0.666	1.50	0.0007	0.0036	0.000	0.000
benzo(k)fluoranthene	1.40E+01	8.88E+00	2.20E+01	0.635	1.58	0.000	0.000	0.000	0.000
Benzo(a)pyrene	1.37E+01	8.70E+00	2.16E+01	0.634	1.58	0.000	0.000	0.000	0.000
Benzo(e)pyrene	1.26E+01	8.00E+00	2.00E+01	0.633	1.58	0.0014	0.0058	0.000	0.000
perylene	1.39E+01	8.79E+00	2.19E+01	0.633	1.58	0.000	0.000	0.000	0.000
indeno(1,2,3-cd)pyrene	2.58E+01	1.66E+01	4.01E+01	0.644	1.55	0.000	0.000	0.000	0.000
dibenz(a,h)anthracene	3.21E+00	1.95E+00	5.28E+00	0.608	1.65	0.000	0.000	0.000	0.000
benzo(ghi)perylene	5.38E+00	3.32E+00	8.72E+00	0.617	1.62	0.000	0.000	0.000	0.000
Average				0.684	1.469				
Total								0.623	0.277
Mortality Data for Dilutions of WSF									
%WSF	48-h								
	48-h Mortality Neat Oil (%)	Mortality Weathered							
59	0	0							
66	10	0							
73	10	10							
81	15	15							
90	30	25							
100	80	10							

Table C3. Measured concentrations and computed toxic units for different exposures (Barata et al. 2005)

PAH	<u>TLM Predictions and Uncertainties for <i>Oithona davisae</i></u>					<u>Exposure Concentration</u>			<u>Toxic Units</u>		
	96 Hr LC50 (µg/L)	Acute HC5 (µg/L)	Acute HC95 (µg/L)	Acute HC5/ 96 Hr LC50	Acute HC95/ 96 Hr LC50	Exposure 1:	Exposure 2:	Exposure 3:	Exposure 1:	Exposure 2:	Exposure 3:
						Nominal 0.5TU (µg/L)	Nominal 1.0TU (µg/L)	Nominal 1.5TU (µg/L)	Nominal 0.5TU	Nominal 1.0TU	Nominal 1.5TU
naphthalene	7.23E+03	2.40E+03	2.18E+04	0.332	3.01	238	462	758	0.033	0.064	0.105
1-methylnaphthalene	2.59E+03	8.42E+02	7.96E+03	0.325	3.07	89.4	167	299	0.035	0.064	0.115
1,2-dimethylnaphthalene	1.44E+03	4.63E+02	4.49E+03	0.321	3.12	32.5	57.7	82.1	0.023	0.040	0.057
phenanthrene	5.75E+02	1.80E+02	1.83E+03	0.314	3.19	21.2	39.5	60.2	0.037	0.069	0.105
1-methylphenanthrene	2.34E+02	7.18E+01	7.63E+02	0.307	3.26	45.0	80.6	117	0.192	0.344	0.498
fluorene	2.18E+03	7.03E+02	6.73E+03	0.323	3.09	71.2	144	227	0.033	0.066	0.104
dibenzothiophene	1.00E+03	3.18E+02	3.16E+03	0.317	3.15	28.3	55.0	84.6	0.028	0.055	0.084
fluoranthene	1.76E+02	5.36E+01	5.79E+02	0.304	3.29	8.39	16.8	25.5	0.048	0.095	0.145
pyrene	2.03E+02	6.19E+01	6.64E+02	0.305	3.27	8.09	14.8	21.5	0.040	0.073	0.106
Average				0.317	3.16						
Total						542	1037	1674	0.468	0.871	1.319

Mortality Data for Exposures

Exposure	Average Mortality (%)
Nominal 0.5 TU	17.9
Nominal 1.0 TU	46.4
Nominal 1.5 TU	79.1

Table C4. Measured concentrations and computed toxic units for No. 2 Fuel Oil and Coal Liquid (States et al. 1982)

PAH	TLM Predictions for <i>Daphnia magna</i> 96 Hr LC50				
	No.2 Fuel Oil 100% WSF (mg/L)	Toxic Units No.2 Fuel Oil 100% WSF	Coal Liquid 100% WSF (mg/L)	Toxic Units Coal Liquid 100% WSF	
C2-benzenes	1.48E+04	40	0.003	500	0.03
C3-benzene (cumene)	6.56E+03	70	0.011	510	0.08
indane	9.76E+03	10	0.001	670	0.07
c4-benzenes (butylbenzene)	1.67E+03	90	0.054	805	0.48
tetralin	6.86E+03	10	0.001	885	0.13
naphthalene	5.89E+03	70	0.012	2630	0.45
C1-naphthalenes	2.08E+03	100	0.048	1730	0.83
c5,6-benzenes (amylbenzene)	5.83E+02	70	0.120	2290	3.93
c2-naphthalene	8.54E+02	40	0.047	480	0.56
C3-naphthalenes	3.26E+02	20	<u>0.061</u>	585	<u>1.79</u>
Total TU:			0.358		8.35

Table C5. Data for exposure of WSF prepared from No. 2 Fuel Oil to *Cyprinodon variegatus* (Anderson et al. 1977)

PAH	Molecular		Chronic		HC5/Chronic		HC95/Chronic		No 2 Fuel Oil (mg/L)	Toxic Units in 100% WSF
	Weight (g/mol)	log K _{ow}	Endpoint (mg/L)	HC5 (µg/L)	HC95 (µg/L)	Endpoint	Endpoint			
ethane	30.00	1.730	21.362	3.27E+03	1.40E+05	0.15	6.54	0.065	0.0030	
propane	44.09	2.370	7.904	1.20E+03	5.19E+04	0.15	6.57	0.065	0.0082	
butane	58.12	2.868	3.562	5.39E+02	2.35E+04	0.15	6.60	0.065	0.0182	
isobutane	58.12	2.869	3.554	5.38E+02	2.35E+04	0.15	6.60	0.065	0.0183	
pentane	72.15	3.471	1.206	1.81E+02	8.02E+03	0.15	6.65	0.065	0.0539	
isopentane	72.15	3.335	1.616	2.43E+02	1.07E+04	0.15	6.64	0.065	0.0402	
cyclopentane	70.0	2.991	3.291	4.98E+02	2.18E+04	0.15	6.61	0.020	0.0061	
methylcyclopentane	84.0	3.571	1.131	1.70E+02	7.53E+03	0.15	6.66	0.019	0.0168	
hexane	86.0	4.053	0.410	6.12E+01	2.75E+03	0.15	6.70	0.014	0.0342	
methylcyclohexane	98.2	3.963	0.568	8.49E+01	3.80E+03	0.15	6.69	0.030	0.0528	
heptane	100.2	4.584	0.152	2.25E+01	1.03E+03	0.15	6.76	0.020	0.1315	
benzene	78.0	1.943	27.305	4.17E+03	1.79E+05	0.15	6.55	0.550	0.0201	
toluene	92.0	2.438	11.082	1.69E+03	7.29E+04	0.15	6.57	1.040	0.0938	
ethylbenzene	106.0	3.006	3.754	5.68E+02	2.48E+04	0.15	6.61	0.950	0.2531	
o-xylene	106.0	2.946	4.272	6.47E+02	2.82E+04	0.15	6.61	0.320	0.0749	
trimethylbenzenes	120.0	3.455	1.615	2.43E+02	1.07E+04	0.15	6.65	0.970	0.6007	
naphthalene	128.0	3.256	1.511	2.28E+02	1.00E+04	0.15	6.63	0.840	0.5558	
1-methylnaphthalene	142.0	3.781	0.541	8.10E+01	3.61E+03	0.15	6.68	0.340	0.6286	
2-methylnaphthalene	142.0	3.788	0.533	7.98E+01	3.56E+03	0.15	6.68	0.480	0.9010	
dimethylnaphthalene	156.0	4.244	0.219	3.26E+01	1.47E+03	0.15	6.72	0.240	1.0956	
trimethylnaphthalene	170.0	4.730	0.084	1.24E+01	5.67E+02	0.15	6.77	0.030	0.3582	
biphenyl	154.0	3.936	0.735	1.10E+02	4.92E+03	0.15	6.69	0.011	0.0150	
methylbiphenyl	168.2	4.259	0.400	5.95E+01	2.69E+03	0.15	6.72	0.014	0.0350	
dimethylbiphenyl	182.0	4.692	0.170	2.51E+01	1.15E+03	0.15	6.77	0.003	0.0176	
fluorene	166.0	3.934	0.455	6.80E+01	3.04E+03	0.15	6.69	0.009	0.0198	
methylfluorene	180.0	4.370	0.193	2.86E+01	1.30E+03	0.15	6.73	0.009	0.0467	
dimethylfluorene	194.0	4.819	0.079	1.16E+01	5.35E+02	0.15	6.79	0.002	0.0254	
dibenzothiophene	184.0	4.341	0.210	3.11E+01	1.41E+03	0.15	6.73	0.004	0.0191	
phenathrene	178.0	4.584	0.120	1.78E+01	8.12E+02	0.15	6.76	0.010	0.0833	
methylphenanthrene	192.0	5.037	0.049	7.16E+00	3.32E+02	0.15	6.81	0.007	0.1434	
dimethylphenanthrene	207.0	5.455	0.021	3.11E+00	1.47E+02	0.15	6.87	<u>0.003</u>	<u>0.1404</u>	
Average						0.15	6.68			
Total								6.325	5.51	
						% Mortality	Toxic Units	Total mg/L		
			100% WSF				5.51	6.325		
			90% WSF		100		4.96	5.69		
			70% WSF		100		3.86	4.43		
			50% WSF		100		2.76	3.16		
			30% WSF		100		1.65	1.90		
			10% WSF		4		0.55	0.63		

Table C6. Concentrations and computed toxic units for prepared mixtures (Rhodes et al. 2005)

PAH	MW (g/mol)	log K _{ow}	Medaka Chronic Endpoint (µg/L)	HC5 (µg/L)	HC95 (µg/L)	HC5/Chronic Endpoint	HC95/Chronic Endpoint
Dibenzothiophene	184.2	4.341	235	5.0	10978	0.02	46.7
phenanthrene	178.2	4.584	135	2.9	6334	0.02	47.0
benz(a)anthracene	228.3	5.744	14	0.29	691.0	0.02	48.8
3,6-dimethylphenanthrene	206.3	5.340	31	0.63	1471	0.02	48.2
4,6-dimethyldibenzothiophene	212.3	5.450	25	0.51	1199	0.02	48.3
7,12-dimethylbenz(a)anthracene	256.3	6.420	3.7	0.07	185.3	0.02	50.1

	Nominal Concentration (µg/L)	Nominal Dibenzothiophene (µg/L)	Nominal Phenanthrene (µg/L)	Nominal Benzo(a)anthracene (µg/L)	Dibenzothiophene Toxic Unit	Phenanthrene Toxic Unit	Benzo(a)anthracene Toxic Unit	Total Toxic Units
	Unmethylated (parent) mixture	0	0	0	0	0	0	0
	12.5	6.25	5.0	1.3	0.027	0.037	0.088	0.15
	25.0	12.50	10.0	2.5	0.053	0.074	0.177	0.30
	50.0	25.00	20.0	5.0	0.106	0.149	0.353	0.61
	100.0	50.00	40.0	10.0	0.213	0.297	0.706	1.22
	200.0	100.00	80.0	20.0	0.426	0.594	1.413	2.43

	Mixture Nominal Concentration	Nominal 4,6-dimethyldi-benzothiophene (µg/L)	Nominal 3,6-dimethyl-phenanthrene (µg/L)	Nominal 7,12-dimethylbenzo(a)-anthracene (µg/L)	4,6-dimethyldibenzo- thiophene Toxic Unit	3,6-dimethylphen- anthrene Toxic Unit	7,12-dimethylbenzo(a)- anthracene Toxic Unit	Total Toxic Units
	Dimethylated mixture	0	0	0	0	0	0	0
	12.5	6.25	5	1.25	0.252	0.164	0.3376	0.75
	25.0	12.5	10	2.5	0.504	0.327	0.6752	1.51
	50.0	25	20	5	1.008	0.655	1.3504	3.01
	100.0	50	40	10	2.016	1.309	2.7009	6.03
	200.0	100	80	20	4.031	2.618	5.4017	12.1

Effect Data	Total PAH (µg/L)	% Normal	% Non-hatch
	unmethylated mixture	0	95.0
12.5		74.9	15
25		92.7	25
50		100.0	2
100		86.8	20
200		49.9	70
methylated mixture	0		10
	12.5		20
	25		10
	50		50
	100		40
	200		70

At TU = 1.0, LC50 = 80 µg/L

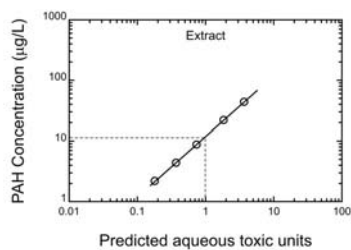
At TU = 1.0, LC50 = 15 µg/L

Table C7. Concentrations and computed toxic units for extract (Rhodes et al. 2005)

PAH	MW (g/mol)	log K_{ow}	Medaka Chronic	HC5 ($\mu\text{g/L}$)	HC95 ($\mu\text{g/L}$)	HC5/Chronic Endpoint	HC95/Chronic Endpoint	Measured Conc ($\mu\text{g/L}$)	TU in 44 $\mu\text{g/L}$	TU in 22 $\mu\text{g/L}$	TU in 8.8 $\mu\text{g/L}$	TU in 4.4 $\mu\text{g/L}$	TU in 2.2 $\mu\text{g/L}$
C2-dibenzothiophene	212.3	5.332	32.0	0.7	1539.9	0.02	48.1	30.39	0.95	0.48	0.19	0.10	0.05
phenanthrene	178.2	4.584	134.6	2.9	6334.4	0.02	47.0	0.35	0.00	0.00	0.00	0.00	0.00
C1-phenanthrene	192.26	5.037	54.7	1.1	2608.9	0.02	47.7	1.35	0.02	0.01	0.00	0.00	0.00
C2-phenanthrene	206.29	5.455	23.8	0.5	1152.5	0.02	48.3	2.37	0.10	0.05	0.02	0.01	0.00
C3-phenanthrene	220.32	5.907	9.6	0.2	472.1	0.02	49.1	2.54	0.26	0.13	0.05	0.03	0.01
C4-phenanthrene	234.34	6.357	3.9	0.1	193.6	0.02	49.9	1.15	0.30	0.15	0.06	0.03	0.01
C5-phenanthrene	248.37	6.700	2.0	0.0	99.3	0.02	50.6	1.37	0.70	0.35	0.14	0.07	0.03
fluoranthene	202.26	5.190	41.4	0.9	1983.2	0.02	47.9	0.08	0.00	0.00	0.00	0.00	0.00
pyrene	202.26	5.126	47.5	1.0	2271.8	0.02	47.8	0.07	0.00	0.00	0.00	0.00	0.00
C1-fluoranthene	216.28	5.257	38.3	0.8	1839.4	0.02	48.0	0.39	0.01	0.01	0.00	0.00	0.00
C2-fluoranthene	230.3	5.557	21.4	0.4	1036.3	0.02	48.5	0.72	0.03	0.02	0.01	0.00	0.00
C3-fluoranthene	244.32	6.384	3.8	0.1	190.6	0.02	50.0	0.67	0.18	0.09	0.04	0.02	0.01
C4-fluoranthene	258.35	6.687	2.1	0.0	106.2	0.02	50.6	0.50	0.24	0.12	0.05	0.02	0.01
chrysene	228.29	5.782	13.0	0.3	637.5	0.02	48.9	0.22	0.02	0.01	0.00	0.00	0.00
C1-chrysene	242.32	6.190	5.75	0.12	285.10	0.02	49.6	0.43	0.07	0.04	0.01	0.01	0.00
C2-chrysene	256.34	6.593	2.55	0.05	128.54	0.02	50.4	0.79	0.31	0.15	0.06	0.03	0.02
C3-chrysene	270.36	6.972	1.19	0.02	60.84	0.02	51.2	0.47	0.40	0.20	0.08	0.04	0.02
benzo(k)fluoranthene	252.32	6.400	3.80	0.08	190.32	0.02	50.0	0.07	0.02	0.01	0.00	0.00	0.00
benzo(e)pyrene	252.32	6.447	3.44	0.07	172.31	0.02	50.1	0.09	0.03	0.01	0.01	0.00	0.00
benzo(a)pyrene	252.31	6.409	3.73	0.07	186.73	0.02	50.0	0.04	0.01	0.01	0.00	0.00	0.00
C1-Benzofluoranthene	266.11	6.743	1.92	0.04	97.16	0.02	50.7	0.14	0.07	0.04	0.01	0.01	0.00
C2-Benzofluoranthene	280.13	7.200	0.75	0.01	38.94	0.02	51.7	0.08	0.11	0.05	0.02	0.01	0.01
perylene	252.31	6.447	3.44	0.07	172.30	0.02	50.1	<u>0.06</u>	<u>0.02</u>	<u>0.01</u>	<u>0.00</u>	<u>0.00</u>	<u>0.00</u>
Total								44.34	3.85	1.92	0.77	0.38	0.19

Effect Data

Total PAH ($\mu\text{g/L}$)	BSD	% Normal
2.2	0.46	83.81
4.4	0.31	85.90
8.8	0.55	86.35
22	1.70	62.34
44	2.99	48.51



At TU = 1.0, LC50 = 10 $\mu\text{g/L}$

Appendix D

Summary of Sediment Data

Table D1. PAH concentrations and effect data for exposure to *R.abronius* (10-day mortality) (Swartz et al. 1997)

Compound	log K _{ow}	MW (g/mole)	TLM Predicted	Dose 1	Dose 2	Dose 3	Dose 4	Dose 5	Dose 6	Dose 7							
			LC50 (µg/g oc)	(mg/goc)	(mg/goc)	(mg/goc)	(mg/goc)	(mg/goc)	(mg/goc)	(mg/goc)	Dose 1 TU	Dose 2 TU	Dose 3 TU	Dose 4 TU	Dose 5 TU	Dose 6 TU	Dose 7 TU
Acenaphthene	3.878	154.21	3260	1.38	0.73	0.87	0.42	0.31	0.21	0.15	0.423	0.224	0.267	0.129	0.095	0.064	0.046
Phenanthrene	4.584	178.2	4060	2.31	1.21	1.01	0.67	0.53	0.38	0.32	0.569	0.298	0.249	0.165	0.131	0.094	0.079
Fluoranthene	5.191	202.26	4920	1.56	0.98	0.72	0.55	0.42	0.32	0.25	0.317	0.199	0.146	0.112	0.085	0.065	0.051
Pyrene	5.126	202.26	4890	0.96	0.61	0.43	0.33	0.26	0.19	0.15	<u>0.196</u>	<u>0.125</u>	<u>0.088</u>	<u>0.067</u>	<u>0.053</u>	<u>0.039</u>	<u>0.031</u>
Total											1.506	0.846	0.750	0.473	0.364	0.262	0.206
	Dose	% Mort	Total PAH (mg/kg)														
	7	100	204.9														
	6	38	109.4														
	5	8	87.9														
	4	11	59.1														
	3	4	42.6														
	2	2	31.9														
	1	3	7.8														

Table D2. PAH concentrations and effect data for exposure to *R.abronius* Halifax harbor (10-day mortality) (Tay et al. 1992)

Concentrations in mg/kg dry wgt															
STATIONS	%TOC	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	Total PAH (mg/kg)
WHIDBEY 1	0.232	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0
DRAKE	1.134	0	0	0	90	70	30	110	90	50	50	70	30	60	0.7
BEDFORD	1.402	0	0	0	0	0	0	210	130	80	0	0	0	0	0.4
CENT BED 1	1.402	0	0	0	190	1100	370	1200	1100	540	640	660	330	730	6.9
CENT BED 2	1.348	0	0	0	0	0	0	2320	2530	1000	0	960	180	1280	8.3
TUFT C1	1.902	0	0	70	60	230	80	460	430	210	190	360	130	280	2.5
TUFT C2	2.384	0	0	0	0	5060	6990	4490	1960	1160	3480	970	0	1320	25.4
IMPEROYAL	1.270	0	0	0	190	0	0	1130	1450	400	0	510	0	690	4.4
E. PASS	1.188	0	0	0	460	990	410	1300	1100	530	520	1100	600	680	7.7
10% SYDNEY	0.705	65400	0	0	14600	91800	0	74600	61700	24800	4900	19300	10100	20500	387.7
WHIDBEY 2	0.232	0	0	0	0	0	0	0	0	0	0	0	0	0	0.0

