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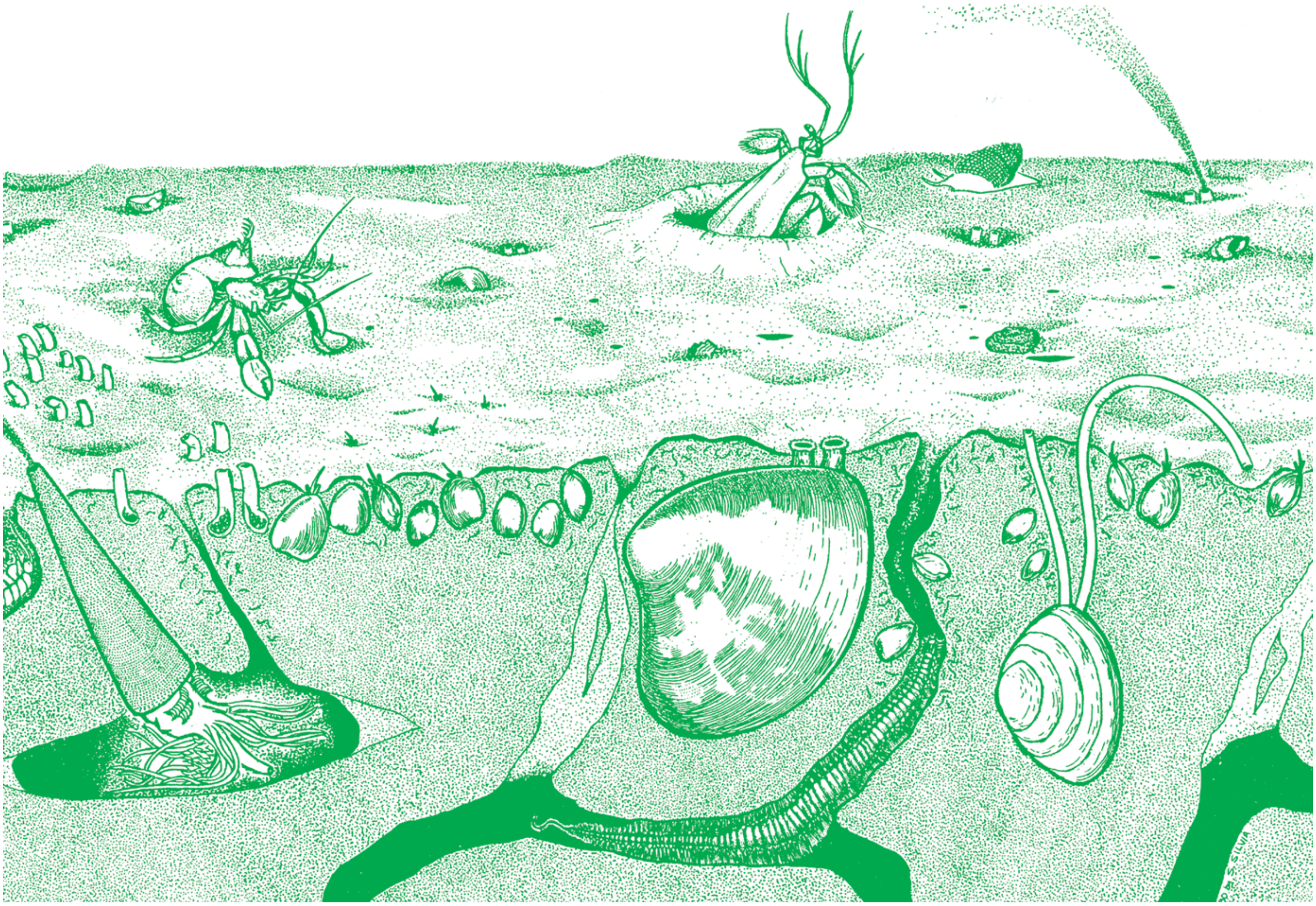
Procedures for the Derivation of Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms

Compendium of Tier 2 Values for Nonionic Organics



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Procedures for the Derivation of Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms: Compendium of Tier 2 Values for Nonionic Organics

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The Office of Research and Development (ORD) has produced this compendium document to provide procedures for the derivation of equilibrium partitioning sediment benchmarks (ESBs) for several nonionic organic chemicals. ESBs may be useful as a complement to existing sediment assessment tools. This document should be cited as:

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This document, and the other ESB documents, can also be found in electronic format at the following web address:

http://www.epa.gov/nheerl/publications/

The information in this document has been funded wholly by the U.S. Environmental Protection Agency. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Abstract

This equilibrium partitioning sediment benchmark (ESB) document describes procedures to derive concentrations for 32 nonionic organic chemicals in sediment which are protective of the presence of freshwater and marine benthic organisms. The equilibrium partitioning (EqP) approach was chosen because it accounts for the varying biological availability of chemicals in different sediments and allows for the incorporation of the appropriate biological effects concentration. This provides for the derivation of benchmarks that are causally linked to the specific chemical, applicable across sediments, and appropriately protective of benthic organisms.

EqP can be used to calculate ESBs for any toxicity endpoint for which there are water-only toxicity data; it is not limited to any single effect endpoint. For the purposes of this document, ESBs for 32 nonionic organic chemicals, including several low molecular weight aliphatic and aromatic compounds, pesticides, and phthalates, were derived using Final Chronic Values (FCV) from Water Quality Criteria (WQC) or Secondary Chronic Values (SCV) derived from existing toxicological data using the Great Lakes Water Quality Initiative (GLI) or narcosis theory approaches. These values are intended to be the concentration of each chemical in water that is protective of the presence of aquatic life. For nonionic organic chemicals demonstrating a narcotic mode of action, ESBs derived using the GLI approach specifically for freshwater organisms were assumed to also be protective of marine organisms. This assumption is based on the similar sensitivity of freshwater and marine organisms to narcotic chemicals like some of the nonionic organics in this document. For this reason, SCVs derived using narcosis theory are protective of both freshwater and marine organisms. For chemicals with more specific modes of action, freshwater and marine organisms were not assumed to be similar in sensitivity, and separate freshwater and marine ESBs were derived as the available data allowed. Because of the lack of a comprehensive toxicity data set and other reasons discussed in this document in detail, values derived here are considered Tier 2 ESBs (ESB_{Tier2}). The presentation of these ESBs is such that updated values could be calculated as new toxicity data become available.

The ESB_{Tier2} is derived by multiplying the FCV or SCV by a chemical's K_{OC}, yielding the concentration in sediment that should provide the same level of protection that the FCV or SCV provides in water. The ESB_{Tier2} should be interpreted as a chemical concentration below which adverse effects are not expected. At concentrations above the ESB_{Tier2}, and assuming equilibrium between phases, effects may occur with increasing severity as the degree of exceedance increases. The document also includes examples demonstrating the calculation of conventionally-derived and narcosis-based ESBs that discuss an approach for addressing mixtures of narcotic chemicals.

ESB documents have also been developed for two pesticides (endrin, dieldrin), polycyclic aromatic hydrocarbon (PAH) mixtures, and metal mixtures.

The ESBs do not intrinsically consider the antagonistic, additive or synergistic effects of other sediment contaminants in combination with the individual nonionic organic chemicals discussed in this document or the potential for bioaccumulation and trophic transfer of these chemicals to aquatic life, wildlife or humans. However, for narcotic chemicals, an approach for considering the toxicity of mixtures is presented. Important assumptions and considerations for applying and interpreting the ESBs are also discussed.

Foreword

Under the Clean Water Act (CWA), the U.S. Environmental Protection Agency (EPA) and the States develop programs for protecting the chemical, physical, and biological integrity of the Nation's waters. To support the scientific and technical foundations of the programs, EPA's Office of Research and Development has conducted efforts to develop and publish equilibrium partitioning sediment benchmarks (ESBs) for some of the 65 toxic pollutants or toxic pollutant categories. Toxic contaminants in bottom sediments of the Nation's lakes, rivers, wetlands, and coastal waters create the potential for continued environmental degradation even where water column contaminant levels meet applicable water quality standards. In addition, contaminated sediments can lead to water quality impacts, even when direct discharges to the receiving water have ceased.

The ESBs and associated methodology presented in this document provide a means to estimate the concentrations of a substance that may be present in sediment while still protecting benthic organisms from the effects of that substance. These benchmarks are applicable to a variety of freshwater and marine sediments because they are based on the biologically available concentration of the substance in the sediments. These ESBs are intended to provide protection to benthic organisms from direct toxicity due to this substance. In some cases, the additive toxicity for specific classes of toxicants (e.g., metal mixtures or polycyclic aromatic hydrocarbon mixtures) is addressed. The ESBs do not intrinsically consider the antagonistic, additive or synergistic effects of other sediment contaminants in combination with the individual nonionic organic chemicals discussed in this document or the potential for bioaccumulation and trophic transfer of these chemicals to aquatic life, wildlife or humans. However, for narcotic chemicals, the ESBs can be used in a framework to evaluate the toxicity of mixtures.

ESBs may be useful as a complement to existing sediment assessment tools, to help evaluate the extent of sediment contamination, to identify chemicals causing toxicity, and to serve as targets for pollutant loading control measures. Both types of ESBs, Tier 1 and Tier 2, are intended for similar applications with the user's understanding that, because of limited data availability, Tier 2 ESBs are likely to have greater uncertainty associated with them as compared to Tier 1 ESBs. As new, high quality toxicological and geochemical data becomes available, it is encouraged that the ESB values are revised and updated.

This document provides technical information to EPA Program Offices, including Superfund, Regions, States, the regulated community, and the public. Decisions about risk management are the purview of individual regulatory programs, and may vary across programs depending upon the regulatory authority and goals of the program. For this reason, each program will have to decide whether the ESB approach is appropriate to that program and, if so, how best to incorporate this technical information into that program's assessment process. While it was necessary to choose specific parameters for the purposes of this document, it is important to realize that the basic science underlying this document can be adapted to a range of risk management goals by adjusting the input parameters. At the same time, the ESBs do not substitute for the CWA or other EPA regulations, nor are they regulation. Thus, they cannot impose legally binding requirements on EPA, States, or the regulated community. EPA and State decision makers retain the discretion to adopt approaches on a case-by-case basis that differ from this technical information where appropriate. It is recommended that the ESBs not be used alone but with other sediment assessment methods to make informed management decisions. EPA may change this technical information in the future. This document has been reviewed by EPA's Office of Research and Development (Atlantic Ecology Division, Narragansett, RI), undergone an external peer review, and approved for publication.

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Executive Summary

This equilibrium partitioning sediment benchmark (ESB) document describes procedures to derive concentrations of 32 nonionic organic chemicals in sediment which are protective of the presence of freshwater and marine benthic organisms. The equilibrium partitioning (EqP) approach was chosen because it accounts for the varying biological availability of chemicals in different sediments and allows for the incorporation of the appropriate biological effects concentration (U.S. EPA 2003a). This provides for the derivation of benchmarks that are causally linked to the specific chemical, applicable across sediments, and appropriately protective of benthic organisms.

EqP theory holds that a nonionic chemical in sediment partitions between sediment organic carbon, interstitial (pore) water and benthic organisms. At equilibrium, if the concentration in any one phase is known, then the concentrations in the others can be predicted. The ratio of the concentration in water to the concentration in organic carbon is termed the organic carbon-water partition coefficient (K_{OC}), which is a constant for each chemical. The ESB Technical Basis Document (U.S. EPA 2003a) demonstrates that biological responses of benthic organisms to nonionic organic chemicals in sediments are different across sediments when the sediment concentrations are expressed on a dry weight basis, but similar when expressed on a µg chemical/g organic carbon basis ($\mu g/g_{OC}$). Similar responses were also observed across sediments when interstitial water concentrations were used to normalize biological availability. The Technical Basis Document (U.S. EPA 2003a) further demonstrates that if the effect concentration in water is known, the effect concentration in sediments on a $\mu g/g_{OC}$ basis can be accurately predicted by multiplying the effect concentration in water by the chemical's K_{OC}.

EqP can be used to calculate ESBs for any toxicity endpoint for which there are water-only toxicity data; it is not limited to any single effect endpoint. For the purposes of this document, ESBs for 32 nonionic organic chemicals, including several low molecular weight aliphatic and aromatic compounds, pesticides, and phthalates, were derived using Final Chronic Values (FCV) from Water Quality Criteria (WQC) or Secondary Chronic Values (SCV) derived from existing toxicological data using the Great Lakes Water Quality Initiative (GLI) or narcosis theory approaches. These values are intended to be the concentration of each chemical in water that is protective of the presence of aquatic life. For nonionic organic chemicals demonstrating a narcotic mode of action, ESBs derived using the GLI approach specifically for freshwater organisms were assumed to also be protective of marine organisms. This assumption is based on the similar sensitivity of freshwater and marine organisms to narcotic chemicals like some of the nonionic organics in this document. For this reason, SCVs derived using narcosis theory are presumed to be protective of both freshwater and marine organisms. For chemicals with other specific modes of action, freshwater and marine organisms were not assumed to have similar sensitivity and separate freshwater and marine ESBs were derived as the available data allowed. For pesticides, only freshwater- and marine-specific FCVs or SCVs were used to derive ESBs because of likely differences between freshwater and marine organism sensitivities. Similarly, for the phthalates, which are not thought to be narcotic, SCVs were derived using the GLI approach and considered protective of freshwater species only. Because of the lack of a comprehensive toxicity data set and other reasons discussed in this document in detail, values derived here are considered Tier 2 ESBs (ESB_{Tier2}). Ancillary analyses conducted as part of this derivation suggest that the sensitivity of benthic/epibenthic organisms is not significantly different from pelagic organisms; for this reason, the FCV or SCV and the resulting ESB_{Tier2} should be fully applicable to benthic organisms. The ESB_{Tier2} is derived by multiplying the FCV or SCV by a chemical's K_{OC}, yielding the concentration in sediment that should provide the same level of protection that the FCV or SCV provides in water. The ESB_{Tier2} should be interpreted as a chemical concentration below which adverse effects are not expected. At concentrations above the ESB_{Tier2}, assuming equilibrium between phases, effects may occur with increasing severity as the degree of exceedance increases. A sediment-specific site assessment (e.g., toxicity testing) would provide further information on chemical bioavailability and the expectation of toxicity relative to the $\text{ESB}_{\text{Tier2}}$ along with associated uncertainties. The document also includes examples demonstrating the calculation of conventionally-derived and narcosis-based ESBs that discuss an approach for addressing mixtures of narcotic chemicals.

As discussed, while this document uses the FCV or SCV, the EqP methodology can be used by environmental managers to derive a benchmark with any desired level of protection, so long as the water-only concentration affording that level of protection is known. Therefore, the resulting benchmark can be species or site-specific if the corresponding water-only information is available. For example, if a water-only effects concentration is known for an economically important benthic species, that value could be used to derive a sediment benchmark commensurate with the protection of that species and endpoint. Another way to increase the site-specificity of an ESB would be to incorporate information on sediment-specific partitioning of chemicals, particularly for sites where the composition and partitioning behavior of the sediment organic carbon may be substantially different than for typical diagenic organic matter (see U.S. EPA 2003b). However, it should also be noted that the ability to predict partitioning based on additional partitioning factors like black carbon is still evolving and may serve to decrease partitioning-related uncertainties in future applications.

The ESBs do not intrinsically consider the antagonistic, additive or synergistic effects of other sediment contaminants in combination with the individual nonionic organic chemicals discussed in this document or the potential for bioaccumulation and trophic transfer of these chemicals to aquatic life, wildlife or humans. However, for narcotic chemicals, ESB values may be used in a framework to evaluate the potential effects of chemical mixtures. Consistent with the recommendations of EPA's Science Advisory Board, publication of these documents does not imply the use of ESBs as stand-alone, pass-fail criteria for all applications; rather, ESB exceedances could be used to trigger the collection of additional assessment data. Similarly, ESBs are supportive of recent recommendations by Wenning et al. (2005), to apply a weight of evidence approach when evaluating contaminated sediments. These ESBs apply only to sediments having $\geq 0.2\%$ total organic carbon by dry weight and nonionic organic chemicals with log K_{OW}s ≥ 2.

Tier 1 and Tier 2 ESB values were developed to reflect differing degrees of data availability and uncertainty. Tier 1 ESBs have been derived for the nonionic organic pesticides endrin and dieldrin (U.S. EPA 2003c,d), polycyclic aromatic hydrocarbon (PAH) mixtures (U.S. EPA 2003e), and metal mixtures (U.S. EPA 2005a). Tier 2 ESBs for several nonionic organic chemicals for freshwater and marine sediments are reported in this document. Both types of ESBs are intended for similar applications with the user's understanding that Tier 2 ESBs are likely to have greater uncertainty associated with them as compared to Tier 1 ESBs. As new, high quality toxicological and geochemical data becomes available, recalculation of the Tier 2 ESB values is encouraged.

Uncertainties associated with $\text{ESB}_{\text{Tier2}}$ values are discussed in detail through-out this document. They include unknown effects of antagonism, synergism and additivity, occurrence of chemical disequilibria, and presence of unusual types of sedimentary carbon, like black carbon, and large particles. Uncertainties for the $\text{ESB}_{\text{Tier2}}$ values can be reduced by conducting additional acute and chronic water-only and spiked sediment toxicity tests to refine water-only effect concentrations and confirm predictions of sediment toxicity, respectively.

