

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

**A Final Report Submitted to
The Coastal Response Research Center**

Submitted By

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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 µg/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 preformed 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 (HC_5 , mmol/L) that considers the variance in the universal narcosis slope and C_L^* . The resulting concentration is the acute HC_5 , 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 HC_5 . The final equation was presented as

$$\log(HC_5) = \log(K_{ow})E\{m\} + E\{\log(C_L^*)\} - E\{\log(ACR)\} - k_Z \sqrt{(log(K_{ow}))^2 V\{m\} + V\{\log C_L^*\} + V\{\log(ACR)\}} \quad (6)$$

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, HC_{95} , the variance term in Equation 8 is added to yield

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

The HC_5 and HC_{95} 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.

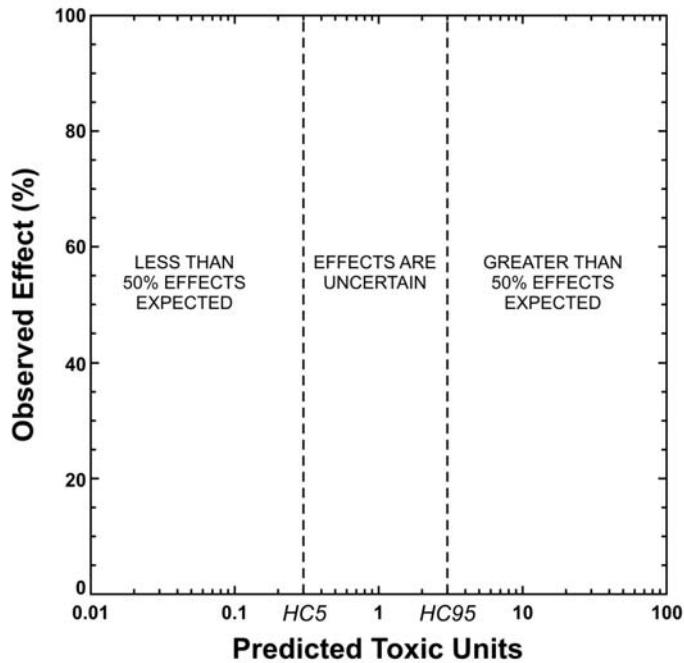


Figure 1. Diagram of how toxicity data from aqueous and sediment tests using mixtures of chemicals will be displayed. Percent effect as a function of predicted total toxic units. Solid lines present 50% effect and total toxic unit of 1.0. Dashed lines represent HC5 and HC95 values.

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., chrysene and fluoranthene) 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 (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.

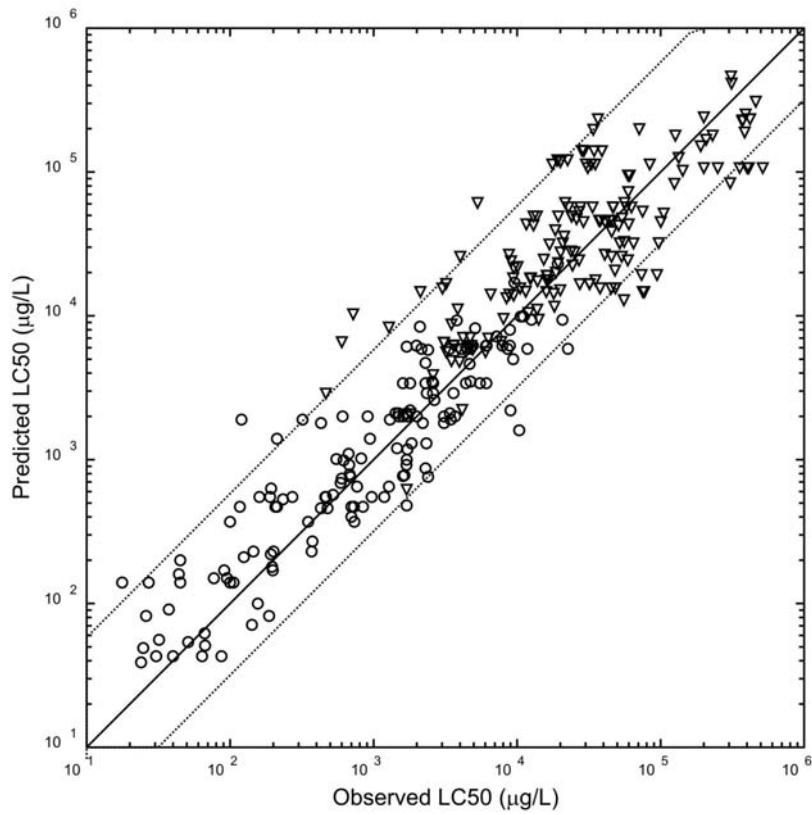


Figure 2. Acute Exposures- Single Compounds - TLM predicted acute LC50 versus observed LC50 for monoaromatic hydrocarbons (▼) and PAHs (○). Solid line represents 1:1 relationship. Dashed lines represent 90% confidence interval