Toxic Unit

STATIONS	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	13 PAH TU	Total PAH TU	% Mortality
WHIDBEY 1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00	0.0
DRAKE	0	0	0	0.00225	0.00152	0.00065	0.00197	0.00162	0.00075	0.00074	0.00089	0.00038	0.00076	0.01153	0.03	5.0
BEDFORD	0	0	0	0.00000	0.00000	0.00000	0.00304	0.00190	0.00097	0.00000	0.00000	0.00000	0.00000	0.00591	0.02	7.0
CENT BED 1	0	0	0	0.00384	0.01932	0.00653	0.01739	0.01605	0.00653	0.00771	0.00677	0.00336	0.00743	0.09494	0.26	21.0
CENT BED 2	0	0	0	0.00000	0.00000	0.00000	0.03496	0.03839	0.01257	0.00000	0.01024	0.00191	0.01355	0.11163	0.31	53.0
TUFT C1	0	0	0.0011	0.00089	0.00298	0.00104	0.00491	0.00463	0.00187	0.00169	0.00272	0.00098	0.00210	0.02494	0.07	4.0
TUFT C2	0	0	0	0.00000	0.05226	0.07249	0.03826	0.01682	0.00825	0.02465	0.00585	0.00000	0.00790	0.22648	0.62	77.0
IMPEROYAL	0	0	0	0.00424	0.00000	0.00000	0.01808	0.02336	0.00534	0.00000	0.00577	0.00000	0.00776	0.06454	0.18	56.0
E. PASS	0	0	0	0.01097	0.02053	0.00854	0.02224	0.01895	0.00757	0.00739	0.01332	0.00722	0.00817	0.12490	0.34	4.0
10% SYDNEY	3.664968914	0	0	0.58625	3.20424	0.00000	2.14864	1.78963	0.59608	0.11729	0.39347	0.20460	0.41487	13.12003	36.08	100.0
WHIDBEY 2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00	3.0

		<i>R. abronius</i> 10-d TLM Endpoint		
Code	PAH	Molecular Weight (g/mol)	log K _{ow}	(μmol/goc)
NAPH	naphthalene	128.17	3.256	19.7
ACENY	acenaphthylene	152.2	3.436	20.1
ACENEN	acenaphthene	154.21	3.878	21.1
FLUENE	fluorene	166.22	3.934	21.2
PHEN	phenanthrene	178.23	4.584	22.8
ANTH	anthracene	178.23	4.546	22.7
FLUOR	fluoranthene	202.26	5.191	24.3
PYRENE	pyrene	202.26	5.126	24.2
B(A)AN	benzo(a)anthracene	228.29	5.744	25.8
CHRY	chrysene	228.29	5.782	25.9
B(B)F	benzo(b)fluoranthene	252.31	6.341	27.6
B(K)F	benzo(k)fluoranthene	252.31	6.4	27.7
B(A)PYR	benzo(a)pyrene	252.31	6.409	27.8

Table D3. PAH concentrations and effect data for exposure to *Leptocheirus plumulosus* and *Eohaustorius estauris* (Dewitt et al. 1992)

Concentrations in ug/kg dry wgt																
Station	%DIL	TOC, %	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	Total PAH
PINK	0	1.82	28	0	0	0	77	0	104	105	85	110	93	0	58	0.7
ORANGE	6	2.386	137	94	1080	892	1952	398	3622	2419	1243	1376	570	0	599	14.4
YELLOW	12	2.657	149	0	1481	1485	2713	589	4835	3066	1126	978	569	0	454	17.4
BLUE	25	2.536	196	214	2439	2944	9219	2205	14257	9536	4273	4497	2740	1999	1745	56.3
GREEN	50	3.584	935	523	8502	10272	50049	6011	30729	22401	10847	12156	7692	5103	4938	170.2
RED	100	4.225	1175.3333	1000	21255	14067.33	71763.7	14332.67	71828	46595	23787	28490	20196	12189.3	12832	339.5

Toxic Units																			
Station	%DIL	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	13 PAH Toxic	Total PAH Toxic Units	<i>E. estauris</i>	<i>L. plumulosus</i>	
PINK	0	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.005	0.01	1	1.7
ORANGE	6	0.002	0.001	0.010	0.008	0.015	0.003	0.023	0.016	0.007	0.007	0.003	0.000	0.003	0.098	0.27	8	15.0	
YELLOW	12	0.002	0.000	0.013	0.012	0.019	0.004	0.028	0.018	0.005	0.005	0.002	0.000	0.002	0.109	0.30	5	0.0	
BLUE	25	0.002	0.002	0.022	0.025	0.067	0.016	0.086	0.058	0.022	0.023	0.012	0.008	0.007	0.351	0.96	14	21.7	
GREEN	50	0.008	0.004	0.055	0.061	0.259	0.031	0.131	0.096	0.039	0.043	0.023	0.015	0.015	0.780	2.15	16	40.0	
RED	100	0.008	0.006	0.116	0.071	0.315	0.063	0.260	0.170	0.072	0.086	0.052	0.031	0.033	1.283	3.53	100	65.0	

Code	PAH	Molecular Weight (g/mol)	log K _{ow}	<i>E. estauris</i>	<i>L. plumulosus</i>
				10-d TLM Endpoint (µmol/goc)	10-d TLM Endpoint (µmol/goc)
NAPH	naphthalene	128.17	3.256	26.2	27.2
ACENY	acenaphthylene	152.2	3.436	26.7	27.8
ACENEN	acenaphthene	154.21	3.878	28.0	29.1
FLUENE	flourene	166.22	3.934	28.2	29.3
PHEN	phenanthrene	178.23	4.584	30.3	31.5
ANTH	anthracene	178.23	4.546	30.1	31.3
FLUOR	fluoranthene	202.26	5.191	32.3	33.6
PYRENE	pyrene	202.26	5.126	32.1	33.4
B(A)AN	benzo(a)anthracene	228.29	5.744	34.3	35.7
CHRY	chrysene	228.29	5.782	34.4	35.8
B(B)F	benzo(b)fluoranthene	252.31	6.341	36.6	38.0
B(K)F	benzo(k)fluoranthene	252.31	6.4	36.8	38.3
B(A)PYR	benzo(a)pyrene	252.31	6.409	36.9	38.3

Table D4. PAH concentrations and effect data for exposure to *R.abronius* (10-day mortality) (Tetrtech, 1986)

Concentrations in mg/kg dry wgt																	
STATIONS	%TOC EST.	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	Total PAH (mg/kg)		
EH01 B1	1	31	0	26	30	140	54	140	160	46	92	34	97	0	0.9		
EH02 B1	2.4	110	0	43	57	240	110	340	380	140	260	150	220	150	2.2		
EH03 V6	0.5	130	0	38	73	240	210	270	260	150	260	130	240	140	2.1		
EH05 V1	1.8	470	110	320	590	2100	1900	5300	5300	2900	5000	1800	2400	1800	30.0		
EH06 V6	1.9	320	51	140	360	1100	1200	1300	1600	730	1400	870	1000	890	11.0		
EH08 V1	0.9	11000	240	23000	32000	58000	22000	60000	50000	12000	6000	4500	5000	4700	288.4		
EH15 V1	1.1	2400	170	980	1800	5400	13000	9800	11000	3000	4700	2100	3000	2300	59.7		
EH16 B1H002	2.4	98	21	39	72	340	180	680	760	370	640	510	590	510	4.8		
BH01 B1 H0	1.3	200	27	54	130	340	0	330	380	100	140	92	100	98	2.0		
BH02 B1	2	0	0	31	44	210	46	170	170	49	70	0	0	0	0.8		
Toxic Units																	
STATIONS		NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	13 PAH Toxic Units	Total PAH Toxic Units	% Mortality
EH01 B1		0.001	0.000	0.001	0.001	0.003	0.001	0.003	0.003	0.001	0.002	0.000	0.001	0.000	0.018	0.05	1.0
EH02 B1		0.002	0.000	0.001	0.001	0.002	0.001	0.003	0.003	0.001	0.002	0.001	0.001	0.001	0.019	0.05	8.0
EH03 V6		0.010	0.000	0.002	0.004	0.012	0.010	0.011	0.011	0.005	0.009	0.004	0.007	0.004	0.089	0.24	5.0
EH05 V1		0.010	0.002	0.005	0.009	0.029	0.026	0.060	0.060	0.027	0.047	0.014	0.019	0.014	0.324	0.89	14.0
EH06 V6		0.007	0.001	0.002	0.005	0.014	0.016	0.014	0.017	0.007	0.012	0.007	0.008	0.007	0.116	0.32	16.0
EH08 V1		0.483	0.009	0.785	1.007	1.587	0.604	1.354	1.137	0.226	0.113	0.072	0.079	0.075	7.530	20.71	100.0
EH15 V1		0.086	0.005	0.027	0.046	0.121	0.292	0.181	0.205	0.046	0.072	0.027	0.039	0.030	1.178	3.24	9.0
EH16 B1H002		0.002	0.000	0.000	0.001	0.003	0.002	0.006	0.006	0.003	0.005	0.003	0.004	0.003	0.038	0.10	10.0
BH01 B1 H0		0.006	0.001	0.001	0.003	0.006	0.000	0.005	0.006	0.001	0.002	0.001	0.001	0.001	0.035	0.10	4.0
BH02 B1		0.000	0.000	0.000	0.001	0.003	0.001	0.002	0.002	0.000	0.001	0.000	0.000	0.000	0.009	0.02	12.0
<i>R. abronius</i>																	
10-d TLM																	
Endpoint																	
Code	PAH	MW (g/mol)	log K _{ow}	(μmol/goe)													
NAPH	naphthalene	128.17	3.256	19.7													
ACENY	acenaphthylene	152.2	3.436	20.1													
ACENEN	acenaphthene	154.21	3.878	21.1													
FLUENE	fluorene	166.22	3.934	21.2													
PHEN	phenanthrene	178.23	4.584	22.8													
ANTH	anthracene	178.23	4.546	22.7													
FLUOR	fluoranthene	202.26	5.191	24.3													
PYRENE	pyrene	202.26	5.126	24.2													
B(A)AN	benzo(a)anthracene	228.29	5.744	25.8													
CHRY	chrysene	228.29	5.782	25.9													
B(B)F	benzo(b)fluoranthene	252.31	6.341	27.6													
B(K)F	benzo(k)fluoranthene	252.31	6.4	27.7													
B(A)PYR	benzo(a)pyrene	252.31	6.409	27.8													

Table D5. PAH concentrations and effect data for exposure to *R.abronius* (10-day mortality) (Swartz et al. unpublished)

Concentrations in µg/kg dry wgt															Total PAH (mg/kg)
STATIONS	%TOC	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	
STA 15-1	2.21	149	129	17	49	295	271	548	928	460	1176	1012	1012	1072	7.1
STA 15-2	2.19	125	133	18	30	209	226	510	1085	470	1152	1122	1122	1174	7.376
STA 15-3	2.09	198	169	31	39	392	296	675	1227	539	1265	1167	1167	1311	8.476
STA 15-4	2.05	133	119	23	56	0	0	460	873	406	1034	886	886	965	5.841
STA 27-1	1.71	119	291	0	0	168	424	581	4290	597	1327	2523	2523	2690	15.533
STA 27-2	1.89	0	379	20	0	277	780	1078	6255	797	2137	3340	3340	3518	21.921
STA 27-3	1.43	106	243	46	59	276	517	1586	3356	1160	1860	2308	2308	2417	16.242
STA 27-4	1.97	150	374	232	265	1326	764	3120	6913	1257	2147	3357	3357	3534	26.796
STA 27-5	1.65	0	212	68	61	464	400	1823	4709	662	1560	2131	2131	2138	16.359
STA 28-1	1.72	0	102	31	54	203	362	658	2697	360	1328	1501	1501	1215	10.012
STA 28-2	1.29	0	120	40	56	0	0	2034	2697	718	1383	1361	1361	1237	11.007
STA 28-3	2.09	0	0	0	0	0	229	302	4223	288	509	1768	1768	1629	10.716
STA 28-4	1.26	80	0	91	71	270	310	1266	2173	401	800	995	995	923	8.375
STA 28-5	2.01	76	107	0	0	131	257	534	3555	302	737	1617.5	1617.5	1510	10.444
STA 28-6	1.44	0	87	121	127	485	406	1456	3312	461	1098	1457	1457	1339	11.806
STA 28X-1	1.5	0	148	41	38	217	234	353	1234	310	835	1317	1317	1320	7.364
STA 28X-2	1.5	0	153	0	0	150	244	282	1360	331	921	1274	1274	1257	7.246
STA 28X-3	1.02	0	114	22	0	150	221	459	967	302	642	1265	1265	1260	6.667
STA 28X-4	1.33	0	140	0	40	228	354	339	920	410	1175	1350	1350	1462	7.768
STA 28X-5	1.25	0	119	0	0	133	198	508	1323	358	654	1353	1353	1398	7.397
STA 33-1	1.13	0	0	0	0	19	11	63	96	18	47	74	74	70	0.472
STA 33-2	1.02	0	0	0	0	0	0	49	99	0	41	64.5	64.5	54	0.372
STA 33-3	0.7	0	0	0	0	0	0	28	45	0	20	40	40	35	0.208
STA 33-4	1.3	0	0	0	0	0	0	61	101	0	51	79	79	69	0.440
STA 33-5	0.85	0	0	0	0	0	0	128	171	112	173	168	168	142	1.062
STA 40-1	0.66	0	16	0	0	16	25	41	67	24	55	100	100	82	0.526
STA 40-2	0.76	0	0	0	0	16	0	54	76	29	64	113	113	90	0.555
STA 40-3	0.77	0	0	0	0	23	45	62	86	37	88	135	135	120	0.731
STA 40-4	0.75	0	0	0	0	0	0	50	84	28	64	114	114	99	0.553
STA 40-5	0.87	0	0	0	0	28	39	80	116	42	83	148	148	133	0.817
STA 13-1	1.44	0	181	0	32	221	346	439	870	459	988	828	828	943	6.135
STA 13-2	1.62	612	238	0	494	949	4300	552	1170	485	1075	951	951	1124	12.901
STA 13-4	1.4	174	185	13	153	348	1406	299	898	326	694	777	777	869	6.919
STA 13-5	1.53	0	191	33	92	505	650	691	1159	435	887	870	870	985	7.368
STA 13-6	1.73	415	252	31	920	1747	8091	708	1147	764	1546	1174	1174	1214	19.183
STA 11-1	0.96	0	0	0	0	86	31	176	223	68	147	188	188	174	1.281
STA 11-2	1.2	0	0	0	0	86	0	194	244	83	155	247	247	232	1.488
STA 11-3	1.28	0	0	0	0	69	44	175	229	91	141	266	266	224	1.505
STA 11-4	1.16	0	0	0	0	46	0	128	172	56	110	204	204	184	1.104
STA 11-5	1.09	0	0	0	0	49	0	124	174	64	128	208	208	203	1.158
STA 11-6	1.34	0	0	0	0	82	34	186	260	94	181	262	262	259	1.620
STA 44-1	0.84	0	73	0	0	69	58	236	425	236	377	297	297	457	2.525
STA 44-2	0.91	0	70	0	0	62	51	241	422	234	324	281	281	431	2.397
STA 44-3	0.7	0	60	0	9	95	63	240	413	220	332	275	275	406	2.388
STA 44-4	0.78	0	0	0	0	50	46	205	316	158	273	234	234	296	1.812
STA 44-5	0.63	0	0	0	0	41	39	161	281	150	238	225	225	320	1.680
STA 44-6	0.65	0	0	0	0	54	53	197	315	163	272	274.5	274.5	358	1.961
YAQ BAY	0.65	0	0	0	5	20	0	0	9	0	0	0	0	0	0.034
STA28 0%	1.85	0	55	9	12	195	72	372	518	272	442	379	379	522	3.227
STA28 13%	1.38	0	80	13	19	126	117	537	1249	429	584	686.5	686.5	1008	5.535
STA28 22%	1.14	0	70	29	27	163	156	658	1610	424	646	861.5	861.5	1030	6.536
STA28 36%	1	36	86	36	42	205	215	817	2194	511	799	1074.5	1074.5	1239	8.329
STA28 60%	0.95	57	132	64	75	322	384	1415	3966	749	1212	1887	1887	2084	14.234
STA28 100%	0.8	100	239	109	127	559	546	2764	7576	1478	2340	3724.5	3724.5	4060	27.347

Table D5. PAH concentrations and effect data for exposure to *R.abronius* (10-day mortality) (Swartz et al. unpublished) (Continued)