Glossary of Abbreviations

ACR	Acute–chronic ratio
AQUIRE	Aquatic Toxicity Information Retrieval
ASTER	ASsessment Tools for the Evaluation of Risk
ASTM	American Society for Testing and Materials
C_L*	Critical lipid concentration
CAS	Chemical Abstracts Service
CWA	Clean Water Act
DOC	Dissolved organic carbon
EC_{50}	Chemical concentration estimated to cause adverse effects to 50% of the test organisms within a specified time period
ECOTOX	ECOTOXicology databases
EMAP	Environmental Monitoring and Assessment Program
EPA	United States Environmental Protection Agency
EqP	Equilibrium partitioning
ESB	Equilibrium partitioning Sediment Benchmark; for nonionic organics, this term usually refers to a value that is organic carbon–normalized (more formally ESB_{OC}) unless otherwise specified
$ESB_{DRY\ WT}$	Equilibrium partitioning Sediment Benchmark; for nonionic organics, expressed on a sediment dry weight basis
ESB_{OC}	Equilibrium partitioning Sediment Benchmark; for nonionic organics, expressed on an organic carbon basis
ESB_{Tier2}	Equilibrium partitioning Sediment Benchmark; for nonionic organics, derived using Tier 2 data; specifically, the values in this document
$ESB_{\ Tier2DRY\ WT}$	Equilibrium partitioning Sediment Benchmark; for nonionic organics, derived using Tier 2 data, expressed on a sediment dry weight basis
$ESB_{Tier2OC}$	Equilibrium partitioning Sediment Benchmark; for nonionic organics, derived using Tier 2 data; expressed on organic carbon basis

ESBTU	Equilibrium Partitioning Sediment Benchmark Toxic Units
FACR	Final acute–chronic ratio
FAV	Final acute value
FCV	Final chronic value
f_{OC}	Fraction of organic carbon in sediment
f_{Solids}	Fraction of solids in sediment
GLI	Great Lakes Water Quality Initiative
GMAV	Genus mean acute value
GMCV	Genus mean chronic value
g_{OC}	Gram organic carbon
HECD	U.S. EPA, Health and Ecological Criteria Division
IC_{50}	Chemical concentration estimated to cause some form of inhibition to 50% of the test organisms within a specified time period
K_{BC}	Black carbon-water partition coefficient
K_{OC}	Organic carbon–water partition coefficient
K_{OW}	Octanol–water partition coefficient
K_P	Sediment–water partition coefficient
LC_{50}	Chemical concentration estimated to be lethal to 50% of test organisms within a specified time period
MC	Moisture content
MDR	Minimum data requirement
NHEERL	U.S. EPA, National Health and Environmental Effects Research Laboratory
OECD	Organization for Economic Cooperation and Development
ORD	U.S. EPA, Office of Research and Development
OST	U.S. EPA, Office of Science and Technology
OSWER	U.S. EPA, Office of Solid Waste and Emergency Response

PAH	Polycyclic aromatic hydrocarbon
PM	Particulate matter
QSAR	Quantitative structure-activity relationship
SACR	Secondary acute-chronic ratio
SAF	Secondary acute factor
SAV	Secondary acute value
SCV	Secondary chronic value
SCV_N	Secondary chronic value based on narcosis theory
SMACR	Species mean acute–chronic ratio
SMAV	Species mean acute value
SPARC	SPARC Performs Automated Reasoning in Chemistry
STORET	EPA’s computerized database for STOrage and RETrieval of water-related data
TIE	Toxicity Identification Evaluation
TOC	Total organic carbon
WQC	Water Quality Criteria

Section 1

Introduction

1.1 General Information

Toxic pollutants in bottom sediments of the Nation's lakes, rivers, wetlands, estuaries, and marine coastal waters create the potential for continued environmental degradation even where water column concentrations comply with established WQC. In addition, contaminated sediments can be a significant pollutant source that may cause water quality degradation to persist, even when other pollutant sources are stopped (Larsson 1985, Salomons et al. 1987, Burgess and Scott 1992). The absence of defensible equilibrium partitioning sediment benchmarks (ESBs) make it difficult to accurately assess the extent of the ecological risks of contaminated sediments and to identify, prioritize, and implement appropriate cleanup activities and source controls (U.S. EPA 1997a, b, c, 2004).

As a result of the need for a procedure to assist regulatory agencies in making decisions concerning contaminated sediment problems, the U.S. Environmental Protection Agency (EPA) Office of Water Office of Science and Technology, Health and Ecological Criteria Division (OST/HECD) and Office of Research and Development National Health and Environmental Effects Research Laboratory (ORD/NHEERL) established a research team to review alternative approaches (Chapman 1987). All of the approaches reviewed had both strengths and weaknesses, and no single approach was found to be applicable for the derivation of guidelines in all situations (U.S. EPA 1989, 1993). The equilibrium partitioning (EqP) approach was selected for nonionic organic chemicals because it presented the greatest promise for generating defensible, national, numeric chemical-specific benchmarks applicable across a broad range of sediment types. The three principal observations that underlie the EqP approach to establishing sediment benchmarks are as follows:

1. The concentrations of nonionic organic chemicals in sediments, expressed on an organic carbon basis, and in interstitial waters correlate to observed biological effects on sediment-dwelling organisms across a range of sediments.
2. Partitioning models can relate sediment concentrations for nonionic organic chemicals on an organic carbon basis to freely-dissolved concentrations in interstitial water.
3. The distribution of sensitivities of benthic organisms to chemicals is similar to that of water column organisms; thus, the currently established water quality criteria (WQC) final chronic values (FCV) or secondary chronic values (SCV) can be used to define the acceptable effects concentration of a chemical freely-dissolved in interstitial water.

The EqP approach, therefore, assumes that (1) the partitioning of the chemical between sediment organic carbon and interstitial water is at or near equilibrium; (2) the concentration in either phase can be predicted using appropriate partition coefficients and the measured concentration in the other phase (assuming the freely-dissolved interstitial water concentration can be accurately measured); (3) organisms receive equivalent exposure from water-only exposures or from any equilibrated phase: either from interstitial water via respiration, from sediment via ingestion or other sediment-integument exchange, or from a mixture of exposure routes; (4) for nonionic chemicals, effect concentrations in sediments on an organic carbon basis can be predicted using the organic carbon partition coefficient (K_{OC}) and effects concentrations in water; (5) the FCV or SCV concentration is an appropriate effects concentration for freely-dissolved chemical in interstitial water; and (6) ESBs derived as the product of the K_{OC} and FCV or SCV are protective of benthic organisms. ESB concentrations presented in this document are expressed as µg chemical/g sediment organic carbon (µg/g_{OC}) and not on an interstitial water basis because (1) interstitial water is difficult to sample and (2) significant amounts of the dissolved chemical may be associated with dissolved organic carbon; thus, total concentrations in interstitial water may overestimate exposure.

1.2 Development of Tier 2 Sediment Benchmarks

Aquatic toxicity values used in this compendium (Table 3-1) were developed in two possible ways: (1) conventionally using Water Quality Criteria (WQC) (when available) and Great Lakes Water Quality Initiative (GLI) generated values, and (2) narcosis theory. This compendium consists of Tier 2 ESBs for 32 chemicals including several low molecular weight aliphatic and aromatic compounds, pesticides and phthalates. Both types of ESBs, Tier 1 and Tier 2, are intended for similar applications with the user's understanding that Tier 2 ESBs are likely to have greater uncertainty associated with them as compared to Tier 1 ESBs. See Section 1.3 for further discussion of Tier 1 and Tier 2 ESBs.

The ESB values are reported in Tables 3-2 and 3-4. In the *References* section, along with the cited sources, the reference U.S. EPA (2001a) contains the sources and tables of data used to derive some of the Tier 2 ESBs.

For many of the chemicals in this document, the Tier 2 ESBs were developed using the GLI (1995) methodology for obtaining secondary chronic values (SCVs). As described in Section 2 and Appendix A, this methodology uses adjustment factors to allow derivation of chronic values when fewer toxicity data are available than are required under the National Ambient Water Quality Criteria methodology (Stephan et al. 1985). Because of these adjustment factors, SCVs are generally expected to be lower than would be likely if a complete data set were available. Consequently, Tier 2 ESBs would tend to be lower (i.e., be more conservative) compared to the Tier 1 ESBs developed exclusively from FCVs. The degree of conservatism will be a function of the database used to derive the SCVs. Further, the presence of these chemicals in mixtures will also affect the conservatism (see Section 4.2.5). The SCVs used in calculating most Tier 2 ESBs were derived using toxicity data primarily for freshwater species. In the toxicity data evaluation for the PAH mixtures ESB (U.S. EPA 2003e), there was no significant difference in sensitivity between freshwater and saltwater species when distributions of data for all species were compared using the approximate randomization (AR) method (Noreen 1989, U.S. EPA 2003e). Like PAHs, many of the Tier 2 ESB chemicals are also narcotics; from this, it is reasonable to presume that these ESBs would be applicable to both freshwater and saltwater sediments.

For pesticides, there are likely to be differences between FCVs or SCVs developed for freshwater and saltwater organisms (e.g., Thursby 1990, U.S. EPA 1980a,b, 1986, 1996, 2005b). Therefore, applying Tier 2 ESB values for pesticides derived using the GLI methodology to saltwater sediments is not recommended and would result in increased uncertainties. To address these uncertainties, Tier 2 ESBs are presented for pesticides for both freshwater and marine organisms based on FCVs from WQC (when available) or SCVs. Similarly, SCVs developed for phthalates in this document using the GLI approach were assumed to be protective only of freshwater species. Unlike the pesticides, WQC FCVs were not available for either freshwater or marine species for the phthalates.

As noted, many of the chemicals for which EPA has developed Tier 2 ESBs are known or suspected to affect aquatic organisms by a narcotic mode of action (Russom et al. 1997). For these compounds, Tier 2 ESBs were also derived using the narcosis theory approach applied to develop ESBs for PAH mixtures (U.S. EPA 2003e). In contrast to the conventional GLI approach, the narcosis approach does not apply adjustment factors. As a consequence, narcosis-based values are often larger in magnitude compared to the GLI-derived values (discussed further in Section 2). In Table 3-1, narcosis-based SCVs are also reported for chemicals with other modes of actions in addition to narcosis (i.e., pesticides and phthalates). For these chemicals, potency via narcosis is generally small compared to the more specific mode(s) of action which would result in narcosis-based ESB values being considerably higher than the conventionally-derived values. Accepting these approaches for developing chronic toxicity values and the associated uncertainties, Tier 2 ESB values for narcotic chemicals, pesticides and phthalates should be meaningful interpretive tools for marine sediments as well as freshwater sediments (Tables 3-2 and 3-4).

With regard to using narcosis to derive ESB values, the approach applied in this document and U.S. EPA (2003e) uses narcosis theory to predict acute toxicity and then empirically based acute-chronic ratios (ACRs) to calculate chronic toxicity values. These chronic values (i.e., SCVs) are then used to calculate the ESBs. Strengthening our mechanistic understanding of the link between acute toxicity based on narcosis and chronic effects potentially caused by other forms of toxicity is an active area of research (e.g., Incardona et al. 2006). Users of this document should recognize deficiencies in our understanding of this link may introduce uncertainties into the narcosis based estimates of ESB values.

Regardless of the approach used to derive the Tier 2 toxicity values, these concentrations have been generated on a single chemical basis; that is, the benchmark addresses effects for that chemical only and does not consider additive effects from other chemicals that may be present in sediment. For that reason, as the number and concentration of other chemicals present increases, single chemical benchmarks would be expected to provide a lesser degree of protection than a mixtures-based approach. EPA has not yet recommended an approach for summing the particular chemicals in this document, but approaches for assessing the toxicity of narcotic mixtures in sediments have been published (Di Toro and McGrath 2000, DiToro et al. 2000), and the Agency has developed methodologies for deriving ESBs for mixtures of PAHs (U.S. EPA 2003e) and metals (U.S. EPA 2005a). The approach discussed in U.S. EPA (2003e) for addressing the toxicity of mixtures of PAHs may be useful for those interested in combining the toxic effects of narcotic chemicals in this compendium (see Section 4.3 for an example).

Values similar to some of those reported in this document were used to evaluate data for EPA’s 1997 and 2004 National Sediment Quality Survey reports to Congress (USEPA 1997a,b,c, 2004). In those documents, the values were called sediment quality advisory levels (SQALs). These SQALs for nonionic organic chemicals were also included as “Ecotox Thresholds” in a 1996 ECO Update bulletin published by EPA’s Office of Solid Waste and Emergency Response (OSWER) (U.S. EPA 1996). In some cases, the Tier 2 ESBs in this document may differ from the SQALs and Ecotox Thresholds because of different data sources. Further, the SQALs and Ecotox Thresholds did not include narcosis-based chronic toxicity values.

Sediment benchmarks generated using the EqP approach are suitable for use in providing technical information to regulatory agencies because they are:

1. Numeric values
2. Chemical specific
3. Applicable to most sediments
4. Predictive of biological effects
5. Protective of benthic organisms

ESBs are derived using the available scientific data to assess the likelihood of significant environmental effects to benthic organisms from chemicals in sediments in the same way that the WQC are derived using the available scientific data to assess the likelihood of significant environmental effects to organisms in the water column. As such, ESBs are intended to protect benthic organisms from the effects of chemicals associated with sediments and, therefore, only apply to sediments permanently inundated with water, to intertidal sediment, and to sediments inundated periodically for durations sufficient to permit development of benthic assemblages. ESBs should not be applied to occasionally inundated soils containing terrestrial organisms, nor should they be used to address the question of possible contamination of upper trophic level organisms or the generic synergistic, additive, or antagonistic effects of multiple chemicals. The application of ESBs under these conditions may result in values lower or higher than those presented in this document. It should be noted that under certain conditions with narcotic chemicals, additivity may be considered.

ESB values presented herein are the concentrations of 32 nonionic organic chemicals in sediment that are not expected to adversely affect most benthic organisms. Just as values in this document can be seen as an update of the SQALs and Ecotox Thresholds, it is recognized (and encouraged) that these ESB values may need to be adjusted to account for new data as they become available. They may also need to be adjusted because of site-specific considerations. For example, in spill situations, where chemical equilibrium between water and sediment has not yet been reached, sediment chemical concentrations less than an ESB may pose risks to benthic organisms. This is because for spills, disequilibrium concentrations in interstitial and overlying water may be proportionally higher relative to sediment concentrations. In systems where biogenic organic carbon dominates, research has shown that the source or 'quality' of total organic carbon (TOC) in natural sediments does not affect chemical partitioning when sediment toxicity was measured as a function of TOC concentration (DeWitt et al. 1992). K_{OC}s for several nonionic chemicals have also been shown to not vary significantly across estuarine sediments with differing organic carbon concentrations and quality (Burgess et al. 2000). However, in systems where other forms of carbon are present at elevated levels, the source or 'quality' of TOC may affect chemical binding despite expressing toxicity as a function of TOC concentration. At some sites, concentrations in excess of an ESB may not pose risks to benthic organisms because the compounds are partitioned to a component of a particulate phase such as black carbon or coal or exceed solubility such as in the case of undissolved oil or chemical (e.g., manufactured gas plant sites) (U.S. EPA 2003e, Cornelissen et al. 2005). In these situations, an ESB would be overly protective of benthic organisms and should not be used unless modified using the procedures outlined in "Procedures for the Derivation of Site-Specific Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms: Nonionic Organics" (U.S. EPA 2003b). It should also be noted that the ability to predict partitioning based on additional factors like black carbon is still evolving and may serve to decrease partitioning-related uncertainties in future applications. If the organic carbon has a low sorptive affinity (e.g., hair, wood chips, hide fragments), an ESB would be under protective. An ESB may also be under protective when the toxicity of other chemicals are additive with an ESB chemical or when species of unusual sensitivity occur at the site.

This document presents the derivation and calculation of Tier 2 ESBs for 32 nonionic organic chemicals. The data that support the EqP approach for deriving ESBs for nonionic organic chemicals are reviewed by Di Toro et al. (1991) and EPA (2003a). Before proceeding through the following text, tables, and calculations, the reader should also consider reviewing Stephan et al. (1985).

1.3 Application of Sediment Benchmarks

ESBs as presented in this document are meant to be used with direct toxicity testing of sediments as a method of sediment evaluation, assuming the toxicity testing species is sensitive to the chemical(s) of interest (e.g., ASTM 1998a,b,c, U.S. EPA 1994, 2000, 2001b). In this way, ESBs are supportive of recent recommendations by Wenning et al. (2005), to apply a weight of evidence approach when evaluating contaminated sediments. Specifically, the ESBs provide a chemical-by-chemical specification of sediment concentrations protective of benthic aquatic life (see Section 4.2.6 for more discussion). The EqP method should be most applicable to nonionic organic chemicals with a log $K_{OW} \geq 2$. However, for chemicals with log K_{OW} between 2 and 3, EqP will function but sedimentary conditions (i.e., f_{OC} and f_{Solids}) should be considered and adjustments to the derivation of the ESB maybe advisable (see Section 3.3). Examples of other chemicals to which the methodology applies include the pesticides endrin and dieldrin (U.S. EPA 2003c,d), metal mixtures (U.S. EPA 2005a), and PAH mixtures (U.S. EPA 2003e).