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

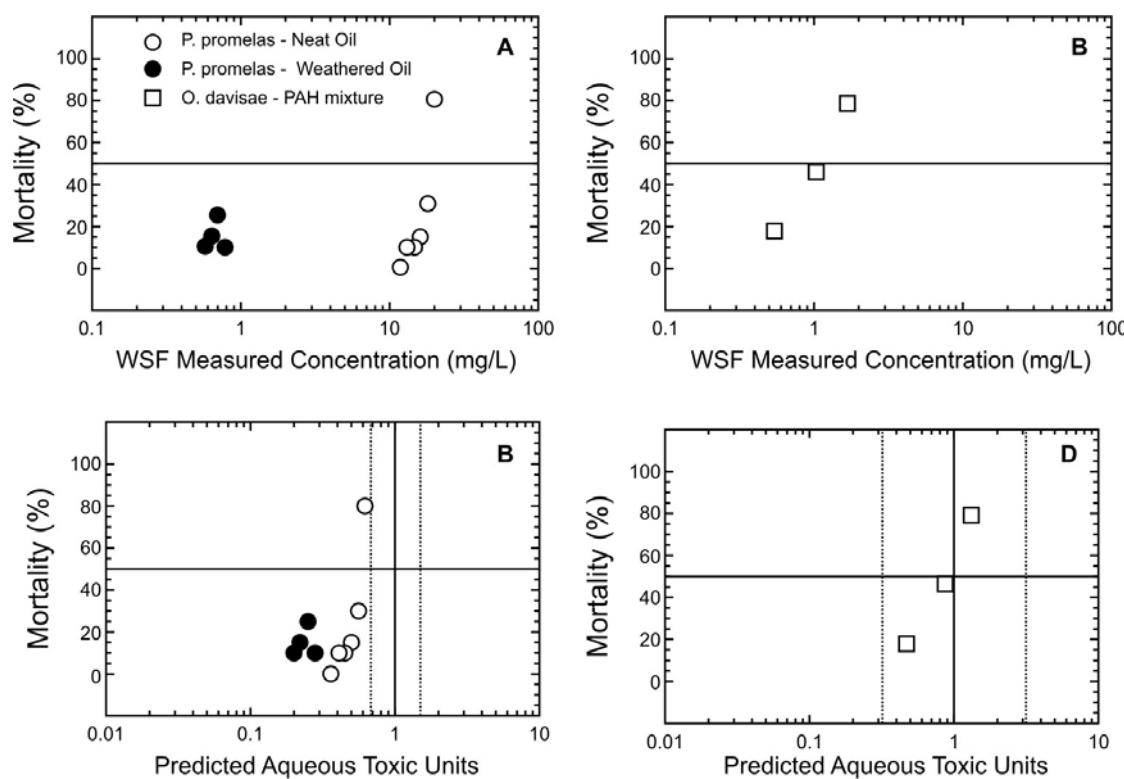


Figure 3. Acute Exposures- Mixtures - Percent mortality as a function of total measured concentration (mg/L) (top panels) and predicted aqueous toxic units (bottom panels). Data on the right is for *Pimephales promelas* exposure to WSFs prepared from neat and weathered Exxon Valdez crude oil (ENSR, 2000). 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 contain 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 fall on the high end 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.

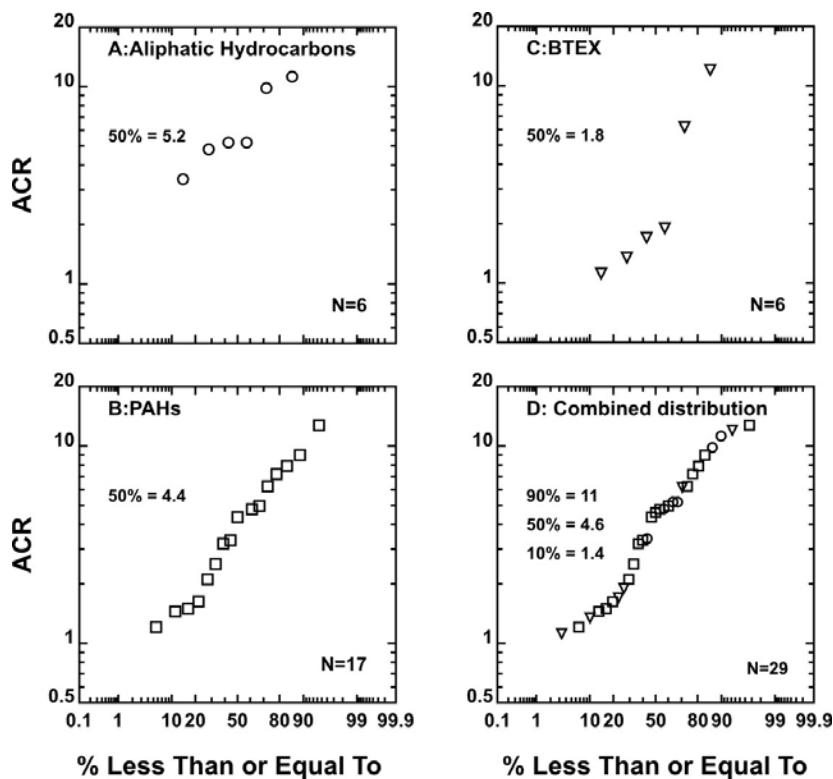


Figure 4. Chronic Effects – Single Compounds - Distribution of acute to chronic ratios (ACRs) for aliphatic hydrocarbons (A), PAHs (B), BTEX (C) and the combined data set (D).

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 variegatus*, *Fundulus heteroclitus* and *Fundulus similis*. A CTLBB is only available for *C. variegatus* 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.

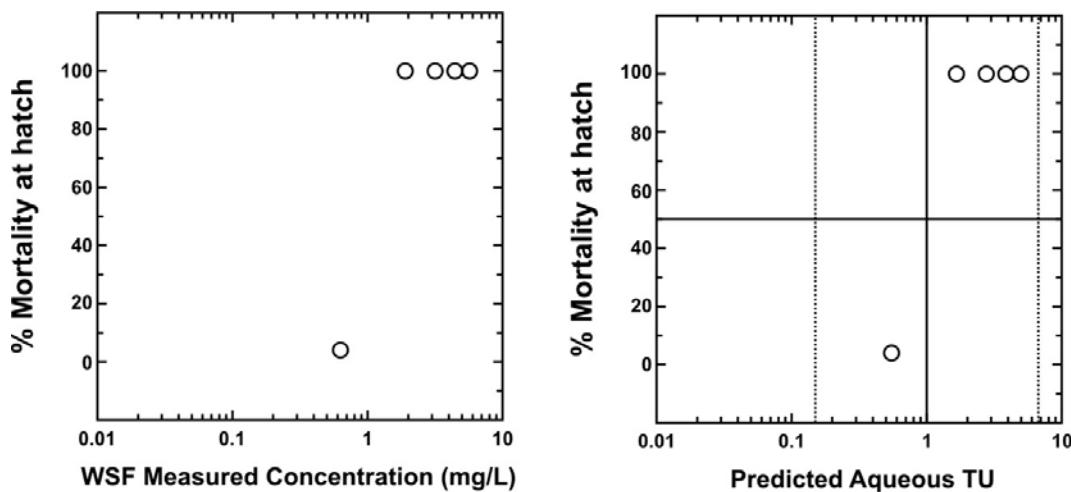


Figure 5. Chronic Effects – Mixtures – Observed mortality as a function of total measured concentration in WSF (mg/L) (left panel) and predicted aqueous toxic units (right panel). Data are for *Cyprinodon variegatus* embryos exposed to WSF prepared from No. 2 fuel oil (Anderson et al. 1977). Dashed lines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