Toxic Units														13 PAH	Total PAH	%Mort
STATIONS	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	Toxic	Toxic	
STA 15-1	0.003	0.002	0.000	0.001	0.003	0.003	0.005	0.009	0.004	0.009	0.007	0.007	0.007	0.058	0.16	15.0
STA 15-2	0.002	0.002	0.000	0.000	0.002	0.003	0.005	0.010	0.004	0.009	0.007	0.007	0.008	0.060	0.16	25.0
STA 15-3	0.004	0.003	0.000	0.001	0.005	0.004	0.007	0.012	0.004	0.010	0.008	0.008	0.009	0.074	0.20	15.0
STA 15-4	0.003	0.002	0.000	0.001	0.000	0.000	0.005	0.009	0.003	0.009	0.006	0.006	0.007	0.050	0.14	5.0
STA 27-1	0.003	0.006	0.000	0.000	0.002	0.006	0.007	0.051	0.006	0.013	0.021	0.021	0.022	0.159	0.44	40.0
STA 27-2	0.000	0.007	0.000	0.000	0.004	0.010	0.012	0.068	0.007	0.019	0.025	0.025	0.027	0.203	0.56	85.0
STA 27-3	0.003	0.006	0.001	0.001	0.005	0.009	0.023	0.048	0.014	0.022	0.023	0.023	0.024	0.201	0.55	80.0
STA 27-4	0.003	0.006	0.004	0.004	0.017	0.010	0.032	0.072	0.011	0.018	0.025	0.024	0.026	0.250	0.69	35.0
STA 27-5	0.000	0.004	0.001	0.001	0.007	0.006	0.022	0.058	0.007	0.016	0.019	0.018	0.018	0.179	0.49	50.0
STA 28-1	0.000	0.002	0.001	0.001	0.003	0.005	0.008	0.032	0.004	0.013	0.013	0.012	0.010	0.103	0.28	100.0
STA 28-2	0.000	0.003	0.001	0.001	0.000	0.000	0.032	0.043	0.009	0.018	0.015	0.015	0.014	0.151	0.42	95.0
STA 28-3	0.000	0.000	0.000	0.000	0.000	0.003	0.003	0.041	0.002	0.004	0.012	0.012	0.011	0.089	0.24	100.0
STA 28-4	0.003	0.000	0.002	0.002	0.005	0.006	0.020	0.035	0.005	0.011	0.011	0.011	0.010	0.123	0.34	100.0
STA 28-5	0.001	0.002	0.000	0.000	0.002	0.003	0.005	0.036	0.003	0.006	0.012	0.011	0.011	0.092	0.25	100.0
STA 28-6	0.000	0.002	0.003	0.002	0.008	0.007	0.021	0.047	0.005	0.013	0.015	0.014	0.013	0.150	0.41	90.0
STA 28X-1	0.000	0.003	0.001	0.001	0.004	0.004	0.005	0.017	0.004	0.009	0.013	0.013	0.013	0.084	0.23	15.0
STA 28X-2	0.000	0.003	0.000	0.000	0.002	0.004	0.004	0.019	0.004	0.010	0.012	0.012	0.012	0.083	0.23	20.0
STA 28X-3	0.000	0.004	0.001	0.000	0.004	0.005	0.009	0.019	0.005	0.011	0.018	0.018	0.018	0.111	0.30	35.0
STA 28X-4	0.000	0.003	0.000	0.001	0.004	0.007	0.005	0.014	0.005	0.015	0.015	0.015	0.016	0.099	0.27	25.0
STA 28X-5	0.000	0.003	0.000	0.000	0.003	0.004	0.008	0.022	0.005	0.009	0.016	0.015	0.016	0.100	0.28	25.0
STA 33-1	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.001	0.001	0.001	0.001	0.007	0.02	0.0
STA 33-2	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.001	0.001	0.001	0.001	0.006	0.02	5.0
STA 33-3	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.000	0.000	0.001	0.001	0.001	0.005	0.01	10.0
STA 33-4	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.000	0.001	0.001	0.001	0.001	0.006	0.02	5.0
STA 33-5	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.004	0.002	0.003	0.003	0.003	0.002	0.021	0.06	30.0
STA 40-1	0.000	0.001	0.000	0.000	0.001	0.001	0.001	0.002	0.001	0.001	0.002	0.002	0.002	0.014	0.04	10.0
STA 40-2	0.000	0.000	0.000	0.000	0.001	0.000	0.001	0.002	0.001	0.001	0.002	0.002	0.002	0.012	0.03	0.0
STA 40-3	0.000	0.000	0.000	0.000	0.001	0.001	0.002	0.002	0.001	0.002	0.003	0.003	0.002	0.016	0.04	15.0
STA 40-4	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.002	0.001	0.001	0.002	0.002	0.002	0.012	0.03	15.0
STA 40-5	0.000	0.000	0.000	0.000	0.001	0.001	0.002	0.003	0.001	0.002	0.002	0.002	0.002	0.016	0.04	15.0
STA 13-1	0.000	0.004	0.000	0.001	0.004	0.006	0.006	0.012	0.005	0.012	0.008	0.008	0.009	0.076	0.21	10.0
STA 13-2	0.015	0.005	0.000	0.009	0.014	0.066	0.007	0.015	0.005	0.011	0.008	0.008	0.010	0.173	0.48	20.0
STA 13-4	0.005	0.004	0.000	0.003	0.006	0.025	0.004	0.013	0.004	0.008	0.008	0.008	0.009	0.098	0.27	0.0
STA 13-5	0.000	0.004	0.001	0.002	0.008	0.011	0.009	0.015	0.005	0.010	0.008	0.008	0.009	0.090	0.25	5.0
STA 13-6	0.009	0.005	0.001	0.015	0.025	0.116	0.008	0.014	0.007	0.015	0.010	0.010	0.010	0.244	0.67	5.0
STA 11-1	0.000	0.000	0.000	0.000	0.002	0.001	0.004	0.005	0.001	0.003	0.003	0.003	0.003	0.023	0.06	10.0
STA 11-2	0.000	0.000	0.000	0.000	0.002	0.000	0.003	0.004	0.001	0.002	0.003	0.003	0.003	0.021	0.06	10.0
STA 11-3	0.000	0.000	0.000	0.000	0.001	0.001	0.003	0.004	0.001	0.002	0.003	0.003	0.002	0.020	0.06	15.0
STA 11-4	0.000	0.000	0.000	0.000	0.001	0.000	0.002	0.003	0.001	0.002	0.003	0.003	0.002	0.016	0.04	0.0
STA 11-5	0.000	0.000	0.000	0.000	0.001	0.000	0.002	0.003	0.001	0.002	0.003	0.003	0.003	0.018	0.05	25.0
STA 11-6	0.000	0.000	0.000	0.000	0.002	0.001	0.003	0.004	0.001	0.002	0.003	0.003	0.003	0.021	0.06	15.0
STA 44-1	0.000	0.003	0.000	0.000	0.002	0.002	0.006	0.010	0.005	0.008	0.005	0.005	0.008	0.053	0.15	0.0
STA 44-2	0.000	0.003	0.000	0.000	0.002	0.001	0.005	0.009	0.004	0.006	0.004	0.004	0.007	0.046	0.13	0.0
STA 44-3	0.000	0.003	0.000	0.000	0.003	0.002	0.007	0.012	0.005	0.008	0.006	0.006	0.008	0.061	0.17	10.0
STA 44-4	0.000	0.000	0.000	0.000	0.002	0.001	0.005	0.008	0.003	0.006	0.004	0.004	0.005	0.040	0.11	0.0
STA 44-5	0.000	0.000	0.000	0.000	0.002	0.002	0.005	0.009	0.004	0.006	0.005	0.005	0.007	0.045	0.12	0.0
STA 44-6	0.000	0.000	0.000	0.000	0.002	0.002	0.006	0.010	0.004	0.007	0.006	0.006	0.008	0.051	0.14	5.0
YAQ BAY	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.00	0.0
STA28 0%	0.000	0.001	0.000	0.000	0.003	0.001	0.004	0.006	0.002	0.004	0.003	0.003	0.004	0.031	0.09	14.0
STA28 13%	0.000	0.002	0.000	0.000	0.002	0.002	0.008	0.019	0.005	0.007	0.007	0.007	0.010	0.070	0.19	32.0
STA28 22%	0.000	0.002	0.001	0.001	0.004	0.003	0.012	0.029	0.006	0.010	0.011	0.011	0.013	0.101	0.28	61.0
STA28 36%	0.001	0.003	0.001	0.001	0.005	0.005	0.017	0.045	0.009	0.013	0.015	0.015	0.018	0.149	0.41	81.0
STA28 60%	0.002	0.005	0.002	0.002	0.008	0.010	0.030	0.085	0.013	0.022	0.029	0.028	0.031	0.268	0.74	93.0
STA28 100%	0.005	0.010	0.004	0.004	0.017	0.017	0.070	0.194	0.031	0.049	0.067	0.067	0.072	0.608	1.67	98.0

Table D5. PAH concentrations and effect data for exposure to *R.abronius* (10-day mortality) (Swartz et al. unpublished) (Continued)

Code	PAH	MW (g/mol)	<i>R. abronius</i> 10-d	
			log K_{ow}	TLM Endpoint ($\mu\text{mol/goc}$)
NAPH	naphthalene	128.17	3.256	19.7
ACENY	acenaphthylene	152.2	3.436	20.1
ACENEN	acenaphthene	154.21	3.878	21.1
FLUENE	flourene	166.22	3.934	21.2
PHEN	phenanthrene	178.23	4.584	22.8
ANTH	anthracene	178.23	4.546	22.7
FLUOR	fluoranthene	202.26	5.191	24.3
PYRENE	pyrene	202.26	5.126	24.2
B(A)AN	benzo(a)anthracene	228.29	5.744	25.8
CHRY	chrysene	228.29	5.782	25.9
B(B)F	benzo(b)fluoranthene	252.31	6.341	27.6
B(K)F	benzo(k)fluoranthene	252.31	6.4	27.7
B(A)PYR	benzo(a)pyrene	252.31	6.409	27.8

Table D6. PAH concentrations and effect data for exposure to *R.abronius* (10-day mortality) (Swartz et al. 1989)

Concentrations in mg/kg dry wgt															
STATIONS	%TOC EST.	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	Total PAH (mg/kg)
EH08	1.4375	460000	86000	890000	651000	412000	35000	422000	126000	67000	10000	64000	27000	34000	3284.0
1600	0.4107143	50	40	350	540	2600	210	1600	900	230	210	90	40	60	6.920
1120	0.4107143	40	40	210	330	1500	110	940	520	130	140	50	40	20	4.070
784	0.4107143	30	10	160	230	1100	70	650	380	80	90	30	0	0	2.830
549	0.4107143	50	20	160	190	770	50	520	310	70	60	20	0	0	2.220
384	0.4107143	30	20	100	120	470	30	330	220	40	30	10	0	0	1.400
269	0.4107143	20	0	60	100	460	30	270	160	40	50	10	10	0	1.210
YB	0.3214286	0	0	0	0	20	0	50	30	0	0	0	0	0	0.100

Toxic Units

STATIONS	NAPH	ACENY	ACENEN	FLUENE	PHEN	ANTH	FLUOR	PYRENE	B(A)AN	CHRY	B(B)F	B(K)F	B(A)PYR	13 TU	Tot TU	%Mort
EH08	12.649	1.953	19.016	12.827	7.056	0.602	5.964	1.793	0.790	0.117	0.640	0.268	0.338	64 ^a	176.04	100
1600	0.005	0.003	0.026	0.037	0.156	0.013	0.079	0.045	0.009	0.009	0.003	0.001	0.002	0.39	1.07	100
1120	0.004	0.003	0.016	0.023	0.090	0.007	0.046	0.026	0.005	0.006	0.002	0.001	0.001	0.23	0.63	100
784	0.003	0.001	0.012	0.016	0.066	0.004	0.032	0.019	0.003	0.004	0.001	-	-	0.16	0.44	90
549	0.005	0.002	0.012	0.013	0.046	0.003	0.026	0.015	0.003	0.002	0.001	-	-	0.13	0.35	13.3
384	0.003	0.002	0.007	0.008	0.028	0.002	0.016	0.011	0.002	0.001	0.000	-	-	0.08	0.22	5.0
269	0.002	-	0.004	0.007	0.028	0.002	0.013	0.008	0.002	0.002	0.000	0.000	-	0.07	0.19	1.7
YB	-	-	-	-	0.002	-	0.003	0.002	-	-	-	-	-	0.01	0.02	3.0

^a The high TU suggests presence of pure product

Code	PAH	MW (g/mol)	log K _{ow}	<i>R. abronius</i> 10-d TLM Endpoint (µmol/goc)
NAPH	naphthalene	128.17	3.256	19.7
ACENY	acenaphthylene	152.2	3.436	20.1
ACENEN	acenaphthene	154.21	3.878	21.1
FLUENE	fluorene	166.22	3.934	21.2
PHEN	phenanthrene	178.23	4.584	22.8
ANTH	anthracene	178.23	4.546	22.7
FLUOR	fluoranthene	202.26	5.191	24.3
PYRENE	pyrene	202.26	5.126	24.2
B(A)AN	benzo(a)anthracene	228.29	5.744	25.8
CHRY	chrysene	228.29	5.782	25.9
B(B)F	benzo(b)fluoranthene	252.31	6.341	27.6
B(K)F	benzo(k)fluoranthene	252.31	6.4	27.7
B(A)PYR	benzo(a)pyrene	252.31	6.409	27.8

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Concentrations in µg/kg dry wgt											
Station	TOC %	Nap	Acny	Acen	Flure	Phen	Anth	Flua	Pyr	B[a]a	Chry
715 00 C51A S001 IS 500 RS 1000 ppb	7.44	721	889	2960	2041	7560	7331	8644	15111	3614	6941
715 00 C51A S002 IS 500 RS 1000 ppb	5.78	6177	7017	3896	13724	18862	431	549955	407555	107415	245
715 00 C51A S003 IS 500 RS 1000 ppb	12.79	7802	10132	31679	59381	86057	953	701330	509179	208874	541
715 00 C51A S004 IS 500 RS 1000 ppb	8.18	9774	6285	2815	2086	5682	8281	19899	73882	11493	20894
715 00 C51A S005 IS 500 RS 1000 ppb	6.79	3304	4171	3082	3126	10546	15327	22493	53132	20164	31703
715 00 C51A S006 IS 500 RS 1000 ppb	3.14	1819	2903	1180	1985	10533	13945	52569	60243	32577	133
715 01 C51A S007 IS 500 RS 1000 ppb	2.15	745	2266	328	555	3116	4828	5370	16416	4320	9564
715 00 C51A S008 IS 500 RS 1000 ppb	4.35	814	2797	824	922	3415	4136	14077	27973	7558	10767
715 00 C51A S009 IS 500 RS 1000 ppb	2.76	4748	4329	929	2621	10717	55665	86448	62330	30445	117
715 00 C51A S010 IS 500 RS 1000 ppb	2.13	235	1582	252	528	2348	3644	6222	10276	5294	10278
715 00 C51A S011 IS 500 RS 1000 ppb	2.20	447	713	358	921	3963	2687	10733	17188	5285	5676
715 00 C51A S012 IS 500 RS 1000 ppb	2.94	3379	4569	773	707	3104	4444	5729	37308	3173	4313
715 00 C51A S013 IS 500 RS 1000 ppb	3.65	3565	1474	2356	1432	4323	4755	4955	23089	2177	3133
715 00 C51A S014 IS 500 RS 1000 ppb	12.35	9638	9627	5244	23816	34633	257032	1709399	1060593	384239	522
715 00 C51A S015 IS 500 RS 1000 ppb	16.05	9817	13804	243201	143711	352302	1196	1360195	816995	298865	679
715 01 C51A S016 IS 500 RS 1000 ppb	7.86	8769	8411	4529	11030	15323	42166	635581	596910	160343	333
715 00 C51A S017 IS 500 RS 1000 ppb	0.87	262	217	0	39	397	558	618	1516	395	525
715 00 C51A S018 IS 500 RS 1000 ppb	2.80	1771	724	919	729	2600	2173	3292	5828	1851	2458
715 00 C51A S019 IS 500 RS 1000 ppb	2.05	0	151	0	29	493	398	930	3727	429	857
715 00 C51A S020 IS 500 RS 1000 ppb	2.88	1854	891	1700	1496	4699	3136	5119	14572	1735	2822
715 00 C51A S021 IS 500 RS 1000 ppb	3.15	6751	2697	4792	5649	16829	17554	11071	41906	5092	8138
715 00 C51A S022 IS 500 RS 1000 ppb	1.49	0	661	78	456	1647	2237	1530	2261	1031	1824
715 00 C51A S023 IS 500 RS 1000 ppb	1.50	0	726	164	171	2257	1549	3786	5868	1495	2949
715 00 C51A S024 IS 500 RS 1000 ppb	4.02	4990	5183	4515	10883	22539	83937	226859	159451	66308	170
715 00 C51A S025 IS 500 RS 1000 ppb	5.12	4410	7873	1882	5203	11515	37094	251039	205996	122655	217
715 00 C51A S026 IS 500 RS 1000 ppb	3.98	4341	2493	2208	2157	7442	8061	10231	65876	7746	9585
715 01 C51A S027 IS 500 RS 1000 ppb	2.91	2551	2668	1268	2764	8643	9286	92661	142954	42731	123
715 00 C51A S028 IS 500 RS 1000 ppb	3.76	1423	2188	691	587	2234	3527	2931	34762	3004	5105
715 00 C51A S029 IS 500 RS 1000 ppb	2.96	1546	1647	672	692	2651	3427	3691	13584	2290	3250
715 00 C51A S030 IS 500 RS 1000 ppb	3.10	5057	1039	1881	838	3492	2316	3816	11430	1642	2832

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Concentrations in µg/kg dry wtg													
Station	B[b+]jFl	B[k]Fl	B[a]P	Ind	Dib[ah]a]	B[ghi]p	Biphen	Triphen	B[e]P	Pery	2-Menap	1-Menap	C2-Nap
715 00 C51A S001 IS 500 RS 1000 ppb	10288	3916	6000	2172	918	2068	85	720	4482	1723	315	527	1137
715 00 C51A S002 IS 500 RS 1000 ppb	53427	21707	36620	12185	4449	10016	614	8855	24598	9985	1860	1398	6463
715 00 C51A S003 IS 500 RS 1000 ppb	143769	46749	74716	24187	8715	18193	2317	14150	56140	18670	7238	1551	14514
715 00 C51A S004 IS 500 RS 1000 ppb	34648	11492	21810	7336	2752	6912	838	2254	15301	6484	2020	2589	6149
715 00 C51A S005 IS 500 RS 1000 ppb	52282	18519	28373	9751	3789	8397	321	5184	22168	7317	909	1223	3099
715 00 C51A S006 IS 500 RS 1000 ppb	42772	15290	22308	7287	2381	5947	354	4841	17716	5691	212	435	2417
715 01 C51A S007 IS 500 RS 1000 ppb	13654	4930	7940	3476	986	2727	42	1252	6354	2278	0	133	487
715 00 C51A S008 IS 500 RS 1000 ppb	13461	3494	7724	3132	339	2838	104	1359	5621	2408	148	300	1002
715 00 C51A S009 IS 500 RS 1000 ppb	22133	8247	13495	4378	1347	3483	535	2510	9073	3880	1365	416	2314
715 00 C51A S010 IS 500 RS 1000 ppb	12221	4209	6107	2682	824	2574	130	1221	5129	1705	100	100	767
715 00 C51A S011 IS 500 RS 1000 ppb	11011	4038	6071	1944	869	1823	0	754	4798	1920	0	0	847
715 00 C51A S012 IS 500 RS 1000 ppb	20096	6785	11819	4219	1356	3628	241	678	8504	3539	938	830	1971
715 00 C51A S013 IS 500 RS 1000 ppb	12221	4658	7144	2780	916	2508	363	417	5576	1761	690	1029	2279
715 00 C51A S014 IS 500 RS 1000 ppb	219056	81448	124842	39596	14940	30870	1177	29981	88214	31017	4112	1892	9341
715 00 C51A S015 IS 500 RS 1000 ppb	169266	60178	95111	29049	10624	22518	4175	23701	65388	24786	6059	3359	133109
715 01 C51A S016 IS 500 RS 1000 ppb	92634	34413	56944	17265	5968	13421	827	13521	36527	14534	2185	1874	5225
715 00 C51A S017 IS 500 RS 1000 ppb	1297	348	807	313	39	220	0	90	536	208	185	0	0
715 00 C51A S018 IS 500 RS 1000 ppb	5139	1728	3126	1499	479	1328	98	229	2387	702	162	448	1118
715 00 C51A S019 IS 500 RS 1000 ppb	1515	491	1005	482	55	351	0	73	765	368	0	0	58
715 00 C51A S020 IS 500 RS 1000 ppb	5192	1685	3147	1208	412	1135	328	446	2441	838	662	690	1985
715 00 C51A S021 IS 500 RS 1000 ppb	23122	7583	14627	5762	1640	5159	1129	831	10575	3804	3474	2478	5477
715 00 C51A S022 IS 500 RS 1000 ppb	2242	756	1354	701	176	524	0	151	1202	450	0	0	0
715 00 C51A S023 IS 500 RS 1000 ppb	4442	1521	2397	1121	380	1024	0	394	1845	754	212	0	466
715 00 C51A S024 IS 500 RS 1000 ppb	44464	15194	23695	6997	2657	5946	793	5948	17902	6609	1990	1134	6401
715 00 C51A S025 IS 500 RS 1000 ppb	92389	30862	47887	14398	5757	11561	752	11506	35637	12452	1682	1299	5482
715 00 C51A S026 IS 500 RS 1000 ppb	25542	7820	14034	4897	1698	4249	202	2304	10525	4132	1110	1066	2880
715 01 C51A S027 IS 500 RS 1000 ppb	44994	14831	23442	7110	2712	5370	180	5404	18531	6054	630	864	1985
715 00 C51A S028 IS 500 RS 1000 ppb	13001	4653	7467	2638	1005	2420	113	712	5312	2298	241	326	1082
715 00 C51A S029 IS 500 RS 1000 ppb	10044	3254	5767	2548	850	1855	86	392	4449	1445	149	381	934
715 00 C51A S030 IS 500 RS 1000 ppb	5676	2129	3412	1443	470	1091	256	242	2757	933	222	1073	1734

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Concentrations in µg/kg dry wt												
Station	C3-Nap	C4-Nap	C1-Flu	C2-Flu A	C2-Flu B	C3-Flu	C1-Phe#1	C1-Phe#2	C2-Phe	C3-Phe	C1-Py	C2-Py
715 00 C51A S001 IS 500 RS 1000 ppb	695	308	2339	381	1802	1890	7582	664	3838	818	8673	4190
715 00 C51A S002 IS 500 RS 1000 ppb	7350	11042	54024	16516	53853	22795	125663	15081	140150	30354	152453	36688
715 00 C51A S003 IS 500 RS 1000 ppb	16099	17035	72289	24207	68348	50941	196532	21955	159364	59102	252840	81026
715 00 C51A S004 IS 500 RS 1000 ppb	3547	253	1768	166	1967	2677	5213	1261	3301	2626	16238	13221
715 00 C51A S005 IS 500 RS 1000 ppb	2214	374	3920	1164	3281	3721	13660	2091	8474	5202	37787	19206
715 00 C51A S006 IS 500 RS 1000 ppb	2329	1175	3434	544	4087	4355	13644	2195	12011	8621	41421	17540
715 01 C51A S007 IS 500 RS 1000 ppb	416	189	444	0	615	766	3991	541	2532	1016	9559	4742
715 00 C51A S008 IS 500 RS 1000 ppb	0	61	565	0	708	763	4263	259	3765	654	11884	4884
715 00 C51A S009 IS 500 RS 1000 ppb	1622	1273	4691	842	6383	6810	17441	2431	15903	7373	34743	11661
715 00 C51A S010 IS 500 RS 1000 ppb	176	101	479	71	349	575	3344	243	2179	1119	8526	3900
715 00 C51A S011 IS 500 RS 1000 ppb	1091	232	1739	131	1272	695	4546	332	2766	825	7432	3664
715 00 C51A S012 IS 500 RS 1000 ppb	1377	236	1274	181	1008	1390	3228	730	2039	1383	11590	7723
715 00 C51A S013 IS 500 RS 1000 ppb	930	154	1464	298	1469	1299	3746	422	2002	628	8131	4556
715 00 C51A S014 IS 500 RS 1000 ppb	11077	22780	85215	25831	84952	61464	187022	22330	183016	146514	528269	161564
715 00 C51A S015 IS 500 RS 1000 ppb	153468	141631	223590	62469	192688	84366	589923	66708	511083	133057	394592	123762
715 01 C51A S016 IS 500 RS 1000 ppb	3816	11333	49586	17641	57274	42880	79115	21736	117772	62780	238531	80036
715 00 C51A S017 IS 500 RS 1000 ppb	0	36	0	0	0	0	0	0	156	53	769	153
715 00 C51A S018 IS 500 RS 1000 ppb	403	115	576	111	379	444	2024	357	969	468	3562	1608
715 00 C51A S019 IS 500 RS 1000 ppb	240	0	0	25	135	178	421	0	210	103	1048	302
715 00 C51A S020 IS 500 RS 1000 ppb	1051	73	1599	183	884	643	3439	459	2226	690	5441	2115
715 00 C51A S021 IS 500 RS 1000 ppb	2186	0	2672	637	698	2004	9665	85	4712	1733	15592	7226
715 00 C51A S022 IS 500 RS 1000 ppb	0	130	248	26	204	187	804	50	425	94	1403	349
715 00 C51A S023 IS 500 RS 1000 ppb	68	92	174	25	183	259	1697	155	690	370	2604	1197
715 00 C51A S024 IS 500 RS 1000 ppb	5485	4459	26123	8284	26126	17159	53817	9081	53561	15172	82824	26282
715 00 C51A S025 IS 500 RS 1000 ppb	5162	3351	17247	7213	17682	12855	40242	7049	38015	19735	133286	43154
715 00 C51A S026 IS 500 RS 1000 ppb	1301	349	2915	891	1020	4091	9104	1854	5258	2630	22009	11608
715 01 C51A S027 IS 500 RS 1000 ppb	2266	996	6351	1951	6762	4908	16073	2545	14518	10284	54572	21459
715 00 C51A S028 IS 500 RS 1000 ppb	770	70	1083	356	1412	1611	2634	663	1585	938	10210	5990
715 00 C51A S029 IS 500 RS 1000 ppb	579	198	781	99	721	636	2344	544	1367	546	5346	3538
715 00 C51A S030 IS 500 RS 1000 ppb	393	317	712	143	468	728	2500	513	1278	348	4204	2033