For the toxic chemicals addressed by the ESB documents, Tier 1 (U.S. EPA, 2003c, d, e, and 2005a) and Tier 2 (this document) values were developed to reflect the differing degrees of data availability and uncertainty. Tier 1 ESBs are more scientifically rigorous and data intensive than Tier 2 ESBs. The minimum requirements to derive a Tier 1 ESB include: (1) each chemical‘s organic carbon-water partition coefficient (K_{OC}) is derived from the octanol-water partition coefficient (K_{OW}) obtained using the SPARC model (Karickhoff et al. 1991) and the K_{OW}-K_{OC} relationship from Di Toro et al. (1991). This K_{OC} has been demonstrated to predict the toxic sediment concentration from the toxic water concentration with less uncertainty than K_{OC} values derived using other methods, (2) the FCV is updated using the most recent toxicological information and is based on the National WQC guidelines (Stephan et al. 1985), and (3) EqP-confirmation tests are conducted to demonstrate the accuracy of the EqP prediction that the K_{OC} multiplied by the effect concentration from a water-only toxicity test predicts the effect concentration from sediment tests (Swartz 1991, DeWitt et al. 1992, Hoke et al. 1994). Using these specifications, Tier 1 ESBs have been derived for the nonionic organic pesticides endrin and dieldrin (U.S. EPA 2003c,d), PAH mixtures (U.S. EPA 2003e), and metals mixtures (U.S. EPA 2005a). In comparison, the minimum requirements for a Tier 2 ESB (this document) are less rigorous: (1) the K_{OW} for the chemical that is used to derive the K_{OC} can be from slow-stir, generator column, shake flask, SPARC or other sources (e.g., Site 2001), (2) FCVs can be from published or draft WQC documents, the Great Lakes Water Quality Initiative (GLI 1995), or developed from AQUIRE (now ECOTOX). Secondary chronic values (SCV) from narcosis theory (Di Toro and McGrath 2000, Di Toro et al. 2000, U.S. EPA 2003e), Suter and Tsao (1996), or other effects concentrations from water-only toxicity tests can also be used. The U.S. EPA methodology for deriving water quality criteria SCVs required for the computation of Tier 2 ESBs is described in *Water Quality Guidance for the Great Lakes System: Supplementary Information Document (SID)* (U.S. EPA 1995a), and (3) EqP confirmation tests are recommended, but are not required for the development of Tier 2 ESBs. Because of these lesser requirements, there is greater uncertainty in the EqP prediction of the sediment effect concentration from the water-only effect concentration, and in the level of protection afforded by Tier 2 ESBs. This uncertainty can be decreased by conducting additional acute and chronic water-only and spiked sediment toxicity tests to evaluate effect concentrations and confirm predicted sediment concentrations, respectively.

1.4 Data Quality Assurance

Data sources, selections and manipulations used to generate K_{OW}s or K_{OC}s and SCV or FCVs are discussed in detail in Section 2. Toxicological data were selected from final and draft Water Quality Criteria, Suter and Tsao

(1996), U.S. EPA (1996), GLI (1995) and U.S. EPA (2001a) or derived using the approach described by Di Toro and McGrath (2000), Di Toro et al. (2000) and U.S. EPA (2003e). K_{OW} values were taken from Karickhoff and Long (1995) as well as other sources. Toxicity data were evaluated for acceptability using the procedures in Stephan et al. (1985), the Great Lakes Water Quality Initiative (GLI 1995), and the approach for deriving narcotic chronic toxicity values (Di Toro and McGrath 2000, Di Toro et al. 2000, U.S. EPA 2003e). Data not meeting criteria for acceptability were rejected. In general, three or four significant figures were used in intermediate calculations to limit the effect of rounding errors, and are not intended to indicate the true level of precision. The time periods covered in the literature searches associated with data in this document can be found in the cited source literature.

Literature searches supporting Suter and Tsao (1996), U.S. EPA (1996), GLI (1995) and U.S. EPA (2001a) were conducted in the mid-1990s. In order to capture more recent data, EPA's ECOTOX database (www.epa.gov/ecotox) was searched for any data pertaining to the chemicals evaluated in this document published after 1995. These data were then sorted to identify sources of acute toxicity data for North American species tested for a period appropriate to the species (Stephan et al. 1985) and for which test concentrations of chemical were measured. In addition, literature sources suggested by peer reviewers of this document were also consulted for data meeting minimum requirements. Fewer than 30 additional data points were identified, and only one of these affected the calculation of an SCV (see footnote in Table 3-1). As new, high quality toxicological and geochemical data becomes available, it is encouraged that the ESB values are revised and updated. See Section 2.5 for further discussion.

The document was reviewed as part of a formal external peer review coordinated at the U.S. EPA National Health and Environmental Effects Research Laboratory, Research Triangle Park, North Carolina and Atlantic Ecology Division, Narragansett, Rhode Island. Any errors of omission or calculation discovered during the peer review process were corrected.

1.5 Overview

This document presents the derivation and calculation of ESBs for 32 nonionic organic chemicals.

Section 2 reviews the toxicological and chemical data used to derive the ESB_{Tier2}s. Section 3 discusses the calculation of the ESB_{Tier2}s. Section 4 "Sediment Benchmark Values: Application and Interpretation" discusses the sediment benchmark values and lists several factors to consider when applying and interpreting these values. Section 5 lists references cited in all sections of this document. Appendix A discusses, in detail, the GLI approach for calculating chronic toxicity values.

Section 2

Derivation of Equilibrium Partitioning Sediment Benchmark Effects Concentrations

2.1 General Introduction

This section outlines the compilation of data used in the derivation of the Tier 2 ESBs presented in this compendium. The section follows the format for calculating the ESB values by first describing the derivation of the K_{OW} values, and then the derivation of the appropriate aquatic toxicity values. The derivation of the K_{OW} values follows procedures outlined in Karickhoff and Long (1996) and in many cases uses values summarized in Karickhoff and Long (1995). Because of the diversity of chemicals discussed in this compendium (i.e., narcotics, pesticides, phthalates), aquatic toxicity values were derived in two possible ways. Conventional aquatic toxicity values were derived either using the procedures detailed in the Great Lakes Water Quality Initiative (GLI, 1995) or taken from existing or draft WQC. For example, marine ESBs for pesticides were based only on FCVs from existing or draft WQC while freshwater ESBs for pesticides were derived using both WQC and GLI toxicity values. Similarly, ESBs for phthalates were derived only for freshwater species using the GLI approach as WQC values were not available. For chemicals designated as being narcotic, toxicity values were also derived using the narcosis theory used to develop ESBs for PAH mixtures (Di Toro et al. 2000, U.S. EPA 2003e). As discussed in Section 1, ESBs derived using either conventional or narcotic approaches, for narcotic chemicals in this document are applicable to both freshwater and marine species based on the concept that these organisms show similar sensitivity to narcotic chemicals. This concept was not exercised for pesticides and phthalates.

2.2 Determination of K_{OW} Values

The determination of K_{ow} values was based on experimental measurements taken primarily by the slow-stir, generator-column, and shake-flask methodologies. The SPARC properties calculator model (Karickhoff and Long 1995) was also used to generate K_{ow} values, when appropriate, for comparison with the measured values. Values that appeared to be considerably different from the rest were classified as outliers and were not used in the calculation. For each chemical, the available log K_{ow} value, based on one of the above mentioned methods, was given preference. If more than one such value was available, the log K_{ow} value was calculated as the arithmetic mean of those values (U.S. EPA 1995b). Most of the log K_{ow} values used in this document are summarized in an internal EPA report (Karickhoff and Long 1995). Subsequent to that evaluation, EPA has published a recommended procedure for selecting K_{ow} values, which can be seen in Karickhoff and Long (1996).

Log K_{ow} values were initially identified in summary texts on physical-chemical properties, such as Howard (1990) and Mackay et al. (1992a,b), and accompanying volumes. Additional compendia of log K_{ow} values were also evaluated including de Bruijn et al. (1989), De Kock and Lord (1987), Doucette and Andren (1988), Isnard and Lambert (1989), Klein et al. (1988), Leo (1993), Noble (1993), and Stephan (1993). To supplement these sources, on-line database searches were conducted in ChemFate, TOXLINE, and Hazardous Substances Data Bank (HSDB) (National Library of Medicine); Internet databases such as EPA's ASsessment Tools for the Evaluation of Risk (ASTER) were also reviewed. Original references were located for the values, and additional values identified. In cases where log K_{ow} values varied over several orders of magnitude or measured values could not be identified, detailed on-line searches were conducted using TOXLIT, Chemical Abstracts, and DIALOG.

2.3 Selection and Determination of Aquatic Toxicity Values

For this discussion, all sources of toxicological information are considered 'conventionally-derived' approaches except for the narcosis source which will be referred to separately as the 'narcosis-based' approach.

A variety of sources were used for selecting conventional chronic toxicity values to be used in the derivation of the ESBs. The following were identified as possible sources to be used for determining chronic toxicity values:

1. Final Chronic Values from the Great Lakes Water Quality Initiative (GLI 1995, U.S. EPA 2001a)
2. Final Chronic Values from National Ambient Water Quality Criteria documents
3. Final Chronic Values from draft freshwater and marine National Ambient Water Quality Criteria documents
4. Final Chronic Values developed from data in AQUIRE (now ECOTOX) and other sources
5. Secondary Chronic Values from Suter and Tsao (1996)
6. Secondary Chronic Values developed from data in AQUIRE (now ECOTOX) and other sources (U.S. EPA 1996, 2001a)

2.3.1 Derivation of Conventional Chronic Toxicity Values

For the nine pesticides discussed in this document, values for freshwater ESBs for the following chemicals:

gamma-BHC/Lindane
diazinon
endosulfan (mixed isomers and alpha and beta forms)
toxaphene

were based on the FCVs from existing or draft National Ambient Water Quality Criteria documents (U.S. EPA 1980a,b, 1986, 2005b). Exceptions were the ESBs for BHCs other than Lindane, malathion and methoxychlor which were derived using SCVs with the GLI approach (GLI 1995, Suter and Tsao 1996, U.S. EPA 1996, 2001a). Marine ESBs for pesticides, in this document, were based only on WQC-derived FCVs. Consequently, marine ESBs for the following chemicals:

diazinon
endosulfan (mixed isomers and alpha and beta forms)
malathion
toxaphene

were derived from FCVs in existing or draft National Ambient Water Quality Criteria documents (Thursby 1990, U.S. EPA 1980b, 1986, 2005b). Similar FCVs for the pesticides BHCs other than Lindane, gamma-BHC/Lindane, and methoxychlor were unavailable and marine ESBs were not derived.

Twelve aquatic toxicity values, including three phthalates, used to develop freshwater SCVs were based on work conducted by Oak Ridge National Laboratories (Suter and Tsao 1996) using the GLI (1995) methodology. This methodology was developed to obtain whole-effluent toxicity screening values based on all available data, but the methodology can also be used to calculate SCVs with fewer toxicity data than are required for the WQC methodology. The SCVs are generally lower than values that are produced by the FCV methodology, reflecting greater uncertainty and use of protective adjustment factors in the absence of additional toxicity data (see Section 2.4). According to GLI (1995), the minimum requirement for deriving an SCV is toxicity data from a single taxonomic family (Daphnidae), provided the data are acceptable. In general, those values from Suter and Tsao (1996), which included at least one daphnid test result in the calculation of the SCV, were included for the derivation of Tier 2 ESBs with the exception of ethylbenzene, toluene, 1,1,1-trichloroethane and trichloroethene. For these four chemicals, daphnids were not used for calculating the SCVs. SCVs from Suter and Tsao (1996) were used to develop Tier 2 ESBs for the following chemicals:

benzene
BHC (other than Lindane)
chlorobenzene
dibenzofuran
diethyl phthalate
di-n-butyl phthalate
ethylbenzene
tetrachloroethane, 1,1,2,2-
tetrachloroethene
toluene
trichloroethane, 1,1,1-
trichloroethene

A preliminary search of data records in the AQUIRE (now ECOTOX) database indicated that the following chemicals, which includes one phthalate, might have sufficient toxicity data for the development of SCVs using the GLI (1995) methodology:

biphenyl
4-bromophenyl phenyl ether
butyl benzyl phthalate
dichlorobenzene, 1,2-
dichlorobenzene, 1,3-
dichlorobenzene, 1,4-
hexachlorethane
malathion
methoxychlor
pentachlorobenzene
tetrachloromethane
tribromomethane
trichlorobenzene, 1,2,4-
m-xylene

The procedure used for deriving SCVs for other chemicals of concern using the GLI (1995) methodology and data from ACQUIRE (now ECOTOX) and other sources is described in detail in Appendix A and U.S. EPA (1996, 2001a).

2.3.2 Derivation of Narcotic Chronic Toxicity Values

Along with the derivation of aquatic toxicity values using conventional techniques (see discussion above), narcosis theory was used to derive SCVs for chemicals determined to be primarily narcotic in their mode of action by ASsessment Tools for the Evaluation of Risk (ASTER) (Russom et al. 1997). These chemicals include:

benzene
biphenyl
4-bromophenyl phenyl ether
chlorobenzene
dibenzofuran
1,2-dichlorobenzene
1,3-dichlorobenzene
1,4-dichlorobenzene
ethylbenzene
hexachloroethane
pentachlorobenzene
1,1,2,2-tetrachloroethane
tetrachloroethene
tetrachloromethane
toluene
tribromomethane
1,2,4-trichlorobenzene
1,1,1-trichloroethane
trichloroethene
m-xylene

It should be noted that for a given chemical multiple modes of action can affect an organism. Therefore, despite the categorization of these chemicals as primarily narcotics, other modes of action may be active. Section 4.3 discusses some of the implications of this issue.

Narcosis-based SCVs were derived using the approach discussed in the *Procedures for the Derivation of Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms: PAH Mixtures* (U.S. EPA 2003e) and Di Toro et al. (2000). In this approach, the SCV for these narcotic chemicals is derived using Equation 2-1:

$$\log(\mathrm{SCV_N}) = \log[\mathrm{C_L}{*}\Delta c_l \div \mathrm{ACR}] - 0.945 \cdot \log(K_{\mathrm{OW}}) \qquad (2\text{-}1)$$

where, $\mathrm{SCV_N}$ is the narcosis-based SCV for a given chemical (mmol/L), $\mathrm{C_L}$* is the critical lipid concentration predicted to cause 50% mortality equaling 35.3 µmol/g octanol, Δc_l is the chemical class specific correction, ACR is the acute-chronic ratio equaling 5.09, -0.945 the universal narcosis slope, and $\mathrm{K_{OW}}$ is specific to the chemical being investigated (Di Toro et al. 2000). This equation can be simplified to:

$$\log(\mathrm{SCV_N}) = \log(6.94) + \Delta c_l - 0.945 \cdot \log(K_{\mathrm{OW}}) \qquad (2\text{-}2)$$

For the narcotic chemicals in this document, the chemical class specific correction value (Δc_l) for halogenated compounds was -0.244. For all other compounds, a correction was not necessary (Di Toro et al. 2000).

Narcosis values were also calculated for chemicals with other toxicological modes of action; specifically, the pesticides and phthalates. In every instance, the narcosis $\mathrm{SCV_N}$ was larger in magnitude than the conventional FCV or SCV. For example, the range of the ratio of narcosis to conventional values was 2.4 for di-n-butyl phthalate to nearly 50,000 for alpha-endosulfan. In general, the ratio of narcosis to conventional values was greater than 1000 and thus the pesticides and phthalates contribute only a small amount of narcotic potency. Despite the utility of knowing the contribution of narcosis to the overall toxicity of the pesticides and phthalates, the narcosis values should be used with caution. The narcosis equation above (Equation 2-2) provides chemical class specific corrections (i.e., Δc_l) for halogenated functional groups. However, several of the pesticides and phthalates contain other functional groups not directly addressed in Equation 2-2 including ester and sulfur groups. At this time, the effects of these types of groups on predictions by Equation 2-2 are unknown.

2.4 Comparison of Narcosis and Conventional Chronic Toxicity Values

For every narcotic chemical in this document, the narcosis-based SCV is greater than the conventionally-derived SCV, although the magnitude of the difference varies among chemicals (also see Table 3-1). Figure 2-1 shows the ratio of the two values, which ranges from 1.1 (1,2,4-trichlorobenzene) to 220 (1,1,1-trichloroethane). Of the 20 chemicals evaluated, four chemicals had ratios below 10, 13 chemicals had ratios between 10 and 50, and three chemicals had ratios greater than 100. To interpret these differences, one must consider the differences in how the two values are derived. There are two features of the conventional SCV derivation that create discrepancies. The first is the use of secondary acute factors (SAFs) to estimate a SAV from existing data (see Section A.5 of Appendix A for more discussion of SAFs). The SAFs applied to the chemicals in question here range from 4 up to 242, depending on the number of minimum data requirements met by the available toxicity data, and is applied to the lowest reported mean acute value available (see Suter and Tsao (1996) and U.S. EPA (2001) for a description of how the conventional SCVs were calculated).

The SAFs were derived based on an analysis of a wide range of chemicals. However, narcotics tend to show a much narrower range in species sensitivity than do many other chemicals; in fact, the total range in species sensitivity reported by Di Toro et al. (2000) is only a factor of 8.3 across a total of 33 species. More importantly, the conventional GLI SCV methodology requires that data for *Daphnia magna* be included in the data set. As shown by Di Toro et al. (2000), the ratio of the estimated SMAV for *Daphnia magna* and the FAV for all species is only a factor 3.1. In the case of rainbow trout, a species for which data were frequently available for the present analysis, that ratio is only 1.7. What this means in terms of SCV derivation for narcotic chemicals is that the generic SAFs are larger than is appropriate for narcotic chemicals in particular; while values of 4 to 242 were used, one would expect the true value to have never been higher than 3.1, and commonly 1.7 or less. This difference in extrapolation therefore accounts for as much as a factor of >10 difference between the conventionally-derived and narcosis-based SAVs, which is directly translated into differences in the SCVs (Figure 2-1).

The second major factor lies in the acute-chronic ratios (ACRs) used to translate the SAV into a SCV. In the conventional approach, calculation of the ACR was based on the geometric mean of at least three ACRs. However, wherever there were less than three species-specific ACRs available, a value of 18 was used to replace the missing data (see Section A.5 of Appendix A for more discussion of ACRs); this value was derived through an analysis of ACRs for a variety of chemicals. For the narcotic chemicals shown in Figure 2-1, availability of chronic toxicity data varied from no measured ACRs to three measured ACRs. Where there were no measured ACRs, the conventionally-derived secondary ACR (SACR) was 18.