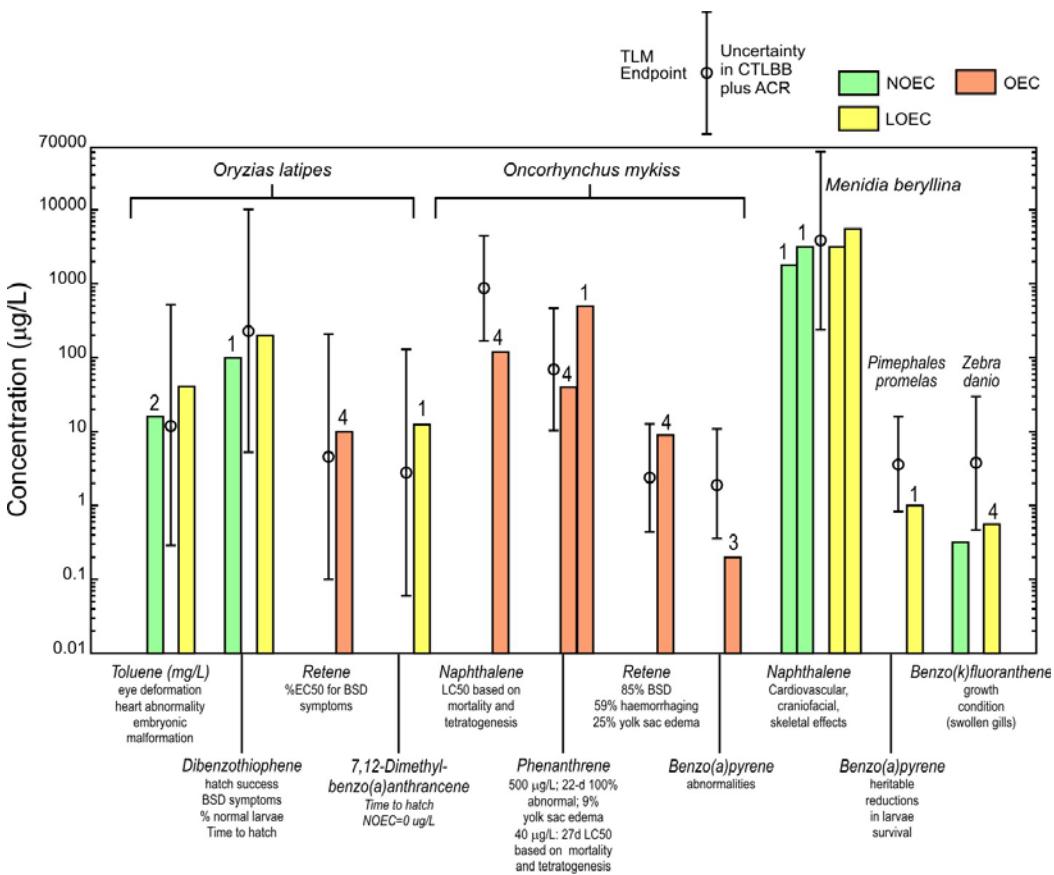


Figure 6. Sublethal effects – Single Compounds – Comparison of OEC/LOEC/NOEC observed from early life stage fish exposures to single compounds to TLM chronic effect concentrations. The effects are those associated with sublethal endpoints such as abnormal larvae development and blue sac disease-like 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 sub-lethal effects in early life stage pink salmon (*Oncorhynchus gorbuscha*) and pacific herring (*Clupea pallasi*) (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 µg TPAH/L, respectively. The TLM chronic endpoint for the parent mixture was 80 µgTPAH/L. The only observed effect from the dimethylated PAH mixture was % hatch, where the NOEC and LOEC values were 25 and 50 µgTPAH/L, respectively. The TLM chronic endpoint for the dimethylated parent mixture was 15 µgTPAH/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 µgTPAH/L, respectively. Hatch length was effected at lower concentrations of the oil sands extract with NOEC and LOEC values of 0 and 2.2 µgTPAH/L, respectively. The TLM chronic endpoint for the oil sands mixture was 10 µg/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 µg/L, which was below the average TLM endpoint of 10 µg/L. However, the HC5 of 0.2 µg/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.

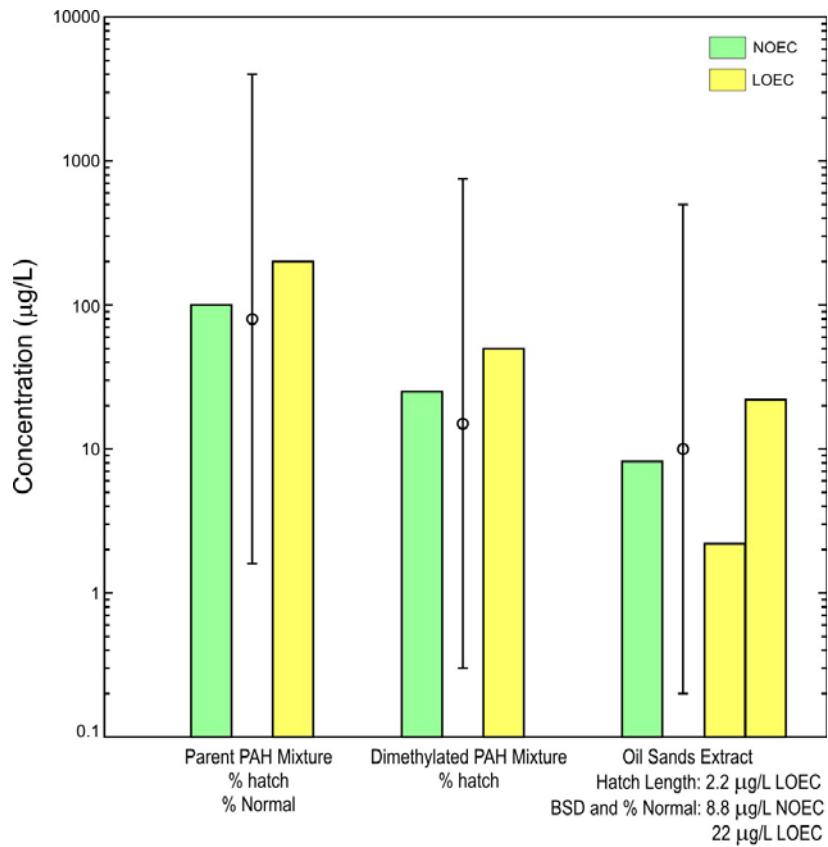


Figure 7. Sublethal effects – Mixtures – Comparison of 18-d NOEC and LOEC from early life stage toxicity tests exposing *Oryzias latipes* to three prepared mixtures of PAHs to TLM chronic endpoints. The symbols represent the TLM effect concentration. The bars represent the 5th and 95% percentiles based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

