

# Importance of Bioavailability for Risk Assessment of Sediment Contaminants at the NASSCO Site – San Diego Bay

Expert Report

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## Summary and Conclusions

The total concentration of a chemical in sediment is not necessarily predictive of adverse biological effects. High concentrations of a chemical do not always lead to a high biological effect and low concentrations of a chemical do not always lead to a low biological effect. The degree to which the chemical is available to organisms (bioavailable) must be integrated into the assessment to achieve a valid prediction of the potential effect of the chemical. The Tentative Cleanup and Abatement Order (California Regional Water Quality Control Board - San Diego Region, 2010a) is deficient in not considering the bioavailability of chemicals in the sediments.

Consider this simple example. Take two pint containers filled with water and place a fish in each. Add 100 grams of copper wire to one container and 1 gram of copper in the form of copper sulfate to the other. The fish in the container to which copper sulfate was added will quickly die, but the fish in the container with the copper wire will not, despite the much greater amount of copper present. If 6 grams of the chemical EDTA is then added to the container with the copper sulfate and another fish is introduced to the container, the new fish will not die. EDTA is a widely used complexing agent that finds application in foods and personal care products, such as shampoos, as well as in industrial applications. It chemically reacts with metals to form stable compounds that resist precipitation. After the addition of the EDTA to the solution containing the copper sulfate, the copper concentration has not changed; there has simply been a change in the chemical form of the copper. Clearly, the form of the chemical is paramount in controlling the effect.

To evaluate the biological effect it is important to consider bioavailability of both metals and organic compounds in addition to the chemical's total concentration. Bioavailability is the fraction of the total concentration that reaches the biological receptor site and is able to interact and cause beneficial or adverse effects. This report considers a number of chemicals that have been measured in sediment or pore water (the water contained within the settled particles), and their bioaccumulation in organisms exposed to sediments from the NASSCO Shipyard. Based on an analysis of the data, and in using scientific

considerations that incorporate bioavailability to produce the best estimate of potential effects, I have reached a number of conclusions.

1. *Metals*. The Board incorrectly concludes that metals in sediments at the NASSCO Shipyard are causing potential risks to aquatic life, i.e. benthic macroinvertebrates. The Board has not considered the bioavailability of the metals in the sediment. The metals in sediment that have been considered are cadmium, copper, lead, mercury, nickel, and zinc. Each of these metals is bound very strongly by sulfide in the sediment. If the concentration of sulfide is greater than that of the metals, the concentration of metal is too low to produce toxicity in benthic organisms. If the concentration of metals exceeds that of sulfide, the excess reacts with organic matter in the sediment. The extent of this reaction must be assessed to determine if the sediment will be toxic. The concentrations of sulfide and of organic matter in the sediments at the NASSCO site are sufficiently high to preclude the metals from causing toxicity.
2. *Polycyclic Aromatic Hydrocarbons (PAH)*. The Board incorrectly concludes that PAHs in sediments at the NASSCO Shipyard are causing potential risks to aquatic life. PAHs are a large class of compounds containing fused benzene rings. They originate from combustion and from petroleum. They are adsorbed by the organic matter component of sediments and the concentration in water can be predicted. Their effect on organisms is caused by Type I narcosis, reaction with the cell membrane. The effects of all narcosis chemicals, on a molar basis, are the same. Thus, an integrated effect for all PAH compounds can be calculated. The PAH concentrations of all NASSCO sediments was less than the narcosis threshold. PAHs in the NASSCO sediments will not be toxic to aquatic organisms.
3. *Bioaccumulation*. The Board has incorrectly interpreted the results of bioaccumulation testing. Bioconcentration factor (BCF) and bioaccumulation factor (BAF) values are frequently applied as generic threshold criteria for the hazard potential of chemicals. They are useful in

programs to rank and prioritize chemicals for possible further consideration including in prioritization for the development of standards. However, they are less useful in providing site-specific information. The Tentative Cleanup and Abatement Order noted that concentrations of arsenic, copper, lead, mercury, zinc, TBT, total PCBs, and high molecular weight PAHs in the *Macoma nasuta* tissue increase with respect to their concentrations in the sediment. This led to the conclusions that bioaccumulation of these compounds are occurring at the Shipyard Sediment Site<sup>1</sup>.

The Regional Board inappropriately selected these chemicals as Indicator Chemicals based primarily on the results of Macoma tissue bioaccumulation. The bioaccumulation results for these organisms, which were collected in Northern California and exposed to sediment from the Shipyard Sediment Site in the laboratory, may not be applicable to organisms present at the Shipyard Sediment Site. This selection of chemicals based on bioaccumulation is contrary to the narrative water quality objective for toxicity applicable to San Diego Bay and the Shipyard Sediment Site which provides that: “All waters shall be maintained free of toxic substances in concentrations that are toxic to, or that produce detrimental physiological responses in human, plant, animal, or aquatic life” (California Regional Water Quality Control Board - San Diego Region, 2010b – Section 1.4.3). The Macoma tissue bioaccumulation testing does not assess the required toxicity or assessment of detrimental physiological responses that are specified in the

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<sup>1</sup> The Tentative Cleanup and Abatement Order indicates “an area extending approximately from the Sampson Street Extension to the north and Chollas Creek to the south and from the National Steel and Shipbuilding Company Shipyard facility (hereinafter ‘NASSCO’) and the BAE Systems San Diego Ship Repair Facility (hereinafter ‘BAE Systems’) shoreline out to the San Diego Bay main shipping channel to the west. This area is hereinafter collectively referred to as the ‘Shipyard Sediment Site’.”

water quality objective. It merely indicates that the chemicals are present in the exposed Macoma. To assess the responses specified in the water quality objective, an appropriate, comprehensive risk assessment evaluating toxicity and detrimental physiological effects must be carried out.

4. *Pore Water.* The Board has incorrectly used the pore water data by comparing the concentrations present in samples from the NASSCO sites to the California Toxics Rule saltwater quality criterion continuous concentration, the highest concentration of a pollutant to which marine aquatic life can be exposed for an extended period of time without deleterious effects. It is inappropriate to compare concentrations of chemicals in pore water to criteria developed for surface water. The Tentative Cleanup and Abatement Order also fails to note that the pore water samples collected at each of the five reference stations exceeded the copper criterion and those from two of the stations exceeded the criterion for total PCBs which indicates that toxicity is predicted for the reference sites, although it was not observed.

The Tentative Cleanup and Abatement Order noted that although several measured concentrations exceeded criterion values, the results may be biased high due to the presence of very fine suspended or colloidal material that had not been removed by centrifugation. The chemistry of pore water can also lead to elevated concentrations. The chemistry of pore water differs, particularly with respect to dissolved organic carbon, for which it is elevated, from that of surface waters for which the criteria have been developed. Dissolved organic carbon enhances release of chemicals from sediment and changes their chemical speciation and consequently their bioavailability. The concentrations of chemicals in pore water have been inappropriately compared to criteria developed for surface water.

The Tentative Cleanup and Abatement Order fails to incorporate bioavailability considerations in its assessment. I have provided appropriate technical assessment of these factors. These should be incorporated into the Board's assessment.

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## **1. Qualifications**

I am Herbert E. Allen a Professor Emeritus of Environmental Engineering and Director of the Center for the Study of Metals in the Environment at the University of Delaware. I taught courses dealing with environmental chemistry and environmental engineering. I retired December 31, 2008 but maintain an active research program. My research is primarily concerned with the fate and effects of chemicals in the environment and with the development of ecological criteria. Because the focus of my research has been the development of criteria that are capable of accurately predicting effects, my research has been sponsored both by government and industry. I began conducting research on bioavailability and chemical speciation in the early 1970s. I have published over 130 papers in the peer reviewed literature as well as a number of books, book chapters, and other publications. I was recently selected as an ISI Highly-Cited Author. Prior to joining the faculty at the University of Delaware in 1989, I served for 6 years as Professor of Chemistry and Director of the Environmental Studies Institute at Drexel University and preceding that I was Professor of Environmental Engineering at Illinois Institute of Technology. My curriculum vita is included as Appendix A to this report.

I was the head of a consortium that conducted most of the extramural research for EPA's sediment quality criteria program. Among the research that I was involved in were the development of the equilibrium partitioning (EqP) approach and the development of the analytical method used for acid volatile sulfide (AVS) and simultaneously extractable metals (SEM). This forms the basis for predicting the toxicity of metals in sediment. I was one of the three individuals that were the organizers of the EPA workshop that resulted in changing water quality criteria for metals from total recoverable to dissolved metal.

I was a member of the team of scientists that formulated the biotic ligand model (BLM) to predict metal toxicity and which conducted the initial chemical and biological studies. Compared to the previously used numerical standards, the BLM sometimes results in greater allowable concentrations of copper, but in other cases it is more restrictive.

Funding for our research on the development of the BLM came both from industry and from the EPA. The approach has been endorsed by resource management agencies, public interest groups, and by EPA's Science Advisory Board.

I headed the EPA-funded Center for the Study of Metals in the Environment. Recently, I have studied the kinetics of metal uptake by soil and presently am conducting research to develop a predictive model of metal toxicity in soil. In addition to EPA funding of this work, I have also been funded by industry for the terrestrial BLM work.

## **2. Bioavailability of Chemicals**

### *2.1. Overview of Bioavailability.*

Bioavailability refers to the degree to which or rate at which a substance is absorbed or becomes available at the site of physiological activity. Comparison of the total concentration of a chemical in different samples of sediment does not by itself provide sufficient information to predict their relative biological effects. That is, a higher concentration may not produce a greater biological effect. This has been known for a long time. Only a fraction of the total amount of a chemical, the bioavailable fraction, that is present in sediment, water or food can reach the biological receptor and interact with it to produce an adverse effect. Other chemicals that are present in the system can increase or decrease the fraction of the chemical that can react with the biological receptor. Some of the factors that affect the bioavailability of chemicals include the concentrations of sulfide and of natural organic matter in sediment, and the pH and dissolved organic matter content of the water. These factors must be included in assessing the bioavailability of chemicals in sediment.

Environmental studies of water, sediments and soils usually report concentrations in terms of mass of chemical (grams or moles) per unit volume (liters) of water or mass (kilograms) of sediment or soil. These units of reporting are useful in locating areas of discharge and deposition of chemicals, but not in determining the effect of the chemicals.

Chemists use harsh means of extraction to determine the total concentration of metals or organic compounds in sediments. These procedures involve digestion of samples with strong acids to remove solubilized metals and extraction with solvents to remove organic compounds. Organisms must also extract the compounds, but they do this using much milder conditions. The fraction of a chemical that a chemist and an organism extract is likely to differ. It is the fraction extracted by the organism that is relevant, not that extracted by the chemist.

The concept of bioavailability is well-known and has been used in agriculture for many years. Fertilization of soil with phosphate is often required to achieve optimum agricultural crop production. The total phosphate content of the unamended soil is not used as the basis to determine the amount of phosphate fertilizer to use. Rather, a sample of soil is extracted with a selective extractant and that concentration provides the basis for deciding the amount of phosphate that is required to be added. The selective extractant releases what is termed “plant available phosphate”; this can be a small fraction of the total amount present in the soil. A large amount of the phosphorus contained in the soil can be present in inorganic and organic chemical forms that are not readily available to support plant growth. That is, they are not bioavailable.

## *2.2. Bioavailability of Metals.*

Metal bioavailability has been extensively studied, most often to explain why the toxicity of a metal differs with the chemistry that is present (Allen, 1993; National Academy of Sciences, 2003; U.S. EPA, 2007a). The different physical and chemical forms of a metal, or other chemical, are termed chemical species. Hence, speciation, the process of ascertaining the different forms of the chemical, is important in assessing its potential biological effect.

In water a toxic level of metal can be rendered nontoxic by the addition of a complexing agent such as EDTA. Natural organic matter in the form of humic and fulvic acids also complex metals and reduce their bioavailability and toxicity. In addition to the effect of complexation by organic matter on the toxicity of metals, other factors also modulate the

toxicity. Prime among these are protons and calcium ions which compete with the toxic metal for reaction with natural organic matter, and also compete with the toxic metal for reaction with the receptor sites on an organism that are responsible for the metal's toxicity. Chemical measurements of total concentrations, together with appropriate equations that account for these reactions, can be used to predict toxicity of a metal for site water chemical conditions. This is the basis of the Biotic Ligand Model (BLM) of metal toxicity (Di Toro et al., 2001) that is the basis for the recently released EPA water quality criteria for copper (U.S. EPA, 2007b). This is one of the best known and most widely used methods to account for the bioavailability of a substance.

### *2.3. Bioavailability of Organic Chemicals.*

Akin to the complexation of metal in water, hydrophobic organic compounds can bind with humic and fulvic acids (Carter and Suffet, 1982). The partitioning of these hydrophobic materials to humic and fulvic acids in the water will reduce their bioavailability and will thus make a chemical less toxic than it would be if the humic and fulvic acids were not present.

### *2.4. Pore Water.*

The bioavailability of chemicals in pore water is not the same as in surface water. The concentration of dissolved organic matter in sediment pore water is greater than that of surface water. Therefore, the fraction of a dissolved metal or hydrophobic organic contaminant in pore water that is bound to the dissolved natural organic material will be greater than it is for surface water. The bioavailability of the contaminant in the pore water will be diminished by this association with organic matter. Comparison of pore water concentrations of a contaminant to a water quality criterion based on toxicity in surface water can present a substantial degree of conservatism.

A principal factor affecting a chemical's bioavailability in sediment is the ability of the chemical to partition to the aqueous phase. Many chemicals partition strongly to the solid phase. Thus, they are detected in sediment analyses. Although the vast majority of the

compound will be on the sediment, the fraction that is present in the pore water can vary greatly. Using the principle of equilibrium partitioning, the biological effect will be related to the concentration of the chemical in the pore water, not to the concentration in the solid phase.

Pore water analyses are difficult. Because of the high concentration of the contaminant in the particulate phase, the results will be biased to too high a value if all particulate matter is not removed. This was noted in the Appendix for Section 15 of the Draft Technical Report (California Regional Water Quality Control Board - San Diego Region, 2010b). Calculation of the pore water concentration in equilibrium with the sediment is more reliable. This requires knowing the partition coefficient for the compound in sediment ( $K_p$  is the ratio of the concentration of the compound in the sediment to its concentration in the pore water). There is great variation of this value among sediments for a single contaminant.

Hydrophobic compounds partition primarily to the organic matter component of sediment. If the partition coefficient is divided by the fraction of organic carbon ( $f_{OC}$ ) in the sediment, the resulting constant,  $K_{OC}$ , is very constant among sediments. The value of  $K_{OC}$  is related to the partition coefficient of the compound between octanol and water ( $K_{OW}$ ) which is readily available. The pore water concentration can be estimated from the concentration of organic carbon in the sediment and the value of  $K_{OC}$  for the contaminant of interest. Therefore bioavailability of the compound depends only on the total concentration of the compound in the sediment,  $K_{OC}$ , and  $f_{OC}$ . This computed bioavailability for an organic contaminant may also be conservative. Although the contaminant is considered to partition to the natural organic matter component of the sediment, a substantial portion will partition to any soot that is present in the sediment. Binding of the contaminant to the soot is much stronger than its binding to the natural organic matter. Therefore, if soot is present the true pore water concentration of the contaminant will be less than computed. This provides further conservatism in predicted effects incorporating bioavailability.

Metals can also partition to the organic matter contained in the sediment. However, they are very strongly bound by any sulfide present. If the molar concentration of sulfide exceeds that of the metals that react with it (Cd, Cu, Hg, Ni, Pb, and Zn) the resulting equilibrium concentration of metal contained in the pore water will be too low to cause toxicity. If the concentration of these metals exceeds that of the sulfide available in the sediment, then the interaction of the excess amount of metals with the organic matter must be taken into account in determining if the bioavailability is sufficiently high to cause toxicity.

### *2.5. Board's Approach.*

The Board has inappropriately used empirical methodologies for Sediment Quality Guidelines for contaminants for which causal methodologies are available.

Section 18.2 of the Draft Technical Report (California Regional Water Quality Control Board - San Diego Region, 2010b) discusses the alternative approaches to developing Sediment Quality Guidelines and their importance in evaluation of potential impacts of contaminants in sediment. The Draft Technical Report (Section 18.2) states:

“Sediment quality guidelines (SQGs) are reference values above which sediment pollutant concentrations could pose a significant threat to aquatic life and can be used to evaluate sediment chemistry data. SQGs are considered one of the most effective methods for attempting to relate sediment chemistry to observed toxic effects and determine whether contaminants are present in amounts that could cause or contribute to adverse effects. ...

Several different approaches, based on empirical or causal correlative methodologies, have been developed for deriving SQG screening levels.... Examples of causal SQGs include the equilibrium partitioning (EqP) approach which uses partitioning theory to relate the dry-weight sediment concentration of a particular chemical that causes an adverse biological effect to the equivalent free chemical concentration in pore water and to the concentration adsorbed to sediment organic carbon or bound to sulfide.... Causal SQGs have a greater ability relative to empirical SQGs to determine the specific contaminants responsible for toxicity (emphasis added). However causal SQGs require more extensive data sets and published values are not available for many contaminants relative to empirical SQGs. By comparison, empirical SQGs can be calculated for a large number of contaminants and only require routine chemical analyses.”

Statistical, empirical approaches to develop SQGs include the effects range–low (ERL) and effects range–median (ERM) values, which are concentrations corresponding to the 10th and 50th percentiles of the distribution observed in toxic samples, respectively. Often these produce conservative evaluations of tolerable pollutant concentrations. However, their very basis allows a percentage of samples that will produce effects to be evaluated as being acceptable. As indicated by the Board, causal relationships are to be preferred over empirical approaches.