In their analysis, Di Toro et al. (2000) calculated a much lower mean ACR of 5.09 for narcotic chemicals specifically. Because narcosis appears to result in a lower ACR than the default value of 18 used in the conventional Tier 2 SCV derivation, one can expect additional conservatism in the conventionally-derived Tier 2 SCVs for those chemicals where little or no chronic data were available. Examples include chemicals like 1,2 dichlorobenzene and pentachlorobenzene, both of which were derived using SACRs of 18 and have correspondingly high ratios of the narcosis-based and conventionally-derived SCV values (Figure 2-1). In contrast, 1,2,4 – trichlorobenzene had enough acute toxicity data to meet all 8 minimum data requirements (MDRs) (so no SAF was applied) and the SACR (with two measured ACRs) was only 6.7, very close to the 5.09 estimated for narcotic chemicals (Di Toro et al. 2000). As a result, the conventionally-derived SCV and the narcosis-based SCVs are very close (Figure 2-1).

The applicability of narcosis theory to the compounds designated here as narcotics can be evaluated by comparing the individual species mean acute values (SMAVs) for each of the compounds to the SMAV one would predict based on narcosis theory. To do this, the individual SMAV values were extracted from the SCV derivation for the 20 narcotic chemicals listed in Section 2.3.2. For those species which also appeared in the dataset compiled by Di Toro et al. (2000), the mean species sensitivity was used along with the K_{OW} of each chemical to predict an LC50 for that species and chemical. These predicted LC50s for all 20 chemicals were compared to the observed SMAVs as shown in Figure 2-2. To allow better discrimination of data for individual chemicals, this same data set was segregated into three groups of chemicals, and replotted as Figures 2-3 through 2-5.

The strong agreement between observed and predicted values, shown by alignment along the one to one line, clearly indicates that the observed toxicity of these chemicals is consistent with a narcosis mode of action. Most of the measured values fall within a factor of two of the predicted value (shown by the dashed lines in Figures 2-2 through 2-5) with no consistent bias from a 1:1 relationship. This in turn suggests that deriving SCVs for these chemicals using narcosis theory is appropriate, and that the differences in the conventionally-derived and narcosis-based SCVs is primarily due to conservatism in the SAFs and default SACRs as discussed above.

Finally, for the three phthalates discussed in this document, ‘FCVs’ derived using the quantitative structure-activity relationship (QSAR) described by Parkerton and Konkel (2000) were compared to conventional SCVs in Table 3-1. ASTER does not classify phthalates as narcotics but there is some evidence they may demonstrate narcotic-like behavior. The QSAR values derived by Parkerton and Konkel (2000) were 60, 62 and 1173 µg/L for butyl benzyl phthalate, di-n-butyl phthalate and diethyl phthalate, respectively. These values compare relatively well to the conventional SCVs of 19, 35 and 270 µg/L for butyl benzyl phthalate, di-n-butyl phthalate and diethyl phthalate, respectively. From this comparison, the conventional values for phthalates in this document appear to be slightly more conservative than the QSAR based numbers but not tremendously different with ratios ranging from 2 to 4. See Adams et al. (1995), Rhodes et al. (1995), Staples et al. (1997), Parkerton and Konkel (2000), and Call et al. (2001) for further discussion of phthalate aquatic toxicity.

2.5 Selection of New and Alternate Aquatic Toxicity Values

As discussed in the *Foreword*, the ESBs are intended primarily as technical information, not as formal guidelines. As such, the aquatic toxicity values used to derive the Tier 2 ESBs reported in this document are principally recommendations. The conventional (based on WQC and GLI) and narcosis approaches were selected to generate aquatic toxicity values for the 32 chemicals in this document because of their wide usage and acceptance by the scientific, regulatory and regulated communities. As new high quality aquatic toxicity data becomes available, it is encouraged that these Tier 2 ESBs be updated and revised. The GLI approach, as discussed in Appendix A, is one method for performing these updates and revisions. Periodic review of aquatic toxicity databases like ECOTOX may provide new high quality aquatic toxicity values for some of the chemicals discussed in this ESB, especially those for which a limited data base was initially available (see Section 2.3.1).

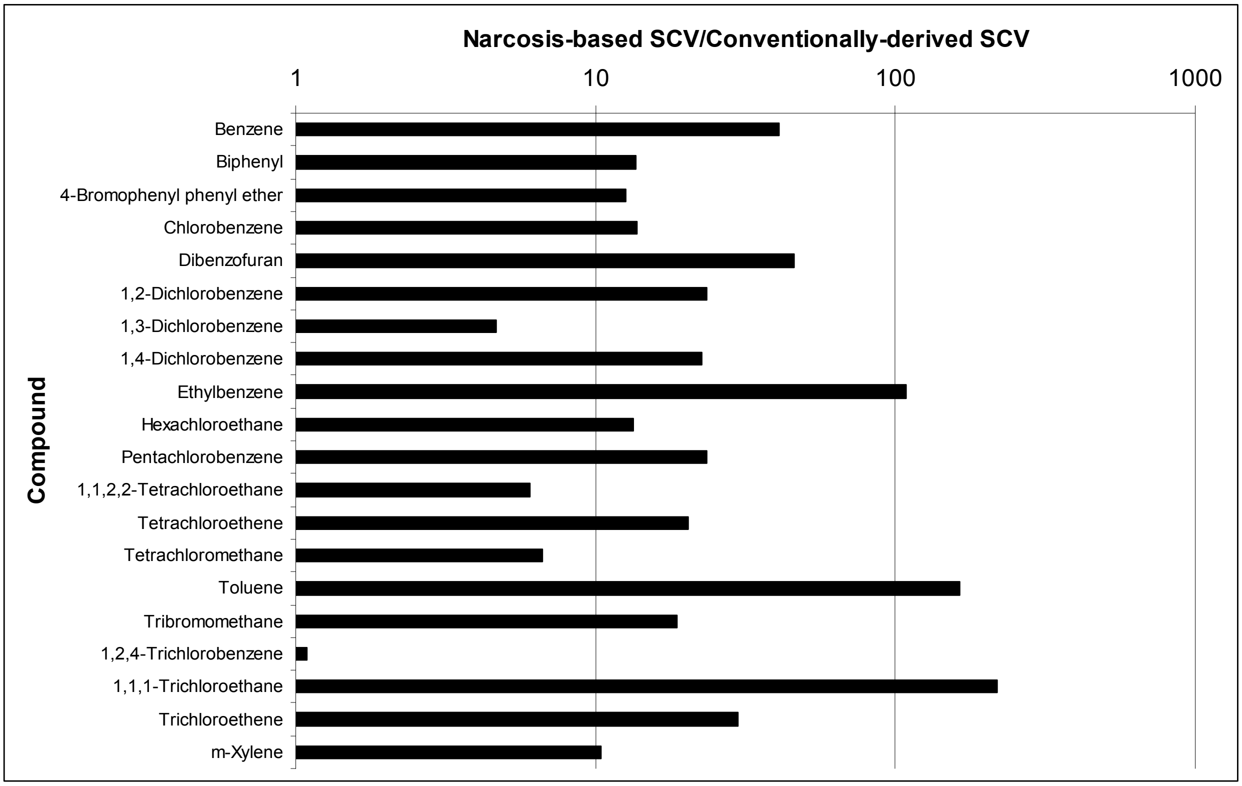

Figure 2-1 Comparison of narcosis-based and conventionally-derived chronic toxicity values. Chemicals with modes of action in addition to narcosis (i.e., pesticides and phthalates) are not shown.

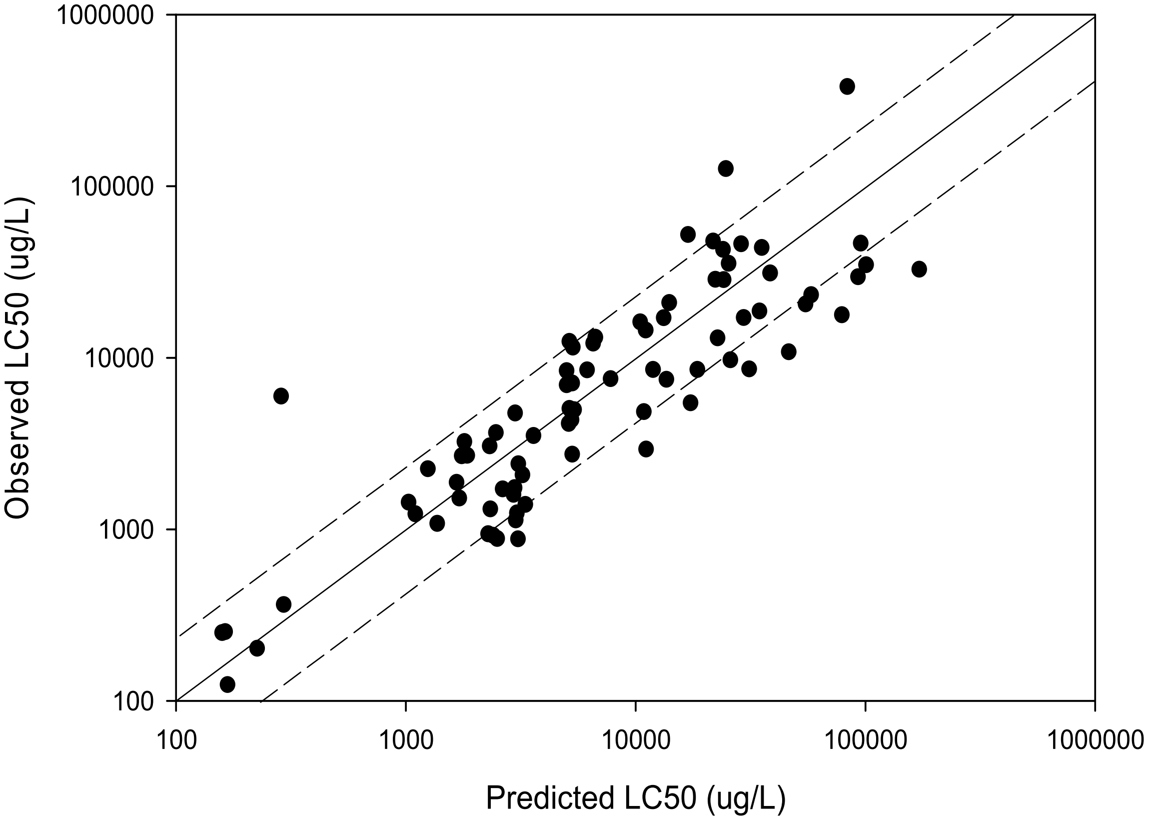

Figure 2-2 Comparison of observed LC_{50} values used in the calculation of secondary chronic values and LC_{50} values predicted using narcosis theory as described by Di Toro et al. (2000) for all 20 narcotic chemicals discussed in this document (including data from Chaisuksant et al. (1998)). Plot shows data for all species that had both measured LC50 values in the SCV derivation and have species-specific sensitivity data as calculated by Di Toro et al. (2000). See discussion in text for more details. The solid line is the one to one line and the dashed lines show ± a factor of two. Chemicals potentially having more specific modes of action (e.g., pesticides and phthalates) are not shown.

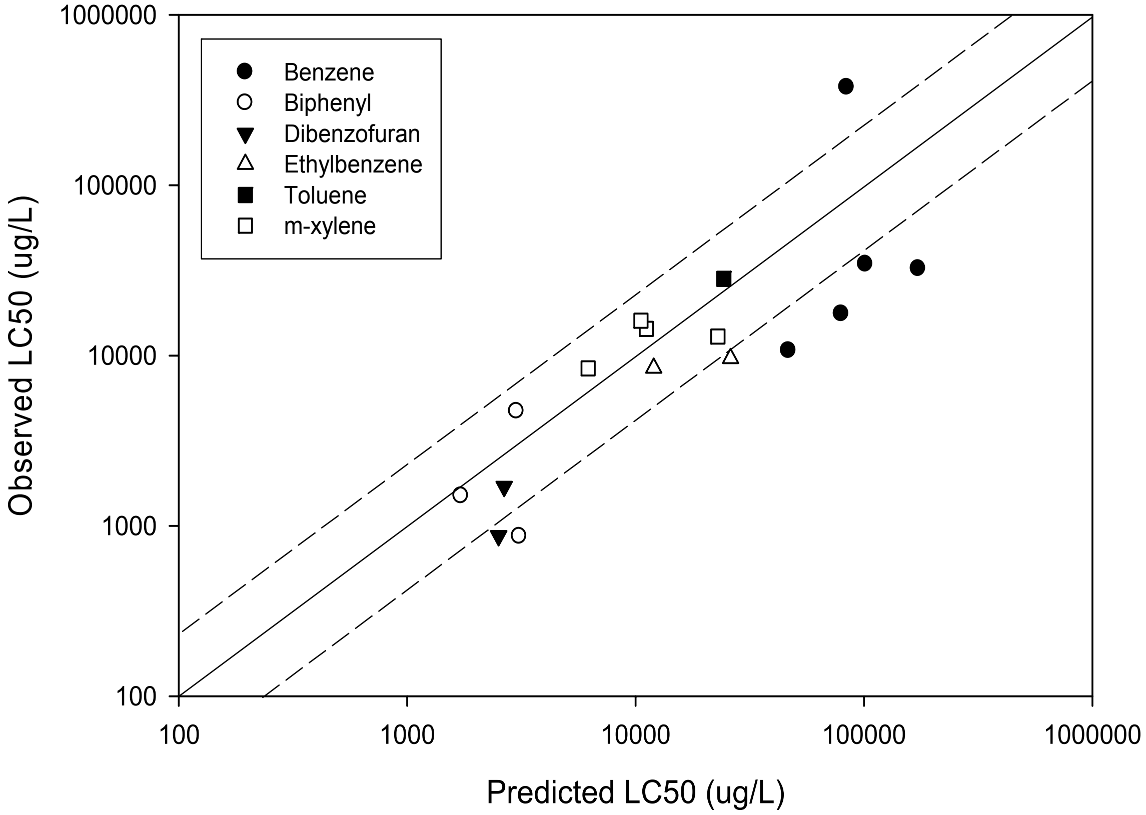

Figure 2-3 Comparison of observed LC_{50} values used in the calculation of secondary chronic values and LC_{50} values predicted using narcosis theory as described by Di Toro et al. (2000) for non-halogenated aromatic narcotic chemicals discussed in this document. Plot shows data for all species that had both measured LC50 data in the SCV derivation and have species-specific sensitivity data as calculated by Di Toro et al. (2000). See discussion in text for more details. The solid line is the one to one line and the dashed lines show ± a factor of two.

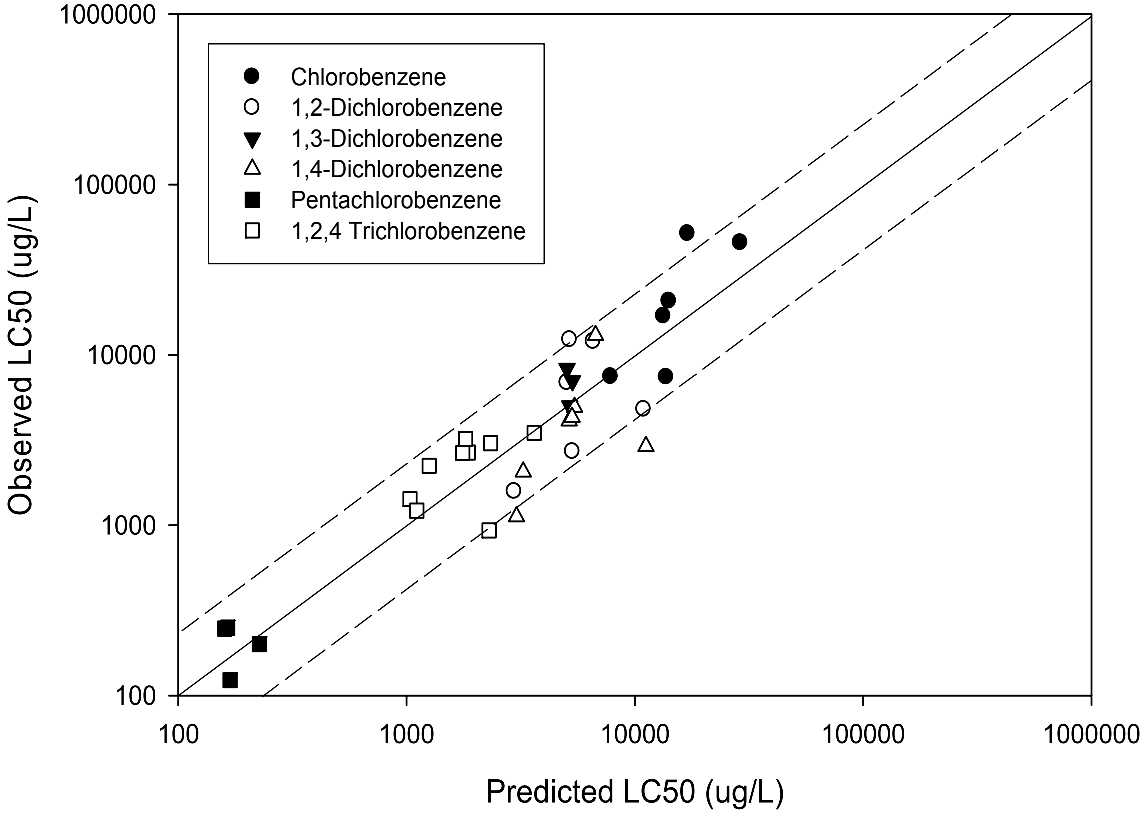

Figure 2-4 Comparison of observed LC_{50} values used in the calculation of secondary chronic values and LC_{50} values predicted using narcosis theory as described by Di Toro et al. (2000) for chlorobenzenes (including Chaisuksant et al. (1998)). Plot shows data for all species that had both measured LC50 data in the SCV derivation and have species-specific sensitivity data as calculated by Di Toro et al. (2000). See discussion in text for more details. The solid line is the one to one line and the dashed lines show ± a factor of two.