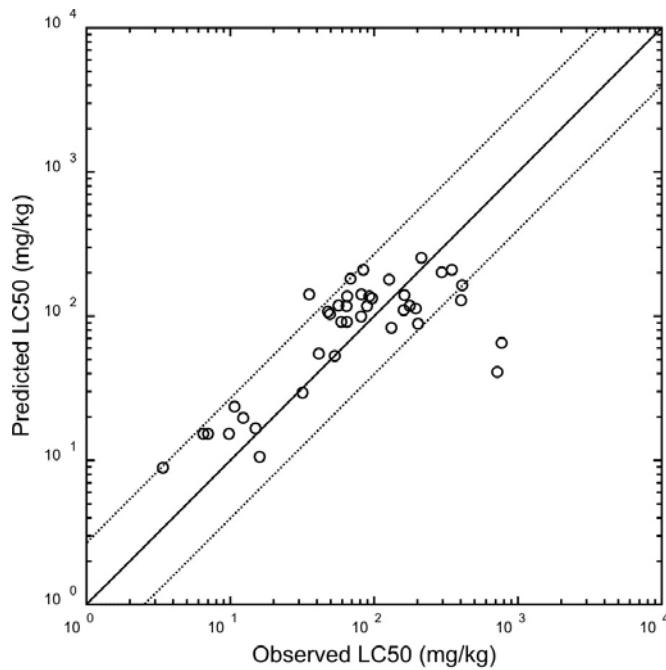


Figure 8. Acute Sediment Exposures – Single Compound - Comparison of observed and TLM predicted sediment effect concentrations (see Table 5 for data). Solid line is 1:1 relationship. The dashed lines are 90% confidence intervals.

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.

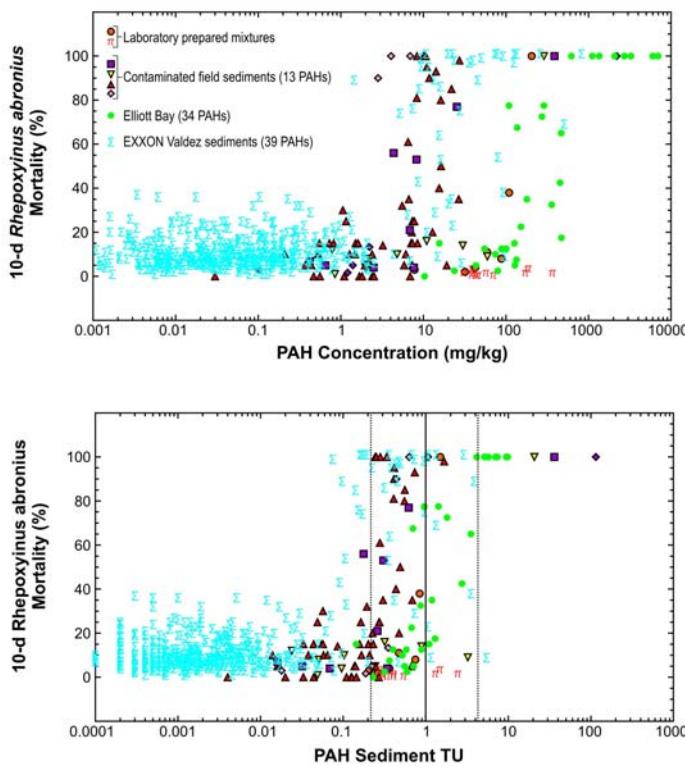


Figure 9. Acute Sediment Exposures – Mixtures – Percent mortality of *Rhepoxyinus abronius* as a function of PAH concentraton (mg/kg) (top panel) and normalized to total PAH sediment toxic units (bottom panel). All data are 10-d exposures. See Table 6 for references. Solid lines at a toxic unit of 1.0 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.

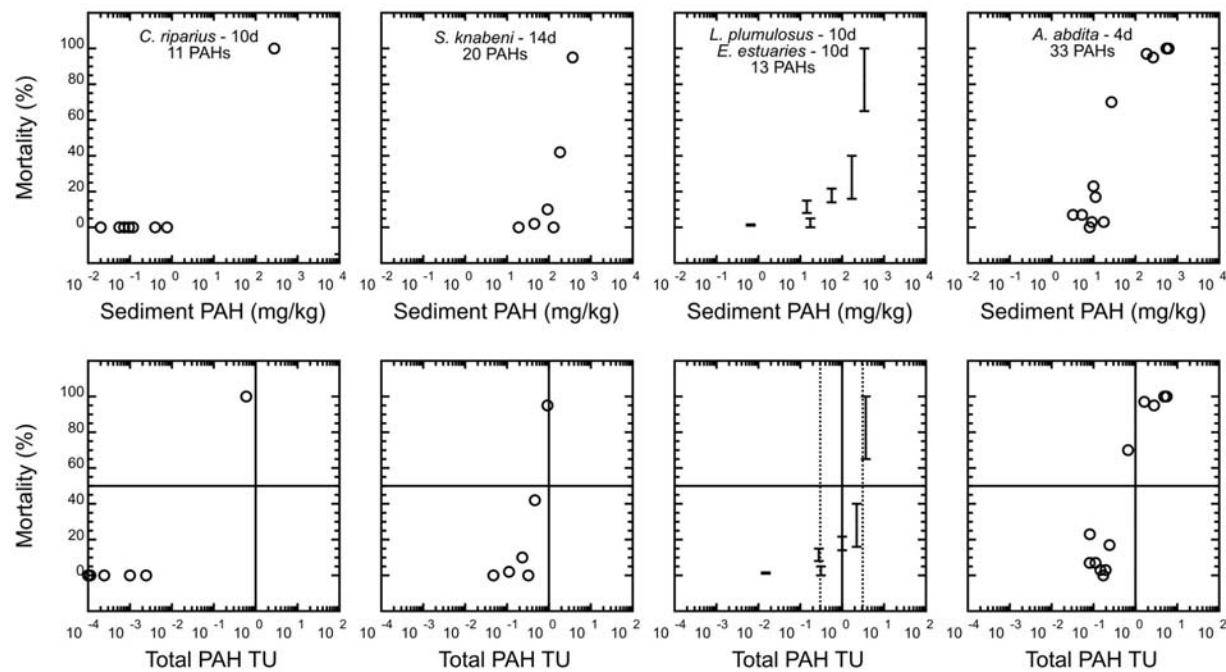


Figure 10. Acute Sediment Exposures – Mixtures – Percent mortality as a function of PAH concentration (mg/kg) (top panel) and normalized to total PAH sediment toxic units (bottom panel). See Table 6 for exposure information. Solid lines at a toxic unit of 1.0 and 50 % mortality are shown for guidance.