#### *2.6. Empirical Sediment Quality Criteria.*

The Board has inappropriately used empirical SQGs rather than causal approaches. SQGs that are based on total concentration are not adequate for prediction of risk. The Draft Technical Report incorrectly equates high concentrations of chemicals with a possible impact to organisms in Table 18-1. That the bioavailability is low is quite clear as adverse biological effects were not observed.

The problem with the use of total metal concentrations to develop SQGs has been discussed by Allen (1996). Sediments which the criteria categorize as likely being harmful may not be; sediments judged as having concentrations of the chemical too low to be harmful may actually be toxic. Thus, use of this type of criteria may result in requiring the unwarranted clean-up of sediments that do not produce adverse biological effect while leaving toxic sediments in place.

Allen analyzed the data used to develop the Canadian freshwater SQG for copper. The data, shown in Figure 1, represent samples in which there was a biological effect and samples in which there was no biological effect. The statistical analysis of the data gave proposed limits of TEL = 35.7 and PEL = 197 mg kg<sup>-1</sup>. The TEL (threshold effect level) is the concentration below which adverse effects are expected to occur rarely. The PEL (probable effect level) is the concentration above which adverse effects are expected to occur frequently. This approach is basically the same as that used by the Board in setting ERM and ERL values.

The maximum concentration that produced no effect in Figure 1 was approximately 8000 mg kg<sup>-1</sup>. This is virtually the same as the maximum concentration for the effect data. The maximum concentration in the no-effect data set is approximately 40-fold greater than the PEL and 200-fold greater than the TEL. There are very high concentrations of copper in sediments that do not cause adverse biological effects. Over one-half of the sediments with concentrations greater than the PEL did not have a biological effect. They would be judged to have an effect whereas they did not adversely affect organisms.

These criteria would not have protected organisms in all of the sediments tested. Of the 115 sediments that were toxic, 10 (8.7%) had copper concentrations less than the TEL and would have been judged to have been acceptable quality. This is clearly a major problem as no toxic sediment should be classified as non-toxic.

It is amply clear that this approach to the establishment of SQGs is inappropriate as it misclassifies a high percentage of the sediments considered. Critical properties of the sediments affecting the chemical and its ability to cause toxicity must be taken into account. This is amply demonstrated by the data in Figure 1. Sediments having copper concentrations as low as 15 mg kg<sup>-1</sup> produced a biological effect whereas sediments having as much as 8000 mg kg<sup>-1</sup> did not.

Long et al. (2000) provided further testing of empirical SQGs that have been developed for use in the U.S. They found that for 9 to 11% of the sediments for which there was acute toxicity in amphipod survival tests no TEL or PEL values were exceeded. This is the same as for the Canadian data set that I have discussed. The data clearly indicate that if empirical SQGs are used, a high percentage of the sediments that have concentrations below the criteria cutoff will actually be acutely toxic. Whether TEL and PEL are exceeded is not predictive of toxicity; bioavailability must be considered.

The bioavailability of copper and other chemicals clearly is not the same in all sediments, and factors that account for the differences in bioavailability must be addressed in SQGs. SQGs that are based on total concentration are not applicable for prediction of risk.

### *2.7. Causal Criteria.*

The Board has correctly indicated that causal criteria are preferred in assessment of sediments. However, they have not applied these criteria in their assessments. Causal criteria incorporate bioavailability as a fundamental consideration. Bioavailability refers to the extent to which humans and ecological receptors are exposed to contaminants in sediment. (Ehlers and Luthy, 2003).

There has been extensive recent research to develop causal relationships between the concentration of chemicals and biological effects. The U.S. EPA has issued procedures for deriving equilibrium partitioning sediment benchmarks for the protection of benthic organisms for metal mixtures (Hansen et al., 2005) and for PAH mixtures (Hansen et al., 2003). My report presents new evaluations of chemicals in sediments at the NASSCO site in San Diego Bay using these procedures. My assessments are based on considering the bioavailability of chemicals.

### *2.8. Conclusions.*

It is not possible to predict the effect of a chemical based solely on its total concentration. Prediction of the effect requires information on both the total concentration and its bioavailability. By incorporating bioavailability it is possible to state whether a biological effect was caused by a specific chemical. Likewise, the same information allows a chemical to be ruled out as the cause of a biological effect.

The Board has inappropriately used empirical Sediment Quality Criteria (SQC) rather than causal approaches. SGQs that are based total concentration are not adequate for prediction of risk.

### **3. Metals**

#### *3.1. Overview.*

The Board has inappropriately failed to incorporate the bioavailability of metals in its evaluation. The metals of concern in San Diego Bay are cadmium (Cd), copper (Cu), lead (Pb), mercury (Hg), nickel (Ni), and zinc (Zn). Their potential for toxicity depends on their binding to the sediment. The principal metal binding material in sediment is sulfide. Metals in excess of the capacity of the sulfide present will bind to the organic matter portion of the sediment. The partitioning of the metal can thus be evaluated and then the concentration of metal in water can be evaluated using the Biotic Ligand Model (BLM). This directly provides an assessment of whether the Cd, Cu, Pb, Hg, Ni, or Zn in the sediment will be toxic to aquatic organisms. These concepts form the basis for the EPA procedure to evaluate metal mixtures in sediments (Hansen et al., 2005). I have followed this procedure in my assessment and have concluded that the metals at the NASSCO site are not toxic.

#### *3.2. Approach.*

The potential for metals in sediment to be toxic to aquatic, sediment-dwelling organisms is dependant on the ability of the metal to partition into sediment pore water. The metals of concern in San Diego Bay are cadmium (Cd), copper (Cu), lead (Pb), mercury (Hg), nickel (Ni), and zinc (Zn). For these metals the strongest binding phase is sulfide which is quantified in sediment as AVS, acid volatile sulfide (Allen et al. 1993). This is the sulfide that is released by cold acid with a relatively short acidification time. The Cd, Cu, Pb, Ni, and Zn that are also solubilized in this procedure are termed Simultaneously Extracted Metals (SEM). Although it was not considered in the development of the initial methodology, Hg can also be included in SEM.

The major reservoir of sulfide in sediment is ferrous sulfide (FeS) which is responsible for the black color of reduced sediment. The addition of Cd, Cu, Pb, Hg, Ni, and/or Zn to sediment causes a reaction between these metals and the FeS. The metal becomes bound by the sulfide, which has a very low solubility, and has been found to be non-toxic to

sediment-dwelling organisms (Di Toro et al., 1992). This finding has led to the use of AVS and SEM, both expressed on a molar basis, for the assessment of potential toxicity of sediment. If  $AVS/SEM > 1$  or  $AVS-SEM > 0$ , no toxicity from metals is predicted. There are metal sulfides that are poorly solubilized under the testing conditions. However, this does not invalidate the AVS/SEM or AVS-SEM criteria because both the metal (SEM) and the sulfide (AVS) will be reduced by the same amount. However, if  $AVS/SEM < 1$  or  $AVS-SEM < 0$ , it does not follow that the metals in the sediment, based on SEM, will be toxic. Under this condition, the strength of binding of the SEM to other materials in addition to sulfide must be considered.

The principal material, other than sulfide, that is responsible for binding metals is natural organic matter, which is characterized by the measurement of Total Organic Carbon (TOC). The potential toxicity of the metals that are bound to organic matter can be predicted using the Biotic Ligand approach (Di Toro et al., 2001) that has recently been incorporated in EPA's Aquatic Life Criteria for Copper (USEPA, 2007b). This approach, accounting for the binding of metals by both sulfide and natural organic matter, has been incorporated into an integrated methodology (Di Toro et al., 2005). The U.S. EPA has adopted this approach for the evaluation of metal mixtures in sediments (Hansen et al., 2005). I have used this approach and have extended it to consider the multiple metal contaminants that are present in sediments at the NASSCO site. The detailed approach and results are described in the following discussion.

### *3.3. Calculations.*

I used the data for SEM, AVS, sediment TOC and sediment pH that were presented in the 2003 Exponent report. I assumed that the total concentration of SEM entered the system in a soluble form and then I allowed these metals to computationally react with the AVS. I computed the composition of the precipitated metal sulfides. Then I subtracted the concentration of each of the metals in the precipitated form from its concentration in the SEM. I then computed the interaction of this excess metal with the TOC in the sediment. The partitioning of the metal between the organic carbon and the sediment pore water was computed using the Biotic Ligand Model and I used this to compute the toxicity of

each metal. I assumed additivity of the toxicities of each of the metals and this was used to compute the overall toxicity. It should be noted that this is an upper level calculation. A portion of the metals entered the sediment not in a soluble form, but rather as smelter slag, a blasting material used in the shipyard.

Sediment samples were collected and analyzed for AVS and SEM. I took these results, which are shown in Table 1 of this report, from Table 4-3 of Volume I of the Exponent study (Exponent, 2003). Also included are the values of sediment pH and TOC from the Exponent report Volume II, Table B1-1.

I determined the metals that were precipitated by the AVS using the chemical equilibrium program MINEQL+ (Schecher and McAvoy, 1992). The input was the values of each of the SEM metals and the AVS. I used the determined pH value except in the cases where pH had not been determined. In those cases the pH was assumed to be 7.5 as I found that the value chosen had little effect on the amount of the metals that were precipitated by the sulfide as can be seen for Sample NA13 in Table 3 for which a pH of 7.0 as well as 7.5. In addition to these input values, I assumed the samples to have the major ion composition of seawater as shown in Table 2.

The concentration of precipitated metals as predicted by MINEQL+ is indicated in Table 3. This table also indicates the mineral species considered as forming the precipitate. In comparison of the data in Tables 1 and 2, it is seen that essentially all of the Hg is precipitated as the sulfide. Hg forms the strongest precipitate with sulfide of any of the metals under consideration. However, because of the very low concentrations of Hg relative to those of AVS, the precipitation of the Hg does little to affect the amount of sulfide available to react with the other metals. The metal forming the next strongest precipitate with sulfide is Cu. If the concentration of AVS is less than that of Cu, all of the available AVS (the AVS in excess of Hg) will react with Cu and an amount of Cu equal to the sulfide will precipitate. This relationship between AVS and Cu is indicated in Table 4. The concentration of each metal that I computed not to have been precipitated by the AVS is indicated in Table 5. These values were computed by subtracting the

concentrations of metal computed to have been precipitated by the AVS which are presented in Table 3 from the total concentration of that metal in the SEM which was presented in Table 1. I divided the concentrations of excess metal by the concentration of organic carbon in the sample to give values of excess metal ( $\mu\text{mole metal/g organic carbon}$ ) which are presented in Table 6.

Criteria values for EC50 ( $\text{SEM}_{x,\text{OC}}^*$ , the concentration of metal in excess of AVS, on an organic carbon normalized basis, resulting in a 50% mortality in seawater as a function of pH) can be calculated using the Biotic Ligand Model (Di Toro et al., 1991). These values are a function of pH as indicated in Figure 2 and Table 7. I computed the number of toxic units of each metal by dividing the concentration of metal in excess of the AVS per g organic carbon from Table 6 by the value for the criteria computed for the sample pH using the equations in Table 7. These results are indicated in Table 8. Toxicity of metals can either be additive or less than additive. I assumed additivity of toxicities and I computed the sum of the toxic units of all metals contained in the samples for each sample (Hansen et al., 2005). In all cases the total toxic units computed for the samples collected at the NASSCO sites was less than one, indicating that metals were not toxic. The values ranged from 0.00 at sites NA09 and NA22 to 0.41 for NA18. The value of toxic units for the SEM metals at the reference sites ranged from 0.00 for sample 2441 to 0.29 for 2243. For the NASSCO sediment samples the average value of toxic units is 0.20 while for the reference station samples the value is 0.14. The number of toxic units of all samples is less than one indicating that the metals in the sediments at the NASSCO and the reference stations are not toxic to benthic organisms.

It should, however, be noted that the value of toxic units for the NASSCO samples is inflated by the inclusion of samples containing appreciable amounts of smelter slag. Metals in slag may be present in the form of stable metal oxides. This fraction of the metal content would not be associated with the AVS. Therefore, the amount of metals not associated with AVS or that are present in the form of stable metal oxide phases is what should be considered to react with the organic matter of the sediment. This consideration

would further reduce the value of toxic units for the NASSCO samples, but not those of the reference station samples.

#### *3.4. Conclusions.*

Binding of the metals Cd, Cu, Pb, Hg, Ni, and Zn in the sediment at the NASSCO is sufficiently strong that they are not toxic to benthic organisms. Total toxic units for each sediment is less than one.

### **4. Polycyclic Aromatic Hydrocarbons (PAH)**

#### *4.1. Overview.*

The Board has inappropriately failed to incorporate the bioavailability of PAHs in its evaluation. PAHs are Type I narcotic compounds. That is, they act by narcosis, a mode of action involving the cell membrane. Toxicity occurs when the molar concentration of the sum of all narcosis chemicals in the lipid of an organism exceeds a threshold value. The PAH compounds partition to the organic carbon of the sediment and the extent of partitioning for any compound is proportional to the fraction organic carbon in the sediment ( $f_{oc}$ ). The sum of the concentrations of PAHs computed for the pore water are compared to the final chronic value water quality criteria. In its derivation of sediment chemistry levels for chemicals of concern (COC), the Board has considered a subset of the PAHs. These are the HPAHs (high molecular weight polynuclear aromatic hydrocarbons). The six HPAH compounds are fluoranthene, perylene, benzo[a]anthracene, crysene, benzo[a]pyrene, and dibenzo[a,h]anthracene.

#### *4.2. Approach.*

Polycyclic aromatic hydrocarbons (PAH) are a large group of chemical compounds characterized by two or more fused benzene rings. The simplest PAH compound, naphthalene, has two rings. The structures of some 2 and 3-ring PAH compounds are shown in Figure 3. The structure of a number of higher molecular weight PAH compounds that contain 4, 5, or 6 rings are shown in Figure 4.

PAHs originate predominantly from two sources, formation during combustion and as constituents of petroleum hydrocarbons. PAHs in petroleum hydrocarbons tend to be enriched in alkylated compounds, for example those containing a methyl group (-CH<sub>3</sub>) attached to the ring. The PAH compounds 2,3,5-trimethylnaphthalene and 1-methylphenanthrene (Figure 3) are examples of alkylated compounds.

PAHs are type I narcotic chemical. That is, they are nonionic organic chemicals having a similar mode of action, i.e., narcosis (Veith and Broderius, 1990). The mechanism of narcosis appears to involve the phospholipids in the cell membrane. For narcosis chemicals mortality occurs when the chemical concentration in the target lipid of the organism reaches a threshold value. This has permitted the development of water quality criteria for a large number of narcosis compounds, including PAHs (Di Toro et al., 2000). It is possible to easily compute the toxicity of type I narcotic chemicals for which specific toxicities have not been determined in the laboratory and when determined in field samples to include these chemicals in the prediction of toxicity.

Because PAHs occur as a mixture, it is important to assess their potential effects as a mixture rather than as individual compounds. The potential effect of a mixture of chemicals can be computed using the concept of toxic units. A toxic unit (TU) is the ratio of the concentration of a compound to the criteria value for the same medium. Thus, toxic units in water (W) and sediment (S) are defined as

$$TU_{Wi} = \frac{C_{W,i}}{C_{WQC,i}} \quad (1)$$

$$TU_{Si} = \frac{C_{S,i}}{C_{SQC,i}} \quad (2)$$

where the subscript *i* indicates the individual chemicals and the denominators are the water quality criteria (WQC) and the sediment quality criteria (SQC) values (Di Toro and McGrath, 2000).

PAHs are hydrophobic organic compounds. Hydrophobic compounds partition almost exclusively to the organic matter contained in soils and sediments (Adams and Li, 1971,

Karickhoff, 1979). The partitioning is directly proportional to the concentration of organic matter in the sediment. Organic matter is general expressed in terms of the organic carbon content of the sediment. The aqueous concentration of a PAH compound in equilibrium with a sediment containing 2% organic carbon will be half that for a sediment containing 1% organic carbon for a system in which the sediment-to-water ratio and the total mass of the PAH is the same for the two sediments. Concentrations of chemicals such as PAHs in sediment expressed on a mass of sediment basis ( $\mu\text{g PAH/kg}$  dry weight) are useful in accounting for material loading. These values can be used to compare the loadings of PAH to different locations. If the potential effects of these loadings (e.g., partitioning to pore water or toxicity) are to be compared the mass basis results must be normalized for the concentration of organic matter (TOC) in the sediment. The concentration of the PAH ( $\mu\text{g PAH/kg}$  dry weight) divided by  $f_{\text{OC}}$ , the fraction of the mass of the sediment that is organic carbon results in the desired quantity,  $\mu\text{g PAH/kg OC}$ ). Potential effects are directly related to these values irrespective of the total PAH concentration.

Sediment toxicity can be predicted using an equilibrium partitioning approach (Di Toro et al., 1991; Di Toro and McGrath, 2000; Hansen et al., 2003). If the sediment is at equilibrium with the pore water, the chemical activity or the fugacity in both the sediment and water phases will be identical. Then, if water-only exposures have been conducted to determine toxicity, this exposure will be identical to that from pore water or from ingesting sediment organic carbon. There route of exposure in the equilibrated system will not matter. I have used this method to evaluate the PAH data for the NASSCO and reference sites.