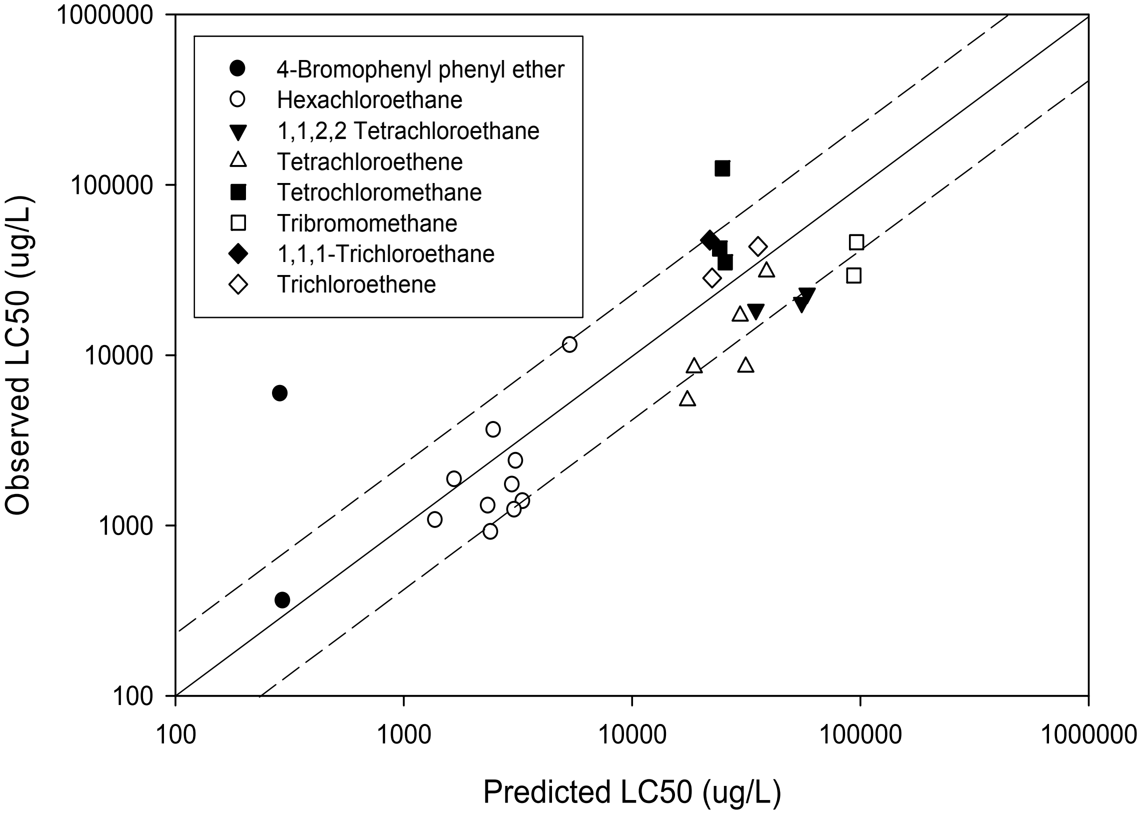

Figure 2-5 Comparison of observed LC_{50} values used in the calculation of secondary chronic values and LC_{50} values predicted using narcosis theory as described by Di Toro et al. (2000) for narcotic chemicals not shown in Figures 2-3 or 2-4, primarily halogenated hydrocarbons. Plot shows data for all species that had both measured LC50 data in the SCV derivation and have species-specific sensitivity data as calculated by Di Toro et al. (2000). See discussion in text for more details. The solid line is the one to one line and the dashed lines show ± a factor of two.

Section 3

Calculation of Equilibrium Partitioning Sediment Benchmarks

3.1 Overview of EqP Methodology

ESBs are the numeric concentrations of individual chemicals that are intended, based on the assumptions discussed in Section 1, to be predictive of biological effects, protective of the presence of benthic organisms, and applicable to the range of natural sediments from lakes, streams, estuaries, and near-coastal marine waters. For nonionic organic chemicals, ESBs are expressed as µg chemical/g_{OC} and apply to sediments having ≥ 0.2% organic carbon by dry weight. A brief overview follows of the concepts that underlie the EqP methodology for deriving ESBs. The methodology is discussed in detail in "Technical Basis for the Derivation of Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms: Nonionic Organics" (U.S. EPA 2003a), hereafter referred to as the ESB Technical Basis Document.

Bioavailability of a chemical at a particular sediment concentration often differs from one sediment type to another. Therefore, a method is necessary to determine ESBs based on the bioavailable chemical fraction in a sediment. For nonionic organic chemicals, the concentration–response relationship for the biological effect of concern can most often be correlated with the interstitial water (i.e., pore water) concentration (µg chemical/L interstitial water) and not with the sediment chemical concentration (µg chemical/g sediment) (Di Toro et al. 1991). This does not mean that all of the exposure is from the interstitial waters but from a purely practical point of view, this correlation suggests that if it were possible to measure the interstitial water chemical concentration, or predict it from the total sediment concentration and the relevant sediment properties, then that concentration could be used to quantify the exposure concentration for an organism. Thus, knowledge of the partitioning of chemicals between the solid and liquid phases in a sediment is a necessary component for establishing ESBs. For this reason, the methodology described below is called the EqP method. As stated above, an ESB can be derived using any given level of protection, in the following discussion the SCVs or FCVs for several nonionic organic chemicals are applied. The EqP approach used here to derive ESBs functions most effectively for nonionic organic chemicals with log K_{OW}s ≥ 2. However, for chemicals with log K_{OW} between 2 and 3, EqP will function but sedimentary conditions (i.e., f_{OC} and f_{Solids}) should be considered and adjustments to the derivation of the ESB maybe advisable (see Section 3.3).

3.2 Derivation of Tier 2 Equilibrium Partitioning Sediment Benchmarks

The ESB Technical Basis Document (U.S. EPA 2003a) demonstrates that benthic species, as a group, have sensitivities similar to all benthic and water column species tested (taken as a group) to derive the WQC concentration for a wide range of chemicals. Thus, an ESB can be established using the FCV, calculated based on the WQC guidelines (Stephan et al. 1985), or a SCV calculated based on other sources like the water quality guidance originally derived for the Great Lakes Water Quality Initiative (GLI 1995), as the acceptable effect concentration in interstitial or overlying water. The appropriate partition coefficient can then be used to relate the interstitial water concentration (i.e., the calculated FCV or SCV) to the sediment concentration via the partitioning equation.

For chemicals discussed in this document, this acceptable concentration in sediment is termed an ESB_{Tier2}.

The methodology for deriving FCVs and SCVs used in the development of these ESBs were taken from existing or draft WQC, the approach developed for the Great Lakes Water Quality Initiative (Tier 1 and 2) and, when necessary, available data were obtained from EPA's AQUIRE database (now ECOTOX accessible at www.epa.gov/ecotox) and other literature (see Section 2).

In addition to deriving FCVs or SCVs based on chemical-specific toxicity data, the likelihood that each chemical would act as a narcotic toxicant (as opposed to a more specific mode of action) was evaluated using the ASTER model (Russom et al. 1997) which predicts mode of toxic action based on chemical structure. For chemicals in this document that were flagged by the ASTER model as acting through a narcotic mode of action, SCVs were also derived using the narcosis model described in U.S. EPA (2003e), Di Toro and McGrath (2000) and Di Toro et al. (2000).

For chemicals evaluated using conventionally-derived SCVs, separate ESB values were calculated for freshwater and marine organisms according to data availability. For chemicals flagged as narcotic toxicants, only single values were calculated, as it is believed that there is little difference in sensitivity between freshwater and marine organisms under this mode of action (U.S. EPA 2003e). A listing of SCVs and FCVs using conventional and narcosis approaches are shown in Table 3-1.

An ESB is calculated as follows. Establishing the SCV or FCV (µg/L) as the acceptable concentration in water for the chemical of interest, the ESB is computed using the partition coefficient, K_P (L/Kg), between sediment and water:

$$ESB_{Tier2} = K_P \cdot SCV \tag{3-1}$$

This is the fundamental equation used to generate an ESB_{Tier2}. Its' utility depends on the existence of a methodology for quantifying K_P.

Organic carbon appears to be the dominant sorption phase for most nonionic organic chemicals in naturally occurring sediments and, thus, controls the bioavailability of these compounds in sediments. Evidence for this can be found in numerous toxicity tests, bioaccumulation studies, and chemical analyses of interstitial water and sediments (Di Toro et al. 1991, U.S. EPA 2003a). The organic carbon binding of a chemical in sediment is a function of that chemical's K_{OC} and the weight fraction of organic carbon (f_{OC}) in the sediment. The relationship is as follows:

$$K_P = f_{OC} \cdot K_{OC} \tag{3-2}$$

It follows that:

$$ESB_{Tier2OC} = K_{OC} \cdot SCV \tag{3-3}$$

where $ESB_{Tier2OC}$ is an ESB_{Tier2} expressed on a sediment organic carbon normalized basis. For nonionic organics, normalization of the "ESB_{Tier2}" to organic carbon is assumed (more formally $ESB_{Tier2OC}$) unless otherwise specified.

Although K_{OC} is not usually measured, it is closely related to the octanol-water partition coefficient (K_{OW}), which has been measured for many compounds, and can be measured very precisely. A chemical's K_{OC} is related to the K_{OW} by the following equation (Di Toro et al. 1991):

$$\text{Log } K_{OC} = 0.00028 + 0.983 \cdot (\log K_{OW}) \tag{3-4}$$

Karickhoff and Long (1996) established a protocol for recommending K_{OW} values for nonionic organic chemicals based on the best available measured, calculated, and estimated data. The recommended $\log_{10}K_{OW}$ values from Karickhoff and Long (1995) were used to derive many of the K_{OC} values for ESB calculation in this document (Table 3-2).

Based on this derivation, ESB_{Tier2} values for 32 nonionic organic chemicals using conventional and narcosis approaches are listed in Table 3-2.

Table 3-1. Chronic toxicity values (µg/L), SCVs and FCVs, used to derive Tier 2 ESBs based on conventional and narcosis approaches. Narcosis values for chemicals with a toxicological mode of action in addition to narcosis are italicized and bolded (e.g., pesticides and phthalates) and are provided for comparison not for use. Values presented with two significant figures except FCVs.

CAS Number	Chemical	log K_{ow}	Conventional* FCV or SCV (µg/L)		Narcosis* SCV (µg/L)
			Freshwater	Marine	
71432	Benzene	2.13	SCV = 130	SCV = 130	5300
319868	BHC other than Lindane	3.78	SCV = 2.2	-	***310***
58899	Gamma-BHC, Lindane	3.73	FCV = 0.080	-	***340***
92524	Biphenyl	3.96	SCV = 14	SCV = 14	190
101553	4-Bromophenyl phenyl ether	5.00	SCV = 1.5	SCV = 1.5	19
85687	Butyl benzyl phthalate	4.84	SCV = 19	-	***58***
108907	Chlorobenzene	2.86	SCV = 64	SCV = 64	880
333415	Diazinon	3.70	FCV = 0.1699	FCV = 0.8185	***670***
132649	Dibenzofuran	4.07	SCV = 3.7	SCV = 3.7	170
95501	1,2-Dichlorobenzene	3.43	SCV = 14	SCV = 14	330
541731	1,3-Dichlorobenzene	3.43	SCV = 71	SCV = 71	330
106467	1,4-Dichlorobenzene	3.42	SCV = 15	SCV = 15	340
84742	Di-n-butyl phthalate	4.61	SCV = 35	-	***85***
84662	Diethyl phthalate	2.50	SCV = 270**	-	***6700***
115297	Endosulfan mixed isomers	4.10	FCV = 0.056	FCV = 0.0087	***210***
959988	Alpha-Endosulfan	3.83	FCV = 0.056	FCV = 0.0087	***390***
33213659	Beta-Endosulfan	4.52	FCV = 0.056	FCV = 0.0087	***86***
100414	Ethylbenzene	3.14	SCV = 7.3	SCV = 7.3	790
67721	Hexachloroethane	4.00	SCV = 12	SCV = 12	160
121755	Malathion	2.89	SCV = 0.097	FCV = 0.1603	***4300***

CAS Number	Chemical	log K_{ow}	Conventional* FCV or SCV (µg/L)		Narcosis* SCV (µg/L)
			Freshwater	Marine	
72435	Methoxychlor	5.08	SCV = 0.019	-	***22***
608935	Pentachlorobenzene	5.26	SCV = 0.47	SCV = 0.47	11
79345	1,1,2,2-Tetrachloroethane	2.39	SCV = 610	SCV = 610	3700
127184	Tetrachloroethene	2.67	SCV = 98	SCV = 98	2000
56235	Tetrachloromethane	2.73	SCV = 240	SCV = 240	1600
108883	Toluene	2.75	SCV = 9.8	SCV = 9.8	1600
8001352	Toxaphene	5.50	FCV = 0.039	FCV = 0.2098	***10***
75252	Tribromomethane (Bromoform)	2.35	SCV = 320	SCV = 320	6000
120821	1, 2, 4-Trichlorobenzene	4.01	SCV = 110	SCV = 110	120
71556	1, 1, 1-Trichloroethane	2.48	SCV = 11	SCV = 11	2400
79016	Trichloroethene	2.71	SCV = 47	SCV = 47	1400
108383	m-Xylene	3.20	SCV = 67***	SCV = 67***	700

- = Not Available.
* = See Section 2.3 for definition.
** = Data summary in Suter and Tsao (1996) did not include a 96-hour LC50 of 131,000 ug/L from Adams et al. (1995). Inclusion of this LC50 in the SCV calculation increased the SCV from 210 to 270 µg/L (Mount 2008).
*** = Value changed from original GLI SCV (Suter and Tsao 1996, U.S. EPA 1996), see Mount (2006).

Table 3-2. Tier 2 ESBs (µg/g_{oc}) based on toxicity values derived using conventional and narcosis approaches (from Table 3-1). K_{OC} based on Equation 3-4. Values presented with two significant figures.

CAS Number	Chemical	Log K_{OC}	Conventional* ESB (µg/g_{OC})		Narcosis* ESB (µg/g_{OC})
			Freshwater	Marine	
71432	Benzene	2.09	16	16	660
319868	BHC other than Lindane	3.72	11	-	^

CAS Number	Chemical	Log K_{OC}	Conventional* ESB (µg/g_{OC})		Narcosis* ESB (µg/g_{OC})
			Freshwater	Marine	
58899	Gamma-BHC, Lindane	3.67	0.37	-	^
92524	Biphenyl	3.89	110	110	1500
101553	4-Bromophenyl phenyl ether	4.92	120	120	1600
85687	Butyl benzyl phthalate	4.76	1100	-	^
108907	Chlorobenzene	2.81	41	41	570
333415	Diazinon	3.64	0.74	3.6	^
132649	Dibenzofuran	4.00	37	37	1700
95501	1,2-Dichlorobenzene	3.37	33	33	780
541731	1,3-Dichlorobenzene	3.37	170	170	780
106467	1,4-Dichlorobenzene	3.36	34	34	780
84742	Di-n-butyl phthalate	4.53	1200	-	^
84662	Diethyl phthalate	2.46	77	-	^
115297	Endosulfan mixed isomers	4.03	0.60	0.093	^
959988	Alpha-Endosulfan	3.77	0.33	0.051	^
33213659	Beta-Endosulfan	4.44	1.6	0.24	^
100414	Ethylbenzene	3.09	8.9	8.9	970
67721	Hexachloroethane	3.93	100	100	1400
121755	Malathion	2.84	0.067	0.11	^
72435	Methoxychlor	4.99	1.9	-	^
608935	Pentachlorobenzene	5.17	70	70	1600
79345	1,1,2,2-Tetrachloroethane	2.35	140	140	830
127184	Tetrachloroethene	2.62	41	41	840
56235	Tetrachloromethane	2.68	120	120	770
108883	Toluene	2.70	5.0	5.0	810

CAS Number	Chemical	Log K_{OC}	Conventional* ESB (µg/g_{OC})		Narcosis* ESB (µg/g_{OC})
			Freshwater	Marine	
8001352	Toxaphene	5.41	10	54	^
75252	Tribromomethane (Bromoform)	2.31	65	65	1200
120821	1, 2, 4-Trichlorobenzene	3.94	960	960	1100
71556	1, 1, 1-Trichloroethane	2.44	3.0	3.0	660
79016	Trichloroethene	2.66	22	22	650
108383	m-Xylene	3.15	94	94	980

* = See Section 2.3 for definition.
- = Not Available.
^ = Not Calculated.

3.3 Effects of Low K_{OW} on Derivation of ESB_{Tier2}

As noted above, the EqP approach used here to derive ESBs functions most effectively for nonionic organic chemicals with log K_{OW}s ≥ 2. However, Fuchsman (2003) demonstrated recently that equilibrium partitioning may inaccurately predict the bioavailable concentration of organic compounds with low log K_{OWs} (i.e., approximately 3). This is because the basic equilibrium partitioning equation (Equation 3-3) assumes that the measured contaminant is associated overwhelmingly with sediment organic carbon and that the amount in the dissolved phase is negligible. However, for chemicals with comparatively low K_{OW} a more substantial fraction of total chemical may be present in the dissolved phase. As a result, the ESB calculation as shown in Equation 3-3, may result in overly protective ESBs.