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 test 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 $\mu\text{g/g}_{\text{oc}}$ for grazing and reproduction, respectively. The 10-d NOECs ranged from 1200 to 3111 $\mu\text{g/g}_{\text{oc}}$. The TLM predicted chronic effect concentration is 1410 $\mu\text{g/g}_{\text{oc}}$, 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 $\mu\text{g/g}_{\text{oc}}$ for reproduction

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

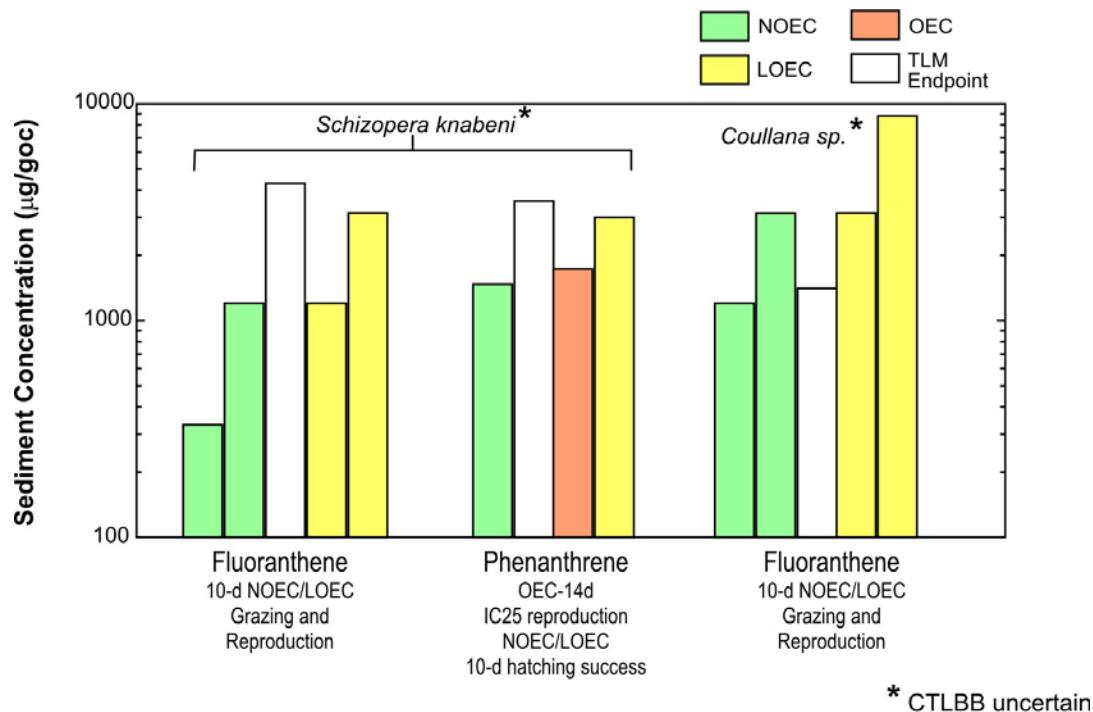


Figure 11. Chronic Sediment Exposures – Single Compounds - Comparison of reported OEC/LOEC/NOEC and TLM effect concentrations from long-term exposures of fluoranthene and phenanthrene to marine copepods *Coullana* sp. and *Schizopera knabeni*. See Table 8 for references.

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 umol/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 Δc 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/KgOC) and a mass basis (i.e., $\mu\text{g/L}$, mg/KgOC). 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.

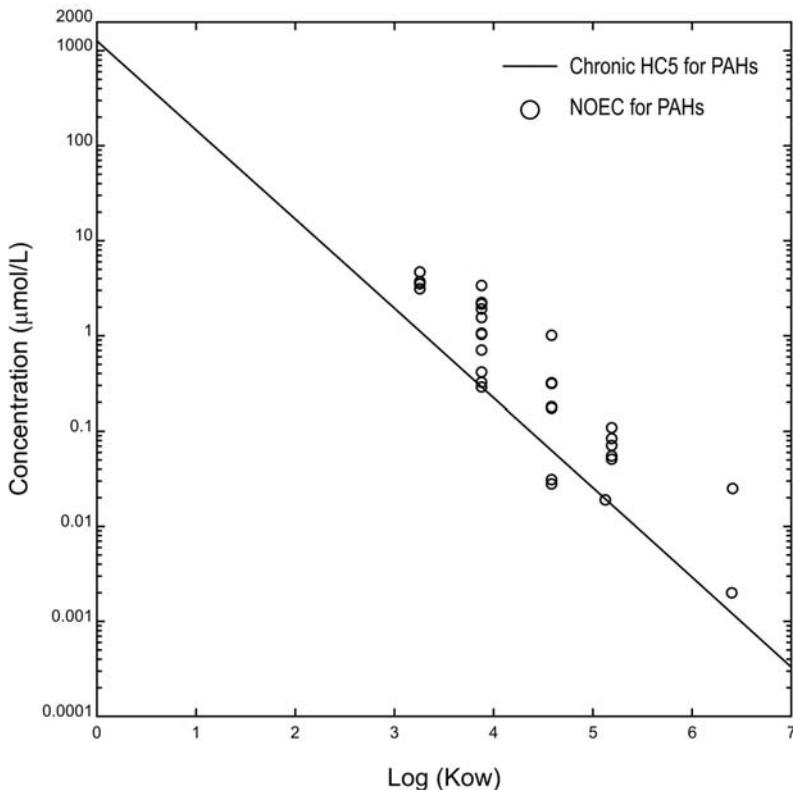


Figure 12. Chronic HC5 concentration for PAHs versus log (K_{ow}). The HC5 concentration is based on the 5th percentile CTLBB for all species in database. The observed NOECs for PAH are denoted with a ○ (Table 10).

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		
			Solid Solubility (µg/L) ^b	Solubility (µg/L) ^{b,d}	Key PAHs ^e
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-methylnaphthalene	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		
			Solid Solubility (µg/L) ^b	Solubility (µg/L) ^{b,d}	Key PAHs ^e
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-fluoranthenes/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-dimethylbenzothiophene	5.450	212.30	53	1100	
C2-phenanthrene/anthracene ^c	5.455	206.29	51	1000	C
C2-fluoranthenes/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-fluoranthenes/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-Chrysene/benzo(a)anthracene ^c	6.593	256.34	1.5	130	C
C4-fluoranthenes/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-Chrysene/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-Chrysene/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 belowSolid solubility computed from Log S = (-1.4136)(LogK_{ow}) + 7.1022 where solubility has units of µmol/LSub-cooled solubility computed from Log S = (-0.8857)(LogK_{ow}) + 5.5367 where solubility has units of µmol/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 ($\mu\text{g/L}$)	Predicted LC50 ($\mu\text{g/L}$)	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 ($\mu\text{g/L}$)	Predicted LC50 ($\mu\text{g/L}$)	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-methylnanthracene	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
<i>Ictalurus punctatus</i>	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
	phenanthrene	unknown	S,M	100	370	Trucco et al. 1983
<i>Lepomis macrochirus</i>	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>Leptochirus plumulosus</i>	acenaphthene	juvenile	S,U	1700	2100	Buccafusco et al. 1981
	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>Menidia beryllina</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>Mysidopsis bahia</i>	acenaphthene	juvenile	R,U	5564 ^a	4700	Thursby, 1991
	acenaphthene	unknown	S,U	2300	4700	Horne et al. 1983
	fluoranthene	unknown	R,U	616 ^a	360	Spehar et al. 1999
	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
<i>Oithona davisae</i>	phenanthrene	immature young adult	S,U	600	740	Rossi and Neff, 1978
	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
<i>Oncorhynchus mykiss</i>	fluoranthene	adult	S,M	196	180	Barata et al. 2005
	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
<i>Palaemonetes pugio</i>	fluoranthene	unknown	S,M	187	82	Horne and Oblad, 1983
	fluoranthene	juvenile	FT,M	26	82	Spehar et al. 1999
	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
<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
<i>Tanytarsus dissimilis</i>	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
	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
<i>Rhepoxygnus abronius</i>	benzo(a)pyrene	unknown	R	13400 ^a	18	Propst et al. 1997
	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-methylnanthracene	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.