#### *4.3. Calculations.*

PAH data for NASSCO and reference sites are given in Table 9. These are the values previously reported by Exponent (2003) in their Table B1-5. I have divided the values of PAH concentrations in Table 9 by the fraction of organic carbon in the sediment to provide the OC normalized value used in EqP. These values are given in Table 10. The table also provides values for  $C_{\text{OC,PAH}_i\text{,FCV}_i}$ , the critical concentration of a PAH in a

sediment which is related to a Final Chronic Value (FCV). This is derived using the EqP procedure (Di Toro et al. 1991; US EPA, 2002). The FCV is computed from Final Acute Values from interpolation of the toxicity data for the four lowest genus mean acute values to provide protection at the 95% level (Stephan et al., 1985). I divided the organic carbon normalized concentration values by the corresponding value of  $C_{OC,PAH_i,FCV_i}$  to compute an Equilibrium Partitioning Sediment Benchmark Toxic Unit ( $ESBTU_{FCV}$ ) value. These values are given in Table 11. The sum of the values for all  $ESBTU_{FCV}$  values is given. This value is less than 1 TU for all samples except for one. A value of TU less than one indicates that the PAHs in the sample will not cause toxicity. Therefore no toxicity is predicted based on the measured PAHs except for the one sample. The one sample having a value greater than one is a split sample for station NA07. The two values of  $ESBTU_{FCV}$  for this station are 1.76 and 0.32. The high variation between these two values indicates that the data should not be used. It is not possible to state what the true value is. I reject both of these results. The next highest values of  $ESBTU_{FCV}$  were 0.53 and 0.43 for the two splits of the sample collected at station NA01 on August 11, 2001. These results show the expected variation of results between splits of the same sample.

The PAH compounds that were analyzed and are reported in Table 9 do not include the alkylated compounds that are present in petrogenic source material. If the PAHs had a large component originating from petroleum, the computed  $ESBTU_{FCV}$  would be lower than they should be. Another sediment sampling was conducted in November 2002 and these samples at both Reference and NASSCO sites. These data, taken from Table B1-6 of Exponent (2003) are given in Table 12. The organic carbon normalized values that I computed are given in Table 13 and the  $ESBTU_{FCV}$  results are presented in Table 14. The value of  $\text{Sum } ESBTU_{FCV_i}$  is less than unity for all Reference samples (0.08 to 0.28) and for all NASSCO site samples (0.22 to 0.41). A value less than unity means that the sediment is not toxic due to PAHs. Therefore, these sediments are not predicted to be toxic.

There is a further conservative factor in the above assessment. In the study of the sediments from San Diego Bay, toxicity was assessed for the amphipod *Eohaustorius*

*estuarius*. As shown in Figure 5, the toxicity of PAH to *Eohaustorius* is only about one-half that of the water quality criteria value. Therefore, the potential for toxicity for *Eohaustorius* is only about one-half of the values indicated above, far less than the values of unity that would cause toxicity by the PAH compounds in the samples.

#### *4.4. Conclusions.*

The concentrations of PAH compounds in the sediments are not sufficiently high to cause toxicity to benthic organisms.

### **5. Bioaccumulation**

#### *5.1. Overview.*

The Board has inappropriately interpreted the bioaccumulation data by not fully evaluating the consequences of any bioaccumulation through an appropriate risk assessment. Bioaccumulation is the increase in the concentration of a chemical in a biological organism over time, compared to the chemical's concentration in the environment. The bioaccumulation factor (BAF) is the ratio of a chemical concentration in an organism to the concentration in water resulting from all possible routes of exposure including dietary absorption and transport across the respiratory surface. The bioconcentration factor (BCF) is the ratio of the concentration of a chemical in an organism to the concentration in water, where the chemical concentration in the aquatic organism, usually determined in laboratory studies, results from exposure to waterborne chemical. Biomagnification describes a process that results in the accumulation of a chemical in an organism at higher levels than are found in its food. It occurs when a chemical becomes more and more concentrated as it moves up through a food chain -- the dietary linkages between single-celled plants and increasingly larger animal species. Both bioaccumulation and biomagnification are important processes, but are distinctly different.

Both bioaccumulation and biomagnification have become important parameters in the evaluation of chemicals for the protection of the environment since the discovery that

DDT and other hydrophobic organic compounds bioaccumulate in algae and then increase in concentration in higher trophic levels in the food chain through biomagnification. It is principally the bioaccumulation of chlorinated pesticides and of PCBs that has led to the use of bioaccumulation as an evaluative criterion. High values of persistent and bioaccumulative organic compounds, including PCBs, may lead to elevated and toxic concentrations in higher levels in higher trophic level species. Metals, with the exception of organometallic compounds (including methyl mercury and TBT), bioaccumulate but they do not biomagnify (U.S. EPA, 2007a).

Bioconcentration factor (BCF) and bioaccumulation factor (BAF) values are frequently applied as generic threshold criteria for the hazard potential of chemicals. They are useful in programs to rank and prioritize chemicals for possible further consideration including in prioritization for the development of standards. They are useful in registration of new chemicals, including development of restrictions of use and the labeling of containers. However, they are less useful in providing site-specific information.

#### *5.2. Bioaccumulation at the Shipyard Sediment Site.*

The Tentative Cleanup and Abatement Order (California Regional Water Quality Control Board - San Diego Region. 2010a) evaluates the laboratory bioaccumulation test data obtained for the clam, *Macoma nasuta*. It is correctly noted that concentrations of arsenic, copper, lead, mercury, zinc, TBT, total PCBs, and high molecular weight PAHs in the *Macoma nasuta* tissue increase with respect to their concentrations in the sediment. This leads to the conclusions that these compounds are bioavailable at the Shipyard Sediment Site and that bioaccumulation is occurring at the site.

These conclusions regarding bioavailability and bioaccumulation are extended to further assessments regarding chemicals. For example, those chemicals that have been selected as Indicator Chemicals. Arsenic, copper, lead, mercury, zinc, TBT, high molecular weight PAHs, and total PCB homologs were selected based solely on the results of *Macoma* tissue bioaccumulation. This is contrary to the narrative water quality objective for toxicity applicable to San Diego Bay and the Shipyard Sediment Site which provides

that: “All waters shall be maintained free of toxic substances in concentrations that are toxic to, or that produce detrimental physiological responses in human, plant, animal, or aquatic life.” The *Macoma* tissue bioaccumulation testing does not assess the required toxicity or assessment of detrimental physiological responses that are specified in the water quality objective. It merely indicates that the chemicals are present in the exposed *Macoma*. To assess the responses specified in the water quality objective, an appropriate risk assessment must be carried out.

### *5.3 Conclusions.*

Bioaccumulation is a normal process for both metals and organic compounds. High levels of bioaccumulation can lead to detrimental responses either in the organism that has bioaccumulated the compound or in consumer organisms. An appropriate risk assessment must be carried out to evaluate if the bioaccumulation produces risk to consumer organisms.

## **6. Pore Water**

### *6.1. Overview.*

The Board has inappropriately used pore water data by comparing concentrations of chemicals in pore water to water quality criteria without accounting for the differences in the chemistry of surface and pore water. Water quality criteria are highly developed and form the basis for water quality standards. However, as discussed in Section 2 of this report, bioavailability has only recently been taken into account in a manner that allows adequate prediction of toxicity. Present water quality standards barely consider bioavailability. Therefore, to appropriately compare a measured concentration to a standard, the fraction of the compound that is bioavailable in a sample should be the same as in the samples that have been used to establish the criteria and thereby the standard.

It is tempting to compare the concentration of compounds in pore water to water quality standards. However, the chemistry of pore water is different from that of surface water. The concentration of dissolved organic carbon in pore water is greater than it is in surface water. Dissolved organic matter binds compounds and reduces their bioavailability.

### *6.2. Pore Water at the Shipyard Sediment Site.*

Pore water samples were collected at four reference stations and at five stations in the NASSCO Shipyard Site. The results for the samples collected at the NASSCO sites and for the reference stations are given in the Exponent report (2003).

The Draft Technical Report (California Regional Water Quality Control Board - San Diego Region, 2010b) compares the concentrations present in samples from the NASSCO sites to the California Toxics Rule saltwater quality criterion continuous concentration, the highest concentration of a pollutant to which marine aquatic life can be exposed for an extended period of time without deleterious effects. All five samples exceeded the criterion for copper and for total PCBs, and two samples exceeded the criterion for lead. The Draft Technical Report (California Regional Water Quality Control Board - San Diego Region, 2010b) uses these results without comment and without comparison of the results to those for samples collected at the reference stations. Although not noted in the Tentative Cleanup and Abatement Order, the pore water samples collected at each of the five reference stations exceeded the copper criterion and those from two of the stations exceeded the criterion for total PCBs. As I have discussed, concentrations of compounds can be compared to water quality criteria and standards only with appropriate consideration for bioavailability. The determination that a pore water concentration is less than the water quality criteria or standard would be a basis for concluding that the pore water would not produce significant biological effect. However, this does not mean that an exceedance does produce a significant biological effect. This is very clearly shown for these data in that many of the samples collected at the reference stations also exceed the water quality criteria and standards. Furthermore, pore water concentrations in reference station samples often exceeded those for the NASSCO sites. The copper concentration at reference station 2231 was exceeded by the concentration of copper at only a single NASSCO site. For total PCBs the concentration in the pore water at two of the NASSCO sites is less than the maximum concentration at reference station 2440.

The Draft Technical Report (California Regional Water Quality Control Board - San Diego Region, 2010b) noted that although several measured concentrations exceeded criterion values, the results may be biased high due to the presence of very fine suspended or colloidal material that had not been removed by centrifugation. Additionally, the chemistry of pore water differs from that of surface waters for which the criteria have been developed. The total organic carbon concentration of seawater used in the development of the toxicity data upon which the criteria are based is much lower than that of these pore water samples. This changes the chemical speciation of the chemicals and consequently their bioavailability. The dissolved organic matter measured in the form of total organic carbon reacts with metals and hydrophobic organic compounds in the pore water and enhances their release from the sediment. However, the additional amount of a chemical that is released from the sediment by virtue of its reaction with the dissolved organic matter is bound to the organic matter and has a lowered bioavailability. Equilibrium partitioning calculations avoid this problem by computing the concentration of the non-chemically bound compound in equilibrium with the sediment. This concentration can be compared to the standard. Among the metals compared to saltwater quality criteria, copper has the greatest propensity to react with dissolved organic matter, followed by lead. The PCB congeners having more chlorine atoms and which are more hydrophobic react more strongly with dissolved organic matter. The importance of organic matter in affecting bioavailability has now been incorporated into the EPA water quality criteria for copper (U.S. EPA, 2007b).

The *Macoma* used in the bioaccumulation testing were not collected in the San Diego area. They were collected from Tomales Bay in Marin County, north of San Francisco (Exponent, 2003). There has been no consideration of the applicability of these organisms to reflect uptake by benthic macroinvertebrates present at the Shipyard Sediment Site. The differences between exposure of organisms to contaminants in the laboratory compared to those exposed in the field has also not been considered (Draft Technical Report (California Regional Water Quality Control Board - San Diego Region, 2010b).

### 6.3. Conclusions.

Concentrations of several chemicals in pore water samples from both NASSCO and reference station sites exceed water quality criteria and standards. The pore water concentrations should not form the basis for decisions. The speciation of compounds in pore water differs from that in surface water. The bioavailability of compounds in pore water is less than in surface water. Consequently, concentrations of chemicals in pore water that exceed the water quality criteria and standards do not indicate that there will be a deleterious effect. This is true for both the reference sites and the NASSCO sites.

## 7. Summary of Expert Opinions

- The Board has inappropriately used empirical SQG rather than causal approaches. SQCs that are based on total concentration are not adequate for prediction of risk. Measuring total sediment pollutant concentrations alone cannot accurately predict risk. By using empirical SQGs based on total sediment pollutant concentrations as screening levels, rather than causal SQGs, the Board has failed to accurately predict risk at the Shipyard Sediment Site.
- The Board has inappropriately failed to consider whether metals are bioavailable in its evaluation. Binding of the metals Cd, Cu, Pb, Hg, Ni, and Zn in the sediment at the NASSCO portion of the Shipyard Sediment Site is sufficiently strong that they are not toxic to benthic organisms because they are not bioavailable at the Shipyard Sediment Site.
- The Board has inappropriately failed to incorporate the bioavailability of PAHs in its evaluation. The concentrations of PAH compounds in the sediments are not sufficiently high to cause toxicity to benthic organisms because of their low bioavailability at the Shipyard Sediment Site. The Board has inappropriately interpreted the bioaccumulation data by not fully evaluating the consequences of any bioaccumulation through an appropriate risk assessment. In the Tier II risk assessment a number of conservative factors were included: high area use factors, bioavailability in food equal to that in the test media, use of uncertainty factors, and use of test data in which the exposure was not from food or water. This Tier II risk assessment should have been followed by a more critical assessment taking into account the site specific conditions.

- The Board has inappropriately used pore water data by comparing concentrations of chemicals in pore water to water quality criteria without accounting for the differences in the chemistry of surface and pore water. Pore water and surface water are chemically different. By comparing concentrations of chemicals in pore water to surface water quality criteria without first accounting for the differences between the chemistry of surface and pore water, the Board has incorrectly assumed there to be risk at Shipyard Sediment Site. Concentrations of chemicals in pore water that exceed the water quality criteria and standards do not indicate that there will be a deleterious effect. There is no comparison of concentrations in pore water at the Shipyard Sediment Site to those at reference sites, The exceedance of copper and PCB concentrations at the reference sites clearly indicates that evaluation of pore water concentrations relative to surface water quality criteria is inappropriate.

Table 1. Sediment AVS, SEM, pH and TOC.

Station <sup>1</sup>	Cd	Cu	Hg	Ni	Pb	Zn	SEM	AVS	pH	TOC
NA01	0.00089	3.32	0.0009	0.141	0.373	4.18	8.02	2.78	7.10	2.10
NA01	0.00089	3.40	0.0008	0.141	0.392	4.13	8.06	2.90	7.49	2.15
NA02	0.00089	2.52	0.0010	0.131	0.325	3.70	6.68	0.75		2.00
NA03	0.00089	3.48	0.0009	0.138	0.397	4.25	8.27	3.68	7.54	2.33
NA04	0.00089	3.79	0.0009	0.170	0.396	4.62	8.98	0.72	7.64	2.04
NA05	0.00178	2.33	0.0005	0.097	0.260	3.06	5.75	0.14	7.92	1.60
NA06	0.00445	5.08	0.0009	0.158	0.462	4.94	10.65	6.49	7.62	2.31
NA07	0.00445	3.87	0.0012	0.152	0.447	4.88	9.35	2.59	7.53	1.98
NA07	0.00445	4.09	0.0011	0.155	0.437	4.64	9.33	3.34	7.71	2.05
NA08	0.00356	4.15	0.0004	0.143	0.349	5.05	9.70	1.68	7.98	2.18
NA09	0.00356	4.06	0.0002	0.148	0.352	5.14	9.70	19.25	7.86	2.26
NA10	0.00178	2.11	0.0004	0.087	0.216	2.71	5.13	0.32	8.19	1.18
NA11	0.00089	2.75	0.0009	0.305	0.294	3.72	7.07	0.56	7.66	1.69
NA12	0.00089	2.39	0.0008	0.121	0.251	3.30	6.06	0.56	7.65	1.48
NA13	0.00089	2.60	0.0006	0.148	0.344	4.21	7.30	3.06		2.10
NA14	0.00178	1.76	0.0003	0.099	0.243	2.92	5.02	1.83		1.82
NA15	0.00089	4.04	0.0008	0.143	0.356	4.83	9.37	0.84	7.63	1.95
NA16	0.00089	3.92	0.0011	0.146	0.375	4.57	9.01	3.87	7.66	1.88
NA17	0.00178	8.42	0.0004	0.170	0.512	11.82	20.92	8.86	7.64	2.33
NA18	0.00267	3.64	0.0005	0.126	0.399	6.55	10.72	0.83	7.38	2.04
NA19	0.00178	4.47	0.0007	0.146	0.410	7.79	12.82	3.93	7.41	1.84
NA20	0.00267	1.42	0.0001	0.072	0.251	3.15	4.90	3.84	7.70	1.42
NA21	0.00356	2.19	0.0001	0.109	0.307	3.53	6.14	2.99		2.15
NA22	0.00356	1.86	0.0000	0.080	0.281	3.29	5.51	5.52	7.65	1.65
Reference										
2441	0.00178	0.49	0.0000	0.087	0.052	1.14	1.77	5.52	7.75	1.10
2433	0.00178	0.53	0.0001	0.066	0.067	1.27	1.93	0.25	7.74	0.67
2440	0.00267	0.67	0.0000	0.058	0.291	1.59	2.61	2.19	7.78	1.62
2231	0.00267	1.26	0.0011	0.099	0.208	2.02	3.59	0.02	7.38	1.30
2243	0.00089	0.65	0.0011	0.045	0.084	1.39	2.17	0.27	7.48	0.51

metals and AVS  $\mu$ moles/g, TOC %

<sup>1</sup> Split samples were analyzed for Stations NA01 and NA07.

Table 2. Major ion composition of seawater (from Table 15.3 of Stumm and Morgan, 1996).

<b>Ion</b>	<b>Average Seawater (mmoles/L)</b>
$\text{HCO}_3^-$	2.38
$\text{SO}_4^{2-}$	28.2
$\text{Cl}^-$	545.0
$\text{Ca}^{2+}$	10.2
$\text{Mg}^{2+}$	53.2
$\text{Na}^+$	468.0
$\text{K}^+$	10.2

Table 3. Concentrations of SEM metals computed by MINEQL+ to have precipitated by AVS.