A modification of the equilibrium partitioning equation (Equation 3-3) can be determined (Fuchsman 2003):

$$ESB_{Tier2DRY\ WT} = SCV\ [(f_{OC}\ K_{OC}) + ((1 - f_{Solids}) \div f_{Solids})] \qquad (3\text{-}5)$$

In which, $ESB_{Tier2DRY\ WT}$ is in units of µg chemical/g dry weight sediment and f_{Solids} is the fraction of sediment present as solids. In the U.S. EPA Environmental Monitoring and Assessment Program (EMAP) data set discussed below, f_{Solids} values for 1024 sediment samples ranged from 0.085 to 0.938 with an average value of 0.553 (U.S. EPA 2007a). In Equation 3-5, the proportion $((1 - f_{Solids}) \div f_{Solids})$, is used to adjust the magnitude of the $ESB_{Tier2DRY\ WT}$ as a function of the amount of solids in the sediment. As K_{OC} increases; that is, the chemical becomes more hydrophobic, the proportion becomes less important and has little effect on the $ESB_{Tier2DRY\ WT}$. Conversely, for low K_{OC} chemicals, the proportion may have a substantial effect on the magnitude of $ESB_{Tier2DRY\ WT}$. The $ESB_{Tier2DRY\ WT}$ is converted to $ESB_{Tier2OC}$ by the following:

$$ESB_{Tier2OC} = ESB_{Tier2DRY\ WT} \div f_{OC} \qquad (3\text{-}6)$$

It should be noted that in aquatic environments, f_{Solids} and f_{OC} are often inversely correlated. For example, in depositional areas, where contaminants discussed in this document frequently accumulate, f_{Solids} is often low and f_{OC} elevated because of the abundance of carbon-rich small particles with large surface area to volume ratios. Conversely, sediments in dynamic areas tend to have low f_{OC} and elevated f_{Solids} because of the dominance of large mineral particles with low surface area to volume ratios and comparatively low carbon content.

An analysis of the effects of low K_{OW} on the ESB calculation is shown in Figure 3-1. The departure of the standard ESB (Equation 3-3) from the modified ESB (Equations 3-5 and 3-6) occurs most substantially at low f_{OC} and low f_{Solids} conditions, starting at a log K_{OW} of approximately 4. Conversely, at high f_{Solids} and high f_{OC} conditions, there is little difference between the calculated values (Figure 3-1a). When high f_{OC} is combined with low f_{Solids} as well as low f_{OC} combined high f_{Solids}, departure between the two approaches for calculating ESBs are observed but at log K_{OW}s of about 2.50 (Figure 3-1b).

Table 3-3 provides examples of the specific effects of f_{Solid} on the derivation of ESBs for four chemicals with a range of K_{OW}s. For this exercise, f_{Solids} was calculated using paired sand and moisture content data from sediment samples collected in several U.S. EPA EMAP estuarine provinces (i.e., Acadian, Carolinian, Virginian) (U.S. EPA 2007a). From the moisture content (MC) data (as %), f_{Solids} was calculated as:

$$f_{Solids} = (100 - MC) \div 100 \qquad (3\text{-}7)$$

and regressed against the sand content (%) to derive the relationship:

$$f_{Solids} = 0.264 + 0.00487 \cdot \text{Sand Content} \qquad (3\text{-}8)$$

For this example, f_{OC} values were set to the environmentally relevant range of 0.002 to 0.05. Examining the extremes, in a sandy sediment

(80% sand), the ESB for low K_{OW} benzene is shown to increase by a factor of three between the standard equation (Equation 3-3) and the modified equation (Equation 3-5) calculations. Conversely, for high K_{OW} toxaphene, there is no difference between the ways of calculating ESBs in the same sandy sediment. For a low sand content sediment (20% sand), benzene ESBs are different by only 20% and again no difference was observed between toxaphene ESBs. The other two chemicals, malathion and 1,2,4-trichlorobenzene with K_{OW}s between benzene and toxaphene, follow similar trends.

Of the 32 chemicals discussed in this document, only four have log K_{OW}s less than 2.5 while 22 have log K_{OWs} that are equal to or less than log 4. In situations where low f_{OC} and low f_{Solids} are known to occur, it is recommended that Equation 3-5 be used to modify the predicted ESB. However, it is most likely chemicals in this document will occur in environments at concentrations of concern when f_{Solids} are low and f_{OC} is high, conditions where departure between the standard and modified ESBs takes place at log K_{OW} of about 2.5, not affecting these chemicals too substantially. It maybe possible under conditions where a contaminated groundwater discharge is occurring into a sedimentary environment for f_{Solids} to be elevated, f_{OC} to be low, and for low K_{OW} chemicals to be present. Under such conditions, the use of Equation 3-5 maybe warranted.

Finally, the value f_{Solids} is not often reported in sediment investigations. In sediments suspected of contamination by low K_{OW} chemicals, it may be important to record this sediment characteris-tic (see Equation 3-8 for predicting f_{Solids} based on sediment sand content). The f_{Solids} values should be available from laboratories conducting chemical analyses on any contaminated sediment samples as part of the determination of moisture content (i.e., Percent Solids = 100% - moisture content (expressed as %)).

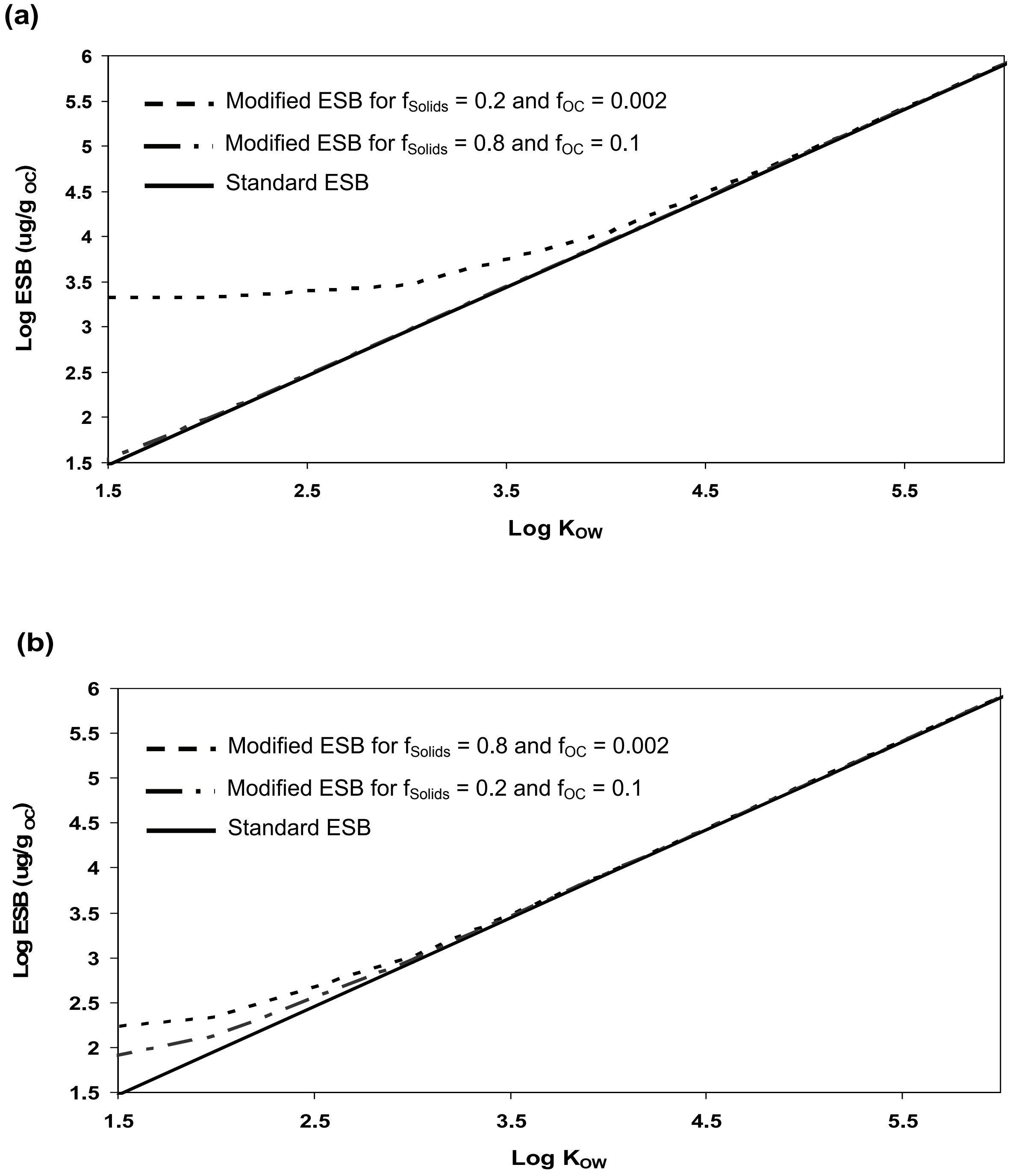

Figure 3-1 **Comparison of ESBs calculated using the standard equation (Equation 3-3) and modified equations which include the effects of low K_{OW} (Equations 3-5 and 3-6): (a) effects of low f_{Solids} and f_{OC} and high f_{Solids} and f_{OC} and (b) effects of high f_{Solids} and low f_{OC} and low f_{Solids} and high f_{OC}. In all cases, the FCV is 1000 ug/L.**

Table 3-3 Example calculations of conventional freshwater standard and modified $ESB_{Tier2DRY\ WT}$ values (µg/g dry weight) for four chemicals under different f_{OC} and f_{Solids} conditions. See text for discussion of the calculation of f_{Solids}. ESB values presented with two significant figures.

Chemical	FCV or SCV (µg/L)	Log K_{OW}:K_{OC}	Standard $ESB_{Tier2DRY\ WT}$: Modified $ESB_{Tier2DRY\ WT}$* (µg/g dry weight)		
			Sediment Characteristics		
			Sand = 80% Silt-Clay = 20% f_{OC} = 0.002 f_{Solids} = 0.65	Sand = 50% Silt-Clay = 50% f_{OC} = 0.025 f_{Solids} = 0.51	Sand = 20% Silt-Clay = 80% f_{OC} = 0.05 f_{Solids} = 0.36
Benzene	130	2.13:2.09	0.032:0.10	0.40:0.52	0.80:1.0
Malathion	0.097	2.89:2.84	0.00013:0.00019	0.0017:0.0018	0.0034:0.0035
1,2,4-Trichlorobenzene	110	4.01:3.94	1.9:2.0	24:24	48:48
Toxaphene	0.039	5.50:5.41	0.02:0.02	0.25:0.25	0.50:0.50

* = See Equation 3-5.

3.4 Conversion to Dry Weight Concentration

Since organic carbon is the major factor controlling the bioavailability of nonionic organic compounds in sediments, ESBs have been developed on an organic carbon normalized basis (e.g., $ESB_{Tier2OC}$) not on a dry weight basis. When the chemical concentrations in sediments are reported as dry weight concentration and organic carbon data are available, it is best to convert the sediment concentration to µg chemical/g organic carbon. These concentrations can then be directly compared to the ESB value. This facilitates comparisons between the ESB and field concentrations relative to identification of hot spots and the degree to which sediment concentrations do or do not exceed ESB values. Conversion from the dry weight to organic carbon-normalized concentration can be performed using the following equations:

$$\mu g\ Chemical/g_{OC} = \mu g\ Chemical/g_{DRY\ WT} \div (\%\ TOC \div 100) \qquad (3\text{-}9)$$

or

$$\mu g\ Chemical/g_{OC} = \mu g\ Chemical/g_{DRY\ WT} \cdot 100 \div \%\ TOC \qquad (3\text{-}10)$$

For example, sediment with a chemical concentration of 0.1 $\mu g/g_{DRY\ WT}$ and 0.5% TOC has an organic carbon-normalized concentration of 20 $\mu g/g_{OC}$ ($0.1\ \mu g/g_{DRY\ WT} \cdot 100 \div 0.5 = 20\ \mu g/g_{OC}$). Another sediment with the same dry weight concentration ($0.1\ \mu g/g_{DRY\ WT}$) but a TOC concentration of 5.0% would have an organic carbon-normalized concentration of 2.0 $\mu g/g_{OC}$ ($0.1\ \mu g/g_{DRY\ WT} \cdot 100 \div 5.0 = 2.0\ \mu g/g_{OC}$).

In situations where TOC values for particular sediments are not available, a range of TOC values may be used in a ‘worst case’ or ‘best case’ analysis. In this situation, the organic carbon-normalized ESB values ($ESB_{Tier2OC}$) may be ‘converted’ to dry weight-normalized ESB values ($ESB_{Tier2DRY\ WT}$). This ‘conversion’ must be performed for each level of TOC of interest:

$$ESB_{Tier2DRY\ WT} = ESB_{Tier2OC}\ (\mu g/g_{OC}) \cdot (\%\ TOC \div 100) \qquad (3\text{-}11)$$

where $ESB_{Tier2DRY\ WT}$ is the dry weight normalized ESB value. Examples of the Tier 2 ESB values ($ESB_{Tier2DRY\ WT}$) using conventional and narcosis approaches normalized to various organic carbon concentrations can be seen in Table 3-4.

Table 3-4. Example Tier 2 ESBs (µg/g dry weight) using freshwater conventional (C) and narcosis (N) approaches normalized to various total organic carbon (TOC) concentrations. Narcosis values for chemicals with a toxicological mode of action in addition to narcosis (e.g., pesticides and phthalates) are not presented. Values presented with two significant figures.

Chemical Name	Approach	Dry Weight Sediment Concentration (µg/g_{DRYWT}) at 0.2% TOC	Dry Weight Sediment Concentration (µg/g_{DRYWT}) at 1.0% TOC	Dry Weight Sediment Concentration (µg/g_{DRYWT}) at 5.0% TOC
Benzene	C	0.032	0.16	0.80
	N	1.3	6.6	33
BHC other than Lindane	C	0.022	0.11	0.55
Gamma-BHC, Lindane	C	0.00074	0.0037	0.019
Biphenyl	C	0.22	1.1	5.5
	N	3.0	15	75
4-Bromophenyl phenyl ether	C	0.24	1.2	6.0
	N	3.2	16	80
Butyl benzyl phthalate	C	2.2	11	55
Chlorobenzene	C	0.082	0.41	2.1
	N	1.1	5.7	29
Diazinon	C	0.0015	0.0074	0.037
Dibenzofuran	C	0.074	0.37	1.9
	N	3.4	17	85
1,2-Dichlorobenzene	C	0.066	0.33	1.7
	N	1.6	7.8	39
1,3-Dichlorobenzene	C	0.34	1.7	8.5
	N	1.6	7.8	39
1,4-Dichlorobenzene	C	0.068	0.34	1.7
	N	1.6	7.8	39
Di-n-butyl phthalate	C	2.4	12	60

Chemical Name	Approach	Dry Weight Sediment Concentration (µg/g$_{DRYWT}$) at 0.2% TOC	Dry Weight Sediment Concentration (µg/g$_{DRYWT}$) at 1.0% TOC	Dry Weight Sediment Concentration (µg/g$_{DRYWT}$) at 5.0% TOC
Diethyl phthalate	C	0.15	0.77	3.85
Endosulfan mixed isomers	C	0.0012	0.006	0.030
Alpha-Endosulfan	C	0.00066	0.0033	0.017
Beta-Endosulfan	C	0.0032	0.016	0.08
Ethylbenzene	C	0.018	0.089	0.45
	N	1.9	9.7	49
Hexachloroethane	C	0.20	1.0	5.0
	N	2.8	14	70
Malathion	C	0.00013	0.00067	0.0034
Methoxychlor	C	0.0038	0.019	0.095
Pentachlorobenzene	C	0.14	0.70	3.5
	N	3.2	16	80
1,1,2,2-Tetrachloroethane	C	0.28	1.4	7.0
	N	1.7	8.3	42
Tetrachloroethene	C	0.082	0.41	2.1
	N	1.7	8.4	42
Tetrachloromethane	C	0.24	1.2	6.0
	N	1.5	7.7	39
Toluene	C	0.01	0.05	0.25
	N	1.6	8.1	41
Toxaphene	C	0.02	0.10	0.50
Tribromomethane (Bromoform)	C	0.13	0.65	3.3
	N	2.4	12	60
1, 2, 4-Trichlorobenzene	C	1.9	9.6	48

Chemical Name	Approach	Dry Weight Sediment Concentration (µg/g$_{DRYWT}$) at 0.2% TOC	Dry Weight Sediment Concentration (µg/g$_{DRYWT}$) at 1.0% TOC	Dry Weight Sediment Concentration (µg/g$_{DRYWT}$) at 5.0% TOC
	N	2.2	11	55
1, 1, 1-Trichloroethane	C	0.006	0.03	0.15
	N	1.3	6.6	33
Trichloroethene	C	0.044	0.22	1.1
	N	1.3	6.5	33
m-Xylene	C	0.19	0.94	4.7
	N	2.0	9.8	49

Section 4

Sediment Benchmark Values: Application and Interpretation

4.1 Benchmarks

Based on the level of protection provided by FCVs or SCVs, the procedures described in this document indicate that benthic organisms should be comparably protected from the adverse effects of the 32 nonionic organic chemicals listed in Table 3-2, when their concentrations in sediment are below the ESB_{Tier2} values. These values are appropriate for the protection of both freshwater and marine sediments based on the assumptions discussed in Section 1, except possibly where a locally important species is very sensitive or sediment organic carbon is <0.2% or the nonionic organic chemical's log K_{OW} is <2 (see Section 3.3 to modify ESB_{Tier2} values).