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 ($\mu\text{g/L}$)	HC5 ($\mu\text{g/L}$)	HC95 ($\mu\text{g/L}$)	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 $\mu\text{g/L}$; NOEC = 100 $\mu\text{g/L}$	240	5.3	10300	1	Rhodes et al. 2005
	4,6-dimethyldibenzothiophene	Static renewal	Nominal	No effects observed at water solubility of 53 $\mu\text{g/L}$		32	0.71	1440	1	Rhodes et al. 2005
	benzo(a)anthracene	Static renewal	Nominal	No effects observed at water solubility of 11 $\mu\text{g/L}$		14	0.31	650	1	Rhodes et al. 2005
	Retene	PCD (partition controlled delivery)-constant	Measured	17 day EC50 for BSD	10 $\mu\text{g/L}$	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 $\mu\text{g/L}$; NOEC = 0 $\mu\text{g/L}$	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 $\mu\text{g/L}$	880	170	4500	4	Black et al. 1983
	Phenanthrene	Flow-through	Measured	27 day LC50; (based on mortality and teratogenesis)	40 $\mu\text{g/L}$	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 $\mu\text{g/L}$	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 $\mu\text{g/L}$	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 ($\mu\text{g/L}$)	HC5 ($\mu\text{g/L}$)	HC95 ($\mu\text{g/L}$)	Ranking ¹	Reference
	Benzo(a)pyrene	Static renewal	Measured	36d - hatching duration; abnormalities	LOEC = 0.37 $\mu\text{g/L}$ (hatch); LOEC = 0.21 $\mu\text{g/L}$	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 $\mu\text{g/L}$; NOEC = 1800 $\mu\text{g/L}$	3900	240	62000	1	Middaugh et al. 1988
				2 to 4 cell stage - LOEC for craniofacial and skeletal effects	LOEC = 5600 $\mu\text{g/L}$; NOEC = 3200 $\mu\text{g/L}$					
<i>Pimephales promelas</i> (fathead minnow)	Benzo(a)pyrene	Static renewal	Nominal	heritable reductions in larvae survival- LOEC	1 $\mu\text{g/L}$	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 $\mu\text{g/L}$; NOEC = 0.23 $\mu\text{g/L}$	3.8	0.47	30	4	Hooftman and Ruiter, 1992a
				42 days - deformities and haemorrhages	LOEC = 1.0 $\mu\text{g/L}$					

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		TLM Predicted LC50 (mg/g _{oc})	TLM Predicted LC50 (mg/kg)	Reference	
					LC50 (mg/kg dry)	TOC (mg/kg)				
<i>Rheoxynius 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 estuaricus</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>Rhepoxygnus abronius</i>	10 day mortality	Swartz et al. 1997
PAH contaminated sediment (Halifax Harbor, Nova Scotia)	13 Parent PAHs	11	<i>Rhepoxygnus 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 estuarium</i>	10 day mortality	DeWitt et al. 1992
PAH contaminated sediment (Eagle Harbor, Washington)	13 Parent PAHs	10	<i>Rhepoxygnus abronius</i>	10 day mortality	Tetratech, 1986
PAH contaminated sediment (San Diego Bay, California)	13 Parent PAHs	54	<i>Rhepoxygnus abronius</i>	10 day mortality	Swartz et al. unpublished data
PAH contaminated sediment (Eagle Harbor, Washington)	13 Parent PAHs	8	<i>Rhepoxygnus abronius</i>	10 day mortality	Swartz et al. 1989
PAH contaminated sediment (Elliott Bay, Washington)	40 PAHs (parent and alkylated)	30	<i>Rhepoxygnus abronius</i> <i>Leptocheirus plumulosus</i>	10 day mortality	Ozretich et al. 2000
Laboratory prepared mixtures	2 to 6 PAHs	12	<i>Rhepoxygnus 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>Rhepoxygnus 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	no	0.559	yes	yes	yes
STA 27-3	80.0	0.201	no	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	no	0.491	yes	yes	yes
STA 28-1	100.0	0.103	no	no	no	0.283	no	no	no
STA 28-2	95.0	0.151	no	no	no	0.417	yes	yes	yes
STA 28-3	100.0	0.089	no	no	no	0.244	no	no	no
STA 28-4	100.0	0.123	no	no	no	0.337	no	no	no
STA 28-5	100.0	0.092	no	no	no	0.253	no	no	no
STA 28-6	90.0	0.150	no	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			
		13 PAH TU	Toxic based on 13 PAH TU	Correct prediction? ¹	Was Criterion Protective? ²		Correct prediction? ¹	Was Criterion Protective? ²	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	no	0.279	no	no	no	
STA28 36%	81.0	0.149	no	no	no	0.410	yes	yes	yes	
STA28 60%	93.0	0.268	no	no	no	0.738	yes	yes	yes	
STA28 100%	98.0	0.608	yes	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 Fleeger and Lotufo, 1999; Lotufo, 1997
			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
			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 ^{Δc_ℓ}	
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-fluorennes	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-fluorennes	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-Chrysenes/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-Chrysenes/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-Chrysenes/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-Chrysenes/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
Phenanthrene	<i>Cyprinodon variegatus</i>	28-d NOEC Survival	520	Ward et al. 1981
	<i>Daphnia magna</i>	21-d NOEC - Reproduction	180	Hooftman and Evers-de Ruiter, 1992b, c
	<i>Daphnia magna</i>	21-d NOEC - Survival	56	Hooftman and Evers-de Ruiter, 1992b, c
	<i>Daphnia magna</i>	21-d NOEC - Growth	32	Hooftman and Evers-de Ruiter, 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 Ruiter, 1992b, c
	<i>Oncornynus mykiss</i>	90-d NOEC - Survival/Growth	5	Call et al. 1986
Fluoranthene	<i>Americamysis bahia</i>	32-d NOEC Survival	5.5	Kuhn and Lussier, 1987
	<i>Brachydanio rerio</i>	41-d NOEC - Growth	22	Hooftman and Evers-de Ruiter, 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 Ruiter, 1992a
Benzo(a)pyrene	<i>Brachydanio rerio</i>	42-d NOEC - Growth	6.3	Hooftman and Evers-de Ruiter, 1992c