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Concentrations in µg/kg dry wgt							
Station	C1-Chry	C2-Chry	Dibthioph	C1-Dibthiophe	C2-Dibthio	C3-Dibthio	Total PAH (mg/kg)
715 00 C51A S001 IS 500 RS 1000 ppb	6462	2863	613	215	238	270	134
715 00 C51A S002 IS 500 RS 1000 ppb	44582	17278	2320	11356	20124	10099	2079
715 00 C51A S003 IS 500 RS 1000 ppb	98509	29185	6764	18231	23852	15393	3259
715 00 C51A S004 IS 500 RS 1000 ppb	16029	7286	549	93	66	221	358
715 00 C51A S005 IS 500 RS 1000 ppb	25689	12441	803	627	684	721	470
715 00 C51A S006 IS 500 RS 1000 ppb	23707	8370	702	673	410	914	452
715 01 C51A S007 IS 500 RS 1000 ppb	6220	3174	149	97	136	131	126
715 00 C51A S008 IS 500 RS 1000 ppb	6874	1471	208	27	202	105	152
715 00 C51A S009 IS 500 RS 1000 ppb	14619	4321	874	1096	2016	1339	467
715 00 C51A S010 IS 500 RS 1000 ppb	1091	98	117	23	24	95	101
715 00 C51A S011 IS 500 RS 1000 ppb	1048	98	408	248	140	165	109
715 00 C51A S012 IS 500 RS 1000 ppb	9125	5442	253	128	125	257	180
715 00 C51A S013 IS 500 RS 1000 ppb	5576	3048	403	119	110	160	128
715 00 C51A S014 IS 500 RS 1000 ppb	175472	61633	3620	17845	28418	18344	5997
715 00 C51A S015 IS 500 RS 1000 ppb	130889	49789	45126	63549	66983	38781	6961
715 01 C51A S016 IS 500 RS 1000 ppb	83966	34284	1643	7893	18420	14135	2722
715 00 C51A S017 IS 500 RS 1000 ppb	351	164	23	25	30	30	10
715 00 C51A S018 IS 500 RS 1000 ppb	1714	998	245	106	78	49	55
715 00 C51A S019 IS 500 RS 1000 ppb	492	149	57	44	0	0	16
715 00 C51A S020 IS 500 RS 1000 ppb	765	865	560	210	78	95	80
715 00 C51A S021 IS 500 RS 1000 ppb	11838	5364	1334	310	232	386	273
715 00 C51A S022 IS 500 RS 1000 ppb	221	139	55	33	57	74	24
715 00 C51A S023 IS 500 RS 1000 ppb	1563	332	157	0	67	0	43
715 00 C51A S024 IS 500 RS 1000 ppb	30877	10515	1891	3230	8582	4748	1113
715 00 C51A S025 IS 500 RS 1000 ppb	55154	16722	788	2720	4878	4129	1349
715 00 C51A S026 IS 500 RS 1000 ppb	15772	6923	562	222	319	745	288
715 01 C51A S027 IS 500 RS 1000 ppb	26135	8841	541	731	1523	1139	619
715 00 C51A S028 IS 500 RS 1000 ppb	7007	3905	245	85	106	365	137
715 00 C51A S029 IS 500 RS 1000 ppb	3802	1806	294	113	100	67	88
715 00 C51A S030 IS 500 RS 1000 ppb	2969	1304	406	70	16	80	74

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Toxic Units For <i>R. abronius</i>										
Station	Nap	Acny	Acen	Flure	Phen	Anth	Flua	Pyr	B[a]a	Chry
715 00 C51A S001 IS 500 RS 1000 ppb	0.004	0.004	0.012	0.008	0.025	0.024	0.024	0.042	0.008	0.016
715 00 C51A S002 IS 500 RS 1000 ppb	0.042	0.040	0.021	0.067	0.080	0.002	1.933	1.443	0.315	0.001
715 00 C51A S003 IS 500 RS 1000 ppb	0.024	0.026	0.076	0.132	0.166	0.002	1.114	0.815	0.277	0.001
715 00 C51A S004 IS 500 RS 1000 ppb	0.047	0.025	0.011	0.007	0.017	0.025	0.049	0.185	0.024	0.043
715 00 C51A S005 IS 500 RS 1000 ppb	0.019	0.020	0.014	0.013	0.038	0.056	0.067	0.160	0.050	0.079
715 00 C51A S006 IS 500 RS 1000 ppb	0.023	0.030	0.012	0.018	0.083	0.110	0.340	0.392	0.176	0.001
715 01 C51A S007 IS 500 RS 1000 ppb	0.014	0.034	0.005	0.007	0.036	0.056	0.051	0.156	0.034	0.075
715 00 C51A S008 IS 500 RS 1000 ppb	0.007	0.021	0.006	0.006	0.019	0.024	0.066	0.132	0.029	0.042
715 00 C51A S009 IS 500 RS 1000 ppb	0.068	0.051	0.010	0.027	0.096	0.499	0.637	0.462	0.187	0.001
715 00 C51A S010 IS 500 RS 1000 ppb	0.004	0.024	0.004	0.007	0.027	0.042	0.059	0.099	0.042	0.082
715 00 C51A S011 IS 500 RS 1000 ppb	0.008	0.011	0.005	0.012	0.044	0.030	0.099	0.160	0.041	0.044
715 00 C51A S012 IS 500 RS 1000 ppb	0.045	0.051	0.008	0.007	0.026	0.037	0.040	0.260	0.018	0.025
715 00 C51A S013 IS 500 RS 1000 ppb	0.039	0.013	0.020	0.011	0.029	0.032	0.028	0.129	0.010	0.014
715 00 C51A S014 IS 500 RS 1000 ppb	0.031	0.025	0.013	0.055	0.069	0.515	2.813	1.758	0.528	0.001
715 00 C51A S015 IS 500 RS 1000 ppb	0.024	0.028	0.465	0.254	0.540	0.002	1.721	1.041	0.316	0.001
715 01 C51A S016 IS 500 RS 1000 ppb	0.044	0.035	0.018	0.040	0.048	0.133	1.643	1.554	0.346	0.001
715 00 C51A S017 IS 500 RS 1000 ppb	0.012	0.008	0.000	0.001	0.011	0.016	0.014	0.036	0.008	0.010
715 00 C51A S018 IS 500 RS 1000 ppb	0.025	0.008	0.010	0.007	0.023	0.019	0.024	0.043	0.011	0.015
715 00 C51A S019 IS 500 RS 1000 ppb	0.000	0.002	0.000	0.000	0.006	0.005	0.009	0.037	0.004	0.007
715 00 C51A S020 IS 500 RS 1000 ppb	0.025	0.010	0.018	0.015	0.040	0.027	0.036	0.104	0.010	0.017
715 00 C51A S021 IS 500 RS 1000 ppb	0.085	0.028	0.047	0.051	0.131	0.138	0.071	0.272	0.027	0.044
715 00 C51A S022 IS 500 RS 1000 ppb	0.000	0.014	0.002	0.009	0.027	0.037	0.021	0.031	0.012	0.021
715 00 C51A S023 IS 500 RS 1000 ppb	0.000	0.016	0.003	0.003	0.037	0.026	0.051	0.080	0.017	0.033
715 00 C51A S024 IS 500 RS 1000 ppb	0.049	0.042	0.034	0.077	0.138	0.516	1.146	0.811	0.280	0.001
715 00 C51A S025 IS 500 RS 1000 ppb	0.034	0.050	0.011	0.029	0.055	0.179	0.995	0.822	0.406	0.001
715 00 C51A S026 IS 500 RS 1000 ppb	0.043	0.020	0.017	0.015	0.046	0.050	0.052	0.339	0.033	0.041
715 01 C51A S027 IS 500 RS 1000 ppb	0.035	0.030	0.013	0.027	0.073	0.079	0.646	1.004	0.249	0.001
715 00 C51A S028 IS 500 RS 1000 ppb	0.015	0.019	0.006	0.004	0.015	0.023	0.016	0.189	0.014	0.023
715 00 C51A S029 IS 500 RS 1000 ppb	0.021	0.018	0.007	0.007	0.022	0.029	0.025	0.094	0.013	0.019
715 00 C51A S030 IS 500 RS 1000 ppb	0.065	0.011	0.019	0.008	0.028	0.018	0.025	0.076	0.009	0.015

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Toxic Units For <i>R. abronius</i>													
Station	B[b+]jFl	B[k]Fl	B[a]P	Ind	Dib[ah]a]	B[ghi]p	Biphen	Triphen	B[e]P	Pery	2-Menap	1-Menap	C2-Nap
715 00 C51A S001 IS 500 RS 1000 ppb	0.020	0.008	0.012	0.004	0.001	0.003	0.000	0.002	0.009	0.003	0.001	0.002	0.004
715 00 C51A S002 IS 500 RS 1000 ppb	0.132	0.054	0.090	0.028	0.009	0.021	0.003	0.026	0.061	0.025	0.011	0.008	0.033
715 00 C51A S003 IS 500 RS 1000 ppb	0.161	0.052	0.083	0.025	0.008	0.018	0.006	0.019	0.062	0.021	0.019	0.004	0.033
715 00 C51A S004 IS 500 RS 1000 ppb	0.061	0.020	0.038	0.012	0.004	0.010	0.003	0.005	0.027	0.011	0.008	0.011	0.022
715 00 C51A S005 IS 500 RS 1000 ppb	0.110	0.039	0.060	0.019	0.007	0.015	0.001	0.013	0.046	0.015	0.004	0.006	0.013
715 00 C51A S006 IS 500 RS 1000 ppb	0.195	0.070	0.101	0.031	0.009	0.023	0.003	0.026	0.080	0.026	0.002	0.005	0.022
715 01 C51A S007 IS 500 RS 1000 ppb	0.091	0.033	0.053	0.022	0.005	0.016	0.001	0.010	0.042	0.015	0.000	0.002	0.007
715 00 C51A S008 IS 500 RS 1000 ppb	0.044	0.011	0.025	0.010	0.001	0.008	0.001	0.005	0.018	0.008	0.001	0.002	0.007
715 00 C51A S009 IS 500 RS 1000 ppb	0.115	0.043	0.070	0.021	0.006	0.016	0.006	0.016	0.047	0.020	0.017	0.005	0.024
715 00 C51A S010 IS 500 RS 1000 ppb	0.082	0.028	0.041	0.017	0.005	0.015	0.002	0.010	0.034	0.011	0.002	0.002	0.010
715 00 C51A S011 IS 500 RS 1000 ppb	0.072	0.026	0.039	0.012	0.005	0.010	0.000	0.006	0.031	0.012	0.000	0.000	0.011
715 00 C51A S012 IS 500 RS 1000 ppb	0.098	0.033	0.057	0.019	0.006	0.015	0.002	0.004	0.041	0.017	0.011	0.010	0.020
715 00 C51A S013 IS 500 RS 1000 ppb	0.048	0.018	0.028	0.010	0.003	0.009	0.003	0.002	0.022	0.007	0.006	0.009	0.018
715 00 C51A S014 IS 500 RS 1000 ppb	0.254	0.094	0.144	0.043	0.014	0.031	0.003	0.042	0.102	0.036	0.011	0.005	0.022
715 00 C51A S015 IS 500 RS 1000 ppb	0.151	0.054	0.085	0.024	0.008	0.017	0.008	0.025	0.058	0.022	0.013	0.007	0.242
715 01 C51A S016 IS 500 RS 1000 ppb	0.169	0.063	0.103	0.029	0.009	0.021	0.003	0.030	0.066	0.026	0.009	0.008	0.019
715 00 C51A S017 IS 500 RS 1000 ppb	0.021	0.006	0.013	0.005	0.001	0.003	0.000	0.002	0.009	0.003	0.007	0.000	0.000
715 00 C51A S018 IS 500 RS 1000 ppb	0.026	0.009	0.016	0.007	0.002	0.006	0.001	0.001	0.012	0.004	0.002	0.005	0.012
715 00 C51A S019 IS 500 RS 1000 ppb	0.011	0.003	0.007	0.003	0.000	0.002	0.000	0.001	0.005	0.003	0.000	0.000	0.001
715 00 C51A S020 IS 500 RS 1000 ppb	0.026	0.008	0.016	0.006	0.002	0.005	0.003	0.003	0.012	0.004	0.008	0.008	0.020
715 00 C51A S021 IS 500 RS 1000 ppb	0.105	0.034	0.066	0.024	0.006	0.020	0.011	0.005	0.048	0.017	0.037	0.026	0.051
715 00 C51A S022 IS 500 RS 1000 ppb	0.022	0.007	0.013	0.006	0.001	0.004	0.000	0.002	0.011	0.004	0.000	0.000	0.000
715 00 C51A S023 IS 500 RS 1000 ppb	0.042	0.015	0.023	0.010	0.003	0.008	0.000	0.005	0.018	0.007	0.005	0.000	0.009
715 00 C51A S024 IS 500 RS 1000 ppb	0.158	0.054	0.084	0.023	0.008	0.018	0.006	0.025	0.063	0.023	0.017	0.009	0.046
715 00 C51A S025 IS 500 RS 1000 ppb	0.258	0.086	0.133	0.038	0.013	0.028	0.004	0.039	0.099	0.035	0.011	0.009	0.031
715 00 C51A S026 IS 500 RS 1000 ppb	0.092	0.028	0.050	0.016	0.005	0.013	0.002	0.010	0.038	0.015	0.009	0.009	0.021
715 01 C51A S027 IS 500 RS 1000 ppb	0.221	0.073	0.115	0.033	0.011	0.023	0.002	0.032	0.090	0.030	0.007	0.010	0.020
715 00 C51A S028 IS 500 RS 1000 ppb	0.049	0.018	0.028	0.009	0.003	0.008	0.001	0.003	0.020	0.009	0.002	0.003	0.008
715 00 C51A S029 IS 500 RS 1000 ppb	0.049	0.016	0.028	0.012	0.003	0.008	0.001	0.002	0.021	0.007	0.002	0.004	0.009
715 00 C51A S030 IS 500 RS 1000 ppb	0.026	0.010	0.016	0.006	0.002	0.004	0.003	0.001	0.013	0.004	0.002	0.012	0.016

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Toxic Units For <i>R. abronius</i>												
Station	C3-Nap	C4-Nap	C1-Flu	C2-Flu A	C2-Flu B	C3-Flu	C1-Phe#1	C1-Phe#2	C2-Phe	C3-Phe	C1-Py	C2-Py
715 00 C51A S001 IS 500 RS 1000 ppb	0.002	0.001	0.008	0.001	0.005	0.005	0.022	0.002	0.010	0.002	0.021	0.009
715 00 C51A S002 IS 500 RS 1000 ppb	0.032	0.042	0.233	0.063	0.205	0.077	0.473	0.057	0.469	0.091	0.480	0.104
715 00 C51A S003 IS 500 RS 1000 ppb	0.032	0.030	0.141	0.042	0.118	0.078	0.334	0.037	0.241	0.080	0.360	0.103
715 00 C51A S004 IS 500 RS 1000 ppb	0.011	0.001	0.005	0.000	0.005	0.006	0.014	0.003	0.008	0.006	0.036	0.026
715 00 C51A S005 IS 500 RS 1000 ppb	0.008	0.001	0.014	0.004	0.011	0.011	0.044	0.007	0.024	0.013	0.101	0.046
715 00 C51A S006 IS 500 RS 1000 ppb	0.019	0.008	0.027	0.004	0.029	0.027	0.094	0.015	0.074	0.047	0.240	0.091
715 01 C51A S007 IS 500 RS 1000 ppb	0.005	0.002	0.005	0.000	0.006	0.007	0.040	0.005	0.023	0.008	0.081	0.036
715 00 C51A S008 IS 500 RS 1000 ppb	0.000	0.000	0.003	0.000	0.004	0.003	0.021	0.001	0.017	0.003	0.050	0.018
715 00 C51A S009 IS 500 RS 1000 ppb	0.015	0.010	0.042	0.007	0.051	0.048	0.137	0.019	0.112	0.046	0.229	0.069
715 00 C51A S010 IS 500 RS 1000 ppb	0.002	0.001	0.006	0.001	0.004	0.005	0.034	0.002	0.020	0.009	0.073	0.030
715 00 C51A S011 IS 500 RS 1000 ppb	0.013	0.002	0.020	0.001	0.013	0.006	0.045	0.003	0.024	0.006	0.062	0.027
715 00 C51A S012 IS 500 RS 1000 ppb	0.012	0.002	0.011	0.001	0.008	0.009	0.024	0.005	0.013	0.008	0.072	0.043
715 00 C51A S013 IS 500 RS 1000 ppb	0.006	0.001	0.010	0.002	0.009	0.007	0.022	0.003	0.011	0.003	0.041	0.020
715 00 C51A S014 IS 500 RS 1000 ppb	0.023	0.041	0.172	0.046	0.152	0.097	0.329	0.039	0.287	0.205	0.779	0.213
715 00 C51A S015 IS 500 RS 1000 ppb	0.243	0.196	0.347	0.086	0.264	0.102	0.799	0.090	0.616	0.143	0.448	0.126
715 01 C51A S016 IS 500 RS 1000 ppb	0.012	0.032	0.157	0.049	0.160	0.106	0.219	0.060	0.290	0.138	0.553	0.166
715 00 C51A S017 IS 500 RS 1000 ppb	0.000	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.003	0.001	0.016	0.003
715 00 C51A S018 IS 500 RS 1000 ppb	0.004	0.001	0.005	0.001	0.003	0.003	0.016	0.003	0.007	0.003	0.023	0.009
715 00 C51A S019 IS 500 RS 1000 ppb	0.003	0.000	0.000	0.000	0.001	0.002	0.004	0.000	0.002	0.001	0.009	0.002
715 00 C51A S020 IS 500 RS 1000 ppb	0.009	0.001	0.014	0.001	0.007	0.004	0.026	0.003	0.015	0.004	0.034	0.012
715 00 C51A S021 IS 500 RS 1000 ppb	0.018	0.000	0.021	0.004	0.005	0.012	0.067	0.001	0.029	0.009	0.090	0.037
715 00 C51A S022 IS 500 RS 1000 ppb	0.000	0.002	0.004	0.000	0.003	0.002	0.012	0.001	0.006	0.001	0.017	0.004
715 00 C51A S023 IS 500 RS 1000 ppb	0.001	0.001	0.003	0.000	0.003	0.003	0.025	0.002	0.009	0.004	0.032	0.013
715 00 C51A S024 IS 500 RS 1000 ppb	0.035	0.025	0.162	0.045	0.143	0.083	0.291	0.049	0.258	0.065	0.375	0.107
715 00 C51A S025 IS 500 RS 1000 ppb	0.026	0.015	0.084	0.031	0.076	0.049	0.171	0.030	0.144	0.066	0.474	0.137
715 00 C51A S026 IS 500 RS 1000 ppb	0.008	0.002	0.018	0.005	0.006	0.020	0.050	0.010	0.026	0.011	0.101	0.048
715 01 C51A S027 IS 500 RS 1000 ppb	0.020	0.008	0.054	0.015	0.051	0.033	0.120	0.019	0.096	0.061	0.341	0.120
715 00 C51A S028 IS 500 RS 1000 ppb	0.005	0.000	0.007	0.002	0.008	0.008	0.015	0.004	0.008	0.004	0.049	0.026
715 00 C51A S029 IS 500 RS 1000 ppb	0.005	0.001	0.007	0.001	0.005	0.004	0.017	0.004	0.009	0.003	0.033	0.019
715 00 C51A S030 IS 500 RS 1000 ppb	0.003	0.002	0.006	0.001	0.003	0.005	0.018	0.004	0.008	0.002	0.025	0.011

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000).