The benchmarks presented in this document are the concentrations of a substance that may be present in sediment while still protecting benthic organisms from the effects of that substance. These benchmarks are applicable to a variety of freshwater and marine sediments because they are based on the biologically available concentration of the substance in those sediments.

The ESBs do not intrinsically consider the antagonistic, additive or synergistic effects of other sediment contaminants in combination with the individual nonionic organic chemicals discussed in this document or the potential for bioaccumulation and trophic transfer of these chemicals to aquatic life, wildlife or humans. However, for narcotic chemicals, the toxicity of mixtures can be considered (see discussion below). Consistent with the recommendations of EPA's Science Advisory Board, publication of this document does not imply the use of ESBs as stand-alone, pass-fail criteria for all applications; rather, when used in a weight of evidence approach (Wenning et al. 2005), exceedances of ESBs could trigger collection of additional assessment data (e.g., benthic community composition, whole sediment toxicity testing, and other sediment quality guideline evaluations (e.g., Long et al. 1995, MacDonald et al. 1996, Long and MacDonald 1998, Swartz 1999, MacDonald et al. 2000a,b, Leung et al. 2005).

4.2 Considerations in the Application and Interpretation of ESBs

4.2.1 Relationship of ESB_{Tier2} to Expected Effects

The ESB_{Tier2} should be interpreted as a chemical concentration below which adverse effects are not expected. In contrast, at concentrations above the ESB_{Tier2}, assuming equilibrium between phases, effects may occur if the chemical is bioavailable as predicted by EqP theory. In general terms, the degree of effect expected increases with increasing exceedance of the ESB_{Tier2}. Because the FCV or SCV is derived as an estimate of the concentration causing chronic toxicity to sensitive organisms, effects of this type may be expected when sediment concentrations are near the ESB_{Tier2}. As sediment concentrations increase beyond the ESB_{Tier2}, one can expect chronic effects on less sensitive species and/or acute effects on sensitive species. See Section 4.2.6 for further discussion.

4.2.2 Use of EqP to Develop Alternative Benchmarks

The FCV or SCV is used to define a threshold for unacceptable effects based on its precedence in establishing unacceptable effects in the development of WQC. However, the use of EqP to assess sediment contamination is not limited to the ESB_{Tier2} and the associated level of protection discussed in this document. As discussed in earlier sections of this document, by substituting water-only effect values other than the FCV or SCV into the ESB equations, other benchmarks may be developed that are useful in evaluating specific types of biological effects, or that better represent the ecological protection goals for specific assessments.

4.2.3 Influence of Unusual Forms of Sediment Organic Carbon

Partition coefficients used for calculating these ESBs are based on estimated and measured partitioning from natural organic carbon in typical field sediments. Some sediments influenced heavily by anthropogenic activity may contain sources of organic carbon whose partitioning properties are not similar to natural organic carbon. The presence of rubber, animal or wood processing wastes, relatively undegraded woody debris or plant matter (e.g., roots, leaves) as well as black carbon (soot) and coal may alter contaminant partitioning and concentrations of chemicals in interstitial waters in unexpected ways (Iglesias-Jimenez et al. 1997, Grathwohl 1990, Xing et al. 1994). Sediments with substantial amounts of these materials may exhibit higher concentrations of chemicals in interstitial water than would be predicted using generic K_{OC} values, thereby making the ESBs under protective. If such a situation is encountered, the applicability of literature K_{OC} values can be evaluated by analyzing for the chemical of interest in both sediment and interstitial water. If the measured concentration in interstitial water is markedly greater (e.g., more than twofold) than that predicted using the K_{OC} values recommended herein (after accounting for dissolved organic carbon (DOC) partitioning in the interstitial water (U.S. EPA 2003b)), then the ESBs would be under protective and calculation of a site-specific ESB should be considered (see U.S. EPA 2001c, 2003b). Conversely, the presence of black carbon or coal in a sediment may result in reduced chemical activity in sediment and correspondingly reduced concentrations of chemical in interstitial water. Under these conditions, the ESB is likely to be over protective and a site-specific ESB may be warranted (U.S. EPA 2001c, 2003b). However, it should also be noted that the ability to predict partitioning based on additional partitioning factors like black carbon is still evolving and may serve to decrease partitioning-related uncertainties in future applications.

The presence of organic carbon in large particles may also influence the apparent partitioning. Large particles may artificially inflate the effect of the organic carbon because of their large mass, but comparatively small surface area; they may also increase variability in TOC measurements by causing sample heterogeneity. The effect of these particles on partitioning can be evaluated by analysis of interstitial water as described above (U.S. EPA 2001c), and site-specific ESBs may be used if required (U.S. EPA 2003b). It may be possible to screen large particles from sediment prior to analysis to reduce their influence on the interpretation of sediment chemistry relative to ESBs.

4.2.4 Relationship to Risks Mediated through Bioaccumulation and Trophic Transfer

As indicated above, ESBs are designed to address direct toxicity to benthic organisms exposed directly to contaminated sediment. They are not designed to address risks that may occur through bioaccumulation and subsequent exposure of pelagic aquatic organisms (e.g., predatory fish), terrestrial or avian wildlife, or humans. No inference can be drawn between attainment of the ESB_{Tier2} and the potential for risk via bioaccumulation and trophic transfer; the potential for those risks must be addressed by separate means.

4.2.5 Exposures to Chemical Mixtures

It is very important that users of this guidance are aware that the ESB_{Tier2} values provided here reflect the expected toxicity of that specific chemical individually; they do not consider the potential interactive toxicity of that chemical with other chemicals in the mixture, whether antagonistic, additive or synergistic. Thus, a sediment may have concentrations of several chemicals at concentrations below the individual ESB_{Tier2} values, but still cause toxicity because of the aggregate effects of the chemicals acting as a mixture. This potential is not explicitly incorporated into the derivation of the ESB_{Tier2} values because the types and concentrations of co-occurring chemicals is infinitely variable, and the expected interaction of those chemicals is therefore not predictable in a general case.

While the potential for mixture effects must be considered for all chemical mixtures, it is of special concern for the chemicals with a primarily narcotic mode of action discussed in this document. Published literature provides a convincing argument that narcotic chemicals do show additive toxicity with other narcotic chemicals (U.S. EPA 2003e). This is especially relevant for interpreting ESB_{Tier2} values because many, if not most, narcotic chemicals tend to co-occur with other narcotic chemicals because they have common sources. For example, benzene, xylene, toluene, and ethylbenzene commonly co-occur in refined petroleum products. Sources of chlorobenzenes often include multiple chlorobenzene compounds with differing levels of chlorination. Also common in sediments is contamination with narcotic chemicals outside those with ESB_{Tier2} values derived here, such as PAHs (see U.S. EPA 2003e).

For these reasons, it is *expected* that narcosis-based ESB_{Tier2} values will be *under protective* if applied as individual values in most sediments, because other narcotic chemicals are likely to co-occur. This issue can be addressed by using ESB_{Tier2} values in the context of a mixture assessment similar to that used for the ESB for PAH mixtures (U.S. EPA 2003e). In this approach, as shown in the examples in Section 4.3, the contribution of each individual narcotic chemical to the toxicity of the overall mixture is assessed by taking the ratio of the measured concentration of that individual chemical in the mixture by the corresponding single chemical ESB_{Tier2} value. This proportion is calculated individually for all narcotic chemicals in the mixture, then the proportions are summed. If the sum of these values is greater than one, then the expected toxicity of the mixture is greater than that associated with an ESB. If the sum of proportions is less than one, then the sediment would not be expected to be toxic to benthos as a result of that mixture of narcotic chemicals. If PAHs are present in the mixture, then the proportions calculated for PAHs according to the PAH mixture ESB (U.S. EPA 2003e) should be added to the proportions calculated for the narcotic ESB_{Tier2} chemicals. In addition, if there are other narcotic chemicals present in the sediment beyond PAHs and the narcotic chemicals with ESB_{Tier2} values given in this document, they can be incorporated into the analysis using parallel procedures as described by Di Toro and McGrath (2000) and Di Toro et al. (2000). Also, U.S. EPA (2003e), and the references within, provides information about narcotic chemicals. Finally, as discussed in Section 4.3, the narcotic contribution of chemicals with modes of action in addition to narcosis (i.e., the pesticides and phthalates) can be included.

While narcosis is generally discussed for chemicals without a more specific mode of action, theory would suggest that all nonionic organic chemicals would contribute to the overall narcotic potency of a mixture. While this is technically true, the impact of these other chemicals (e.g., pesticides) on the overall narcotic potency of a mixture would be dependent on the toxicity of the chemical acting through a specific mode of action compared to its narcotic potency. If a chemical has a very high conventional potency (low FCV/SCV) compared to its narcosis SCV, then it would exceed the conventional chemical-specific ESB before it was present in sufficient concentration to contribute significantly to the narcotic potency of a mixture. One can make this comparison by examining the ratios between conventionally-derived FCV/SCV values and the narcosis SCV as given in Table 3-1. Most of these comparisons show that the conventional FCV/SCV is generally 100-fold or more lower than the narcosis SCV; accordingly, these chemicals could not contribute more than 1% to an exceedance of a narcosis mixture ESB without simultaneously violating the conventionally-derived ESB_{Tier2}. For this reason, the contribution of most non-narcotic chemicals discussed in this document can be ignored in the calculation of the narcotic potency of mixtures without substantial error. The exceptions are some of the phthalates, for which the conventionally-derived ESB_{Tier2} values are much higher relative to the narcosis SCV. Where these chemicals occur near their conventionally-derived ESB_{Tier2} concentrations, it may be worth considering the potential for them to contribute to the narcotic potency of that mixture.

4.2.6 Interpreting ESB_{Tier2}s in Combination with Toxicity Tests

Sediment toxicity tests provide an important complement to ESBs in interpreting overall risk from contaminated sediments. Toxicity tests have different strengths and weaknesses compared to chemical-specific guidelines, and the most powerful inferences can be drawn when both are used together.

Unlike chemical-specific guidelines, toxicity tests are capable of detecting any toxic chemical, if it is bioavailable in toxic amounts; one does not need to know what chemicals of concern are present to monitor the toxicity of sediment. Toxicity tests are also useful for detecting the combined effects of chemical mixtures, if those effects are not considered in the formulation of the applicable chemical-specific guideline or benchmark.

On the other hand, toxicity tests also have weaknesses; they provide information only for the species tested, and only for the endpoints measured. This is particularly critical given that a majority of the sediment toxicity tests conducted at the time of this writing primarily measure short-term lethality (in some cases growth), although the use of chronic sediment toxicity tests is becoming more common. Chronic sediment toxicity test procedures have been developed and published for some species (e.g., U.S. EPA 2001b), but these procedures are more resource-intensive as compared to acute tests. In contrast, the ESB_{Tier2} is intended to protect most species against both acute and chronic effects.

Many assessments may involve comparison of sediment chemistry (relative to ESBs or other sediment quality guidelines) and toxicity test results. In cases where results using these two methods agree (either both positive or both negative), the interpretation is clear. In cases where the two disagree, the interpretation is more complex and requires further evaluation.

Individual ESBs address only the effects of the chemical or group of chemicals for which they are derived. For this reason, if a sediment shows toxicity but does not exceed the ESB_{Tier2} value for a chemical of interest, it is likely that the cause of toxicity is a different chemical or chemicals (although the chemical of interest maybe contributing to observed toxicity as a component of a mixture). This result might also occur if the partitioning of the chemical in a sediment is different from that assumed by the K_{OC} value used (see Section 4.2.3 *Influence of Unusual Forms of Sediment Organic Carbon* above).

In other instances, it may be that an ESB_{Tier2} is exceeded but the sediment is not toxic. As explained above, these findings are not mutually exclusive, because the inherent sensitivity of the two measures is different. Four possible circumstances may account for this result. First, the ESB_{Tier2} is intended to protect relatively sensitive species against both acute and chronic effects, whereas toxicity tests are performed with species that may or may not be sensitive to chemicals of concern, and often do not encompass the most sensitive endpoints (e.g., growth or reproduction). As such, one may not expect a nonionic organic chemical concentration near the ESB_{Tier2} to cause lethality in a short-term toxicity test. Second, a GLI-based SCV, because of the use of SAFs, may overestimate a contaminant's toxicity compared to the intended level of protection, as described in Section 2.4. Third, site-specific conditions may result in lower bioavailability than assumed based on equilibrium partitioning (see Section 4.2.3). Finally, the organism may avoid the sediment or have other mechanisms to reduce exposure relative to that assumed by the EqP approach. To distinguish these potential explanations, species- and endpoint-specific toxicity information could be used to better interpret toxicity test results, and SCV derivation could be reviewed. Spiked sediment tests could also be used to verify the exposure-response relationship for that particular organism and contaminant. If these lines of evidence do not account for the discrepancy between predicted and observed toxicity, then site-specific chemical partitioning could be investigated (U.S. EPA 2003b).

As discussed above, a good method for evaluating the results of toxicity tests is to calculate effect concentrations in sediment that are species and endpoint specific. For some species contained in the water-only toxicity data for the 32 nonionic organic chemicals discussed here, effect concentrations in sediment can be calculated that are specific for that organism (U.S. EPA 2003e). These values could then be used to directly judge whether the absence of toxicity in the test would be expected from the concentration of nonionic organics chemicals present. As noted above, the magnitude of error between toxicity test results and predicted effects is made larger because of the use of SCVs, and SAFs, to derive some ESB_{Tier2} values (see discussion in Section 2.4).

If the exceedance of an ESB is sufficient that one would expect effects in a toxicity test but they are not observed, it is prudent to evaluate the partitioning behavior of the chemical in the sediment. This is performed by isolating interstitial water from the sediment and analyzing it for the chemicals of interest. Predicted chemical concentrations in the interstitial water can be calculated from the measured concentrations in the solid phase (normalized to organic carbon) as follows:

$$\mu\text{g chemical/L} = (\mu\text{g chemical/g}_{OC}) \cdot (10^3\text{g}_{OC}/\text{Kg}_{OC} \div K_{OC}) \qquad (4\text{-}1)$$

For chemicals with log K_{OW} greater than 5.5, corrections for DOC partitioning in the interstitial water will be necessary (see Gschwend and Wu 1985, Burkhard 2000, U.S. EPA 2003b). See U.S. EPA (2003b) for a discussion of the effects of DOC on ESB derivation. If the measured chemical in the interstitial water is substantially less (e.g., 2-3 fold lower or more), it suggests organic carbon in that sediment may not partition similarly to more typical natural organic carbon, and derivation of site-specific ESBs based on interstitial water may be warranted (U.S. EPA 2003b).

Finally, in addition to the use of sediment toxicity tests for interpreting ESB_{Tier2} values, the generation of acute and chronic water-only data with benthic organisms for the nonionic organic chemicals discussed in this document would be very beneficial. Further, acute and chronic whole sediment toxicity data sets with these chemicals would also complement the interpretation of the ESBs.

4.2.7 Effects of Disequilibrium Conditions

As discussed throughout this document, the EqP is based on an assumption of chemical equilibrium between the solid phase of sediment and the interstitial water. In natural settings, equilibrium may not always exist or may be disturbed by episodic events. As such, the potential for disequilibrium and its impact on the interpretation of the equilibrium-based ESBs should be considered. For purposes of this discussion, two types of disequilibria are discussed: 1) disequilibrium between the solid phase sediment and interstitial water; and 2) disequilibrium between the sediment and overlying water column.

With regard to the first, ESBs are based on an assumption that nonionic organic chemicals are in equilibrium with the sediment and interstitial water and are associated with sediment primarily through absorption to sediment organic carbon. When new chemical is introduced to a sediment, time is required for the chemical to distribute itself between interstitial water and sediment organic carbon. The time required for equilibrium to be achieved is dependent on the characteristics and concentration of the chemical. Sediment spiking experiments suggest that this is typically in the range of weeks.

In areas where sediment erosion and deposition are highly dynamic, equilibrium may be frequently disturbed. The degree to which this would affect the applicability of ESBs depends on the degree and frequency of equilibrium disruption. As noted above, even high K_{ow} nonionic organic compounds come to equilibrium in clean sediment in a period of days, weeks or months. Equilibrium times should be even shorter for mixtures of two sediments that each have previously been at equilibrium. This is particularly relevant in tidal situations where large volumes of sediments are eroded and deposited, even though near equilibrium conditions may predominate over large areas. While the potential for disequilibrium is recognized, it is probably unwise to deviate from the equilibrium assumption without strong evidence that disequilibrium exists over the long term to a sufficient degree to change the expected toxicity of sediment contamination. Recognize that even if there are short-term disturbances to equilibrium between sediment and interstitial water, conditions may quickly re-approach equilibrium between disturbances, such that an equilibrium-based approach is still reasonable, even if there are periods of disturbance/disequilibrium. If it is shown that disequilibrium exists to such an extent that equilibrium-based ESBs are inappropriate, site-specific experimentation may be useful in developing a modified approach (U.S. EPA 2003b).

Even where equilibrium exists between the solid phase sediment and interstitial water, there is often disequilibrium between the sediment and overlying water. This is particularly true for legacy pollution where input of new contamination to the water body has ceased or greatly decreased, and the sediment is now a source of contamination to the overlying water. Some have argued that such disequilibrium reduces exposure of sediment organisms, particularly for those that interact substantially with the overlying water. While the theoretical possibility is clear, the quantitative data from which an appropriate compensation could be calculated is lacking. Moreover, many toxicity test procedures used in the development and testing of EqP theory involve renewal of overlying water and thus include some degree of disequilibrium between the sediment and overlying water. Nonetheless, results from these tests are generally explicable through EqP predictions (e.g., Swartz et al. 1990, DeWitt et al. 1992, Hoke et al. 1994), suggesting that the degree to which this disequilibrium affects exposure is not exceptional, at least for those organisms. In instances where it is determined that EqP does not apply for a particular sediment because of the disequilibrium situations discussed above, site-specific experimentation may be useful in developing a modified approach (U.S. EPA 2003b).