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Appendix A

Regression Coefficients for Target Lipid Model

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-Yakooob 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				x
Khan et al. 1994		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				x
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		x		
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			
Niederlechner 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	
Niederlechner 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		x	
Rice and Thomas, 1989				
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

⁴ Toxic effects not observed for all organisms

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

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

⁷ May also be a phototoxicity issue.

⁸ Contaminant 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			x	
Winkler et al. 1983			x	
Woodward et al. 1981	x		x	

Table B2. Summary of Sediment Literature reviewed

Reference	Did not conform to EPA Guidelines for performing								No Organic Carbon measurement	Mixture Concentrations/Endpoints reported as Total PAHs/TPH/Total Oil/%WSF
	Acute Data	Chronic Data	Accepted	Not Accepted	Feeding issue	Spiked sediments not at equilibrium	Spiked sediment stored too long (greater than 120 days)			
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 Dillon, 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					
Huusonen 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			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							

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			
Bhattacharya 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					
Hyotylainen 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	Did not conform to EPA Guidelines for performing								
	Acute Data	Chronic Data	Accepted	Not Accepted	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
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			
Wilcoxen 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					
Verrhest 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	Predicted	Reference
		LC50 (mg/L)	LC50 (mg/L)	
<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
<i>Lepomis macrochirus</i>	biphenyl	4.0	4.8	Di Toro et al. 2000
	benzene	22	121	Di Toro et al. 2000
	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	McGrath et al. 2004
	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
<i>Daphnia pulex</i>	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>Tetrahymena elliotti</i>	benzene	305	84	Di Toro et al. 2000
	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	
<i>Carassius auratus</i>	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	
	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	
<i>Palaemonetes pugio</i>	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	
<i>Poecilia reticulata</i>	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	
	benzene	27.0	53	Di Toro et al. 2000	
	toluene	9.5	21	Di Toro et al. 2000	
<i>Hydra oligactis</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	
<i>Xenopus laevis</i>	ethylbenzene	97	32	Di Toro et al. 2000	
	benzene	34	197	Di Toro et al. 2000	
	benzene	190	151	Di Toro et al. 2000	
	benzene	231	179	Di Toro et al. 2000	
	benzene	370	225	Di Toro et al. 2000	
<i>Lymnaea stagnalis</i>	Gambusia affinis	386	188	Di Toro et al. 2000	
	Ambystoma mexicanum	toluene	56	13	Di Toro et al. 2000
	Mysidopsis bahia	benzene	28.3	141	Di Toro et al. 2000
	Leucisus idus melanotus	benzene	20.0	117	Di Toro et al. 2000
	Oryzias latipes	toluene	54.0	48	Di Toro et al. 2000
<i>Scenedemus subspicatus</i>	toluene	125	83	McGrath et al. 2004	
	Selenastrum capricornutum	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 Predicted		Reference
		LC50 (mg/L)	LC50 (mg/L)	
<i>Oncorhynchus mykiss</i>	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
	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 C3. Measured concentrations and computed toxic units for different exposures (Barata et al. 2005)

PAH	TLM Predictions and Uncertainties for <i>Oithona davisae</i>					Exposure Concentration			Toxic Units		
	96 Hr LC50 ($\mu\text{g/L}$)	Acute HC5 ($\mu\text{g/L}$)	Acute HC95 ($\mu\text{g/L}$)	Acute HC5/ 96 Hr LC50	Acute HC95/ 96 Hr LC50	Exposure 1: Nominal 0.5TU ($\mu\text{g/L}$)	Exposure 2: Nominal 1.0TU ($\mu\text{g/L}$)	Exposure 3: Nominal 1.5TU ($\mu\text{g/L}$)	Exposure 1: Nominal 0.5TU	Exposure 2: Nominal 1.0TU	Exposure 3: 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		Toxic Units No.2 Fuel Oil 100% WSF	Coal Liquid 100% WSF	Toxic Units Coal Liquid 100% WSF
	for <i>Daphnia magna</i> 96 Hr LC50 (mg/L)	No.2 Fuel Oil 100% WSF (mg/L)			
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 Weight	log K _{ow}	Chronic Endpoint (mg/L)	HC5/Chronic HC95/Chronic				No 2 Fuel Oil (mg/L)	Toxic Units in 100% WSF
	(g/mol)			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
phenanthrene	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	0.003	0.1404
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		HC5 (µg/L)	HC95 (µg/L)	HC5/Chronic Endpoint	HC95/Chronic Endpoint
	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
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-dimethylbenzothiophene	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	
Unmethylated (parent) mixture	0	0	0	0	0	0	0	0.00
	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- benzothiophene (µg/L)	Nominal 3,6- phenanthrene (µg/L)	Nominal 7,12- dimethylbenzo(a)- anthracene (µg/L)	4,6-dimethylbenzo- 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	0.00
	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								
unmethylated mixture	Total PAH (µg/L)	% Normal	% Non-hatch					
	0	95.0	10					
	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						

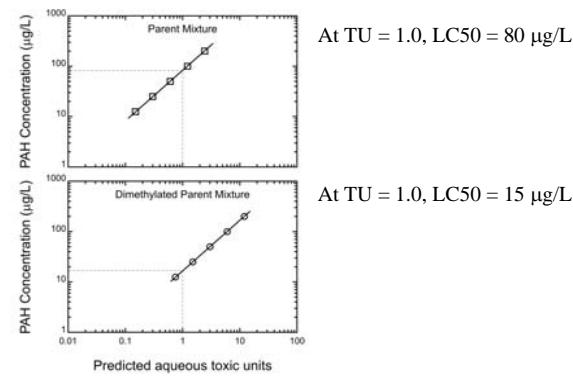
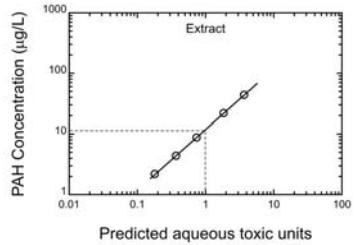