Toxic Units For <i>R. abronius</i>										
Station	C1-Chry	C2-Chry	Dibthioph	C1-Dibthiophe	C2-Dibthio	C3-Dibthio	R. abronius Total PAH Toxic Units	L. plumulosus Total PAH Toxic Units	R. abronius Mortality (%)	L. plumulosus Mortality (%)
715 00 C51A S001 IS 500 RS 1000 ppb	0.013	0.005	0.002	0.001	0.001	0.001	0.347	0.252	5	10
715 00 C51A S002 IS 500 RS 1000 ppb	0.117	0.041	0.010	0.042	0.066	0.030	7.078	5.127	100	100
715 00 C51A S003 IS 500 RS 1000 ppb	0.117	0.031	0.013	0.031	0.036	0.020	4.987	3.613	100	100
715 00 C51A S004 IS 500 RS 1000 ppb	0.030	0.012	0.002	0.000	0.000	0.000	0.832	0.603	0	65
715 00 C51A S005 IS 500 RS 1000 ppb	0.058	0.025	0.003	0.002	0.002	0.002	1.242	0.900	5	30
715 00 C51A S006 IS 500 RS 1000 ppb	0.115	0.037	0.005	0.005	0.002	0.005	2.623	1.900	25	60
715 01 C51A S007 IS 500 RS 1000 ppb	0.044	0.020	0.002	0.001	0.001	0.001	1.052	0.762	0	30
715 00 C51A S008 IS 500 RS 1000 ppb	0.024	0.005	0.001	0.000	0.001	0.000	0.646	0.468	15	30
715 00 C51A S009 IS 500 RS 1000 ppb	0.081	0.022	0.008	0.009	0.014	0.008	3.370	2.441	65	65
715 00 C51A S010 IS 500 RS 1000 ppb	0.008	0.001	0.001	0.000	0.000	0.001	0.847	0.614	5	20
715 00 C51A S011 IS 500 RS 1000 ppb	0.007	0.001	0.005	0.002	0.001	0.001	0.918	0.665	85	70
715 00 C51A S012 IS 500 RS 1000 ppb	0.047	0.026	0.002	0.001	0.001	0.001	1.136	0.823	20	50
715 00 C51A S013 IS 500 RS 1000 ppb	0.023	0.011	0.003	0.001	0.001	0.001	0.683	0.494	0	10
715 00 C51A S014 IS 500 RS 1000 ppb	0.216	0.069	0.007	0.031	0.044	0.025	9.384	6.798	100	100
715 00 C51A S015 IS 500 RS 1000 ppb	0.124	0.043	0.069	0.085	0.080	0.041	9.007	6.524	100	100
715 01 C51A S016 IS 500 RS 1000 ppb	0.163	0.060	0.005	0.022	0.045	0.031	6.683	4.841	100	100
715 00 C51A S017 IS 500 RS 1000 ppb	0.006	0.003	0.001	0.001	0.001	0.001	0.221	0.160	0	0
715 00 C51A S018 IS 500 RS 1000 ppb	0.009	0.005	0.002	0.001	0.001	0.000	0.384	0.278	5	20
715 00 C51A S019 IS 500 RS 1000 ppb	0.004	0.001	0.001	0.000	0.000	0.000	0.137	0.100	30	0
715 00 C51A S020 IS 500 RS 1000 ppb	0.004	0.004	0.005	0.002	0.001	0.001	0.569	0.413	5	0
715 00 C51A S021 IS 500 RS 1000 ppb	0.057	0.023	0.010	0.002	0.001	0.002	1.734	1.256	55	90
715 00 C51A S022 IS 500 RS 1000 ppb	0.002	0.001	0.001	0.000	0.001	0.001	0.303	0.220	0	5
715 00 C51A S023 IS 500 RS 1000 ppb	0.016	0.003	0.003	0.000	0.001	0.000	0.530	0.384	10	0
715 00 C51A S024 IS 500 RS 1000 ppb	0.117	0.036	0.012	0.017	0.041	0.020	5.510	3.992	100	100
715 00 C51A S025 IS 500 RS 1000 ppb	0.164	0.045	0.004	0.011	0.018	0.014	4.924	3.567	100	100
715 00 C51A S026 IS 500 RS 1000 ppb	0.060	0.024	0.003	0.001	0.002	0.003	1.364	0.988	90	65
715 01 C51A S027 IS 500 RS 1000 ppb	0.137	0.042	0.005	0.005	0.010	0.007	3.965	2.872	100	100
715 00 C51A S028 IS 500 RS 1000 ppb	0.028	0.014	0.002	0.000	0.001	0.002	0.671	0.486	75	60
715 00 C51A S029 IS 500 RS 1000 ppb	0.020	0.008	0.002	0.001	0.001	0.000	0.557	0.403	10	15
715 00 C51A S030 IS 500 RS 1000 ppb	0.015	0.006	0.003	0.000	0.000	0.000	0.500	0.362	5	15

Table D7. PAH concentrations and effect data for Elliott Bay (Ozretich et al. 2000) (Continued)

Code	PAH	log K _{ow}	MW (g/mol)	<i>R. abronius</i> 10-d	<i>L. plumulosus</i> 10-d	<i>R. abronius</i>		Acute HC95 (µg/L)	Acute HC5/96 Hr LC50	Acute HC95/96 Hr LC50	
				TLM Endpoint (µmol/goc)	TLM Endpoint (µmol/goc)	10-d TLM Endpoint (µg/L)	Acute HC5 (µg/L)				
Nap	Naphthalene	3.256	128.17	19.7	27.2	1592.834	405.947	6249.878	0.255	3.92	
Acny	Acenaphthylene	3.436	152.20	20.1	27.8	1283.272	324.850	5069.374	0.253	3.95	
Acen	Acenaphthene	3.878	154.21	21.1	29.1	501.539	124.699	2017.183	0.249	4.02	
Flure	Fluorene	3.934	166.22	21.2	29.3	479.137	118.842	1931.739	0.248	4.03	
Phen	Phenanthrene	4.584	178.23	22.8	31.5	126.578	30.462	525.972	0.241	4.16	
Anth	Anthracene	4.546	178.23	22.7	31.3	137.380	33.123	569.792	0.241	4.15	
Flua	Fluoranthene	5.191	202.26	24.3	33.6	38.827	9.053	166.530	0.233	4.29	
Pyr	Pyrene	5.126	202.26	24.2	33.4	44.666	10.451	190.895	0.234	4.27	
B[a]a	Benzo(a)anthracene	5.744	228.29	25.8	35.7	13.308	3.006	58.909	0.226	4.43	
Chry	Chrysene	5.782	228.29	25.9	35.8	12.261	2.764	54.399	0.225	4.44	
B[b+j]Fl	Benzo(b+j)fluoranthene	6.38	252.32	27.7	38.2	3.735	0.811	17.196	0.217	4.60	
B[k]Fl	Benzo(k)fluoranthene	6.4	252.32	27.7	38.3	3.577	0.776	16.492	0.217	4.61	
B[a]P	Benzo(a)pyrene	6.409	252.32	27.8	38.3	3.509	0.761	16.184	0.217	4.61	
Ind	Indeno(1,2,3-cd)pyrene	6.158	276.34	27.0	37.3	6.600	1.454	29.964	0.220	4.54	
Dib[ah]a]	Dibenz(a,h)anthracene	7.129	278.35	30.0	41.4	0.820	0.169	3.970	0.207	4.84	
B[ghi]p	Benzo(g,h,i)perylene	6.886	276.34	29.2	40.4	1.375	0.289	6.544	0.210	4.76	
Biphen	Biphenyl	3.936	154.21	21.2	29.3	774.491	192.083	3122.795	0.248	4.03	
Triphen	Triphenylene	5.63	228.30	25.5	35.2	17.015	3.870	74.814	0.227	4.40	
B[e]P	Benzo(e)pyrene	6.447	252.32	27.9	38.5	3.233	0.699	14.948	0.216	4.62	
Pery	Perylene	6.447	252.32	27.9	38.5	3.233	0.699	14.948	0.216	4.62	
2-Menap	2-methylnaphthalene	3.789	142.20	20.9	28.9	560.268	139.828	2244.902	0.250	4.01	
1-Menap	1-methylnaphthalene	3.781	142.20	20.9	28.8	570.011	142.307	2283.177	0.250	4.01	
C2-Nap	C2-naphthalenes	4.244	156.23	22.0	30.3	230.877	56.474	943.866	0.245	4.09	
C3-Nap	C3-naphthalenes	4.730	170.25	23.2	32.0	88.269	21.087	369.481	0.239	4.19	
C4-Nap	C4-naphthalenes	5.220	184.28	24.4	33.7	33.232	7.736	142.761	0.233	4.30	
C1-Flu	C1-fluorenes	4.370	180.25	22.3	30.7	203.028	49.369	834.936	0.243	4.11	
C2-Flu A	C2-fluorenes	4.819	194.27	23.4	32.3	83.142	19.772	349.611	0.238	4.20	
C2-Flu B	C2-fluorenes	4.819	194.27	23.4	32.3	83.142	19.772	349.611	0.238	4.20	
C3-Flu	C3-fluorenes	5.318	208.30	24.7	34.1	30.412	7.041	131.357	0.232	4.32	
C1-Phe#1	C1-phenanthrenes	5.037	192.26	23.9	33.0	51.435	12.093	218.773	0.235	4.25	
C2-Phe	C2-phenanthrenes	5.455	206.29	25.0	34.6	22.418	5.150	97.582	0.230	4.35	
C3-Phe	C3-phenanthrenes	5.907	220.32	26.3	36.3	9.039	2.022	40.404	0.224	4.47	
C1-Py	C1-pyrenes	5.582	216.29	25.4	35.0	17.877	4.077	78.384	0.228	4.38	
C2-Py	C2-pyrenes	6.027	230.13	26.6	36.8	7.290	1.619	32.825	0.222	4.50	
C1-Chry	C1-chrysenes	6.190	242.32	27.1	37.4	5.402	1.188	24.573	0.220	4.55	
C2-Chry	C2-chrysenes	6.593	256.34	28.3	39.1	2.398	0.514	11.193	0.214	4.67	
Dibthioph	Dibenzothiophene	4.341	184.26	22.2	30.6	220.930	53.796	907.311	0.243	4.11	
C1-Dibthiophe	C1-Dibenzothiophene	4.859	198.29	23.5	32.4	77.853	18.476	328.049	0.237	4.21	
C2-Dibthio	C2-Dibenzothiophene	5.332	212.31	24.7	34.1						
C3-Dibthio	C3-Dibenzothiophene	5.810	226.34	26.0	35.9						
									Average	0.23	4.32

Table D8. PAH concentrations and effect data for laboratory prepared mixtures (Boese et al. 1999)

Compound	Measured Sed (µg/kg)	Measured Sed (µmol/kg)	Measured TOC (%)	Measured Sed (µmol/kg)	log K _{ow}	log k _{oc}	MW (g/mol)	<i>R. abronius</i> 10-d TLM Endpoint (µmol/goc)	Total TU	# Initial Mortality
Mixture: 6 @0.25 sol										3
Anthracene	5109	28.665208	2.659	1.0780447	4.546	4.47	178.23	22.7	0.05	
2-Methylanthracene	3493	18.168106	2.659	0.6832684	5.001	4.92	192.26	23.8	0.03	
3,6-Dimethylphenanthrene	16613	80.53226	2.659	3.0286672	5.455	5.36	206.29	25.0	0.12	
Benzo(a)anthracene	7250	31.757852	2.659	1.1943532	5.744	5.65	228.29	25.8	0.05	
Chrysene	4885	21.398222	2.659	0.804747	5.782	5.68	228.29	25.9	0.03	
Benzo(b)fluroanthene	1584	6.2777425	2.659	0.2360941	6.341	6.23	252.32	27.6	0.01	
Sum all	38.934			7.0251745					0.28	
Mixture: 6 @0.25 sol +Flu										0
Anthracene	5010	28.109746	2.512	1.1190185	4.546	4.47	178.23	22.7	0.05	
2-Methylanthracene	3805	19.790908	2.512	0.7878546	5.001	4.92	192.26	23.8	0.03	
3,6-Dimethylphenanthrene	16196	78.510834	2.512	3.1254313	5.455	5.36	206.29	25.0	0.12	
Benzo(a)anthracene	6671	29.221604	2.512	1.1632804	5.744	5.65	228.29	25.8	0.05	
Chrysene	4755	20.82877	2.512	0.8291708	5.782	5.68	228.29	25.9	0.03	
Benzo(b)fluroanthene	1509	5.980501	2.512	0.2380773	6.341	6.23	252.32	27.6	0.01	
Fluoranthene	5846	28.903392	2.512	1.1506127	5.191	5.10	202.26	24.3	0.05	
Sum all	43792			8.4134457					0.34	
Mixture: 6 @1.0 sol										1
Anthracene	26200	147.00107	2.56	5.7422291	4.546	4.47	178.23	22.7	0.25	
2-Methylanthracene	15705	81.686258	2.56	3.1908695	5.001	4.92	192.26	23.8	0.13	
3,6-Dimethylphenanthrene	72728	352.55223	2.56	13.771572	5.455	5.36	206.29	25.0	0.55	
Benzo(a)anthracene	30403	133.1771	2.56	5.2022304	5.744	5.65	228.29	25.8	0.20	
Chrysene	17836	78.128696	2.56	3.0519022	5.782	5.68	228.29	25.9	0.12	
Benzo(b)fluroanthene	8938	35.423272	2.56	1.3837216	6.341	6.23	252.32	27.6	0.05	
Sum all	171810			32.342524					1.31	
Mixture: 6 @1.0 sol + Flu										3
Anthracene	23322	130.85339	2.45	5.3409548	4.546	4.47	178.23	22.7	0.24	
2-Methylanthracene	15072	78.393842	2.45	3.1997486	5.001	4.92	192.26	23.8	0.13	
3,6-Dimethylphenanthrene	70976	344.05933	2.45	14.043238	5.455	5.36	206.29	25.0	0.56	
Benzo(a)anthracene	27419	120.10601	2.45	4.9022859	5.744	5.65	228.29	25.8	0.19	
Chrysene	16935	74.181962	2.45	3.0278352	5.782	5.68	228.29	25.9	0.12	
Benzo(b)fluroanthene	7219	28.610495	2.45	1.1677753	6.341	65.23	252.32	27.6	0.04	
Fluoranthene	24500	121.13122	2.45	4.9441313	5.191	5.10	202.26	24.3	0.20	
Sum all	185443			36.625969					1.48	

Table D8. PAH concentrations and effect data for laboratory prepared mixtures (Boese et al. 1999) (Continued)

Compound	Measured Sed (µg/kg)	Measured Sed (µmol/kg)	Measured TOC (%)	Measured Sed (µmol/kg)	log K_{ow}	log k_{oc}	MW (g/mol)	<i>R. abronius</i> 10-d TLM Endpoint (µmol/goc)	Total TU	# Initial Mortality
Benzo(a)anthracene	34433	150.83008	2.56	5.8918002	5.744	5.65	228.29	25.8	0.23	1
Chrysene	15208	66.617022	2.56	2.6022274	5.782	5.68	228.29	25.9	0.10	0
Benzo(b)fluroanthene	8518	33.758719	2.56	1.3187	6.341	6.23	252.32	27.6	0.05	0
9,10-Dimethylanthracene	389893	1890	2.56	73.828125	5.408	5.32	206.29	24.9	2.96	0
3,6-Dimethylphenanthrene	65911	319.50652	2.56	12.480723	5.455	5.36	206.29	25.0	0.50	0
Sum all	513963								3.84	
2-Methylanthracene + Fluoranthene	13991	72.771247	2.56	2.8426268	5.001	4.92	192.26	23.8	0.12	0
Sum all	24492	121.09166	2.56	4.7301431	5.191	5.10	202.26	24.3	0.19	
	38483			7.57277					0.31	
9,10-Dimethylanthracene+ Fluoranthene	338632	1642	2.56	64.140625	5.408	5.32	206.29	24.9	2.57	1
Sum all	26722	132.11708	2.56	5.1608233	5.191	5.10	202.26	24.3	0.21	
	365354			69.283236					2.79	
Benzo(a)anthracene+ Fluoranthene	31678	138.7621	2.56	5.4203946	5.744	5.65	228.29	25.8	0.21	1
Sum all	25434	125.74904	2.56	4.9120717	5.191	5.10	202.26	24.3	0.20	
	57112			10.332466					0.41	
3,6-Dimethylphenanthrene+ Fluoranthene	48578	235.48403	2.56	9.1985948	5.455	5.36	206.29	25.0	0.37	0
Sum all	21719	107.38159	2.56	4.1945933	5.191	5.10	202.26	24.3	0.17	
	70297			13.393188					0.54	
Benzo(b)fluroanthene+ Fluoranthene	6987	27.691027	2.56	1.0816808	6.341	6.23	252.32	27.6	0.04	1
Sum all	23699	117.17097	2.56	4.5769909	5.191	5.10	202.26	24.3	0.19	
	30686			5.6586717					0.23	
Chrysene+ Fluoranthene	16143	70.71269	2.56	2.7622145	5.782	5.68	228.29	25.9	0.11	1
Sum all	24663	121.93711	2.56	4.7631684	5.191	5.10	202.26	24.3	0.20	
	40806			7.5253828					0.30	
Anthracene+ Fluoranthene	23225	130.30915	2.56	5.0902012	4.546	4.457202	178.23	22.7	0.22	0
Sum all	22851	112.97834	2.56	4.4132166	5.191	4.997852	202.26	24.3	0.18	
	46076			9.5034178					0.41	

Table D9. PAH concentrations for sediment contaminated from asphalt (Huuskonen et al. 1998)

Concentrations in ng/g dry wgt								
	Vehendi (ng/g)	Salu (ng/g)	Joesuu (ng/g)	Mustajogi (ng/g)	Baltic TPP (ng/g)	Riigikula 1 (ng/g)	Riigikula 2 (ng/g)	Hoytiainen 1 (ng/g)
% OC	14.1	4.4	2.1	3.8	4.3	23.1	3.7	0.3
Phenanthrene	15.3	53	0.5	9.5	15.1	29.2	38700	10
Anthracene	0.4			1.1	0.2	5.1		0.9
Fluoranthene	9.1	23.9	2.1	9.5	2	97	29600	13
Pyrene	31.5	150	4.9	6	19	460	174500	9.5
Benzo(a)anthracene	3.9	14.8	2.8	3.1	1.9	38.8	24400	
Chrysene	5	38.1	4.9	9.9	4.8	34.4	8360	
Benzo(e)pyrene+ B(b)fl	4.7	40.4	5.2	11.5	8.2	18	1690	54
Benzo(k) fluoranthene	1.6	9.5				11.3	372	
Benzo(a)pyrene	1.5	16.7	1.1	1.4	7.3	20.3	373	7.5
Benzo(ghi)perylene	7.4	49.1			10.3	30.2	405	23
Total Measured PAH (mg/kg)	0.0804	0.3955	0.0215	0.052	0.0688	0.7443	278.4	0.1179
Toxic Units								
	Vehendi TU	Salu TU	Joesuu TU	Mustajogi TU	Baltic TPP TU	Riigikula 1 TU	Riigikula 2 TU	Hoytiainen 1 TU
Phenanthrene	3.76E-06	4.17E-05	8.24E-07	8.65E-06	1.22E-05	4.38E-06	3.62E-02	1.15E-04
Anthracene	9.86E-08		0.00E+00	1.01E-06	1.62E-07	7.67E-07	0.00E+00	1.04E-05
Fluoranthene	1.84E-06	1.55E-05	2.86E-06	7.14E-06	1.33E-06	1.20E-05	2.29E-02	1.24E-04
Pyrene	6.43E-06	9.81E-05	6.71E-06	4.54E-06	1.27E-05	5.73E-05	1.36E-01	9.11E-05
Benzo(a)anthracene	6.59E-07	8.02E-06	3.18E-06	1.94E-06	1.05E-06	4.00E-06	1.57E-02	0.00E+00
Chrysene	8.42E-07	2.06E-05	5.54E-06	6.18E-06	2.65E-06	3.54E-06	5.36E-03	0.00E+00
Benzo(e)pyrene+ B(b)fl	6.66E-07	1.84E-05	4.95E-06	6.05E-06	3.81E-06	1.56E-06	9.13E-04	3.60E-04
Benzo(k) fluoranthene	2.28E-07	4.34E-06	0.00E+00	0.00E+00	0.00E+00	9.83E-07	2.02E-04	0.00E+00
Benzo(a)pyrene	2.14E-07	7.62E-06	1.05E-06	7.39E-07	3.41E-06	1.76E-06	2.02E-04	5.02E-05
Benzo(ghi)perylene	9.13E-07	1.94E-05	0.00E+00	0.00E+00	4.17E-06	2.28E-06	1.91E-04	1.33E-04
Sum TU 13PAH	0.00002	0.00023	0.00003	0.00004	0.00004	0.00009	0.21732	0.00088
Total TU PAH	0.00004	0.00064	0.00007	0.00010	0.00011	0.00024	0.59763	0.00243