Station <sup>1</sup>	Concentration of Precipitates from MINEQL+ mmole/kg sediment						Total ppt S	AVS	pH	TOC
	Cd Greenockite	Cu Covellite	Hg Cinnabar	Ni Millerite	Pb Galena	Zn Sphalerite				
NA01		2.78	0.0009				2.78	2.78	7.10	2.10
NA01		2.90	0.0008				2.90	2.90	7.49	2.15
NA02		0.750	0.0010				0.75	0.75	7.5 est	2.00
NA03		3.48	0.0009			0.1990	3.68	3.68	7.54	2.33
NA04		0.720	0.0009				0.72	0.72	7.64	2.04
NA05		0.140	0.0005				0.14	0.14	7.92	1.60
NA06	0.004270	5.08	0.0009			0.4620	6.43	6.49	7.62	2.31
NA07		2.59	0.0012				2.59	2.59	7.53	1.98
NA07		3.34	0.0011				3.34	3.34	7.71	2.05
NA08		1.68	0.0004				1.68	1.68	7.98	2.18
NA09	0.003560	4.06	0.0002	0.1480	0.3520	5.1400	9.70	19.25	7.86	2.26
NA10		0.320	0.0004				0.32	0.32	8.19	1.18
NA11		0.560	0.0009				0.56	0.56	7.66	1.69
NA12		0.560	0.0008				0.56	0.56	7.65	1.48
NA13		2.60	0.0006			0.3410	3.06	3.06	7.0 est	2.10
NA13	0.000606	2.60	0.0006			0.3430	3.00	3.06	7.5 est	2.10
NA14	0.000221	1.76	0.0003			0.0695	1.83	1.83	7.5 est	1.82
NA15		0.839	0.0008				0.84	0.84	7.63	1.95
NA16		3.87	0.0011				3.87	3.87	7.66	1.88
NA17	0.000970	8.42	0.0004			0.4390	8.86	8.86	7.64	2.33
NA18		0.829	0.0005				0.83	0.83	7.38	2.04
NA19		3.93	0.0007				3.93	3.93	7.41	1.84
NA20	0.002530	1.42	0.0001			0.2510	3.85	3.84	7.70	1.42
NA21	0.003280	2.19	0.0001			0.3060	2.93	2.99	7.5 est	2.15
NA22	0.003570	1.86		0.0800	0.2810	3.2900	5.51	5.52	7.65	1.65
Reference										
2441	0.001780	0.490		0.0870	0.0520	1.1400	1.77	5.52	7.75	1.10
2433		0.250	0.0001				0.25	0.25	7.74	0.67
2440	0.002570	0.670			0.2910	1.2300	2.19	2.19	7.78	1.62
2231		0.019	0.0011				0.02	0.02	7.38	1.30
2243		0.269	0.0011				0.27	0.27	7.48	0.51

<sup>1</sup> Split samples were analyzed for NA01 and NA07. Calculations were performed at both pH 7.5 and 7.0 for NA13.

Table 4. Relationship between the concentration Cu contained in the SEM, AVS and the fraction of the Cu calculated by MINEQL+ to have precipitated.

Station	AVS	Total Cu	ppt'd Cu	AVS-Total Cu	% Cu ppt'd
NA01	2.78	3.32	2.78	-0.54	83.7
NA01	2.90	3.40	2.90	-0.50	85.3
NA02	0.75	2.52	0.750	-1.77	29.8
NA03	3.68	3.48	3.48	0.20	100
NA04	0.72	3.79	0.720	-3.07	19.0
NA05	0.14	2.33	0.140	-2.19	6.0
NA06	6.49	5.08	5.08	1.41	100
NA07	2.59	3.87	2.59	-1.28	66.9
NA07	3.34	4.09	3.34	-0.75	81.7
NA08	1.68	4.15	1.68	-2.47	40.5
NA09	19.25	4.06	4.06	15.19	100
NA10	0.32	2.11	0.320	-1.79	15.2
NA11	0.56	2.75	0.560	-2.19	20.4
NA12	0.56	2.39	0.560	-1.83	23.4
NA13	3.06	2.60	2.60	0.46	100
NA14	1.83	1.76	1.76	0.07	100
NA15	0.84	4.04	0.839	-3.20	20.8
NA16	3.87	3.92	3.87	-0.05	98.7
NA17	8.86	8.42	8.42	0.44	100
NA18	0.83	3.64	0.829	-2.81	22.8
NA19	3.93	4.47	3.93	-0.54	87.9
NA20	3.84	1.42	1.42	2.42	100
NA21	2.99	2.19	2.19	0.80	100
NA22	5.52	1.86	1.86	3.66	100
Reference					
2441	5.52	0.49	0.490	5.03	100
2433	0.25	0.53	0.250	-0.28	47.2
2440	2.19	0.67	0.670	1.52	100
2231	0.02	1.26	0.019	-1.24	1.5
2243	0.27	0.65	0.269	-0.38	41.4

Table 5. Concentrations of metals that were computed not to have been precipitated by the AVS.

Station	pH*	TOC	Cd	Cu	Hg	Ni	Pb	Zn
NA01	7.10	2.10	0.00089	0.54	0	0.141	0.373	4.18
NA01	7.49	2.15	0.00089	0.5	0	0.141	0.392	4.13
NA02	<b>7.50</b>	2.00	0.00089	1.77	0	0.131	0.325	3.7
NA03	7.54	2.33	0.00089	0	0	0.138	0.198	4.25
NA04	7.64	2.04	0.00089	3.07	0	0.17	0.396	4.62
NA05	7.92	1.60	0.00178	2.19	0	0.097	0.26	3.06
NA06	7.62	2.31	0.00018	0	0	0.158	0	4.054
NA07	7.53	1.98	0.00445	1.28	0	0.152	0.447	4.88
NA07	7.71	2.05	0.00445	0.75	0	0.155	0.437	4.64
NA08	7.98	2.18	0.00356	2.47	0	0.143	0.349	5.05
NA09	7.86	2.26	0	0	0	0	0	0
NA10	8.19	1.18	0.00178	1.79	0	0.087	0.216	2.71
NA11	7.66	1.69	0.00089	2.19	0	0.305	0.294	3.72
NA12	7.65	1.48	0.00089	1.83	0	0.121	0.251	3.3
NA13	<b>7.50</b>	2.10	0.000284	0.00	0	0.148	10.00000	4.15
NA14	<b>7.50</b>	1.82	0.001559	0.00	0	0.099	0.1735	2.92
NA15	7.63	1.95	0.00089	3.20	0	0.143	0.356	4.83
NA16	7.66	1.88	0.00089	0.05	0	0.146	0.375	4.57
NA17	7.64	2.33	0.00081	0.00	0	0.17	0.073	11.82
NA18	7.38	2.04	0.00267	2.81	0	0.126	0.399	6.55
NA19	7.41	1.84	0.00178	0.54	0	0.146	0.41	7.79
NA20	7.70	1.42	0.00014	0.00	0	0.072	0	0.97
NA21	<b>7.50</b>	2.15	0.00028	0.00	0	0.109	0.001	3.10
NA22	7.65	1.65	-0.00001	0.00	0	0	0	0.00
Reference								
2441	7.75	1.10	0	0.00	0	0	0	0.00
2433	7.74	0.67	0.00178	0.28	0	0.066	0.067	1.27
2440	7.78	1.62	0.0001	0.00	0	0.058	0	0.36
2231	7.38	1.30	0.00267	1.24	0	0.099	0.208	2.02
2243	7.48	0.51	0.00089	0.38	0	0.045	0.084	1.39

\* pH values in boldface were not determined. A value of 7.50 was assumed for the purpose of calculation.

Table 6. Concentration of SEM in excess of AVS divided by the concentration of TOC ( $\mu\text{moles metal/g organic carbon}$ ).

Station	pH*	TOC	Cd <sup>#</sup>	Cu <sup>#</sup>	Ni <sup>#</sup>	Pb <sup>#</sup>	Zn <sup>#</sup>
NA01	7.10	2.10	0.0424	25.71	6.71	17.76	199.05
NA01	7.49	2.15	0.0414	23.26	6.56	18.23	192.09
NA02	<b>7.50</b>	2.00	0.0445	88.5	6.55	16.25	185
NA03	7.54	2.33	0.0382	0	5.92	8.5	182.4
NA04	7.64	2.04	0.0436	150.49	8.33	19.41	226.47
NA05	7.92	1.60	0.1113	136.88	6.06	16.25	191.25
NA06	7.62	2.31	0.0078	0	6.84	0	175.5
NA07	7.53	1.98	0.2247	64.65	7.68	22.58	246.46
NA07	7.71	2.05	0.2171	36.59	7.56	21.32	226.34
NA08	7.98	2.18	0.1633	113.3	6.56	16.01	231.65
NA09	7.86	2.26	0	0	0	0	0
NA10	8.19	1.18	0.1508	151.69	7.37	18.31	229.66
NA11	7.66	1.69	0.0527	129.59	18.05	17.4	220.12
NA12	7.65	1.48	0.0601	123.65	8.18	16.96	222.97
NA13	<b>7.50</b>	2.10	0.0135	0	7.05	0.05	197.77
NA14	<b>7.50</b>	1.82	0.0857	0	5.44	9.53	160.44
NA15	7.63	1.95	0.0456	164.15	7.33	18.26	247.69
NA16	7.66	1.88	0.0473	2.66	7.77	19.95	243.09
NA17	7.64	2.33	0.0348	0	7.3	3.13	507.3
NA18	7.38	2.04	0.1309	137.79	6.18	19.56	321.08
NA19	7.41	1.84	0.0967	29.35	7.93	22.28	423.37
NA20	7.70	1.42	0.0099	0	5.07	0	68.31
NA21	<b>7.50</b>	2.15	0.013	0	5.07	0.05	144.09
NA22	7.65	1.65	-0.0006	0	0	0	0
<b>Reference</b>							
2441	7.75	1.10	0	0	0	0	0
2433	7.74	0.67	0.2657	41.79	9.85	10	189.55
2440	7.78	1.62	0.0062	0	3.58	0	22.22
2231	7.38	1.30	0.2054	95.46	7.62	16	155.38
2243	7.48	0.51	0.1745	74.71	8.82	16.47	272.55

\* pH values in boldface were not determined. A value of 7.50 was assumed for the purpose of calculation.

<sup>#</sup>metal values  $\mu\text{moles/g OC}$

Table 7. Values for excess simultaneously extracted metals concentration causing a 50% mortality for seawater ( $SEM_{x,OC}^*$ ) at varying pH. Data are from Di Toro et al. (2005) and the plots of the data are shown in Figure 2.

Metal	Equation
Cadmium	$SEM_{x,OC}^* = -614.01 + 101.74 \text{ pH}$
Copper	$SEM_{x,OC}^* = -3463.3 + 587.0 \text{ pH}$
Nickel	$SEM_{x,OC}^* = -3194.9 + 651.8 \text{ pH}$
Lead	$SEM_{x,OC}^* = -4372.3 + 1119.8 \text{ pH}$
Zinc	$SEM_{x,OC}^* = -3189.3 + 612.6 \text{ pH}$

Table 8. Computed toxic units for each metal contained in the SEM.

Toxic Units = Excess metal per g OC/Criteria

Station	pH*	TOC	Cd	Cu	Ni	Pb	Zn	SUM
NA01	7.10	2.10	0.00	0.04	0.00	0.00	0.17	0.21
NA01	7.49	2.15	0.00	0.02	0.00	0.00	0.14	0.16
NA02	<b>7.50</b>	2.00	0.00	0.09	0.00	0.00	0.13	0.22
NA03	7.54	2.33	0.00	0.00	0.00	0.00	0.13	0.13
NA04	7.64	2.04	0.00	0.15	0.00	0.00	0.15	0.30
NA05	7.92	1.60	0.00	0.12	0.00	0.00	0.12	0.24
NA06	7.62	2.31	0.00	0.00	0.00	0.00	0.12	0.12
NA07	7.53	1.98	0.00	0.07	0.00	0.01	0.17	0.25
NA07	7.71	2.05	0.00	0.03	0.00	0.01	0.15	0.19
NA08	7.98	2.18	0.00	0.09	0.00	0.00	0.14	0.23
NA09	7.86	2.26	0.00	0.00	0.00	0.00	0.00	0.00
NA10	8.19	1.18	0.00	0.11	0.00	0.00	0.13	0.24
NA11	7.66	1.69	0.00	0.13	0.01	0.00	0.15	0.29
NA12	7.65	1.48	0.00	0.12	0.00	0.00	0.15	0.27
NA13	<b>7.50</b>	2.10	0.00	0.00	0.00	0.00	0.14	0.14
NA14	<b>7.50</b>	1.82	0.00	0.00	0.00	0.00	0.11	0.11
NA15	7.63	1.95	0.00	0.16	0.00	0.00	0.17	0.33
NA16	7.66	1.88	0.00	0.00	0.00	0.00	0.16	0.16
NA17	7.64	2.33	0.00	0.00	0.00	0.00	0.34	0.34
NA18	7.38	2.04	0.00	0.16	0.00	0.01	0.24	0.41
NA19	7.41	1.84	0.00	0.03	0.00	0.01	0.31	0.35
NA20	7.70	1.42	0.00	0.00	0.00	0.00	0.04	0.04
NA21	<b>7.50</b>	2.15	0.00	0.00	0.00	0.00	0.10	0.10
NA22	7.65	1.65	0.00	0.00	0.00	0.00	0.00	0.00
Reference								
2441	7.75	1.10	0.00	0.00	0.00	0.00	0.00	0.00
2433	7.74	0.67	0.00	0.04	0.01	0.00	0.12	0.17
2440	7.78	1.62	0.00	0.00	0.00	0.00	0.01	0.01
2231	7.38	1.30	0.00	0.11	0.00	0.00	0.12	0.23
2243	7.48	0.51	0.00	0.08	0.01	0.00	0.20	0.29

\* pH values in boldface were not determined. A value of 7.50 was assumed for the purpose of calculation.

Table 9. Concentration of PAH compounds (µg/kg dry weight) in sediment samples (Exponent. 2003, Table B1-5).