Table C7. Concentrations and computed toxic units for extract (Rhodes et al. 2005)

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
fluroanthene	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	0.06	0.02	0.01	0.00	0.00	0.00
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 LC50 (µg/g oc)	Dose 1 (mg/goc)	Dose 2 (mg/goc)	Dose 3 (mg/goc)	Dose 4 (mg/goc)	Dose 5 (mg/goc)	Dose 6 (mg/goc)	Dose 7 (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	0.196	0.125	0.088	0.067	0.053	0.039	0.031
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 D5. PAH concentrations and effect data for exposure to *R.abronius* (10-day mortality) (Swartz et al. unpublished) (Continued)

Code	PAH	MW (g/mol)	log K _{ow}	<i>R. abronius</i> 10-d TLM Endpoint (μ mol/goc)	
				TLM Endpoint (μ mol/goc)	TLM Endpoint (μ 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	antracene	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	C1-Chry	C2-Chry	Dibthioph	C1-Dibthiophe	C2-Dibthio	Total PAH (mg/kg)	
715 00 C5IA S001 IS 500 RS 1000 ppb	6462	2863	613	215	238	270	134
715 00 C5IA S002 IS 500 RS 1000 ppb	44582	17278	2320	11356	20124	10099	2079
715 00 C5IA S003 IS 500 RS 1000 ppb	98509	29185	6764	18231	23852	15393	3259
715 00 C5IA S004 IS 500 RS 1000 ppb	16029	7286	549	93	66	221	358
715 00 C5IA S005 IS 500 RS 1000 ppb	25689	12441	803	627	684	721	470
715 00 C5IA S006 IS 500 RS 1000 ppb	23707	8370	702	673	410	914	452
715 01 C5IA S007 IS 500 RS 1000 ppb	6220	3174	149	97	136	131	126
715 00 C5IA S008 IS 500 RS 1000 ppb	6874	1471	208	27	202	105	152
715 00 C5IA S009 IS 500 RS 1000 ppb	14619	4321	874	1096	2016	1339	467
715 00 C5IA S010 IS 500 RS 1000 ppb	1091	98	117	23	24	95	101
715 00 C5IA S011 IS 500 RS 1000 ppb	1048	98	408	248	140	165	109
715 00 C5IA S012 IS 500 RS 1000 ppb	9125	5442	253	128	125	257	180
715 00 C5IA S013 IS 500 RS 1000 ppb	5576	3048	403	119	110	160	128
715 00 C5IA S014 IS 500 RS 1000 ppb	175472	61633	3620	17845	28418	18344	5997
715 00 C5IA S015 IS 500 RS 1000 ppb	130889	49789	45126	63549	66983	38781	6961
715 01 C5IA S016 IS 500 RS 1000 ppb	83966	34284	1643	7893	18420	14135	2722
715 00 C5IA S017 IS 500 RS 1000 ppb	351	164	23	25	30	30	10
715 00 C5IA S018 IS 500 RS 1000 ppb	1714	998	245	106	78	49	55
715 00 C5IA S019 IS 500 RS 1000 ppb	492	149	57	44	0	0	16
715 00 C5IA S020 IS 500 RS 1000 ppb	765	865	560	210	78	95	80
715 00 C5IA S021 IS 500 RS 1000 ppb	11838	5364	1334	310	232	386	273
715 00 C5IA S022 IS 500 RS 1000 ppb	221	139	55	33	57	74	24
715 00 C5IA S023 IS 500 RS 1000 ppb	1563	332	157	0	67	0	43
715 00 C5IA S024 IS 500 RS 1000 ppb	30877	10515	1891	3230	8582	4748	1113
715 00 C5IA S025 IS 500 RS 1000 ppb	55154	16722	788	2720	4878	4129	1349
715 00 C5IA S026 IS 500 RS 1000 ppb	15772	6923	562	222	319	745	288
715 01 C5IA S027 IS 500 RS 1000 ppb	26135	8841	541	731	1523	1139	619
715 00 C5IA S028 IS 500 RS 1000 ppb	7007	3905	245	85	106	365	137
715 00 C5IA S029 IS 500 RS 1000 ppb	3802	1806	294	113	100	67	88
715 00 C5IA S030 IS 500 RS 1000 ppb	2969	1304	406	70	16	80	74

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

ID	log Kow	MW (g/mol)	<i>R. abronius</i>		
			10-d TLM Endpoint ($\mu\text{mol/goc}$)	HC5 $\mu\text{mol/goc}$	HC95 $\mu\text{mol/goc}$
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) (Continued)

PAH	<i>A. abdita</i>		
	MW (g/mol)	log K _{ow}	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-Chrysenes	242.32	6.190	46.8
C2-Chrysenes	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-Chrysenes	270.36	6.972	50.9
C4-Chrysenes	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 g/mole

Phenanthrene Physical Chemical Properties (Table 1)

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

TLM Coefficients (Table A)

$$\text{Log CTLBB} = \log (c_L^*) = 2.087$$

$$\text{SE} (\log (c_L^*)) = 0.044$$

$$\text{Variance} (\log (c_L^*)) = \text{SE} (\log (c_L^*))^2 = (0.044)^2 = 0.001936$$

$$k_z = 1.87$$

$$\text{ACR} = 3.83$$

$$\text{SE(ACR)} = 0.324$$

$$\text{Variance ACR} = \text{SE(ACR)}^2 = (.324)^2 = 0.105$$

$$m = \text{slope} = -0.936$$

$$\text{SE slope} = 0.015$$

$$\text{Variance slope} = (\text{SE slope})^2 = (0.015)^2 = 0.000225$$

$$\Delta C \text{ MAH chemical class correction} = -0.109$$

$$\Delta C \text{ PAH chemical class correction} = -0.352$$

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

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

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

$$\log(\text{LC50}) = 0.159$$

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

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

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

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

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

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

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

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

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

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

$$TU_{\text{mixture}} = 0.009 + 2.000$$

$$TU_{\text{mixture}} = 2.009$$

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

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

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

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

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

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

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

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

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

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

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

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

$$\log(\text{HC}_{95}) = [(-0.936)(1.943)] + [2.087 - 0.109] - \log(3.83) + 1.87 \sqrt{(0.000225)(1.943)^2 + 0.001936 + 1.05}$$

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

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

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

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

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

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

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

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

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-fluorennes	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 (µmol/L)	Chronic HCS5 (µg/L)	Solid Solubility (µg/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-dimethylbenzothiophene	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-Chrysene/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-Chrysene/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-Chrysene/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-Chrysene/benzo(a)anthracene	7.421	7.295	284.38	-0.352	-6.875	0.00013	0.038	0.12	2.63	748