Table D9. PAH concentrations for sediment contaminated from asphalt (Huuskonen et al. 1998) (Continued)

	Molecular Weight (g/mol)	log K_{ow}	<i>C. riparius</i> 10-d TLM Endpoint (μmol/goc)
Phenanthrene	178.23	4.584	162.1
Anthracene	178.23	4.546	161.4
Fluoranthene	202.26	5.191	173.1
Pyrene	202.26	5.126	171.9
Benzo(a)anthracene	228.29	5.744	183.8
Chrysene	228.29	5.782	184.5
Benzo(e)pyrene+ B(b)fl	252.31	6.447	198.3
Benzo(k) fluoranthene	252.31	6.4	197.3
Benzo(a)pyrene	252.31	6.409	197.5
Benzo(ghi)perylene	276.33	6.886	207.9

In this experiment- 100 mortality was observed for the Riigikula 2 sediment. All other sediments - no difference in mortality or growth

Table D10. PAH concentrations and effect data for Diesel Fuel (Fleeger and Lotufo, 1999)

	log K _{ow}	Log K _{oc}	MW (g/mol)	Sub cooled Solubility (μmol/L)	Acute S. knabeni Endpoint (μmol/goc)	TOC (%)	Undiluted Sediment (mg/kg)	Undiluted Sediment (μmol/goc)	Undiluted Sediment TU
Naphthalene	3.256	3.201	128.17	241.83	68.0	1.5	2.601	1.3528907	0.02
1-methylnaphthalene	3.781	3.717	142.20	196.91	71.9	1.5	44.054	20.65354	0.29
C2-naphthalenes	4.244	4.172	156.23	59.95	75.6	1.5	143.537	61.250293	0.81
C3-naphthalenes	4.730	4.650	170.25	22.25	79.7	1.5	141.64	55.463534	0.70
C4-naphthalenes	5.220	5.132	184.28	8.19	84.1	1.5	84.171	30.450402	0.36
Fluorene	3.934	3.867	166.22	11.43	73.1	1.5	6.843	2.7445554	0.04
Phenanthrene	4.584	4.506	178.23	6.17	78.5	1.5	17.321	6.4788943	0.08
C1-phenanthrenes	5.037	4.952	192.26	11.8968	82.4	1.5	53.68	18.613683	0.23
C2-phenanthrenes	5.455	5.363	206.29	5.0723	86.2	1.5	56.659	18.310469	0.21
C3-phenanthrenes	5.907	5.807	220.32	2.0178	90.6	1.5	38.957	11.788005	0.13
Dibenzothiophene	4.341	4.267	184.26	49.1899	76.4	1.5	5.169	1.8701834	0.02
C1-Dibenzothiophene	4.859	4.777	198.29	17.1034	80.8	1.5	23.93	8.0454553	0.10
C2-Dibenzothiophene	5.332	5.242	212.31	6.5185	85.1	1.5	52.212	16.394894	0.19
Fluoranthene	5.191	5.103	202.26	1.19	83.8	1.5	0.825	0.2719272	0.00
Pyrene	5.126	5.039	202.26	0.6520	83.2	1.5	3.839	1.265368	0.02
Benzo(a)anthracene	5.744	5.647	228.29	0.0482	89.0	1.5	0.105	0.0306628	0.00
Chrysene	5.782	5.684	228.29	0.0088	89.3	1.5	0.026	0.0075927	0.00
Benzo(b)fluoranthene	6.380	6.272	252.32	0.0060	95.3	1.5	0.007	0.0018495	0.00
Benzo(k)fluoranthene	6.400	6.291	252.32	0.0032	95.5	1.5	0.002	0.0005284	0.00
Benzo(a)pyrene	6.409	6.300	252.32	0.0151	95.6	1.5	<u>0.005</u>	0.0013211	<u>0.00</u>
Total							675.583		3.20
	Sediment Conc (mg/kg)	Dilution	Equivalent TU	% Mortality					
	370	0.54	1.723	95					
	185	0.27	0.861	42					
	130	0.19	0.605						
	93	0.14	0.433	10					
	45	0.07	0.210	2					
	19	0.03	0.088						
From Fig 3.3 in Lotufo and Fleeger, 1999			NOEC reproduction =	45 mg/kg	TU = (.21*3.83) =	.80)			
			LOEC reproduction =	93 mg/kg	TU = (0.43*3.83) =	1.7)			

Table 11D. Summary of Total PAH concentrations, TU and % Mortality for Exxon Valdez field sediment (Page et al. 2002)

The original database contained PAH data for 648 sediment samples. In each sample, more than 70 parameters were measured. There were more than 45,000 datapoints in the database. After processing the data and eliminating all sediments with TOC < 0.2%, 470 sediment samples remained for inclusion. Due to the large size of the database, only a summary of the data is presented. Please contact David Page for complete data set (dpage@bowdoin.edu).

Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival	Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival	Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival
00BI01	3.69	3430190	0.6748	1E-20	00SR04	0.23	335348	0.0776	98	0SRMB4	3.73	7702	0.0015	89
00BI01	1.6	2241006	0.4910	4	00SR04	0.56	23027	0.0043	88	0SRMB4	0.23	15261	0.0038	88
00BI01	1.52	3276849	0.7282	2	00SR04	0.22	131591	0.0237	96	0SRMB4	0.8	12184	0.0026	93
00BI01	0.43	5200047	1.0595	1E-20	00SR05	0.22	20614864	3.8400	12	0SRMB4	6.21	17709	0.0034	85
00BI01	0.29	530759	0.0955	90	00SR05	0.51	5396431	0.9554	26	0SRMB4	6.02	6420	0.0015	88
00BI01	1.75	5213663	1.0401	1	00SR05	0.25	2737808	0.4658	94	0SRMB4	5.09	8462	0.0019	93
00BI01	0.34	116468	0.0212	92	00SR05	0.36	54228	0.0095	86	A03501	0.24	5292	0.0012	98
00BI01	1.76	17610	0.0032	83	00SR05	0.75	18917	0.0036	91	A03501	0.31	1158	0.0004	90
00BI01	0.66	22452	0.0042	77	00SR05	1.53	7571	0.0012	92	A03501	0.24	1583	0.0005	98
00BI01	0.91	21627	0.0042	82	00SR05	1.04	19045	0.0036	93	A03501	0.25	2248	0.0007	100
00BI01	0.93	32925	0.0066	87	00SR05	1.35	3701	0.0008	89	A03501	0.26	1842	0.0006	98
00BI01	0.97	65227	0.0127	88	00SR05	0.91	7704	0.0017	88	A03501	0.31	3448	0.0009	74
00MB01	0.4	4000	0.0016	92	00SR05	1.42	8789	0.0018	91.5	A04800	1.43	146755	0.0275	86
00MB01	1.8	4833	0.0019	69	00SR05	0.22	116082	0.0232	91	A04800	0.36	2917	0.0010	95
00MB01	0.28	20714	0.0082	99	00SR05	0.2	7390500	1.1521	92	A04800	0.42	37567	0.0062	93
00MB01	0.49	3714	0.0011	82	00SR06	0.2	3950	0.0013	99	A04800	0.46	413957	0.0717	92
00MB01	0.23	18609	0.0046	88	00SR06	0.32	50688	0.0099	95	A04800	0.57	169649	0.0273	78
00MB01	0.39	5410	0.0017	78	00SR06	0.33	54870	0.0108	94	A04800	0.39	5315	0.0012	95
00MB01	0.27	8370	0.0023	97	00SR06	0.23	33843	0.0077	85	A05903	0.28	205614	0.0362	95
00MB01	0.29	14690	0.0052	88	00SR06	0.34	34853	0.0069	87	A05903	0.29	178552	0.0312	88
00MB01	0.3	0	0.0000	88	00SR06	0.22	17305	0.0043	91	A05903	0.21	199000	0.0171	96
00MB01	0.33	11848	0.0044	88	00SR07	0.34	28192699	5.4116	92	A05903	0.34	118985	0.0208	94
00MB01	0.34	1882	0.0007	95	00SR07	0.27	22830	0.0047	98	A05903	0.25	128792	0.0223	91
00MB01	0.6	17050	0.0061	87	00SR07	0.28	176293	0.0322	83	A35107	0.33	1170	0.0005	88
00MB01	0.42	8071	0.0030	82	00SR07	0.25	3480	0.0010	92	A35107	0.34	27818	0.0053	94
00MB01	0.56	11125	0.0038	91	00SR07	0.27	8396	0.0018	95	A35107	0.2	51490	0.0092	83
00SL01	1.24	716097	0.1402	16	00SR07	0.29	57534	0.0098	94	A35107	0.5	159540	0.0274	90
00SL01	0.62	130742	0.0238	79	00SR07	0.26	2438	0.0009	97	A35107	0.37	4305	0.0012	93
00SL01	0.93	793968	0.1525	25	00SR07	0.27	10578	0.0024	92	A35107	0.77	7600	0.0014	97
00SL01	0.51	12567	0.0026	92	0E11SA	0.4	5596014	1.0471	78	C12102	0.55	2436247	0.4508	12
00SL01	0.47	25145	0.0048	90	0E11SA	0.38	3609196	0.7315	72	C12102	0.24	23144	0.0041	94
00SL01	0.44	29332	0.0055	96	0E11SA	0.38	60255	0.0119	66	C12102	1.89	1617	0.0004	80
00SL01	0.41	65429	0.0123	93	0E11SA	0.36	30692	0.0070	83	C15903	0.77	1225977	0.2229	6
00SL01	0.45	13707	0.0030	91	0E11SA	0.38	4803	0.0015	81	C15903	0.94	2519856	0.4727	3
00SL01	0.61	6826	0.0018	98	0E11SA	0.39	8026	0.0030	95	C15903	0.39	348705	0.0615	80
00SL01	0.37	24076	0.0048	88	0E11SA	0.41	2156	0.0008	92	C15903	0.26	59965	0.0111	80
00SL01	0.37	30916	0.0063	92	0E11SA	0.39	6687	0.0024	93	C15903	0.22	80105	0.0165	93
00SL01	0.37	41189	0.0079	90	0E11SA	0.35	6814	0.0023	92	C15903	0.22	6714	0.0015	94
00SL01	0.38	29321	0.0061	92	0E11SA	0.38	6368	0.0022	94	C15903	0.28	14961	0.0028	92
00SL01	0.4	41450	0.0082	89	0E11SA	0.36	8833	0.0024	95	C15903	0.34	42965	0.0083	97
00SL01	0.34	23274	0.0057	88	0SRE11	15.77	1642270	0.3575	1E-20	C16102	0.57	16206640	3.5226	63
00SR03	0.28	2318	0.0008	93	0SRE11	15.99	842718	0.1817	1E-20	C16102	0.59	13253220	2.8628	1E-20
00SR03	0.44	23632	0.0051	65	0SRE11	0.33	27152	0.0063	96	C16102	0.61	845981	0.1705	27
00SR03	0.54	10463	0.0027	86	0SRE11	0.36	20228	0.0048	96	C16102	0.33	291952	0.0511	86
00SR03	0.3	10757	0.0026	97	0SRE11	0.37	23924	0.0055	93	C16102	0.39	72226	0.0146	81
00SR04	0.97	19175	0.0030	93	0SRE11	0.39	6118	0.0015	78	C16102	0.37	87805	0.0168	69
00SR04	2.45	11660	0.0019	80	0SRE11	0.38	10834	0.0031	91	C16102	0.37	68641	0.0122	96
00SR04	0.77	35116	0.0065	81	0SRE11	0.39	9297	0.0026	96	C19106	0.26	555488	0.0965	12
00SR04	2.69	16078	0.0026	89	0SRE11	0.41	10637	0.0026	79	C19106	0.25	170552	0.0298	72
00SR04	1.58	5483	0.0010	94	0SRE11	0.37	12022	0.0030	94	C19106	0.76	2030364	0.3646	37
00SR04	0.32	160438	0.0424	92	0SRE11	0.42	643	0.0002	82	C19106	0.23	5322	0.0014	76

Table 11D. Summary of Total PAH concentrations, TU and % Mortality for Exxon Valdez field sediment (Page et al. 2002) (Continued)

Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival	Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival	Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival
C19106	0.23	3900	0.0012	76	M03601	0.47	23362	0.0046	94	P25101	0.65	123	0.0000	76
C19106	0.63	749	0.0002	88	M03601	0.31	12016	0.0027	92	P25101	0.58	0	0.0000	89
C19106	0.25	2148	0.0006	90	M03601	0.38	19161	0.0043	91	P25101	1.07	869	0.0002	87
C19106	0.25	1456	0.0006	90	M03601	0.36	6861	0.0019	93	P25101	2.04	1078	0.0002	96
C19106	0.24	1529	0.0005	95	M27013	0.52	1396	0.0003	92	P25101	2.66	2808	0.0005	77
C19106	0.24	2196	0.0006	98	M27013	0.52	37654	0.0075	85	P25101	3.63	120008	0.0224	91
C19106	0.23	26913	0.0053	92	M27013	1.18	10458	0.0019	74	P25101	2.75	3124	0.0005	95
C19106	0.29	890	0.0003	93	M27013	0.43	253860	0.0440	92	P25101	2.57	125	0.0000	87.5
D00300	0.21	123952	0.0264	96	M27013	0.39	70538	0.0128	95	P25101	0.6	1083	0.0002	83
D00300	0.2	7400	0.0023	96	M27013	0.42	47231	0.0090	96	P25101	0.57	228	0.0001	96
D00601	0.2	5290	0.0013	90	O18010	0.37	20270	0.0047	93	P25101	1.15	539	0.0001	91
D00601	0.26	3223	0.0010	94	O18010	0.36	15856	0.0039	84	P33908	0.82	256	0.0001	92
D00601	0.28	5282	0.0013	93	O18010	0.3	9170	0.0026	93	P33908	0.38	947	0.0004	96
D00601	0.21	3948	0.0011	91	O18010	0.37	10876	0.0029	86	P33908	2.24	317	0.0001	85
D00601	0.3	8287	0.0018	89	O18010	0.39	4118	0.0013	92	P33908	0.42	3643	0.0009	93
D00601	0.23	2087	0.0006	85	O18010	0.35	3903	0.0013	92	P33908	1.45	910	0.0002	90
D04100	0.61	2840	0.0006	94	O18010	0.41	5012	0.0015	96	P33908	2.79	3699	0.0007	90
D04100	0.58	5283	0.0011	93	O18010	0.42	5281	0.0015	92	P33908	3.52	4537	0.0008	94
D04100	0.62	17693	0.0032	91	O18010	0.43	17047	0.0044	93	P33908	2.78	5475	0.0011	95
D04100	0.63	6984	0.0015	88	O18010	0.39	13192	0.0033	91	P33908	1.83	4981	0.0010	95
D04100	0.57	1132	0.0003	81	O65505	0.39	1256	0.0005	95	P33908	2.9	3649	0.0006	82
D04100	0.52	21067	0.0040	82	O65505	1.54	548	0.0001	96	P33908	2.83	7343	0.0014	91
D04100	1.5	83333	0.0152	93	O65505	0.62	516	0.0002	85	00B101	5.24	2379050	0.4391	4
D04100	0.68	22782	0.0041	87	O65505	0.37	676	0.0003	87	00B101	7.91	6354867	1.3274	32
D04100	0.75	19749	0.0035	96	O65505	0.29	6966	0.0014	91	00B101	12.85	6361479	1.3423	1E-20
D04100	3.48	61658	0.0106	98	O65505	0.2	2930	0.0007	96	00B101	2.45	27073	0.0046	81
D04100	0.75	7820	0.0013	92	O65505	0.25	880	0.0003	81	00B101	1.1	1979736	0.4140	66
D04100	0.59	11717	0.0021	95	O65505	0.29	6448	0.0014	88	00B101	1.47	174438	0.0298	95
D05000	1.01	1089663	0.1802	81	O75507	0.39	6564	0.0016	96	00B101	9.88	292436	0.0518	95
D05000	2.06	959347	0.1597	1E-20	O75507	0.34	6162	0.0014	91	00B101	9.74	2980	0.0005	69
D05000	0.29	40866	0.0068	86.5	O75507	0.26	4385	0.0013	80	00B101	1.11	103151	0.0171	92
D05000	0.46	21365	0.0035	95	O75507	0.4	3625	0.0010	92	00B101	9.48	9910	0.0016	89
D05000	0.35	32380	0.0050	98	O75507	0.36	1750	0.0007	89	00B101	8.87	4495	0.0008	97
D05000	0.25	55684	0.0086	92	O75507	0.35	1686	0.0006	95	00B101	11.04	5537	0.0009	88
D05000	0.2	35675	0.0059	95	O75507	0.3	2167	0.0007	95	00B101	0.61	3170	0.0006	88
D05000	0.2	71375	0.0113	99	O75507	0.44	1295	0.0004	91	00B101	1.08	102	0.0000	89
D05000	0.21	35557	0.0057	98	O75507	0.4	3000	0.0009	93	00B101	1.18	3919	0.0007	86
M00200	0.51	9367	0.0019	89	O75507	0.34	3765	0.0011	98	00MB01	1.86	151	0.0001	75
M00200	0.54	16535	0.0032	91	O75507	0.34	8588	0.0031	98	00MB01	2.01	134	0.0001	84
M00200	0.53	1402	0.0004	96.5	O89109	0.53	3879	0.0009	88	00MB01	0.48	1271	0.0005	65
M00200	0.42	6148	0.0014	91	O89109	0.52	1675	0.0004	82	00MB01	1.32	106	0.0000	90
M00200	0.48	2425	0.0007	98	O89109	0.59	35066	0.0065	98	00MB01	1.05	291	0.0001	90
M00200	0.37	4243	0.0013	94	O89109	0.59	6056	0.0014	93	00MB01	1.04	163	0.0001	100
M03601	0.44	6830	0.0012	87	O89109	1.47	17267	0.0031	99	00MB01	5.44	814	0.0002	96
M03601	0.32	82456	0.0130	84	O89109	0.46	1317	0.0004	94	00MB01	2.04	495	0.0001	95
M03601	0.53	2182698	0.3803	6	O89109	1.37	8832	0.0021	84	00MB01	0.65	908	0.0002	94
M03601	0.4	3493	0.0008	79	O89109	3.04	2799	0.0007	91	00MB01	0.74	608	0.0001	93
M03601	0.31	4677	0.0010	75	O89109	1.93	11176	0.0023	92	00MB01	0.57	1404	0.0003	98
M03601	0.38	9742	0.0019	76	O89109	0.51	2086	0.0006	96	00MB01	3.66	237	0.0000	97
M03601	0.47	19006	0.0037	80	O89109	0.49	2249	0.0007	96	00MB01	1.66	1000	0.0002	92
M03601	0.4	39595	0.0070	87	O89109	0.56	1016	0.0003	82	00MB01	0.62	1016	0.0002	92

Table 11D. Summary of Total PAH concentrations, TU and % Mortality for Exxon Valdez field sediment (Page et al. 2002) (Continued)

Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival	Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival	Sitecode	TOC (%)	Total PAH µg/kgoc	Total PAH TU	Amphipod % Survival
00MB01	1.09	1669	0.0003	96	00SR05	2.1	6051	0.0012	100	OSRMB4	2.04	2833	0.0005	85
00SL01	0.85	4629235	0.9447	3	00SR05	0.51	29727	0.0056	92	OSRMB4	6.17	3125	0.0006	98
00SL01	1.1	972850	0.1965	1E-20	00SR05	3.08	20935	0.0038	82	OSRMB4	13.56	4338	0.0007	96
00SL01	1.05	1513124	0.3141	15	00SR06	0.36	0	0.0000	91	OSRMB4	3.78	6907	0.0014	92
00SL01	0.45	9929	0.0019	94	00SR06	0.23	2965	0.0005	95	OSRMB4	6.86	4875	0.0009	97
00SL01	0.47	10183	0.0017	87	00SR06	0.31	22194	0.0042	84	OSRMB4	7.27	7598	0.0014	91
00SL01	0.39	19969	0.0040	90	00SR06	0.83	5711	0.0010	93	O18010	0.37	9441	0.0022	85
00SL01	0.46	1780	0.0004	95	00SR06	0.5	4098	0.0007	95	O18010	0.36	11147	0.0026	79
00SL01	0.38	9789	0.0013	98	00SR06	3.5	23876	0.0035	96	O18010	0.4	5388	0.0014	96
00SL01	0.38	19871	0.0030	94	00SR06	0.29	20621	0.0035	84	O18010	0.38	3042	0.0008	95
00SL01	0.34	11203	0.0017	91	00SR06	0.3	24880	0.0039	96	O18010	0.43	3727	0.0010	95
00SL01	0.32	14859	0.0020	95	00SR06	0.22	9059	0.0016	89	O18010	0.44	5252	0.0014	87
00SL01	0.37	17703	0.0027	96	00SR07	0.61	36972	0.0061	81	O18010	0.46	6178	0.0016	94
00SL01	0.37	30749	0.0045	100	00SR07	1.06	121930	0.0203	74	O18010	0.47	5228	0.0013	92
00SL01	0.39	135603	0.0254	97	00SR07	0.33	269691	0.0498	95	O18010	0.48	7102	0.0017	98
00SL01	0.4	45418	0.0075	91	00SR07	0.23	19922	0.0031	95	O18010	0.43	6807	0.0017	97
00SR03	0.86	1874353	0.3470	48	00SR07	0.23	34574	0.0055	90	O18010	0.45	8609	0.0020	94
00SR03	0.72	284534	0.0473	97	00SR07	0.22	28550	0.0046	76	O18010	0.46	6822	0.0017	94
00SR03	0.53	129642	0.0205	91	00SR07	0.23	526	0.0001	94	O65505	0.55	7358	0.0012	96
00SR03	1.12	1539	0.0003	95	00SR07	0.27	3026	0.0004	97	O65505	0.84	2270	0.0005	96
00SR03	0.55	2456	0.0005	90	00SR07	0.28	4596	0.0008	92	O65505	0.86	939	0.0003	93
00SR03	0.65	1106	0.0002	95	00SR07	0.26	565	0.0001	95	O65505	15.87	795	0.0001	83
00SR03	1.03	89	0.0000	82	00SR07	0.3	16757	0.0026	89	O65505	3.36	494	0.0001	94
00SR03	1.62	99	0.0000	74	OE11SA	15.94	498779	0.1057	47	O65505	6.09	1005	0.0002	97
00SR03	2.26	71	0.0000	81	OE11SA	9.42	781313	0.1703	1E-20	O65505	3.52	595	0.0002	77
00SR03	2.64	163	0.0000	86	OE11SA	3.82	527577	0.1087	68	O65505	2.92	402	0.0001	93
00SR03	0.88	93	0.0000	71	OE11SA	0.45	3902	0.0010	65	O65505	0.32	1613	0.0005	98
00SR03	2.31	121	0.0000	83	OE11SA	0.33	8724	0.0017	78	O65505	0.98	979	0.0003	99
00SR03	4.06	3715	0.0008	76	OE11SA	0.32	1069	0.0003	64	O65505	1.43	512	0.0001	91
00SR03	4.67	874	0.0002	76	OE11SA	0.3	1430	0.0004	95	O65505	3.53	1500	0.0003	91
00SR03	5.03	0	0.0000	87	OE11SA	0.38	368	0.0001	97	P25101	0.3	690	0.0003	93
00SR04	2.43	22366	0.0036	91	OE11SA	0.33	270	0.0001	94	P25101	0.69	490	0.0002	79
00SR04	0.77	46390	0.0074	78	OE11SA	0.31	306	0.0001	18	P25101	0.65	897	0.0003	87
00SR04	0.46	56233	0.0093	90	OE11SA	0.34	474	0.0002	95	P25101	1.12	1213	0.0002	88
00SR04	5.91	32504	0.0057	90	OE11SA	0.38	126	0.0000	97	P25101	1.13	796	0.0002	77
00SR04	2.46	19230	0.0030	86	OSR01N	0.26	3696	0.0007	92	P25101	3.86	656	0.0001	96
00SR04	4.25	5209	0.0009	97	OSR01N	0.3	2659	0.0005	90	P25101	0.84	413	0.0001	95
00SR04	5.74	2690	0.0005	84	OSR01N	0.38	3787	0.0007	83	P25101	5.04	546	0.0001	95
00SR04	5.96	4579	0.0010	88	OSR01N	0.31	8642	0.0016	94	P25101	3.99	749	0.0002	88
00SR04	6.17	6015	0.0013	83	OSR01N	0.31	1713	0.0004	85	P25101	1.49	298	0.0001	91
00SR04	2.26	5854	0.0011	94	OSRE11	1.71	501153	0.0903	58	P25101	1.08	152	0.0001	89
00SR04	2.32	4069	0.0007	99	OSRE11	1.57	411617	0.0704	73	P25101	1.42	413	0.0001	87
00SR04	4.25	9901	0.0019	96	OSRE11	2.1	440443	0.0744	2	P33908	0.2	2235	0.0007	98
00SR05	1.11	196119	0.0321	94	OSRE11	0.36	53694	0.0094	87	P33908	0.24	2967	0.0009	95
00SR05	0.64	1086002	0.1995	94	OSRE11	0.35	11071	0.0020	94	P33908	0.35	2474	0.0007	89
00SR05	0.54	112594	0.0175	92	OSRE11	0.42	10371	0.0018	92	P33908	2.85	2200	0.0005	97
00SR05	7.93	18700	0.0031	90	OSRE11	0.47	5338	0.0010	82	P33908	1.04	1911	0.0005	92
00SR05	2.77	3667	0.0006	96	OSRE11	0.47	796	0.0002	96	P33908	3.87	2725	0.0005	98
00SR05	4.21	44675	0.0074	93	OSRE11	0.46	4552	0.0009	90	P33908	3.53	2320	0.0006	93
00SR05	1.54	78	0.0000	96	OSRE11	0.34	18771	0.0035	94	P33908	2.93	2072	0.0004	92
00SR05	4.98	17396	0.0032	82	OSRE11	0.46	637	0.0002	87	P33908	6.35	2362	0.0005	94
00SR05	2.98	22279	0.0042	88	OSRE11	0.48	1429	0.0004	89	P33908	3.21	2532	0.0005	93
00SR05	0.64	3308	0.0007	86	OSRMB4	3.93	23	0.0000	100	P33908	4.56	1717	0.0004	100
00SR05	3.98	4892	0.0010	90	OSRMB4	1.98	1374	0.0003	97	P33908	3.89	3833	0.0007	96
00SR05	2.97	43260	0.0080	93	OSRMB4	2.39	293	0.0001	99					

Table 11D. Summary of Total PAH concentrations, TU and % Mortality for Exxon Valdez field sediment (Page et al. 2002) (Continued)

ID	log Kow	<i>R. abronius</i>			
		MW (g/mol)	10-d TLM Endpoint (µmol/goc)	HC5 µmol/goc	HC95 µmol/goc
Naphthalene	3.256	128.17	19.74	8.51	46
2-methylnaphthalene	3.789	142.2	20.91	8.90	49
1-methylnaphthalene	3.781	142.2	20.89	8.89	49
C1-naphthalenes	3.785	142.2	20.90	8.89	49
C2-naphthalenes	4.244	156.23	21.97	9.23	52
C3-naphthalenes	4.73	170.25	23.15	9.59	56
C4-naphthalenes	5.22	184.28	24.41	9.95	60
Biphenyl	3.936	154.21	21.25	9.01	50
Acenaphthylene	3.436	152.2	20.13	8.64	47
Acenaphthene	3.878	154.21	21.11	8.96	50
Fluorene	3.934	166.22	21.24	9.00	50
C1-fluorenes	4.37	180.25	22.27	9.32	53
C2-fluorenes	4.819	194.27	23.38	9.66	57
C3-fluorenes	5.318	208.3	24.67	10.02	61
Phenanthrene	4.584	178.23	22.79	9.48	55
Anthracene	4.546	178.23	22.70	9.45	54
C1-phenanthrenes	5.037	192.26	23.93	9.82	58
C2-phenanthrenes	5.455	206.29	25.04	10.13	62
C3-phenanthrenes	5.907	220.32	26.30	10.46	66
C4-phenanthrenes	6.357	234.35	27.61	10.79	71
Dibenzothiophene	4.341	184.26	22.20	9.30	53
C1-Dibenzothiophene	4.859	198.29	23.48	9.69	57
C2-Dibenzothiophene	5.332	212.31	24.71	10.03	61
C3-Dibenzothiophene	5.81	226.34	26.02	10.39	65
Fluoranthene	5.191	202.26	24.34	9.93	60
Pyrene	5.126	202.26	24.17	9.88	59
C1-fluoranthene	5.582	216.29	25.39	10.22	63
Benzo(a)anthracene	5.744	228.29	25.84	10.34	65
Chrysene	5.782	228.29	25.94	10.37	65
C1-chrysenes	6.19	242.32	27.12	10.67	69
C2-chrysenes	6.593	256.34	28.32	10.97	73
C3-chrysenes	6.972	270.37	29.51	11.25	77
C4-chrysenes	7.421	284.4	30.98	11.59	83
Benzo(b)fluoranthene	6.341	252.32	27.56	10.78	70
Benzo(k)fluoranthene	6.4	252.32	27.74	10.83	71
Benzo(e)pyrene	6.447	252.32	27.88	10.86	72
Benzo(a)pyrene	6.409	252.32	27.77	10.83	71
Perylene	6.447	252.32	27.88	10.86	72
Indeno(1,2,3-cd)pyrene	6.158	276.34	27.02	10.65	69
Dibenz(a,h)anthracene	7.129	278.35	30.02	11.37	79
Benzo(g,h,i)perylene	6.886	276.34	29.24	11.19	76

Table 12D. PAH Concentrations and effect data from North Cape Oil Spill (Ho et al. 1999)

Concentration in ng/g dry wgt															
	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E2	ST E2	ST E2	ST E2	ST E2	ST E2
Sample Collection Date	21-Jan-96	25-Jan-96	01-Feb-96	21-Feb-96	21-Mar-96	30-May-96	26-Jul-96	15-Oct-96	21-Jan-96	25-Jan-96	21-Feb-96	21-Mar-96	30-May-96	26-Jul-96	15-Oct-96
days from Jan 19:	2	6	13	33	62	132	189	270	2	6	33	62	132	189	270
Naphthalene	0	39.6	0	0	0	0	0	0	0	105	260	130	74	0	0
Sum C-1 Naphthalenes	717	3342	245	132	0	0	0	0	863	9665	2610	1048	754	0	0
Sum C-2 Naphthalenes	2790	11870	1520	252	0	0	25	19	3770	43400	16050	7150	3376	0	22
Sum C-3 Naphthalenes	4805	18785	5220	472	20	0	84	26	5850	74250	37000	22650	5140	58	207
Fluorene	14.3	46.4	6.7	1.6	0	3	0	3	16.7	119	346	94.5	120	0	0
Sum C1 Fluorenes	758	2770	734	55	125	112	197	129	1030	7550	24650	14750	6895	205	342
Sum C2 Fluorenes	1850	5935	2180	156	492	194	286	167	2520	15850	54000	44500	14540	388	1016
Sum C3 Fluorenes	2190	6195	2300	191	1192	327	674	258	2890	16150	65000	64750	19475	999	1885
Dibenzothiophene	9.7	32.9	8.7	1.8	0.7	3	4	7	12.6	82.9	248	119	67	3	5
Phenanthrene	69.9	213	48.1	29.5	0	31	41	51	88.4	491	1340	724	388	10	9
Anthracene	5.2	9.6	10.0	7.2	0	10	10	27	8.8	19.9	138	44.3	27	7	5
Sum C-1 Dibenzothiophenes	672	2310	844	85	243	131	210	263	936	6110	21100	16150	8315	281	552
Sum C-1 Phen./Anthracenes	2755	8510	3430	374	712	292	535	714	3380	21150	70400	58950	19400	513	1142
Sum C-2 Dibenzothiophenes	986	3550	1200	87.5	689	243	441	298	1400	8895	38750	34050	12200	564	984
Sum C-2 Phen./Anthracenes	3440	10725	4700	447	2120	686	1230	900	4490	26350	105400	102050	31400	1595	3190
Sum C-3 Dibenzothiophenes	843	3105	892	73.5	1034	465	792	378	1250	7135	38400	38000	14340	830	1289
Sum C-3 Phen./Anthracenes	1960	6150	1940	154	2080	873	1340	740	2730	15200	80150	78850	27500	1690	3075
Sum C-4 Phen./Anthracenes	812	2340	803	68.4	1171	609	944	751	1220	6040	34800	38600	12900	1148	1795
Fluoranthene	69.0	66.3	14.9	64.3	32.7	60	142	95	94.0	76.5	224	172	125	56	47
Pyrene	81.5	138	43.2	60.1	43.2	56	119	126	113	258	1045	880	321	60	63
Sum C-1 Fluor./Pyrenes	733	1900	509	185	759	538	883	1571	1180	4030	24000	21100	6115	732	1094
Benzo[a]anthracene	12.6	9.3	0	10.1	13.1	36	53	66	20.9	15.2	44.8	74.3	81	24	24
Chrysene	18.1	13.3	6.4	11.0	16.5	45	68	197	26.3	21.3	73.1	156	134	38	40
Sum C-1 Chrysenes	113	190	102	238	296	360	686	856	200	355	1385	3205	1475	486	524
Sum C-2 Chrysenes	29.9	86.0	59.2	31.9	162	144	276	277	63.6	218	932	1970	854	200	269
Benzo[b]fluoranthene	13.5	9.2	2.6	8.8	6.0	19	26	43	18.2	16.0	20.4	53.8	35	15	22
Benzo[k]fluoranthene	11.6	8.8	3.1	8.3	6.3	20	18	21	18.8	10.0	32.6	29.6	34	10	11
Benzo[e]pyrene	10.3	7.0	2.5	7.2	5.4	14	18	26	15.9	10.6	21.9	29.0	28	11	14
Benzo[a]pyrene	13.5	9.0	2.2	8.1	4.0	15	20	34	19.6	12.9	19.9	27.7	29	11	13
Perylene	5.2	3.9	1.6	4.9	3.4	9	10	12	9.1	6.3	16.0	12.6	18	6	8
Indeno[123-cd]pyrene	8.3	7.1	1.6	4.7	1.8	12	14	18	13.0	9.7	11.3	9.5	27	8	9
Dibenz[ah]anthracene	2.3	2.8	0	2.3	0	6	6	8	4.8	3.7	4.6	3.3	11	3	3
Benzo[ghi]perylene	9.8	8.1	2.0	5.7	2.3	14	11	13	13.5	11.3	13.5	8.1	33	7	6
SUM PAHs (ppb) ng/g	24,675	85,928	26,082	2,586	9,877	3976	6810	4728	34,966	258,563	590,642	522,609	176,910	8,288	15,515

Table 12D. PAH Concentrations and effect data from North Cape Oil Spill (Ho et al. 1999) (Continued)

Toxic Units															
	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E1	ST E2	ST E2	ST E2	ST E2	ST E2	ST E2
Sample Collection Date	21-Jan-96	25-Jan-96	01-Feb-96	21-Feb-96	21-Mar-96	30-May-96	26-Jul-96	15-Oct-96	21-Jan-96	25-Jan-96	21-Feb-96	21-Mar-96	30-May-96	26-Jul-96	15-Oct-96
days from Jan 19:	2	6	13	33	62	132	189	270	2	6	33	62	132	189	270
Naphthalene	0.00000	0.00181	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00186	0.00457	0.00228	0.00129	0.00000	0.00000
Sum C-1 Naphthalenes	0.02794	0.13023	0.00955	0.00514	0.00000	0.00000	0.00000	0.00000	0.01294	0.14488	0.03912	0.01571	0.01130	0.00000	0.00000
Sum C-2 Naphthalenes	0.09421	0.40081	0.05133	0.00851	0.00000	0.00000	0.00084	0.00065	0.04896	0.56364	0.20844	0.09286	0.04384	0.00000	0.00028
Sum C-3 Naphthalenes	0.14126	0.55225	0.15346	0.01386	0.00059	0.00000	0.00246	0.00077	0.06615	0.41836	0.25610	0.05812	0.00066	0.00000	0.00235
Fluorene	0.00047	0.00152	0.00022	0.00005	0.00000	0.00011	0.00000	0.00010	0.00021	0.00150	0.00437	0.00119	0.00151	0.00000	0.00000
Sum C1 Fluorenes	0.02187	0.07997	0.02119	0.00158	0.00361	0.00322	0.00569	0.00372	0.01144	0.08384	0.27371	0.16378	0.07656	0.00228	0.00379
Sum C2 Fluorenes	0.04719	0.15144	0.05563	0.00398	0.01255	0.00494	0.00728	0.00426	0.02473	0.15555	0.52996	0.43672	0.14270	0.00380	0.00997
Sum C3 Fluorenes	0.04938	0.13968	0.05186	0.00431	0.02686	0.00737	0.01520	0.00581	0.02506	0.14005	0.56367	0.56150	0.16888	0.00866	0.01635
Dibenzothiophene	0.00027	0.00093	0.00025	0.00005	0.00025	0.00008	0.00011	0.00021	0.00014	0.00090	0.00270	0.00130	0.00073	0.00003	0.00005
Phenanthrene	0.00199	0.00609	0.00137	0.00084	0.00000	0.00087	0.00117	0.00145	0.00097	0.00539	0.01470	0.00794	0.00425	0.00010	0.00010
Anthracene	0.00015	0.00027	0.00029	0.00021	0.00000	0.00028	0.00030	0.00079	0.00010	0.00022	0.00152	0.00049	0.00030	0.00007	0.00006
Sum C-1 Dibenzothiophenes	0.01673	0.05750	0.02101	0.00212	0.00605	0.00325	0.00521	0.00654	0.00896	0.05849	0.20199	0.15460	0.07960	0.00269	0.00528
Sum C-1 Phen./Anthracenes	0.06938	0.21430	0.08637	0.00942	0.01792	0.00735	0.01347	0.01797	0.03274	0.20485	0.68185	0.57096	0.18790	0.00496	0.01106
Sum C-2 Dibenzothiophenes	0.02177	0.07841	0.02651	0.00193	0.01521	0.00536	0.00973	0.00657	0.01189	0.07557	0.32920	0.28927	0.10365	0.00479	0.00836
Sum C-2 Phen./Anthracenes	0.07716	0.24058	0.10543	0.01002	0.04755	0.01539	0.02759	0.02018	0.03874	0.22733	0.90933	0.88043	0.27090	0.01376	0.02752
Sum C-3 Dibenzothiophenes	0.01659	0.06110	0.01755	0.00145	0.02035	0.00914	0.01558	0.00743	0.00946	0.05400	0.29062	0.28759	0.10853	0.00628	0.00975
Sum C-3 Phen./Anthracenes	0.03920	0.12300	0.03880	0.00308	0.04160	0.01746	0.02680	0.01479	0.02100	0.11692	0.61655	0.60655	0.21154	0.01300	0.02365
Sum C-4 Phen./Anthracenes	0.01453	0.04191	0.01438	0.00123	0.02096	0.01091	0.01690	0.01344	0.00840	0.04161	0.23972	0.26589	0.08886	0.00791	0.01236
Fluoranthene	0.00162	0.00156	0.00035	0.00151	0.00077	0.00140	0.00333	0.00224	0.00085	0.00069	0.00202	0.00155	0.00113	0.00051	0.00042
Pyrene	0.00193	0.00326	0.00102	0.00142	0.00102	0.00132	0.00281	0.00299	0.00103	0.00235	0.00953	0.00802	0.00293	0.00055	0.00058
Sum C-1 Fluor./Pyrenes	0.01602	0.04153	0.01113	0.00404	0.01658	0.01175	0.01929	0.03434	0.00992	0.03388	0.20177	0.17739	0.05141	0.00615	0.00920
Benz[a]anthracene	0.00029	0.00021	0.00000	0.00023	0.00030	0.00083	0.00122	0.00153	0.00018	0.00013	0.00040	0.00066	0.00072	0.00021	0.00021
Chrysene	0.00035	0.00026	0.00012	0.00022	0.00032	0.00088	0.00133	0.00385	0.00020	0.00016	0.00055	0.00117	0.00101	0.00029	0.00030
Sum C-1 Chrysenes	0.00200	0.00335	0.00180	0.00419	0.00521	0.00635	0.01210	0.01510	0.00136	0.00241	0.00939	0.02174	0.01001	0.00329	0.00355
Sum C-2 Chrysenes	0.00048	0.00137	0.00094	0.00051	0.00258	0.00229	0.00440	0.00442	0.00039	0.00134	0.00572	0.01209	0.00524	0.00122	0.00165
Benzo[b]fluoranthene	0.00023	0.00015	0.00004	0.00015	0.00010	0.00031	0.00043	0.00071	0.00012	0.00010	0.00013	0.00034	0.00022	0.00010	0.00014
Benzo[k]fluoranthene	0.00019	0.00015	0.00005	0.00014	0.00010	0.00032	0.00030	0.00036	0.00012	0.00006	0.00021	0.00019	0.00021	0.00007	0.00007
Benzo[e]pyrene	0.00017	0.00012	0.00004	0.00012	0.00009	0.00022	0.00030	0.00044	0.00010	0.00007	0.00014	0.00018	0.00018	0.00007	0.00009
Benzo[a]pyrene	0.00022	0.00015	0.00004	0.00013	0.00007	0.00025	0.00033	0.00056	0.00012	0.00008	0.00013	0.00018	0.00019	0.00007	0.00009
Perylene	0.00009	0.00006	0.00003	0.00008	0.00006	0.00014	0.00017	0.00020	0.00006	0.00004	0.00010	0.00008	0.00011	0.00004	0.00005
Indeno[123-cd]pyrene	0.00013	0.00011	0.00003	0.00007	0.00003	0.00018	0.00021	0.00028	0.00008	0.00006	0.00007	0.00006	0.00016	0.00005	0.00005
Dibenz[ah]anthracene	0.00003	0.00004	0.00000	0.00003	0.00000	0.00008	0.00008	0.00011	0.00003	0.00002	0.00002	0.00002	0.00006	0.00002	0.00002
Benzo[ghi]perylene	0.00014	0.00012	0.00003	0.00008	0.00003	0.00020	0.00016	0.00019	0.00007	0.00006	0.00007	0.00004	0.00018	0.00004	0.00003
Sum Total TUs:	0.664	2.334	0.671	0.081	0.241	0.112	0.195	0.172	0.337	2.758	5.561	4.819	1.634	0.082	0.147
% Mortality :	no data	no data	70	7	17	7	3	0	no data	95	100	100	97	23	3

organic carbon for HR1 (ST E1) is 0.5%
organic carbon for HR2 (ST E2) is 1.3%

Table 12D. PAH Concentrations and effect data from North Cape Oil Spill (Ho et al. 1999) (Continued)