Station	Sample Number	Date	TOC %	f <sub>oc</sub>	Naphth-alene	Acenaph-thylene	Acenaph-thene	Fluorene	Phenanthrene	Anthracene	Fluor-anthene	Pyrene	Benz[a]-anthracene	Chrysene	Benzo[b]-fluoran-thene	Benzo[k]-fluoran-thene	Benzo[a]-pyrene	Benzo[e]-pyrene	Indeno-[1,2,3-cd]-pyrene	Dibenz[a,h]-anthracene	Benzo[g,h,i]-perylene	Perylene	1-Methyl-Naphth-alene	2-Methyl-Naphth-alene	2,6-Dimethyl-Naphth-alene	1,3,5-Trimethyl-Naphth-alene	1-Methyl-phenanthrene	
<b>Reference</b>																												
2229	SD0103	9/9/2002	0.55	0.0055	7.5	7.5	7.5	7.5	14.0	10.0	60.0	100.0	60.0	68.0	57.0	56.0	92.0	56.0	55.0	8.3	52.0		7.5	7.5	7.5	7.5	7.5	7.5
2230	SD0104	9/9/2002	0.37	0.0037	7.5	7.5	7.5	7.5	13.0	7.5	34.0	34.0	23.0	33.0	29.0	27.0	31.0	22.0	24.0	7.5	21.0		7.5	7.5	7.5	7.5	7.5	7.5
2231	SD0013	8/8/2001	1.30	0.0130	12.0	12.0	12.0	12.0	20.0	19.0	59.0	59.0	45.0	81.0	85.0	59.0	81.0	59.0	75.0	14.0	66.0		12.0	12.0	12.0	12.0	12.0	12.0
2231	SD0134	9/14/2002	1.25	0.0125	13.0	13.0	13.0	13.0	17.0	13.0	52.0	68.0	39.0	67.0	76.0	60.0	79.0	66.0	66.0	13.0	64.0		13.0	13.0	13.0	13.0	13.0	13.0
2240	SD0125	9/12/2002	1.09	0.0109	13.0	13.0	13.0	13.0	13.0	13.0	34.0	46.0	20.0	32.0	38.0	34.0	39.0	35.0	33.0	13.0	35.0		13.0	13.0	13.0	13.0	13.0	13.0
2241	SD0128	9/12/2002	0.25	0.0025	6.8	6.8	6.8	6.8	6.8	6.8	9.3	12.0	6.8	13.0	14.0	13.0	13.0	13.0	12.0	6.8	12.0		6.8	6.8	6.8	6.8	6.8	6.8
2243	SD0049	8/14/2001	0.51	0.0051	7.8	7.8	7.8	7.8	7.8	7.8	15.0	20.0	12.0	18.0	23.0	18.0	21.0	17.0	25.0	7.8	25.0		7.8	7.8	7.8	7.8	7.8	7.8
2243	SD0124	9/12/2002	0.63	0.0063	8.0	8.0	8.0	8.0	8.0	8.0	18.0	23.0	10.0	17.0	25.0	21.0	24.0	22.0	21.0	8.0	22.0		8.0	8.0	8.0	8.0	8.0	8.0
2244	SD0126	9/12/2002	1	0.55	0.0055	8.1	8.1	8.1	8.1	8.1	8.1	21.0	23.0	10.0	16.0	26.0	21.0	22.0	21.0	8.1	22.0		8.1	8.1	8.1	8.1	8.1	8.1
2244	SD0126	9/12/2002	2	0.51	0.0051	7.8	7.8	7.8	7.8	7.8	11.0	14.0	7.8	11.0	16.0	13.0	15.0	14.0	15.0	7.8	14.0		7.8	7.8	7.8	7.8	7.8	7.8
2265	SD0107	9/9/2002	0.70	0.0070	8.6	8.6	8.6	8.6	8.6	8.6	19.0	23.0	14.0	24.0	28.0	23.0	27.0	23.0	22.0	8.6	21.0		8.6	8.6	8.6	8.6	8.6	8.6
2433	SD0041	8/12/2001	0.67	0.0067	8.0	8.0	8.0	8.0	16.0	12.0	43.0	45.0	35.0	60.0	55.0	48.0	58.0	39.0	48.0	8.5	41.0		8.0	8.0	8.0	8.0	8.0	8.0
2433	SD0130	9/13/2002	0.69	0.0069	8.1	8.1	8.1	8.1	9.7	8.1	32.0	39.0	29.0	48.0	49.0	40.0	47.0	37.0	31.0	8.1	30.0		8.1	8.1	8.1	8.1	8.1	8.1
2435	SD0102	9/9/2002	0.37	0.0037	7.0	7.0	7.0	7.0	7.0	7.0	9.7	12.0	7.0	12.0	12.0	10.0	10.0	8.4	8.4	7.0	7.8		7.0	7.0	7.0	7.0	7.0	7.0
2440	SD0043	8/13/2001	1.62	0.0162	10.0	11.0	26.0	29.0	200.0	100.0	540.0	580.0	210.0	290.0	220.0	230.0	230.0	170.0	170.0	32.0	170.0		8.1	8.1	8.1	8.1	8.1	15.0
2440	SD0131	9/13/2002	1.07	0.0107	15.0	8.2	42.0	35.0	330.0	99.0	530.0	550.0	250.0	350.0	230.0	230.0	280.0	180.0	150.0	25.0	120.0		8.2	8.2	8.2	8.2	8.2	28.0
2441	SD0034	8/11/2001	1.10	0.0110	8.9	8.9	8.9	8.9	8.9	11.0	16.0	33.0	24.0	30.0	47.0	41.0	34.0	35.0	24.0	28.0	8.9	21.0		8.9	8.9	8.9	8.9	8.9
2441	SD0123	9/12/2002	1.28	0.0128	9.9	9.9	9.9	9.9	43.0	23.0	130.0	110.0	68.0	110.0	88.0	81.0	88.0	63.0	47.0	9.9	38.0		9.9	9.9	9.9	9.9	9.9	
<b>NASSCO</b>																												
NA01	SD0030	8/11/2001	1	2.10	0.0210	14.0	93.0	14.0	24.0	190.0	270.0	570.0	550.0	630.0	1200.0	1200.0	980.0	1300.0	790.0	960.0	190.0	700.0	14.0	14.0	14.0	14.0	14.0	27.0
NA01	SD0031	8/11/2001	2	2.15	0.0215	15.0	100.0	15.0	25.0	150.0	270.0	470.0	490.0	490.0	960.0	1000.0	740.0	1000.0	660.0	830.0	160.0	630.0	15.0	15.0	15.0	15.0	15.0	22.0
NA02	SD0033	8/11/2001		2.00	0.0200	15.0	38.0	15.0	15.0	66.0	95.0	240.0	250.0	230.0	390.0	340.0	310.0	440.0	230.0	310.0	61.0	220.0	15.0	15.0	15.0	15.0	15.0	15.0
NA03	SD0032	8/11/2001		2.33	0.0233	15.0	79.0	15.0	30.0	160.0	230.0	470.0	480.0	470.0	820.0	850.0	730.0	910.0	590.0	700.0	130.0	530.0	15.0	15.0	15.0	15.0	15.0	20.0
NA04	SD0035	8/11/2001		2.04	0.0204	15.0	56.0	15.0	15.0	60.0	110.0	210.0	220.0	470.0	560.0	390.0	510.0	370.0	450.0	82.0	360.0	15.0	15.0	15.0	15.0	15.0	15.0	
NA05	SD0044	8/13/2001		1.60	0.0160	12.0	30.0	12.0	12.0	62.0	97.0	200.0	210.0	190.0	370.0	360.0	340.0	400.0	290.0	340.0	70.0	320.0	12.0	12.0	12.0	12.0	12.0	
NA06	SD0020	8/9/2001		2.31	0.0231	14.0	34.0	14.0	14.0	94.0	120.0	330.0	370.0	350.0	690.0	590.0	520.0	610.0	420.0	470.0	99.0	410.0	14.0	14.0	14.0	14.0	14.0	
NA07	SD0017	8/8/2001	1	1.98	0.0198	14.0	40.0	14.0	16.0	140.0	130.0	490.0	500.0	370.0	550.0	630.0	500.0	670.0	420.0	490.0	110.0	370.0	14.0	14.0	14.0	14.0	14.0	17.0
NA07	SD0018	8/8/2001	2	2.05	0.0205	14.0	150.0	17.0	27.0	320.0	390.0	4300.0	4200.0	2100.0	2400.0	3700.0	2300.0	3500.0	2200.0	2200.0	1600.0	14.0	14.0	14.0	14.0	14.0	61.0	
NA08	SD0055	8/14/2001		2.18	0.0218	16.0	36.0	16.0	16.0	78.0	120.0	280.0	220.0	440.0	520.0	390.0	470.0	350.0	410.0	78.0	360.0	16.0	16.0	16.0	16.0	16.0	16.0	
NA09	SD0054	8/14/2001		2.28	0.0228	17.0	29.0	17.0	17.0	66.0	77.0	200.0	260.0	180.0	320.0	400.0	310.0	380.0	260.0	64.0	320.0	17.0	17.0	17.0	17.0	17.0	17.0	
NA10	SD0056	8/14/2001		1.18	0.0118	11.0	25.0	11.0	11.0	38.0	62.0	110.0	160.0	96.0	190.0	250.0	220.0	270.0	190.0	240.0	43.0	220.0	11.0	11.0	11.0	11.0	11.0	
NA11	SD0021	8/9/2001		1.89	0.0189	13.0	25.0	13.0	13.0	120.0	86.0	240.0	260.0	200.0	370.0	360.0	310.0	400.0	260.0	300.0	56.0	260.0	13.0	13.0	13.0	13.0	13.0	
NA12	SD0027	8/10/2001		1.48	0.0148	13.0	27.0	13.0	13.0	62.0	81.0	180.0	180.0	150.0	270.0	250.0	220.0	260.0	180.0	210.0	44.0	190.0	13.0	13.0	13.0	13.0	13.0	
NA13	SD0036	8/11/2001		2.10	0.0210	14.0	14.0	14.0	14.0	40.0	32.0	140.0	160.0	110.0	220.0	180.0	170.0	180.0	150.0	28.0	130.0	14.0	14.0	14.0	14.0	14.0	14.0	
NA14	SD0051	8/14/2001		1.82	0.0182	12.0	12.0	12.0	12.0	32.0	21.0	110.0	110.0	86.0	190.0	130.0	120.0	140.0	110.0	120.0	20.0	100.0	12.0	12.0	12.0	12.0	12.0	
NA15	SD0037	8/12/2001		1.95	0.0195	14.0	52.0	14.0	14.0	81.0	100.0	220.0	260.0	210.0	390.0	500.0	380.0	500.0	350.0	420.0	80.0	370.0	14.0	14.0	14.0	14.0	14.0	
NA16	SD0038	8/12/2001		1.88	0.0188	18.0	52.0	32.0	29.0	180.0	120.0	340.0	350.0	240.0	390.0	540.0	390.0	540.0	380.0	470.0	87.0	400.0	14.0	14.0	14.0	14.0	14.0	
NA17	SD0039	8/12/2001		2.33	0.0233	15.0	60.0	15.0	15.0	100.0	130.0	370.0	680.0	220.0	390.0	510.0	420.0	480.0	380.0	410.0	85.0	370.0	15.0	15.0	15.0	15.0	15.0	
NA18	SD0053	8/14/2001		2.04	0.0204	14.0	31.0	14.0	14.0	53.0	72.0	170.0	190.0	150.0	280.0	350.0	280.0	360.0	250.0	300.0	59.0	270.0	14.0	14.0	14.0	14.0	14.0	
NA19	SD0042	8/12/2001		1.84	0.0184	14.0	50.0	14.0	14.0	51.0	93.0	190.0	200.0	170.0	330.0	500.0	350.0	460.0	340.0	410.0	76.0	330.0	14.0	14.0	14.0	14.0	14.0	
NA20	SD0028	8/10/2001		1.42	0.0142	9.2	34.0	9.2	9.2	92.0	99.0	310.0	420.0	210.0	320.0	420.0	330.0	390.0	270.0	260.0	57.0	230.0	9.2	9.2	9.2	9.2	9.2	

Table 10. Concentration of PAH compounds ( $\mu\text{g/g OC}$ ) in sediment samples normalized to the concentration of organic carbon.

Station	Sample Number	Sample Date	TOC Split %	$f_{oc}$	Naphthalene	Acenaphthylene	Acenaphthene	Fluorene	Phenanthrene	Anthracene	Fluoranthene	Pyrene	Benz[a]anthracene	Chrysene	Benzo[b]fluoranthene	Benzo[k]fluoranthene	Benzo[a]pyrene	Benzo[e]pyrene	Indeno[1,2,3-cd]pyrene	Dibenz[a,h]anthracene	Benzo[g,h,i]perylene	Perylene	1-Methyl Naphthalene	2-Methyl Naphthalene	2,6-Dimethyl Naphthalene	1,3,5-Trimethyl Naphthalene	1-Methyl phenanthrene			
<b>Reference</b>																														
2229	SD0103	9/9/2002	0.55	0.0055	1.3636	1.3636	1.3636	1.3636	2.5455	1.8182	10.9091	18.1818	10.9091	12.3636	10.3636	10.1818	16.7273	10.1818	10.0000	1.5091	9.4545									
2230	SD0104	9/9/2002	0.37	0.0037	2.0270	2.0270	2.0270	2.0270	3.5135	2.0270	9.1892	9.1892	6.2162	8.9189	7.8378	7.2973	8.3784	5.9459	6.4865	2.0270	5.6757									
2231	SD0013	8/8/2001	1.30	0.0130	0.9231	0.9231	0.9231	0.9231	1.5385	1.4615	4.5385	4.5385	3.4615	6.2308	6.5385	4.5385	6.2308	4.5385	5.7692	1.0769	5.0769									
2231	SD0134	9/14/2002	1.25	0.0125	1.0400	1.0400	1.0400	1.0400	1.3600	1.0400	4.1600	4.1600	3.1200	5.3600	6.0800	4.8000	6.2000	5.2800	5.2800	1.0400	5.1200									
2240	SD0125	9/12/2002	1.09	0.0109	1.1927	1.1927	1.1927	1.1927	1.1927	1.1927	3.1193	4.2202	1.8349	2.9358	3.4862	3.1193	3.5780	3.2110	3.0275	1.1927	3.2110									
2241	SD0128	9/12/2002	0.25	0.0025	2.7200	2.7200	2.7200	2.7200	2.7200	2.7200	3.7200	4.8000	2.7200	5.2000	5.6000	5.2000	5.2000	5.2000	4.8000	2.7200	4.8000									
2243	SD0049	8/14/2001	0.51	0.0051	1.5294	1.5294	1.5294	1.5294	1.5294	1.5294	2.9412	3.9216	2.3529	3.5294	4.5098	3.5294	4.1176	3.3333	4.9020	1.5294	4.9020									
2243	SD0124	9/12/2002	0.63	0.0063	1.2698	1.2698	1.2698	1.2698	1.2698	1.2698	2.8571	3.6508	1.5873	2.6984	3.9683	3.3333	3.8095	3.4921	3.3333	1.2698	3.4921									
2244	SD0126	9/12/2002	1	0.55	0.0055	1.4727	1.4727	1.4727	1.4727	1.4727	3.8182	4.1818	1.8182	2.9091	4.7273	3.8182	4.0000	3.8182	4.0000	1.4727	4.0000									
2244	SD0126	9/12/2002	2	0.51	0.0051	1.5294	1.5294	1.5294	1.5294	1.5294	2.1569	2.7451	1.5294	2.1569	3.1373	2.5490	2.9412	2.7451	2.9412	1.5294	2.7451									
2265	SD0107	9/9/2002	0.70	0.0070	1.2286	1.2286	1.2286	1.2286	1.2286	1.2286	2.7143	3.2857	2.0000	3.4286	4.0000	3.2857	3.8571	3.2857	3.1429	1.2286	3.0000									
2433	SD0041	8/12/2001	0.67	0.0067	1.1940	1.1940	1.1940	1.1940	2.3881	1.7910	6.4179	6.7164	5.2239	8.9552	8.2090	7.1642	8.8567	5.8209	7.1642	1.2687	6.1194									
2433	SD0130	9/13/2002	0.89	0.0089	1.1739	1.1739	1.1739	1.1739	1.4058	1.1739	4.6377	5.6522	4.2029	6.9965	7.1014	5.7971	6.8116	5.3623	4.4928	1.1739	4.3478									
2435	SD0102	9/9/2002	0.37	0.0037	1.8919	1.8919	1.8919	1.8919	1.8919	1.8919	2.6216	3.2432	1.8919	3.2432	3.2432	2.7027	2.7027	2.2703	2.2703	1.8919	2.1081									
2440	SD0043	8/13/2001	1.62	0.0162	0.6173	0.6173	0.6173	0.6173	12.3457	1.6173	33.3333	35.8025	12.9630	17.9012	13.5802	14.1975	14.7025	10.4938	10.4938	1.9753	10.4938									
2440	SD0131	9/13/2002	1.07	0.0107	1.4019	1.4019	1.4019	1.4019	3.9252	3.2710	30.8411	9.2523	49.5327	51.4019	23.3645	32.7103	21.4953	26.1682	16.8224	14.0187	2.3364	11.2150								
2441	SD0034	8/11/2001	1.10	0.0110	0.8091	0.8091	0.8091	0.8091	1.0000	1.4545	3.0000	2.1818	2.7273	3.7273	3.0909	3.1818	1.8181	2.5455	0.8091	1.9091	0.8091									
2441	SD0123	9/12/2002	1.28	0.0128	0.7734	0.7734	0.7734	0.7734	3.3594	1.7969	10.1563	8.5938	5.3125	8.5938	6.8750	6.3281	6.8750	4.9219	3.6719	0.7734	2.9688									
<b>NASSCO</b>																														
NA01	SD0030	8/11/2001	1	2.10	0.0210	0.6667	4.4286	0.6667	1.1429	9.0476	12.8571	27.1429	26.1905	30.0000	57.1429	57.1429	46.6667	61.9048	37.6190	45.7143	9.0476	33.3333								
NA01	SD0031	8/11/2001	2	2.15	0.0215	0.6977	4.6512	0.6977	1.1628	6.9767	12.5581	21.8605	22.7907	22.7907	44.6512	46.5116	34.4186	46.5116	38.6047	7.4419	29.3023									
NA02	SD0033	8/11/2001	2.00	0.0200	0.7500	1.9000	0.7500	0.7500	3.3000	4.7500	12.0000	12.5000	11.5000	19.5000	17.0000	15.5000	22.0000	11.5000	15.5000	3.0500	11.0000									
NA03	SD0032	8/11/2001	2.33	0.0233	0.6438	3.3906	0.6438	1.2676	6.8670	9.8712	20.1717	20.6009	20.1717	35.1931	36.4807	31.3305	39.0558	25.3219	30.0429	5.5794	22.7468									
NA04	SD0035	8/11/2001	2.04	0.0204	0.7353	2.7451	0.7353	0.7353	2.9412	5.3922	10.2941	10.7843	23.0392	27.4510	19.1176	25.0000	18.1373	22.0588	4.0196	17.6471	0.7353	17.6471								
NA05	SD0044	8/13/2001	1.60	0.0160	0.7500	1.8750	0.7500	0.7500	3.8750	6.0625	12.5000	13.1250	11.8750	23.1250	22.5000	21.2500	25.0000	18.1250	21.2500	4.3750	20.0000									
NA06	SD0020	8/9/2001	2.31	0.0231	0.6061	1.4719	0.6061	0.6061	4.0693	5.1948	14.2857	16.0173	14.2857	29.8701	25.5411	22.5108	26.4069	18.1818	20.3463	4.2857	17.7489									
NA07	SD0017	8/8/2001	1	1.98	0.0198	0.7071	2.0202	0.7071	0.8081	7.0707	6.5657	24.7475	25.2525	18.6869	27.7778	31.8182	25.2525	33.8384	21.2121	24.7475	5.5556	18.6869								
NA07	SD0018	8/8/2001	2	2.05	0.0205	0.6829	7.3171	0.6829	1.3171	15.6098	19.0244	209.756	204.8780	117.0732	180.4878	112.1951	170.7317	107.3171	107.3171	24.8780	78.0468									
NA08	SD0055	8/14/2001	2.18	0.0218	0.7339	1.6514	0.7339	0.7339	3.5780	5.5046	11.4679	17.4312	10.0917	20.1835	23.8532	17.8899	21.5596	16.0550	18.8073	3.5780	16.5138									
NA09	SD0054	8/14/2001	2.26	0.0226	0.7522	1.2832	0.7522	0.7522	2.9204	3.4071	8.8496	11.5044	7.9646	14.1593	17.6991	13.7168	16.8142	12.8319	15.9292	2.8319	14.1593									
NA10	SD0056	8/14/2001	1.18	0.0118	0.9322	2.1186	0.9322	0.9322	3.2203	5.2542	9.3220	13.5593	8.1356	16.1017	21.1864	18.6441	22.8814	16.1017	20.3390	6.6441	18.6441									
NA11	SD0021	8/9/2001	1.69	0.0169	0.7692	1.4793	0.7692	0.7692	7.1006	5.0888	14.2012	15.3846	11.8343	21.8935	21.3018	18.3432	23.6686	15.3846	17.7515	3.9136	15.3846									
NA12	SD0027	8/10/2001	1.48	0.0148	0.8784	1.8243	0.8784	0.8784	4.1892	5.4730	12.1622	12.1622	10.1351	18.2432	16.8919	14.8649	17.5676	12.1622	14.1892	2.9370	12.8378									
NA13	SD0036	8/11/2001	2.10	0.0210	0.6667	0.6667	0.6667	0.6667	1.9048	1.5238	6.6667	7.6190	5.2381	10.4762	8.5714	8.0952	8.5714	7.1429	7.1429	1.3333	6.1905									
NA14	SD0051	8/14/2001	1.82	0.0182	0.6593	0.6593	0.6593	0.6593	1.7582	1.1538	6.0440	6.0440	4.7253	10.4396	7.1429	6.5934	7.6923	6.0440	6.5934	1.0989	5.4945									
NA15	SD0037	8/12/2001	1.95	0.0195	0.7179	2.6667	0.7179	0.7179	4.1538	5.1282	11.2821	13.3333	10.7692	20.0000	25.6410	19.4872	25.6410	17.9487	21.5385	4.1026	18.9744									
NA16	SD0038	8/12/2001	1.88	0.0188	0.9574	2.7660	1.7021	1.5426	9.5745	6.3830	18.0851	18.6170	12.7660	20.7447	28.7234	20.7447	28.7234	20.2128	25.0000	4.6277	21.2766									
NA17	SD0039	8/12/2001	2.33	0.0233	0.6438	2.5751	0.6438	0.6438	4.2918	5.5794	15.8798	29.1845	9.4421	16.7382	21.8884	18.0258	20.6009	16.3090	17.5966	3.6481	15.8798									
NA18	SD0053	8/14/2001	2.04	0.0204	0.6863	1.5196	0.6863	0.6863																						

Table 11. Equilibrium Partitioning Sediment Benchmark Toxic Units (ESBTU) relative to the Final Chronic Value (FCV) for the sediment samples.