PAH	MW (g/mol)	log K _{ow}	<i>A. abdita</i> TLM Endpoint (μmol/goc)
naphthalene	128.17	3.256	34.1
C1-naphthalenes	142.20	3.788	36.1
C2-naphthalenes	156.23	4.244	37.9
C3-naphthalenes	170.25	4.730	40.0
fluorene	166.22	3.930	36.6
C1-fluorenes	180.25	4.370	38.4
C2-fluorenes	194.27	4.819	40.3
C3-fluorenes	208.30	5.318	42.6
Dibenzothiophene	184.20	4.340	38.3
phenanthrene	178.23	4.584	39.3
anthracene	178.23	4.546	39.2
C1-Dibenzothiophene	198.30	4.859	40.5
C1-phenanthrenes	192.26	5.037	41.3
C2-Dibenzothiophene	212.30	5.332	42.6
C2-phenanthrenes	206.29	5.455	43.2
C3-Dibenzothiophene	226.30	5.810	44.9
C3-phenanthrenes	220.32	5.907	45.4
C4-phenanthrenes	234.34	6.357	47.7
fluoranthene	202.26	5.190	42.0
Pyrene	202.26	5.126	41.7
C1-fluoranthenes	216.28	5.257	42.3
benzo(a)anthracene	195.00	5.744	44.6
chrysene	228.29	5.782	44.8
C1-Chyrsenes	242.32	6.190	46.8
C2-Chyrsenes	256.34	6.593	48.9
benzo(b)fluoranthene	252.32	6.341	47.6
benzo(k)fluoranthene	252.32	6.400	47.9
Benzo(e)pyrene	252.31	6.447	48.1
Benzo(a)pyrene	252.31	6.409	47.9
perylene	252.31	6.447	48.1
indeno(1,2,3-cd)pyrene	276.34	6.158	46.6
dibenz(a,h)anthracene	278.35	7.129	51.8
benzo(ghi)perylene	276.34	6.886	50.5
C4-naphthalenes	184.28	5.220	42.1
biphenyl	154.21	3.936	64.2
acenaphthylene	152.20	3.436	34.7
acenaphthene	154.21	3.878	36.4
C3-Chyrsenes	270.36	6.972	50.9
C4-Chyrsenes	284.38	7.421	53.5

Appendix E

Example Calculations

APPENDIX E

EXAMPLE CALCULATIONS

Example calculations using fathead minnows, benzene and phenanthrene.

Benzene Physical Chemical Properties (Table 1)

$\log K_{OW} = 1.943$
 $MW = 78.11 \text{ g/mole}$

TLM Coefficients (Table A)

$\log CTLBB = \log (c_L^*) = 2.087$
 $SE (\log (c_L^*)) = 0.044$
 $Variance (\log (c_L^*)) = SE (\log (c_L^*))^2 = (0.044)^2 = 0.001936$
 $k_z = 1.87$

$m = \text{slope} = -0.936$
 $SE \text{ slope} = 0.015$
 $Variance \text{ slope} = (SE \text{ slope})^2 = (0.015)^2 = 0.000225$
 $\Delta C \text{ MAH chemical class correction} = -0.109$
 $\Delta C \text{ PAH chemical class correction} = -0.352$

(1) What is water-only acute LC50 of benzene?

$$\log(C_{W_1}^*) = \log(LC50) = m \log(K_{OW}) + \log(C_L^*) + \Delta C \quad (\text{Equation 1})$$

$$\log(LC50) = (-0.936)(1.943) + (2.087) + (-0.109)$$

$$\log(LC50) = 0.159$$

$$LC50 = 1.44 \text{ mmol/L} = 112 \text{ mg/L}$$

Phenanthrene Physical Chemical Properties (Table 1)

$\log K_{OW} = 4.584$
 $MW = 178.23 \text{ g/mole}$

$$ACR = 3.83$$

$$SE(ACR) = 0.324$$

$$Variance ACR = SE(ACR)^2 = (0.324)^2 = 0.105$$

(2) What is the water-only acute LC50 of phenanthrene?

$$\log(\text{LC50}) = m \log(K_{OW}) + \log(C_L^*) + \Delta C \quad (\text{Equation 1})$$

$$\log(\text{LC50}) = (-0.936)(4.584) + (2.087) + (-0.352)$$

$$\log(\text{LC50}) = -2.56$$

$$\text{LC50} = 0.00278 \text{ mmol/L} = 0.50 \text{ mg/L}$$

(3) What are the Toxic units of a mixture of 1 mg/L benzene and 1 mg/L phenanthrene?

$$\text{TU}_{\text{benzene}} = \frac{C_{w,\text{benzene}}}{C_{w,\text{benzene}}^*} = \frac{1 \text{ mg/L}}{112 \text{ mg/L}} = 0.009 \quad (\text{Equation 8})$$

$$\text{TU}_{\text{phen}} = \frac{C_{w,\text{phen}}}{C_{w,\text{phen}}^*} = \frac{1 \text{ mg/L}}{0.5 \text{ mg/L}} = 2$$

$$\text{TU}_{\text{mixture}} = \sum_i \text{TU}_{W,i} = \text{TU}_{\text{benzene}} + \text{TU}_{\text{phen}} \quad (\text{Equation 9})$$

$$\text{TU}_{\text{mixture}} = 0.009 + 2.000$$

$$\text{TU}_{\text{mixture}} = 2.009$$

(4) What is the water-only chronic effect concentration of benzene?

$$\text{ACR} = \frac{\text{Acute Effect Concentration}}{\text{Chronic Effect Concentration}} \quad (\text{Equation 2})$$

$$\text{Chronic Effect Concentration} = \frac{\text{Acute Effect Concentration}}{\text{ACR}}$$

$$\text{Chronic Effect Concentration} = \frac{112 \text{ mg/L}}{3.83}$$

$$\text{Chronic Effect Concentration} = 29.2 \text{ mg/L}$$

(5) What are the HC5 and HC95 of benzene on a chronic basis?

$$\log(\text{HC}_5) = \log(K_{ow})E\{m\} + E\{\log(C_L^*)\} - E\{\log(\text{ACR})\} - k_Z \sqrt{(\log(K_{ow}))^2 V\{m\} + V\{\log(C_L^*)\} + V\{\log(\text{ACR})\}} \quad (\text{Equation 6})$$

$$\log(\text{HC}_5) = [(-0.936)(1.943)] + [2.087 - 0.109] - (\log(3.83)) - 1.87 \sqrt{(0.000225)(1.943)^2 + 0.001936 + 0.105}$$

$$\log(\text{HC}_5) = -0.4238 - 1.87 \sqrt{0.10778}$$

$$\log(\text{HC}_5) = -1.0377$$

$$\text{HC}_5 = 0.092 \text{ mmol/L} = 7.2 \text{ mg/L}$$

$$\log(\text{HC}_{95}) = \log(K_{ow})E\{m\} + E\{\log(C_L^*)\} - E\{\log(\text{ACR})\} + k_Z \sqrt{(\log(K_{ow}))^2 V\{m\} + V\{\log(C_L^*)\} + V\{\log(\text{ACR})\}} \quad (\text{Equation 7})$$

$$\log(\text{HC}_{95}) = [(-0.936)(1.943)] + [2.087 - 0.109] - \log(3.83) + 1.87 \sqrt{(0.000225)(1.943)^2 + 0.001936 + 0.105}$$

$$\log(\text{HC}_{95}) = -0.4238 + 1.87 \sqrt{0.10778}$$

$$\log(\text{HC}_{95}) = 0.190$$

$$\text{HC}_{95} = 1.55 \text{ mmol/L} = 121 \text{ mg/L}$$

(6) What is the acute sediment effect concentration of benzene?

$$\log(C_s^*) = 0.00028 + 0.047(\log K_{OW}) + \log(C_L^*) + \Delta C \quad (\text{Equation 5})$$

$$\log(C_s^*) = 0.00028 + (0.047)(1.943) + 2.087 - 0.109$$

$$\log(C_s^*) = 2.0696$$

$$(C_s^*) = 117 \mu\text{mol/g}_{OC} = 9100 \text{ mg/Kg}_{OC}$$

Appendix F

**HC5 and HC95
Summary Calculations for PAHs**

Table F1. Calculation of MAH and PAH HC5 for aquatic toxicity and sediment toxicity

slope	-0.936
Average log (C _L [*])	2.088
average log (ACR)	0.583
k _Z ¹	2.3
variance of slopes	0.000225
variance log (C _L [*])	0.104
variance of log (ACR)	0.105

¹ k_Z based on number of ACRs

Chemical	log K _{ow}	log (K _{oc})	Molecular Weight (g/mol)	Chemical class adjustment factor	Chronic log HC5 (mmol/L)	Chronic HC5 (µmol/L)	Chronic HC5 (µg/L)	Solid Solubility (µg/L)	Chronic HC5 (mmol/kgoc)	Chronic HC5 (mg/kgoc)
benzene	1.943	1.910	78.11	-0.109	-1.476	33	2609	1780000	2.72	212
toluene	2.438	2.397	92.14	-0.109	-1.941	11.4602	1056	515000	2.86	263
o-xylene	2.946	2.896	106.17	-0.109	-2.418	3.8209	406	220000	3.01	319
ethylbenzene	3.006	2.955	106.17	-0.109	-2.474	3.3558	356	152000	3.03	321
m-xylene	3.032	2.981	106.17	-0.109	-2.499	3.1723	337	160000	3.03	322
p-xylene	3.051	2.999	106.17	-0.109	-2.516	3.0446	323	215000	3.04	323
naphthalene	3.256	3.201	128.19	-0.352	-2.952	1.1167	143	31000	1.77	227
acenaphthylene	3.436	3.378	152.20	-0.352	-3.121	0.7564	115	16100	1.81	275
C3-benzenes	3.455	3.397	120.00	-0.109	-2.896	1.2703	152	19700	3.17	380
1-methylnaphthalene	3.781	3.717	142.20	-0.352	-3.446	0.3585	51.0	28000	1.87	266
C1-naphthalenes	3.788	3.724	142.20	-0.352	-3.452	0.3531	50.2	7900	1.87	266
2-methylnaphthalene	3.789	3.725	142.20	-0.352	-3.453	0.3523	50.1	25000	1.87	266
acenaphthene	3.878	3.812	154.21	-0.352	-3.537	0.2906	44.8	3800	1.89	291
fluorene	3.930	3.863	166.20	-0.352	-3.586	0.2596	43.1	1900	1.90	315
biphenyl	3.936	3.869	154.21	-0.109	-3.348	0.4484	69.2	7000	3.32	512
2-chloronaphthalene	3.940	3.873	162.64	-0.691	-3.934	0.1164	18.9	5500	0.87	141
1-chloronaphthalene	3.950	3.883	162.64	-0.691	-3.943	0.1139	18.5	5400	0.87	142
C2-naphthalenes	4.244	4.172	156.23	-0.352	-3.881	0.1315	20.5	1970	1.95	305
1,3-dimethylnaphthalene	4.257	4.185	156.23	-0.352	-3.893	0.1279	20.0	8000	1.96	306
methylbiphenyl	4.259	4.187	168.23	-0.109	-3.652	0.2228	37.5	4050	3.43	576
2,6-dimethylnaphthalene	4.270	4.198	156.23	-0.352	-3.905	0.1243	19.4	1700	1.96	306
1,2-dimethylnaphthalene	4.270	4.198	156.23	-0.352	-3.905	0.1243	19.4	1800	1.96	306
dibenzothiophene	4.340	4.267	184.26	-0.352	-3.971	0.1068	19.7	1110	1.97	364
1-methylfluorene	4.370	4.296	180.25	-0.352	-4.000	0.1001	18.0	1090	1.98	357
C1-fluorenes	4.370	4.296	180.25	-0.352	-4.000	0.1001	18.0	1510	1.98	357
anthracene	4.546	4.469	178.20	-0.352	-4.165	0.0684	12.2	45	2.01	359
2,3,5-trimethylnaphthalene	4.570	4.493	170.20	-0.352	-4.188	0.0649	11.0	580	2.02	343
2,3,6-trimethylnaphthalene	4.570	4.493	170.20	-0.352	-4.188	0.0649	11.0	740	2.02	343
phenanthrene	4.584	4.506	178.23	-0.352	-4.201	0.0630	11.2	1100	2.02	360
dimethylbiphenyl	4.692	4.613	182.00	-0.109	-4.060	0.0872	15.9	530	3.57	650

Table F1. Calculation of MAH and PAH HC5 for aquatic toxicity and sediment toxicity (Continued)

Chemical	log K_{ow}	log (K_{oc})	Molecular Weight (g/mol)	Chemical class adjustment factor	Chronic log HC5 (mmol/L)	Chronic HC5 (μ mol/L)	Chronic HC5 (μ g/L)	Solid Solubility (μ g/L)	Chronic HC5 (mmol/kgoc)	Chronic HC5 (mg/kgoc)
C3-naphthalenes	4.730	4.650	170.25	-0.352	-4.338	0.0459	7.81	440	2.05	349
C2-fluorenes	4.819	4.737	194.27	-0.352	-4.422	0.0378	7.35	380	2.07	401
C1-Dibenzothiophene	4.859	4.777	198.30	-0.352	-4.460	0.0347	6.88	340	2.07	411
9-methylanthracene	4.996	4.911	192.26	-0.352	-4.589	0.0258	4.96	261	2.10	404
1-methylphenanthrene	5.036	4.951	192.26	-0.352	-4.626	0.0236	4.54	270	2.11	406
C1-phenanthrene/anthracene	5.037	4.952	192.26	-0.352	-4.627	0.0236	4.53	180	2.11	406
2-methylphenanthrene	5.040	4.955	192.26	-0.352	-4.630	0.0234	4.50	180	2.11	406
pyrene	5.126	5.039	202.26	-0.352	-4.711	0.0194	3.93	132	2.13	430
fluoranthene	5.190	5.102	202.26	-0.352	-4.771	0.0169	3.42	260	2.14	433
C4-naphthalenes	5.220	5.132	184.28	-0.352	-4.800	0.0159	2.92	97	2.15	396
C1-fluoranthene/pyrene	5.257	5.168	216.28	-0.352	-4.835	0.0146	3.17	101	2.15	466
C3-fluorenes	5.318	5.228	208.30	-0.352	-4.892	0.0128	2.67	80	2.17	451
C2-Dibenzothiophene	5.332	5.242	212.30	-0.352	-4.905	0.0124	2.64	78	2.17	461
3,6-dimethylphenanthrene	5.340	5.250	206.29	-0.352	-4.913	0.0122	2.52	73	2.17	448
4,6-dimethyldibenzothiophene	5.450	5.358	212.30	-0.352	-5.016	0.0096	2.04	53	2.19	466
C2-phenanthrene/anthracene	5.455	5.363	206.29	-0.352	-5.021	0.0095	1.97	51	2.20	453
C2-fluoranthene/pyrene	5.557	5.463	230.31	-0.352	-5.117	0.0076	1.76	40	2.22	510
Triphenylene	5.630	5.535	228.30	-0.352	-5.186	0.0065	1.49	43	2.23	509
benzo(a)anthracene	5.744	5.647	228.29	-0.352	-5.293	0.0051	1.16	11	2.26	515
chrysene	5.782	5.684	228.29	-0.352	-5.329	0.0047	1.07	2	2.26	517
C3-Dibenzothiophene	5.810	5.712	226.30	-0.352	-5.356	0.0044	1.00	17	2.27	514
C3-phenanthrene/anthracene	5.907	5.807	220.32	-0.352	-5.447	0.0036	0.787	12	2.29	505
Retene	6.120	6.016	234.34	-0.352	-5.648	0.0023	0.527	6.6	2.34	547
indeno(1,2,3-cd)pyrene	6.158	6.054	276.34	-0.352	-5.684	0.00207	0.573	6.9	2.34	648
C1-Chrysenes/benzo(a)anthracene	6.190	6.085	242.32	-0.352	-5.714	0.00193	0.468	5.4	2.35	570
C4-phenanthrene/anthracene	6.357	6.249	234.34	-0.352	-5.871	0.00135	0.315	3	2.39	559
benzo(b)fluoranthene	6.341	6.233	252.32	-0.352	-5.856	0.00139	0.351	1.5	2.38	602
C3-fluoranthene/pyrene	6.384	6.276	244.34	-0.352	-5.897	0.00127	0.310	2.9	2.39	585
benzo(k)fluoranthene	6.400	6.291	252.32	-0.352	-5.912	0.00123	0.309	0.8	2.40	605
benzo(a)pyrene	6.409	6.300	252.31	-0.352	-5.920	0.00120	0.303	3.8	2.40	605
7,12-dimethylbenzo(a)anthracene	6.420	6.311	256.35	-0.352	-5.931	0.00117	0.301	50	2.40	616
Benzo(e)pyrene	6.447	6.338	252.30	-0.352	-5.956	0.00111	0.279	4	2.41	607
perylene	6.447	6.338	252.31	-0.352	-5.956	0.00111	0.279	0.4	2.41	607
C2-Chrysenes/benzo(a)anthracene	6.593	6.481	256.34	-0.352	-6.094	0.00081	0.207	1.5	2.44	625
C4-fluoranthene/pyrene	6.687	6.574	258.35	-0.352	-6.183	0.00066	0.170	1.1	2.46	636
C5-phenanthrene/anthracene	6.700	6.586	248.37	-0.352	-6.195	0.00064	0.159	1.1	2.46	612
C1-benzofluoranthene	6.743	6.629	266.11	-0.352	-6.235	0.00058	0.155	1	2.47	658
benzo(ghi)perylene	6.886	6.769	276.34	-0.352	-6.370	0.00043	0.118	0.26	2.51	692
C3-Chrysenes/benzo(a)anthracene	6.972	6.854	270.36	-0.352	-6.451	0.00035	0.096	0.47	2.53	683
dibenz(a,h)anthracene	7.129	7.008	278.35	-0.352	-6.600	0.00025	0.070	0.6	2.56	713
C2-benzofluoranthene	7.200	7.078	280.13	-0.352	-6.667	0.00022	0.060	0.23	2.58	722
C4-Chrysenes/benzo(a)anthracene	7.421	7.295	284.38	-0.352	-6.875	0.00013	0.038	0.12	2.63	748