Station	Sample Number	Date	Spit	TOC %	f <sub>oc</sub>	Naphthalene	Acenaphthylene	Acenaphthene	Fluorene	Phenanthrene	Anthracene	Fluoranthene	Pyrene	Benz[a]-anthracene	Chrysene	Benzo[b]-fluoranthene	Benzo[k]-fluoranthene	Benzo[a]pyrene	Benzo[e]pyrene	Indeno[1,2,3-cd]pyrene	Dibenz[a,h]anthracene	Benzo[g,h,i]perylene	SUM ESBTU/FCVI
<b>Reference</b>																							
2229	SD0103	9/9/2002		0.55	0.0055	0.00354	0.00302	0.00278	0.00253	0.00427	0.00306	0.01543	0.03046	0.01297	0.01465	0.01059	0.01038	0.01733	0.01053	0.00897	0.00134	0.00863	0.16048
2230	SD0104	9/9/2002		0.37	0.0037	0.00526	0.00448	0.00413	0.00377	0.00590	0.00341	0.01300	0.01539	0.00739	0.01057	0.00801	0.00744	0.00868	0.00615	0.00582	0.00180	0.00518	0.11638
2231	SD0013	8/8/2001		1.30	0.0130	0.00240	0.00204	0.00188	0.00172	0.00258	0.00246	0.00642	0.00760	0.00412	0.00738	0.00668	0.00463	0.00646	0.00469	0.00517	0.00096	0.00464	0.07183
2231	SD0134	9/14/2002		1.25	0.0125	0.00270	0.00230	0.00212	0.00193	0.00228	0.00175	0.00588	0.00911	0.00371	0.00635	0.00621	0.00489	0.00655	0.00546	0.00474	0.00093	0.00468	0.07159
2240	SD0125	9/12/2002		1.09	0.0109	0.00310	0.00264	0.00243	0.00222	0.00200	0.00201	0.00441	0.00707	0.00218	0.00348	0.00356	0.00318	0.00371	0.00332	0.00272	0.00106	0.00293	0.05202
2241	SD0128	9/12/2002		0.25	0.0025	0.00706	0.00602	0.00554	0.00506	0.00456	0.00458	0.00526	0.00804	0.00323	0.00616	0.00572	0.00530	0.00539	0.00538	0.00430	0.00242	0.00438	0.08840
2243	SD0049	8/14/2001		0.51	0.0051	0.00397	0.00338	0.00311	0.00284	0.00257	0.00257	0.00416	0.00657	0.00280	0.00418	0.00461	0.00360	0.00427	0.00345	0.00440	0.00136	0.00448	0.06232
2243	SD0124	9/12/2002		0.63	0.0063	0.00330	0.00281	0.00259	0.00236	0.00213	0.00214	0.00404	0.00612	0.00189	0.00320	0.00405	0.00340	0.00395	0.00361	0.00299	0.00113	0.00319	0.05290
2244	SD0126	9/12/2002	1	0.55	0.0055	0.00383	0.00326	0.00300	0.00274	0.00247	0.00248	0.00540	0.00700	0.00216	0.00345	0.00483	0.00389	0.00415	0.00395	0.00359	0.00131	0.00365	0.06116
2244	SD0126	9/12/2002	2	0.51	0.0051	0.00397	0.00338	0.00311	0.00284	0.00257	0.00257	0.00305	0.00460	0.00182	0.00256	0.00320	0.00280	0.00305	0.00284	0.00264	0.00136	0.00251	0.04867
2265	SD0107	9/9/2002		0.70	0.0070	0.00319	0.00272	0.00250	0.00228	0.00206	0.00207	0.00384	0.00550	0.00238	0.00406	0.00409	0.00335	0.00400	0.00340	0.00282	0.00109	0.00274	0.05209
2433	SD0041	8/12/2001		0.67	0.0067	0.00310	0.00264	0.00243	0.00222	0.00201	0.00302	0.00908	0.01125	0.00621	0.01061	0.00839	0.00730	0.00897	0.00602	0.00643	0.00113	0.00559	0.09840
2433	SD0130	9/13/2002		0.69	0.0069	0.00305	0.00260	0.00239	0.00218	0.00236	0.00198	0.00656	0.00947	0.00500	0.00824	0.00725	0.00591	0.00706	0.00555	0.00403	0.00105	0.00397	0.07865
2435	SD0102	9/9/2002		0.37	0.0037	0.00491	0.00419	0.00385	0.00352	0.00317	0.00319	0.00371	0.00543	0.00225	0.00384	0.00331	0.00276	0.00280	0.00235	0.00204	0.00168	0.00193	0.05493
2440	SD0043	8/13/2001		1.82	0.0182	0.00180	0.00150	0.00327	0.00333	0.02071	0.01039	0.04715	0.05997	0.01541	0.02121	0.01387	0.01447	0.01471	0.01085	0.00941	0.00176	0.00958	0.25919
2440	SD0131	9/13/2002		1.07	0.0107	0.00364	0.00170	0.00799	0.00608	0.05175	0.01558	0.07006	0.08610	0.02778	0.03876	0.02196	0.02191	0.02712	0.01740	0.01257	0.00208	0.01024	0.42272
2441	SD0034	8/11/2001		1.10	0.0110	0.00210	0.00179	0.00165	0.00150	0.00168	0.00245	0.00424	0.00365	0.00324	0.00506	0.00381	0.00315	0.00330	0.00226	0.00228	0.00072	0.00174	0.04462
2441	SD0123	9/12/2002		1.28	0.0128	0.00201	0.00171	0.00158	0.00144	0.00564	0.00303	0.01437	0.01439	0.00632	0.01018	0.00702	0.00645	0.00712	0.00509	0.00329	0.00069	0.00271	0.09304
<b>NASSCO</b>																							
NA01	SD0030	8/11/2001	1	2.10	0.0210	0.00173	0.00980	0.00136	0.00212	0.01518	0.02164	0.03839	0.04387	0.03567	0.06770	0.05837	0.04757	0.06415	0.03890	0.04100	0.00806	0.03044	0.52595
NA01	SD0031	8/11/2001	2	2.15	0.0215	0.00181	0.01029	0.00142	0.00216	0.01171	0.02114	0.03092	0.03818	0.02710	0.05290	0.04751	0.03509	0.04820	0.03175	0.03462	0.00663	0.02676	0.42819
NA02	SD0033	8/11/2001		2.00	0.0200	0.00195	0.00420	0.00153	0.00139	0.00554	0.00800	0.01697	0.02094	0.01367	0.02310	0.01736	0.01580	0.02280	0.01189	0.01390	0.00272	0.01005	0.19181
NA03	SD0032	8/11/2001		2.33	0.0233	0.00167	0.00750	0.00131	0.00239	0.01152	0.01662	0.02853	0.03451	0.02399	0.04170	0.03726	0.03194	0.04047	0.02619	0.02694	0.00497	0.02077	0.35828
NA04	SD0035	8/11/2001		2.04	0.0204	0.00191	0.00607	0.00150	0.00137	0.00493	0.00908	0.01456	0.01724	0.01282	0.02730	0.02804	0.01949	0.02591	0.01876	0.01978	0.00358	0.01612	0.22846
NA05	SD0044	8/13/2001		1.60	0.0160	0.00195	0.00415	0.00153	0.00139	0.00650	0.01021	0.01768	0.02198	0.01412	0.02740	0.02298	0.02166	0.02591	0.01874	0.01906	0.00390	0.01826	0.23742
NA06	SD0020	8/9/2001		2.31	0.0231	0.00157	0.00326	0.00123	0.00113	0.00683	0.00875	0.02021	0.02683	0.01699	0.03539	0.02609	0.02295	0.02736	0.01880	0.01825	0.00382	0.01621	0.25567
NA07	SD0017	8/8/2001	1	1.98	0.0198	0.00184	0.00447	0.00144	0.00150	0.01186	0.01105	0.03500	0.04230	0.02222	0.03291	0.03250	0.02574	0.03507	0.02194	0.02220	0.00495	0.01707	0.32406
NA07	SD0018	8/8/2001	2	2.05	0.0205	0.00177	0.01619	0.00169	0.00245	0.02619	0.03203	0.29668	0.34318	0.12181	0.13871	0.18436	0.11437	0.17692	0.11098	0.09625	0.02215	0.01728	1.75701
NA08	SD0055	8/14/2001		2.18	0.0218	0.00191	0.00365	0.00149	0.00136	0.00600	0.00927	0.01622	0.02920	0.01200	0.02391	0.02436	0.01824	0.02234	0.01660	0.01687	0.00319	0.01508	0.22169
NA09	SD0054	8/14/2001		2.26	0.0226	0.00195	0.00284	0.00153	0.00140	0.00490	0.00574	0.01252	0.01927	0.00947	0.01678	0.01808	0.01398	0.01742	0.01327	0.01429	0.00252	0.01293	0.16889
NA10	SD0056	8/14/2001		1.18	0.0118	0.00242	0.00469	0.00190	0.00173	0.00540	0.00885	0.01319	0.02271	0.00967	0.01908	0.02164	0.01901	0.02371	0.01665	0.01824	0.00324	0.01703	0.20916
NA11	SD0021	8/9/2001		1.69	0.0169	0.00200	0.00327	0.00157	0.00143	0.01191	0.00857	0.02009	0.02577	0.01407	0.02594	0.02176	0.01870	0.02453	0.01591	0.01592	0.00295	0.01405	0.22844
NA12	SD0027	8/10/2001		1.48	0.0148	0.00228	0.00404	0.00179	0.00163	0.00703	0.00921	0.01720	0.02037	0.01205	0.02162	0.01725	0.01515	0.01820	0.01258	0.01273	0.00265	0.01172	0.18750
NA13	SD0036	8/11/2001		2.10	0.0210	0.00173	0.00148	0.00136	0.00124	0.00320	0.00257	0.00943	0.01276	0.00623	0.01241	0.00876	0.00825	0.00888	0.00739	0.00641	0.00119	0.00565	0.09894
NA14	SD0051	8/14/2001		1.82	0.0182	0.00171	0.00146	0.00134	0.00123	0.00295	0.00194	0.00855	0.01012	0.00562	0.01237	0.00730	0.00672	0.00797	0.00625	0.00591	0.00098	0.00502	0.08744
NA15	SD0037	8/12/2001		1.95	0.0195	0.00186	0.00590	0.00146	0.00133	0.00697	0.00863	0.01596	0.02233	0.01281	0.02370	0.02619	0.01986	0.02657	0.01856	0.01932	0.00365	0.01733	0.23243
NA16	SD0038	8/12/2001		1.88	0.0188	0.00249	0.00612	0.00347	0.00287	0.01606	0.01075	0.02558	0.03118	0.01518	0.02458	0.02934	0.02115	0.02977	0.02090	0.02242	0.00412	0.01943	0.28541
NA17	SD0039	8/12/2001		2.33	0.0233	0.00167	0.00570	0.00131	0.00120	0.00720	0.00939	0.02246	0.04889	0.01123	0.01983	0.02236	0.01837	0.02135	0.01687	0.01578	0.00325	0.01450	0.24136
NA18	SD0053	8/14/2001		2.04	0.0204	0.00178	0.00336	0.00140	0.00128	0.00436	0.00594	0.01179	0.01560	0.00874	0.01626	0.01752	0.01399	0.01829	0.01267	0.01319	0.00258	0.01209	0.16084
NA19	SD0042	8/12/2001		1.84	0.0184	0.00198	0.00601	0.00155	0.00141	0.00465	0.00851	0.01461	0.01821	0.01099	0.02125	0.02776	0.01939	0.02591	0.01911	0.01998	0.00368	0.01638	0.22138
NA20	SD0028	8/10/2001		1.42	0.0142	0.00168	0.00530	0.00132	0.00120														

Table 12. Concentration of alkylated and non-alkylated PAH compounds ( $\mu\text{g}/\text{kg}$  dry weight) in sediment samples (Exponent. 2003, Table B1-5).

Sample Number	Date	TOC %	$f_{\text{OC}}$	Naphthalene	1-Methylnaphthalene	2-Methylnaphthalene	C2-Naphthalenes	C3-Naphthalenes	C4-Naphthalenes	Acenaphthylene	Acenaphthene	Fluorene	C1-Fluorene	C2-Fluorene	C3-Fluorene	Phenanthrene	Anthracene	C1-Phenanthrenes/Anthracenes	C2-Phenanthrenes/Anthracenes	C3-Phenanthrenes/Anthracenes	C4-Phenanthrenes/Anthracenes	
<b>Reference</b>																						
2231	SD0168	11/6/2002	1.20	0.0120	12	12	12	12	12	12	12	12	12	12	12	12	13	12	12	12	12	
2243	SD0176	11/7/2002	0.64	0.0064	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	8.5	
2433	SD0167	11/6/2002	0.70	0.0070	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	14	8.3	15	16	10	
2440	SD0175	11/7/2002	0.87	0.0087	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	8.3	52	40	26	28	23	
2441	SD0166A	11/6/2002	1.26	0.0126	9.9	9.9	9.9	9.9	9.9	9.9	9.9	9.9	9.9	9.9	9.9	17	16	11	12	9.9	9.9	
<b>NASSCO</b>																						
NA01	SD0179	11/7/2002	2.20	0.0220	14	14	14	15	15	15	14	26	15	15	15	22						
NA06	SD0181	11/7/2002	2.04	0.0204	14	14	14	20	19	14	19	14	14	15	14	160	150	120	100	79	37	
NA13	SD0183	11/8/2002	1.80	0.0180	14	14	14	14	14	14	14	14	14	14	14	92	72	57	70	68	35	
NA16	SD0182	11/7/2002	2.13	0.0213	15	15	15	16	16	16	24	15	16	16	16	45	38	38	39	28	15	
NA17	SD0184	11/8/2002	1.52	0.0152	10	10	10	10	10	10	12	10	10	10	10	54	51	50	59	46	16	
																44	29	37	47	47	10	
<b>COC,PAHI,FCVI</b>					385	446	447	510	581	657	452	491	538	611	686	769	596	594	670	770	829	913
Station	Sample Number	Date	TOC %	$f_{\text{OC}}$	Fluoranthene	Pyrene	C1-Fluoranthrenes/Pyrenes	Benz[a]anthracene	Chrysene	C1-Benz[a]anthracenes/Chrycenes	C2-Benz[a]anthracenes/Chrycenes	C3-Benz[a]anthracenes/Chrycenes	C4-Benz[a]anthracenes/Chrycenes	Benzo[b]fluoranthrene	Benzo[k]fluoranthrene	Perylene	Benzo[a]pyrene	Benzo[e]pyrene	Indeno[1,2,3-cd]pyrene	Dibenz[a,h]anthracene	Benzo[g,h,i]perylene	
<b>Reference</b>																						
2231	SD0168	11/6/2002	1.20	0.0120	44	56	36	37	64	36	26	12	80	54	16	74	59	73	12	63		
2243	SD0176	11/7/2002	0.64	0.0064	16	19	11	9.7	15	9.3	9.9	8.5	21	16	8.5	20	16	20	8.5	18		
2433	SD0167	11/6/2002	0.70	0.0070	59	77	59	50	61	43	30	16	60	54	14	73	49	48	8.3	41		
2440	SD0175	11/7/2002	0.87	0.0087	170	200	140	110	150	100	79	47	50	140	99	30	120	96	95	15	79	
2441	SD0166A	11/6/2002	1.26	0.0126	69	77	62	56	90	48	28	12	9.9	74	56	14	61	44	41	9.9	30	
<b>NASSCO</b>																						
NA01	SD0179	11/7/2002	2.20	0.0220	340	390	560	440	840	560	350	120	130	880	610	170	910	570	610	120	420	
NA06	SD0181	11/7/2002	2.04	0.0204	260	330	280	200	330	270	210	80	77	620	330	90	480	370	340	63	240	
NA13	SD0183	11/8/2002	1.80	0.0180	160	200	180	140	250	180	130	54	48	370	210	68	320	240	250	42	200	
NA16	SD0182	11/7/2002	2.13	0.0213	160	220	190	150	250	220	190	83	85	470	300	79	430	320	360	64	280	
NA17	SD0184	11/8/2002	1.52	0.0152	140	180	150	110	160	160	180	91	90	350	250	54	320	200	230	43	170	
<b>COC,PAHI,FCVI</b>					770	697	770	841	844		929	1008	1112	1214	979	981	967	965	967	111	112	
																			5	3		

Table 13. Concentration of alkylated and non-alkylated PAH compounds ( $\mu\text{g/g OC}$ ) in sediment samples normalized to the concentration of organic carbon.

Station	Sample Number	Date	TOC %	f <sub>oc</sub>	Naphthalene	1-Methyl-Naphthalene	2-Methyl-Naphthalene	C2-Naphthalenes	C3-Naphthalenes	C4-Naphthalenes	Acenaphthylene	Acenaphthene	Fluorene	C1-Fluorene	C2-Fluorene	C3-Fluorene	Phenanthrene	Anthracene	C1-Phenanthrenes/Anthracenes	C2-Phenanthrenes/Anthracenes	C3-Phenanthrenes/Anthracenes	C4-Phenanthrenes/Anthracenes		
<b>Reference</b>																								
	2231	SD0168	11/6/2002	1.20	0.0120	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0833	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	
	2243	SD0176	11/7/2002	0.64	0.0064	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	1.3281	
	2433	SD0167	11/6/2002	0.70	0.0070	1.1857	1.1857	1.1857	1.1857	1.1857	1.1857	1.1857	1.1857	1.1857	1.1857	1.1857	1.1857	2.0000	1.1857	2.1429	2.2857	1.4286	1.1857	
	2440	SD0175	11/7/2002	0.87	0.0087	0.9540	0.9540	0.9540	0.9540	0.9540	0.9540	0.9540	0.9540	0.9540	0.9540	0.9540	0.9540	5.9770	4.5977	2.9885	3.2184	2.6437	1.9540	
	2441	SD0166A	11/6/2002	1.26	0.0126	0.7857	0.7857	0.7857	0.7857	0.7857	0.7857	0.7857	0.7857	0.7857	0.7857	0.7857	0.7857	1.3492	1.2698	0.8730	0.9524	0.7857	0.7857	
<b>NASSCO</b>																								
	NA01	SD0179	11/7/2002	2.20	0.0220	0.6364	0.6364	0.6364	0.6818	0.6818	0.6818	1.5909	0.6364	1.1818	0.6818	0.6818	1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	NA06	SD0181	11/7/2002	2.04	0.0204	0.6863	0.6863	0.6863	0.9804	0.9314	0.6863	0.9314	0.6863	0.6863	0.7353	0.6863	7.8431	7.3529	5.8824	4.9020	3.8725	1.8137	1.8137	
	NA13	SD0183	11/8/2002	1.80	0.0180	0.7778	0.7778	0.7778	0.7778	0.7778	0.7778	0.7778	0.7778	0.7778	0.7778	0.7778	5.1111	4.0000	3.1667	3.8889	3.7778	1.9444	1.9444	
	NA16	SD0182	11/7/2002	2.13	0.0213	0.7042	0.7042	0.7042	0.7512	0.7512	0.7512	1.1268	0.7042	0.7512	0.7512	0.7512	2.1127	1.7840	1.7840	1.8310	1.3146	0.7042	0.7042	
	NA17	SD0184	11/8/2002	1.52	0.0152	0.6579	0.6579	0.6579	0.6579	0.6579	0.7895	0.6579	0.6579	0.6579	0.6579	0.6579	3.5526	3.3553	3.2895	3.8816	3.0263	1.0526	1.0526	
<b>COC,PAH,FCVI</b>						385	446	447	510	581	657	452	491	538	611	686	769	596	594	670	770	829	913	
Station	Sample Number	Date	TOC %	f <sub>oc</sub>	Fluoranthene	Pyrene	C1-Fluoranthrenes/Pyrenes	Benz[a]anthracene	Chrysene	C1-Benz[a]anthracenes/Chrycenes	C2-Benz[a]anthracenes/Chrycenes	C3-Benz[a]anthracenes/Chrycenes	C4-Benz[a]anthracenes/Chrycenes	Benzo[b]fluoranthrene	Benzo[k]fluoranthrene	Perylene	Benzo[a]pyrene	Benzo[e]pyrene	Indeno[1,2,3-cd]pyrene	Dibenz[a,h]anthracene	Benzo[g,h,i]perylene			
<b>Reference</b>																								
	2231	SD0168	11/6/2002	1.20	0.0120	3.6667	4.6667	3.0000	3.0833	5.3333	3.0000	2.1667	1.0000	1.0000	6.6667	4.5000	1.3333	6.1667	4.9167	6.0833	1.0000	5.2500		
	2243	SD0176	11/7/2002	0.64	0.0064	2.5000	2.9688	1.7188	1.5156	2.3438	1.4531	1.5469	1.3281	3.2813	2.5000	1.3281	3.1250	2.5000	3.1250	1.3281	2.6125			
	2433	SD0167	11/6/2002	0.70	0.0070	8.4286	11.0000	8.4286	7.1429	8.7143	6.1429	4.2857	2.2857	1.1857	8.5714	7.7143	2.0000	10.4286	7.0000	6.8571	1.1857	5.8571		
	2440	SD0175	11/7/2002	0.87	0.0087	19.5402	22.9885	16.0920	12.6437	17.2414	11.4943	9.0805	5.4023	5.7471	16.0920	11.3793	3.4483	13.7931	11.0345	10.9195	1.7241	9.0805		
	2441	SD0166A	11/6/2002	1.26	0.0126	5.4762	6.1111	4.9206	4.4444	7.1429	3.8095	2.2222	0.9524	0.7857	5.8730	4.4444	1.1111	4.8413	3.4921	3.2540	0.7857	2.3810		
<b>NASSCO</b>																								
	NA01	SD0179	11/7/2002	2.20	0.0220	15.4545	17.7273	25.4545	20.0000	38.1818	25.4545	15.9091	5.4545	5.9091	40.0000	27.7273	7.7273	41.3636	25.9091	27.7273	5.4545	19.0909		
	NA06	SD0181	11/7/2002	2.04	0.0204	12.7451	16.1765	13.7255	9.8039	16.1765	13.2353	10.2941	3.9216	3.7745	30.3922	16.1765	4.4118	23.5294	18.1373	16.6667	3.0882	11.7647		
	NA13	SD0183	11/8/2002	1.80	0.0180	8.8889	11.1111	10.0000	7.7778	13.8889	10.0000	7.2222	3.0000	2.6667	20.5556	11.6667	3.7778	17.7778	13.3333	13.8889	2.3333	11.1111		
	NA16	SD0182	11/7/2002	2.13	0.0213	7.5117	10.3286	8.9202	7.0423	11.7371	10.3286	8.9202	3.8967	3.9906	22.0657	14.0845	3.7089	20.1878	15.0235	16.9014	3.0047	13.1455		
	NA17	SD0184	11/8/2002	1.52	0.0152	9.2105	11.8421	9.8684	7.2368	10.5263	11.8421	5.9868	5.9211	23.0263	16.4474	3.5526	21.0526	13.1579	15.1316	2.8289	11.1842			
<b>COC,PAH,FCVI</b>						770	697	770	841	844	929	1008	1112	1214	979	981	967	965	967	1115	1123	1095		

Table 14. Equilibrium Partitioning Sediment Benchmark Toxic Units (ESBTU) relative to the Final Chronic Value (FCV) for the sediment samples for which alkylated and non-alkylated PAH compounds were determined.

Station	Sample Number	Date	TOC %	f <sub>oc</sub>	Naphthalene	1-Methyl-Naphthalene	2-Methyl-Naphthalene	C2-Naphthalenes	C3-Naphthalenes	C4-Naphthalenes	Acenaphthylene	Acenaphthene	Fluorene	C1-Fluorene	C2-Fluorene	C3-Fluorene	Phenanthrene	Anthracene	C1-Phenanthrenes/Anthracenes	C2-Phenanthrenes/Anthracenes	C3-Phenanthrenes/Anthracenes	C4-Phenanthrenes/Anthracenes
<b>Reference</b>																						
2231	SD0168	11/6/2002	1.20	0.0120	0.0026	0.00224	0.00224	0.00196	0.00172	0.00152	0.00221	0.00204	0.00186	0.00164	0.00146	0.0013	0.00182	0.00168	0.00149	0.0013	0.00121	0.0011
2243	SD0176	11/7/2002	0.64	0.0064	0.00345	0.00298	0.00297	0.0026	0.00229	0.00202	0.00294	0.0027	0.00247	0.00217	0.00194	0.00173	0.00223	0.00224	0.00198	0.00172	0.0016	0.00145
2433	SD0167	11/6/2002	0.70	0.0070	0.00308	0.00266	0.00265	0.00232	0.00204	0.0018	0.00262	0.00241	0.0022	0.00194	0.00173	0.00154	0.00336	0.002	0.0032	0.00297	0.00172	0.0013
2440	SD0175	11/7/2002	0.87	0.0087	0.00248	0.00214	0.00213	0.00187	0.00164	0.00145	0.00211	0.00194	0.00177	0.00156	0.00139	0.00124	0.01003	0.00774	0.00446	0.00418	0.00319	0.00214
2441	SD0166A	11/6/2002	1.26	0.0126	0.00204	0.00176	0.00176	0.00154	0.00135	0.0012	0.00174	0.0016	0.00146	0.00129	0.00115	0.00102	0.00226	0.00214	0.0013	0.00124	0.00095	0.00086
<b>NASSCO</b>																						
NA01	SD0179	11/7/2002	2.20	0.0220	0.00165	0.00143	0.00142	0.00134	0.00117	0.00104	0.00352	0.0013	0.0022	0.00112	0.00099	0.0013	0	0	0	0	0	0
NA06	SD0181	11/7/2002	2.04	0.0204	0.00178	0.00154	0.00154	0.00192	0.0016	0.00104	0.00206	0.0014	0.00128	0.00112	0.00107	0.00089	0.01316	0.01238	0.00878	0.00637	0.00467	0.00199
NA13	SD0183	11/8/2002	1.80	0.0180	0.00202	0.00174	0.00174	0.00153	0.00134	0.00118	0.00172	0.00158	0.00145	0.00127	0.00113	0.00101	0.00858	0.00673	0.00473	0.00505	0.00456	0.00213
NA16	SD0182	11/7/2002	2.13	0.0213	0.00183	0.00158	0.00158	0.00147	0.00129	0.00114	0.00249	0.00143	0.00131	0.00123	0.0011	0.00098	0.00354	0.003	0.00266	0.00238	0.00159	0.00077
NA17	SD0184	11/8/2002	1.52	0.0152	0.00171	0.00148	0.00147	0.00129	0.00113	0.001	0.00175	0.00134	0.00122	0.00108	0.00096	0.00086	0.00596	0.00565	0.00491	0.00504	0.00365	0.00115
COC,PAH,FCVI					385	446	447	510	581	657	452	491	538	611	686	769	596	594	670	770	829	913
Station	Sample Number	Date	TOC %	f <sub>oc</sub>	Fluoranthene	Pyrene	C1-Fluoranthrenes/Pyrenes	Benz[a]anthracene	Chrysene	C1-Benz[a]anthracenes/Chrycenes	C2-Benz[a]anthracenes/Chrycenes	C3-Benz[a]anthracenes/Chrycenes	C4-Benz[a]anthracenes/Chrycenes	Benzo[b]fluoranthrene	Benzo[k]fluoranthrene	Perylene	Benzo[a]pyrene	Benzo[e]pyrene	Indeno[1,2,3-cd]pyrene	Dibenz[a,h]anthracene	Benzo[g,h,i]perylene	SUM ESBTUFCVI
<b>Reference</b>																						
2231	SD0168	11/6/2002	1.20	0.0120	0.00476	0.0067	0.0039	0.00367	0.00632	0.00323	0.00215	0.0009	0.00082	0.00681	0.00459	0.00138	0.00639	0.00508	0.00546	0.00089	0.00479	0.09923
2243	SD0176	11/7/2002	0.64	0.0064	0.00325	0.00426	0.00223	0.0018	0.00278	0.00156	0.00153	0.00119	0.00109	0.00335	0.00255	0.00137	0.00324	0.00259	0.0028	0.00118	0.00257	0.08082
2433	SD0167	11/6/2002	0.70	0.0070	0.01095	0.01578	0.01095	0.00849	0.01033	0.00681	0.00425	0.00206	0.00098	0.00876	0.00786	0.00207	0.01081	0.00724	0.00615	0.00106	0.00535	0.16124
2440	SD0175	11/7/2002	0.87	0.0087	0.02538	0.03298	0.0209	0.01503	0.02043	0.01237	0.00901	0.00486	0.00473	0.01844	0.0116	0.00357	0.01429	0.01141	0.00979	0.00154	0.00829	0.27608
2441	SD0166A	11/6/2002	1.26	0.0126	0.00711	0.00877	0.00639	0.00528	0.00846	0.0041	0.0022	0.00086	0.00065	0.006	0.00453	0.00115	0.00502	0.00381	0.00292	0.0007	0.00217	0.09658
<b>NASSCO</b>																						
NA01	SD0179	11/7/2002	2.20	0.0220	0.02007	0.02543	0.03306	0.02378	0.04524	0.0274	0.01578	0.00491	0.00487	0.04086	0.02826	0.00799	0.04286	0.02679	0.02487	0.00486	0.01743	0.41294
NA06	SD0181	11/7/2002	2.04	0.0204	0.01855	0.02321	0.01783	0.01166	0.01917	0.01425	0.01021	0.00353	0.00311	0.03104	0.01649	0.00456	0.02438	0.01876	0.01495	0.00275	0.01074	0.30778
NA13	SD0183	11/8/2002	1.80	0.0180	0.01154	0.01594	0.01299	0.00925	0.01646	0.01076	0.00716	0.0027	0.0022	0.021	0.01189	0.00391	0.01842	0.01379	0.01246	0.00208	0.01015	0.23219
NA16	SD0182	11/7/2002	2.13	0.0213	0.00976	0.01482	0.01158	0.00837	0.01391	0.01112	0.00885	0.0035	0.00329	0.02254	0.01436	0.00384	0.02092	0.01554	0.01516	0.00268	0.01201	0.22362
NA17	SD0184	11/8/2002	1.52	0.0152	0.01196	0.01699	0.01282	0.0086	0.01247	0.01133	0.01175	0.00538	0.00488	0.02352	0.01677	0.00367	0.02182	0.01361	0.01357	0.00252	0.01021	0.24352
COC,PAH,FCVI					770	697	770	841	844	929	1008	1112	1214	979	981	967	965	967	1115	1123	1095	

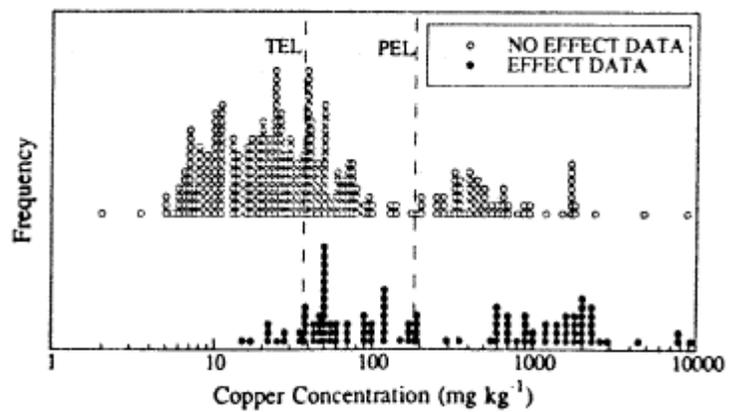


Figure 1. Distribution of effect and no-effect data used to derive the Canadian Sediment Quality Guidelines for copper in freshwater sediments. TEL is the threshold effects concentration and PEL is the probable effects level. Figure from Allen (1996).

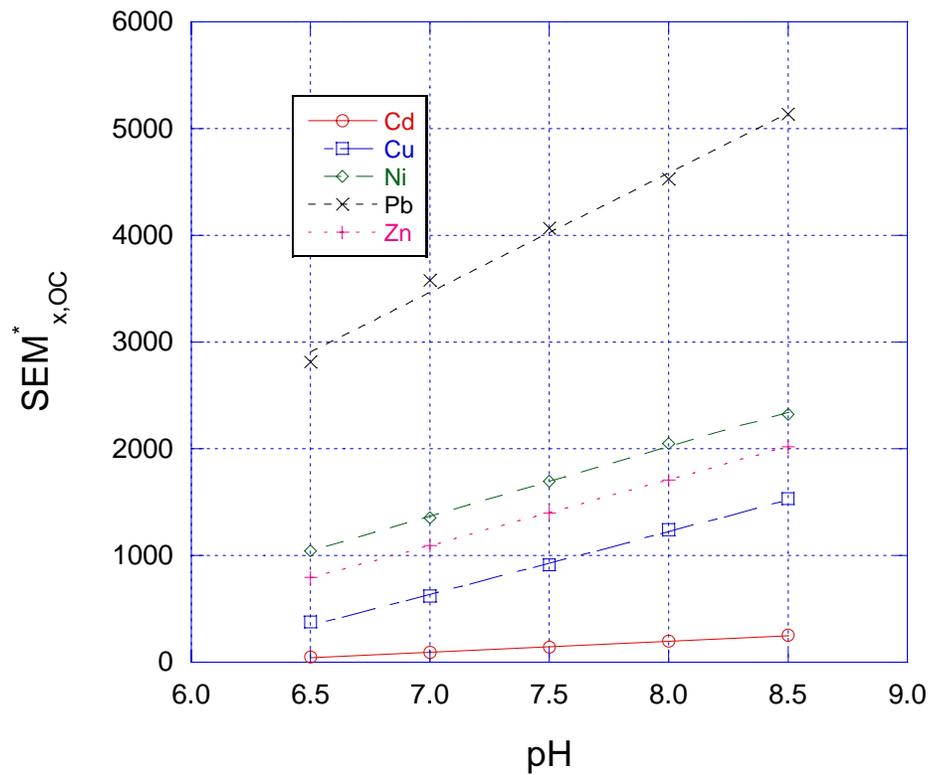


Figure 2. Values for excess simultaneously extracted metals concentration causing a 50% mortality for seawater ( $SEM^*_{x,OC}$ ) at varying pH. Data are from Di Toro et al. (2005) and the equations for the plots of the data are given in Table 7.

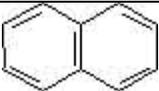
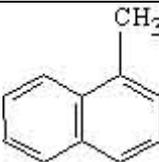
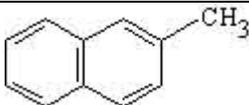
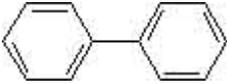
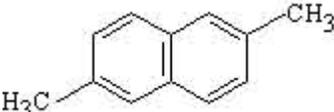
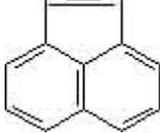
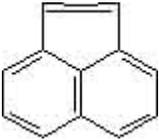
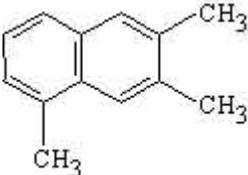
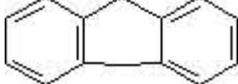
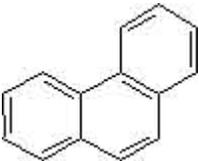
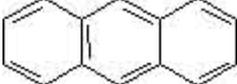
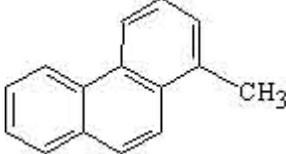
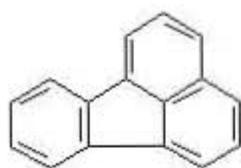
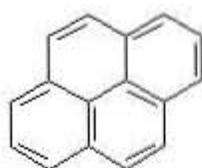
 <p><b>Naphthalene</b> CAS No: 91-20-3 Formula: C<sub>10</sub>H<sub>8</sub> MW: 128</p>	 <p><b>1-Methylnaphthalene</b> CAS No: 90-12-0 Formula: C<sub>11</sub>H<sub>10</sub> MW: 142</p>	 <p><b>2-Methylnaphthalene</b> CAS No: 91-57-6 Formula: C<sub>11</sub>H<sub>10</sub> MW: 142</p>
 <p><b>Biphenyl</b> CAS No: 92-52-4 Formula: C<sub>12</sub>H<sub>10</sub> MW: 154</p>	 <p><b>2,6-Dimethylnaphthalene</b> CAS No: 581-42-0 Formula: C<sub>12</sub>H<sub>12</sub> MW: 156</p>	 <p><b>Acenaphthylene</b> CAS No: 208-96-8 Formula: C<sub>12</sub>H<sub>8</sub> MW: 152</p>
 <p><b>Acenaphthene</b> CAS No: 83-32-9 Formula: C<sub>12</sub>H<sub>10</sub> MW: 154</p>	 <p><b>2,3,5-Trimethylnaphthalene</b> CAS No: 2245-38-7 Formula: C<sub>13</sub>H<sub>14</sub> MW: 170</p>	 <p><b>Fluorene</b> CAS No: 86-73-7 Formula: C<sub>13</sub>H<sub>10</sub> MW: 166</p>
 <p><b>Phenanthrene</b> CAS No: 85-01-8 Formula: C<sub>14</sub>H<sub>10</sub> MW: 178</p>	 <p><b>Anthracene</b> CAS No: 120-12-7 Formula: C<sub>14</sub>H<sub>10</sub> MW: 178</p>	 <p><b>1-Methylphenanthrene</b> CAS No: 832-69-9 Formula: C<sub>15</sub>H<sub>12</sub> MW: 192</p>

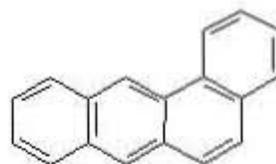
Figure 3. Low molecular weight polycyclic aromatic hydrocarbons.



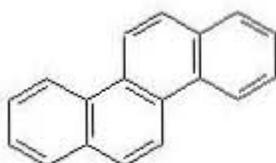
Fluoranthene



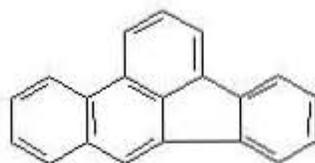
Pyrene



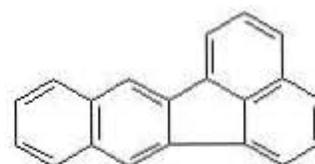
Benz[a]anthracene



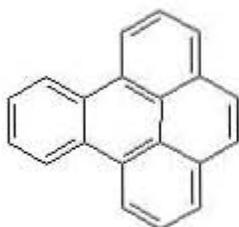
Chrysene



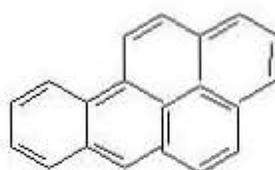
Benzofluoranthene



Benzofluoranthene



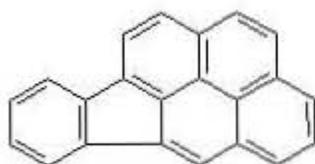
Benz[e]pyrene



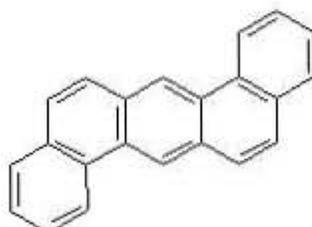
Benzofluoranthene



Perylene



Indeno[1,2,3-cd]pyrene



Dibenz[a,h]anthracene



Benzofluoranthene

Figure 4. High molecular weight polycyclic aromatic hydrocarbons.

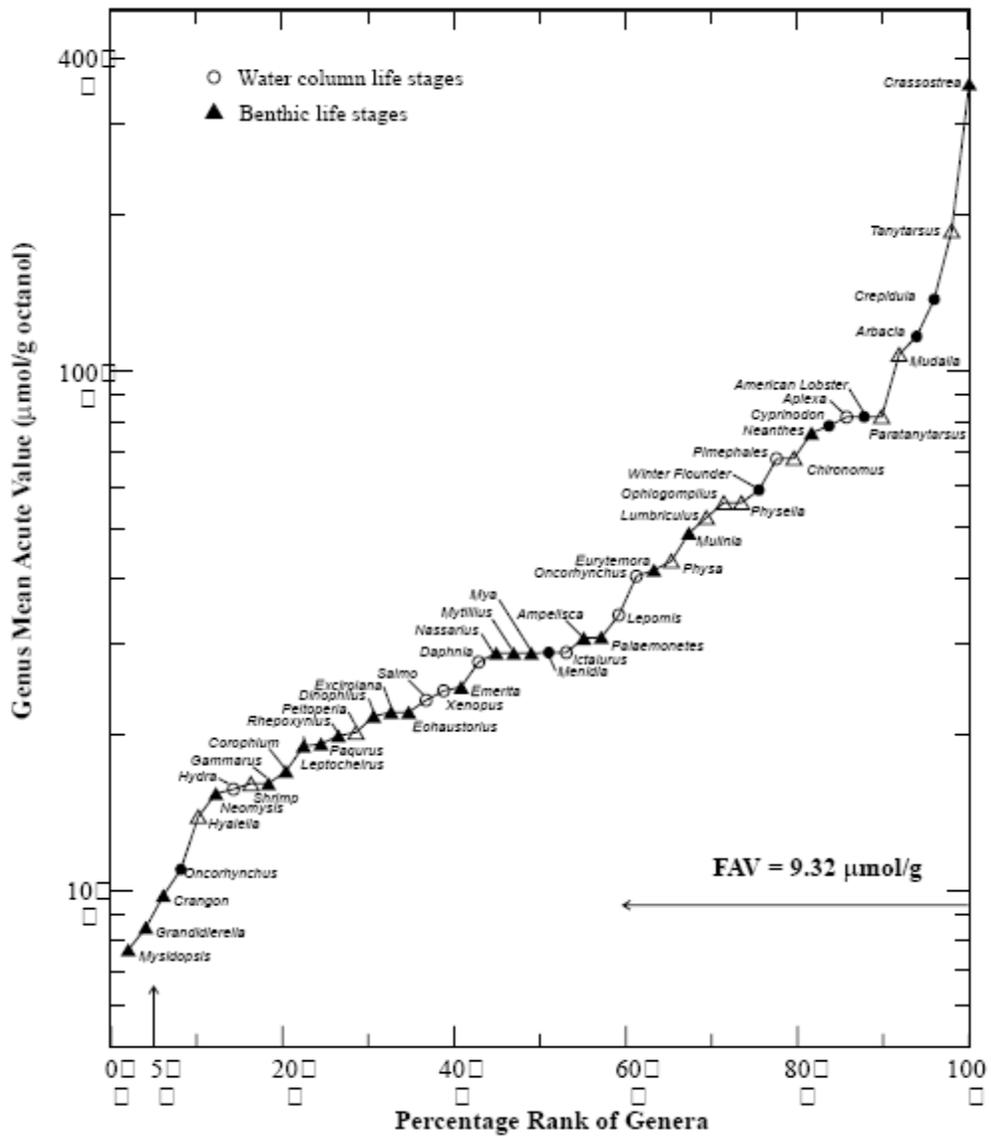


Figure 5. Ranking of sensitivity of organisms to PAHs .

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## Appendix A

### Herbert E. Allen Biographical Information

**Herbert E. Allen**

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Herbert E. Allen is a Professor Emeritus of Environmental Engineering at the University of Delaware and Director of the Center for the Study of Metals in the Environment. He retired from the tenured faculty on December 31, 2008, but maintains an active research program. Before joining the faculty of the University of Delaware in 1989 he was the Director of the Environmental Studies Institute and Professor of Chemistry at Drexel University and preceding that he was on the faculty of the Department of Environmental Engineering at the Illinois Institute of Technology. Dr. Allen received his Ph.D. and B.S. from the University of Michigan and his M.S. from Wayne State University.

Dr. Allen's research has been primarily concerned with fate and effects of trace metals in aquatic and soil environments, specializing in metal speciation and bioavailability. He has authored more than 160 journal papers and book chapters and he has edited 8 books and has prepared numerous reports and proceedings papers. He is listed as a Highly Cited Researcher by ISI. He has been the Principal or Co-Principal Investigator for over 70 research projects funded by government and by industry. He headed a multi-university consortium of universities, supported by EPA from 1994 until 2000 which conducted research on fate and effects of metals and organics in natural water systems and currently heads the multi-university EPA Center for the Study of Metals in the Environment. Dr. Allen was a member of the organizing committee for the 1993 EPA Annapolis workshop and of the 1996 SETAC Pellston conference to review Water Quality Criteria for metals. He served as the Chairman of the Organizing Committee for the Workshop on Metal Speciation that was held in Jekyll Island, Georgia every two years from 1987 through 1995. He has served as a consultant to a number of industrial companies, to government agencies, and to the World Health Organization.

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**RESEARCH INTERESTS**

Environmental chemistry; fate and effects of pollutants in water, sediment and soil environments; bioavailability of trace metals; development of environmental standards; ecological risk assessment; and analytical chemistry

**EDUCATION**

Ph.D., Environmental Chemistry, University of Michigan, 1974  
M.S., Analytical Chemistry, Wayne State University, 1967  
B.S., Chemistry, University of Michigan, 1962

**EXPERIENCE**

Director, Center for the Study of Metals in the Environment, 2001-2011 (funded by U.S. Environmental Protection Agency; University of Delaware lead in cooperation with other institutions).  
University of Delaware, Professor Emeritus of Environmental Engineering, 2009-present;  
Professor of Environmental Engineering, 1989-2008; Joint Professor of Oceanography, The Graduate College of Marine Studies, 1996-2008  
Drexel University, Professor of Chemistry and Director of Environmental Studies Institute, 1983-89  
Illinois Institute of Technology, Professor, 1980-84; Associate Professor, 1976-80; and Assistant Professor of Environmental Engineering, 1974-76  
Visiting Professor, Water Research Centre, Medmenham, England, 1980-81  
Faculty Associate, Argonne National Laboratory, 1978-79  
Lecturer, Department of Environmental and Industrial Health, University of Michigan, 1970-74  
Chemist, U.S. Bureau of Commercial Fisheries, 1962-70

**AWARDS AND HONORS**

ISI Highly Cited Researcher, 2006  
World Health Organization traveling fellowship for The Netherlands and Germany, 1981  
Visiting Professor, Department of Environmental Science, Nankai University, Tianjin, People's Republic of China, 1993  
Who's Who in America, 43rd – current edition  
Distinguished Service Award of the American Chemical Society, Div. Environmental Chemistry, 1987  
Sigma Xi, member 1973-present, president Drexel University chapter 1985-86

## **PROFESSIONAL ACTIVITIES (selected)**

World Health Organization, consultant to Regional Office for Europe, Technical Advisor to governments of Argentina, Brazil, Hungary, India, Jamaica, Mexico, Poland and Turkey, 1969-85; International Program on Chemical Safety, 1996

Environmental Protection Agency, Chemistry and Physics Grant Review Panel, 1980 - 1992; Science Advisory Board Consultant, 1994 - 2001

Delaware River Basin Committee, Member Toxics Advisory Committee, 1995 - 1999

International Copper Assoc., International Lead Zinc Research Org. and Nickel Producers Environmental Research Org.; Member International Technical Advisory Panel on Ecotoxicology, 1995 - 1999

National Research Council, Committee on Environmental Management Technologies (CEMT) Subcommittee on Subsurface Contaminants, 1997 - 1999

National Research Council, Committee on the Superfund Site Assessment and Remediation in the Coeur d'Alene River Basin, 2003 - 2005

National Research Council, Committee on Earth Science and Public Health, 2004 - 2006

Government of The Netherlands, Consultant on Soil Standards, 1996 - 1997

CSIR Division of Water Technology, South Africa, Advisor on Environmental Quality Standards, 1997

International Copper Association, Environmental Advisory Panel, 1998 - 2005; Advisor on Environmental Studies, Latin America and Asia programs, 1996 - 2003

U.S. Borax, Boron Ecotoxicology Advisory Group, 2002-2004

American Chemical Society, Div. Environmental Chemistry, Treasurer, 1972-75; Chairman, 1977-78

Associate Editor, **Ecotoxicology and Environmental Safety**, 2003 - present

Editorial Advisory Board Member, **Chemical Speciation and Bioavailability**, 1988-1999

Editorial Board Member, **Water Environment Research**, 1992-1994

Editorial Board Member, **Environmental Toxicology and Chemistry**, 1994-1996

Editorial Board Member, **Environmental Pollution**, 2002 - 2005

Editorial Board Member, **Journal of Environmental Science and Health - Part B - Pesticides, Food Contaminants, and Agricultural Wastes**, 2002 - present

## **SELECTED PUBLICATIONS (from over 160; books + recent selected papers)**

H.E. Allen ed. **Bioavailability of Metals in Terrestrial Ecosystems: Importance of Partitioning for Bioavailability to Invertebrates, Microbes and Plants**. SETAC Press, Pensacola, FL, 2002, 158 p.

H.E. Allen, A.W. Garrison and G.W. Luther, III eds. **Metals in Surface Waters**, Ann Arbor Press Chelsea, MI, 1998, 262 p.

H.E. Allen, ed. **Metal Contaminated Aquatic Sediments**, Ann Arbor Press. Chelsea, MI, 1995, 292 p.

H.E. Allen, C.P. Huang, G.W. Bailey, and A.R. Bowers, eds. **Metal Speciation and Contamination of Soil**, Lewis Publishers. Boca Raton, FL, 1994, 358 p.

H.E. Allen, E.M. Perdue, and D. Brown, eds. **Metals in Groundwater**, Lewis Publishers. Chelsea, MI, 1993, 437 p.

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### **SELECTED PROJECTS (from over 70)**

Principal Investigator – “Improving Understanding of the Fate and Transport of Munitions Constituents to Enhance Sustainability of Operational Ranges,” Strategic Environmental Research and Development Program, (2009-2013).

Principal Investigator – “Center for the Study of Metals in the Environment,” U.S. Environmental Protection Agency (University of Delaware lead in cooperation with 6 other institutions; 2001-2009).

Principal Investigator – The Development of a Terrestrial Biotic Ligand Model (TBLM), International Copper Association, (2002-2004).

Principal Investigator – Nickel Chemistry and Bioavailability in Soils, Nickel Producers Environmental Research Association, (2003-2004).

Principal Investigator - “Development of a Model to Predict the Fate of Fragrance Materials in Sludge-Amended Soils,” Research Institute for Fragrance Materials (2000-2003).

Principal Investigator - “Characterization of Zinc Partitioning, Desorption and Adsorption at the NVF Site in Yorklyn, DE” - Richards, Layton & Finger (2001-2002)

Principal Investigator - “Prediction and Assessment of the Bioavailability of Heavy Metals in Soil,” International Copper Association and International Lead Zinc Research Association (1998-2001).

Principal Investigator - “Development of Soil Screening Levels for Heavy Metals Based on Prediction of Soil-Water Partitioning, Aqueous Speciation and Bioavailability,” Environmental Protection Agency (1999-2001).

Principal Investigator - “Development of a Quantitative Risk Assessment Framework for Copper,” Subcontract from HydroQual (funding from International Copper Association) (1996-2002).

Principal Investigator - “Aquatic Toxicity of Copper: Effects of Chemical Speciation,” International Copper Association (1996-1998).

Principal Investigator - “Speciation, Bioavailability and Fate of Contaminants in the Aquatic Environment” (University of Delaware Lead Institution of Eight Universities), Environmental Protection Agency - Office of Water (1994-2000).

Principal Investigator - “Pollutant Quantitation with Passive Samplers,” Delaware Research Partnership/Gore Industries (1995-1996).

Principal Investigator - “Innovative Physicochemical Treatment of Explosives Contaminated Soil: Feasibility Investigation,” U.S. Army Environmental Center (1995-1996).

Principal Investigator - “Analysis and Reactions of Degradation Products of Sulfur Mustard in the Environment,” U.S. Army Environmental Center (1995-1997).

Principal Investigator - “Adsorption of Metals to New Jersey Soils,” New Jersey Department of Environmental Protection (1990-1997).