A special case may be in spill situations, where there is a sudden, dramatic influx of new chemical into a system. Immediately following a spill, it can be expected that one or both types of disequilibrium might exist, that the overlying water might have higher chemical activity than in the sediment, and that the solid-phase sediment may not be in equilibrium with the interstitial water. In this situation there is a high potential for ESBs to be under protective.

In sediments where particles of undissolved chemical occur, disequilibrium exists and the benchmarks may be over protective in the sense that chemical concentrations in interstitial water may be lower than would be predicted based on chemical concentrations in sediment and f_{oc}. However, it is also true that in this situation basing an assessment solely on chemical concentrations in the interstitial water might under-represent the degree of contamination. This is because sufficient chemical exists to contaminate a larger mass of sediment if the sediment containing as yet undissolved chemical is later mixed with other, less contaminated sediment.

Clearly, situations where substantial disequilibrium exists can result in several complexities for interpreting sediment chemistry in the context of ESBs. While it is true that ESBs may be less accurate for such situations, it is also important that an alternate assessment approach be developed that adequately accounts for the site-specific conditions. Disequilibrium should not be used as an excuse to dismiss ESB values without developing an alternate conceptual model on which to base the assessment.

4.3 Example Application of ESB_{Tier2}s Using Conventional and Narcosis Approaches and EqP-based Interpretation

Table 4-1 shows sediment chemistry data (in ug/g_{OC}) for four example marine sediments (i.e., A, B, C, D) along with the corresponding conventional and narcosis ESB_{Tier2} values. The sediment concentrations have been normalized for a TOC of 4.5% using Equation 3-9. Assuming a f_{Solids} of 0.20, ESB_{Tier2} values for benzene, 1,1,2,2-tetrachloroethane, and tetrachloroethene were adjusted using Equations 3-5 and 3-6. These values were compared to measured sediment chemistry. For each of the four sediments, Table 4-1 also shows the ratios of the measured concentration in sediment to the conventional and narcosis ESB_{Tier2}s. For the chemicals with modes of action in addition to narcosis (i.e., the pesticides in these examples), their narcosis contribution is not reported but was calculated to be very small and did not substantially affect the sum narcosis ESBTUs (see discussion in Section 2.3.2).

In sediment A (Table 4-1), all measured chemicals were below their conventional and narcosis ESB_{Tier2} values. In addition, the sum of the ratios of the measured concentrations to their narcosis ESB_{Tier2} (sum narcosis ESBTUs) was only 0.01, far below a value of 1 which would indicate concern for a narcotic effect caused by a mixture of chemicals. While these results themselves indicate no reason to suspect adverse effects to benthic organisms from these chemicals, it must be remembered that this conclusion is limited to the effects of these specific chemicals. It is, of course, still possible that other chemicals could be present in the sediment at concentrations that could cause adverse effects. Toxicity testing would be one way to address the potential for toxicity caused by unmeasured chemicals.

Sediment B (Table 4-1) has the same concentrations of all measured chemicals as in sediment A, except for diazinon and malathion, which exceed their conventional ESB_{Tier2} by factors of 3.9 and 11, respectively. These exceedances suggest concern for adverse effects of these chemicals on benthic organisms, subject to the assumptions underlying the ESB approach as discussed elsewhere in this document. Toxicity testing, particularly with species sensitive to these chemicals, could be used to further evaluate the presence of toxicity, as well as assessing the potential presence of toxicity from unmeasured chemicals. In addition, spiked sediment tests with these chemicals and/or sediment Toxicity Identification Evaluation (TIE) studies (U.S. EPA 2007b) may also be useful in evaluating the expected contribution of these chemicals at these concentrations to sediment toxicity.

For sediment C (Table 4-1), concentrations of the pesticides diazinon, alpha endosulfan and malathion are all below their conventional ESB_{Tier2} values, but three of the other measured chemicals, benzene, ethylbenzene and toluene, exceed their corresponding conventional ESB_{Tier2} values by factors of 4.3, 5.1, and 7.6, respectively. In contrast, these same chemicals do not exceed their narcosis ESB values, nor does the sum of narcosis ESBTUs exceed 1. The exceedance of the conventional ESB_{Tier2}s suggests that the levels of benzene, ethylbenzene, and toluene are high enough to be of potential concern when evaluated by the GLI

Tier 2 assessment approach (GLI 1995). However, the fact that the sum of narcosis ESBTUs does not exceed one raises the possibility that the exceedances for these chemicals may be influenced by conservatism in the GLI Tier 2 paradigm, particularly as it relates to narcotic chemicals (see Section 2.4 for additional discussion). Another issue to be considered relates to the likelihood that other narcotic chemicals, not listed in Table 4-1 may be present and contribute to an overall mixture toxicity. In particular, the elevated concentrations of benzene, ethylbenzene and toluene may suggest contamination with hydrocarbons such as refined petroleum products that may also contain PAHs or other hydrocarbons that could contribute to a narcotic mixture effect. Further analytical chemistry and toxicity testing would be logical supplements to the information in Table 4-1 for determining the overall likelihood of risk to benthic organisms. If PAHs are present, separate ESB guidance for PAH mixtures (U.S. EPA 2003e) can provide an approach to evaluate their potential contribution to narcotic toxicity. The theory underlying narcotic toxicity (Di Toro and McGrath 2000, Di Toro et al. 2000, U.S. EPA 2003e) suggests that the sum of ESBTUs for PAHs could be added to the sum of narcosis Tier 2 ESBTUs in Table 4.1 to assess the combined potency of those chemicals.

Finally, in sediment D (Table 4-1), concentrations of measured pesticides are again low, but concentrations of both BTEX compounds (i.e., benzene, toluene, ethylbenzene, xylene) and the measured chlorinated compounds are higher than for sediment C. Conventional $\mathrm{ESB}_{\mathrm{Tier2}}$s are exceeded for several compounds; although no individual narcosis $\mathrm{ESB}_{\mathrm{Tier2}}$ values are exceeded, the sum of narcosis ESBTUs does exceed 1. In this case, both the conventional $\mathrm{ESB}_{\mathrm{Tier2}}$s and the narcosis mixture analysis suggests the potential for adverse effects to benthic organisms. Also, the finding that many compounds, including BTEX, chlorinated benzenes, and other chlorinated hydrocarbons are all present in concentrations approaching their narcosis $\mathrm{ESB}_{\mathrm{Tier2}}$s makes it likely that other, unmeasured chemicals in these families may also be present at toxicologically significant concentrations in this sediment, because typical sources of these chemicals to the environment often include many different related compounds (e.g., other di-, tri-, tetra-and hexachloro-benzenes). While this document does not address these additional compounds specifically, an approach for addressing their contribution in a way similar to that used in this document is provided by Di Toro and McGrath (2000) and Di Toro et al. (2000).

Table 4-1 Example applications of ESB_{Tier2} values with several nonionic organic chemicals using conventional and narcosis approaches. In this example, four marine sediments with 4.5% TOC and f_{Solids} of 0.20 are assessed. Sediment concentrations are shown with organic carbon normalization using Equation 3-9. ESB_{Tier2} values modified with Equations 3-5 and 3-6 to account for f_{Solids} for benzene, 1,1,2,2-tetrachloroethane and tetrachloroethene are shown rather than ESB_{Tier2} values in Table 3-1.

Sediment A	Conventional* ESB (µg/g_{OC})	Narcosis* ESB (µg/g_{OC})	Sediment Concentration (µg/g_{OC})	Sediment Concentration/ Conventional ESB	Sediment Concentration/ Narcosis ESB
Benzene	28	1100	0.95	0.0339	0.0009
Ethylbenzene	8.9	970	0.23	0.0258	0.0002
Toluene	5	810	0.32	0.0640	0.0004
m-Xylene	94	980	0.42	0.0045	0.0004
Chlorobenzene	41	570	0.67	0.0163	0.0012
1,2-Dichlorobenzene	33	780	1.2	0.0364	0.0015
Pentachlorobenzene	70	1600	2.3	0.0329	0.0014
Tetrachloromethane	120	770	1.5	0.0125	0.0019
1,1,2,2-Tetrachloroethane	190	1200	1.3	0.0068	0.0011
Hexachloroethane	100	1400	0.89	0.0089	0.0006
Trichloroethene	22	650	0.51	0.0232	0.0008
Tetrachloroethene	50	1000	0.53	0.0106	0.0005
Diazinon	3.6	^	0.02	0.0056	^
Alpha-Endosulfan	0.051	^	0.01	0.1961	^
Malathion	0.11	^	0.01	0.0909	^
Sum Narcosis ESBTUs					0.0111

Sediment B	Conventional* ESB (µg/g_{OC})	Narcosis* ESB (µg/g_{OC})	Sediment Concentration (µg/g_{OC})	Sediment Concentration/ Conventional ESB	Sediment Concentration/ Narcosis ESB
Benzene	28	1100	0.95	0.0339	0.0009
Ethylbenzene	8.9	970	0.23	0.0258	0.0002
Toluene	5	810	0.32	0.0640	0.0004
m-Xylene	94	980	0.42	0.0045	0.0004
Chlorobenzene	41	570	0.67	0.0163	0.0012
1,2-Dichlorobenzene	33	780	1.2	0.0364	0.0015
Pentachlorobenzene	70	1600	2.3	0.0329	0.0014

Tetrachloromethane	120	770	1.5	0.0125	0.0019
1,1,2,2-Tetrachloroethane	190	1200	1.3	0.0068	0.0011
Hexachloroethane	100	1400	0.89	0.0089	0.0006
Trichloroethene	22	650	0.51	0.0232	0.0008
Tetrachloroethene	50	1000	0.53	0.0106	0.0005
Diazinon	3.6	^	13.9	**3.8611**	^
Alpha-Endosulfan	0.051	^	0.01	0.1961	^
Malathion	0.11	^	1.2	**10.9091**	^
Sum Narcosis ESBTUs					0.0111

Sediment C	Conventional * ESB (µg/g$_{OC}$)	Narcosis* ESB (µg/g$_{OC}$)	Sediment Concentration (µg/g$_{OC}$)	Sediment Concentration/ Conventional ESB	Sediment Concentration/ Narcosis ESB
Benzene	28	1100	120	**4.2857**	0.1091
Ethylbenzene	8.9	970	45	**5.0562**	0.0464
Toluene	5	810	38	**7.6000**	0.0469
m-Xylene	94	980	31	0.3298	0.0316
Chlorobenzene	41	570	1.3	0.0317	0.0023
1,2-Dichlorobenzene	33	780	3.7	0.1121	0.0047
Pentachlorobenzene	70	1600	8.8	0.1257	0.0055
Tetrachloromethane	120	770	1.1	0.0092	0.0014
1,1,2,2-Tetrachloroethane	190	1200	0.66	0.0035	0.0006
Hexachloroethane	100	1400	0.43	0.0043	0.0003
Trichloroethene	22	650	0.19	0.0086	0.0003
Tetrachloroethene	50	1000	0.21	0.0042	0.0002
Diazinon	3.6	^	0.02	0.0056	^
Alpha-Endosulfan	0.051	^	0.01	0.1961	^
Malathion	0.11	^	0.01	0.0909	^
Sum Narcosis ESBTUs					0.2493

Sediment D	Conventional * ESB (µg/g$_{OC}$)	Narcosis* ESB (µg/g$_{OC}$)	Sediment Concentration (µg/g$_{OC}$)	Sediment Concentration/ Conventional ESB	Sediment Concentration/ Narcosis ESB
Benzene	28	1100	410	**14.6429**	0.3727
Ethylbenzene	8.9	970	320	**35.9551**	0.3299
Toluene	5	810	290	**58.0000**	0.3580

m-Xylene	94	980	360	**3.8298**	0.3673
Chlorobenzene	41	570	250	**6.0976**	0.4386
1,2-Dichlorobenzene	33	780	140	**4.2424**	0.1795
Pentachlorobenzene	70	1600	87	**1.2429**	0.0544
Tetrachloromethane	120	770	12	0.1000	0.0156
1,1,2,2-Tetrachloroethane	190	1200	16	0.0842	0.0133
Hexachloroethane	100	1400	31	0.3100	0.0221
Trichloroethene	22	650	27	**1.2273**	0.0415
Tetrachloroethene	50	1000	15	0.3000	0.0150
Diazinon	3.6	^	0.02	0.0056	^
Alpha-Endosulfan	0.051	^	0.01	0.1961	^
Malathion	0.11	^	0.01	0.0909	^
Sum Narcosis ESBTUs					**2.2081**

* = See Section 2.3 for definition.
^ = Not Reported.

Section 5

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Appendix A

Description of the Derivation of Conventional Freshwater Chronic Toxicity Values using the Great Lakes Water Quality Initiative (GLI 1995) Approach

A.1 Acquisition and Review of Conventional Aquatic Toxicity Data

As discussed above, when possible, conventional ESBs were based on FCVs for aquatic life (Stephan et al.1985). When FCVs could not be derived, the ESBs were calculated from SCVs for aquatic life using the GLI approach (Suter and Mabrey 1994, GLI 1995, Suter and Tsao 1996). The purpose of this section is to describe the procedure used to derive SCVs from data in AQUIRE (now ECOTOX) and other sources.

The following restrictions on toxicity data and reference sources used were applied:

1. Acute toxicity data for only freshwater species were used (GLI, 1995), whereas acute-chronic ratios (ACRs) for both freshwater and saltwater species were used in order to expand the number of available ACRs.

2. Only the following were used as sources of references:

   a. U.S. Environmental Protection Agency's AQUIRE (now ECOTOX) database.
   b. Tables in existing documents from EPA's Office of Research and Development.

A preliminary review was conducted on test results obtained by means of a search of AQUIRE (now ECOTOX). Only information that could be retrieved from AQUIRE (now ECOTOX) was used in this review. Each test result was rejected if one or more of the reasons listed below applied. The first three reasons for rejection given below were addressed in the search strategy used to find test results in AQUIRE (now ECOTOX). All pertinent test results were printed and reviewed manually using the "Reasons for Rejection of a Test Result Based on Information in AQUIRE." For each test result that was not rejected, a copy of the original report was reviewed as described in the next section of this report, "Data Rejection Checklist."

Reasons for Rejection of a Test Result Based on Information in AQUIRE (now ECOTOX):

___ The test was not conducted in the laboratory (i.e., **Site** was not LAB).
___ Poor documentation (the documentation code (**Dc**) was not 1 or 2).
___ The endpoint was not reported (i.e., **Endpt** was left blank or was "NR").
___ The purity of the test chemical was less than 80% (i.e., **Chem_char** < 80%).
___ The test species (**Latin, Species**) was not an aquatic animal.
___ The test species (**Latin, Species**) was not a resident North American species.
___ The test species was *Wyeomyia smithii* (i.e., the pitcher plant mosquito) or was in the genus *Artemia* (i.e., it was a brine shrimp).

The following reasons for rejection applied only to acute toxicity tests:

___ The test exposure was not static, renewal, or flow-through (i.e., **Extype** was not S, R, or F).
___ The test was not conducted in freshwater (i.e., **Media** was not FW).
___ If the test species was Cladoceran (CLAD, water flea), copepod (COPE), midge or phantom midge (insect, family Chironomidae, order Diptera, DIPT), the **Duration** was less than 2 days (48 hr).
___ For all other animal species, the **Duration** was less than 4 days (96 hrs).
___ The **endpoint** was not LC_{50} or EC_{50} or IC_{50}.
___ The **effect** was not EQU, IMM, and/or MOR, except that SHD (incompletely developed shells, change in the ability to grow a shell) was acceptable for bivalve molluscs.

The following reasons for rejection applied only to chronic toxicity tests:

___ The concentrations of test material were not measured (i.e., **Method** was not M) in the test solution.
___ The test exposure was not flow-through or renewal (i.e., **Extype** was not F or R).

If the test species was a Cladoceran (CLAD, water flea) or copepod (COPE):

___ The **Life stage** was older than 24 hr.
___ The **Duration** was less than 21 days (except less than 7 days for *Ceriodaphnia*).
___ For all other species, the **Duration** was less than 24 days.

Stephan et al. (1985), references cited therein, and other pertinent publications (e.g., the American Fisheries Society guidebook series for North American fishes, molluscs, and crustacea) were used to determine whether a vertebrate or invertebrate aquatic species is resident in North America. Because of various constraints, some species listed below were assumed to be nonresident if a limited search did not demonstrate that they were resident. Any species that was said to have been field-collected in North America was considered resident.

Examples of resident species not in Stephan et al. (1985):

Chironomus riparius	midge
Gila elegans	bonytail
Gillia attilis	buffalo pebblesnail
Lestes congener	damselfly
Sigara alternata	water boatman
Stenonema interpunctatum	mayfly
Umbra pygmaea	eastern mudminnow

Examples of nonresident species not in Stephan et al. (1985):

Anguilla anguilla	common eel (assumed nonresident)
Anodonta anatina	fresh-water mussel
Anodonta cyanea	swan mussel
Barbus ticto	two-spotted; tic tac toe barb
Carassius carassius	Crucian carp
Chana punctatus or *gachua*	snake-head catfish
Cirrhinus mrigala	carp, hawkfish
Heteropneustes fossilis	Indian catfish
Macrobrachiu rosenbergii	giant freshwater prawn
Mystus vittatus	catfish
Notopterus notopterus	featherback
Paratelphusa jacquemontii	crab (probably)
Rasbora heteromorpha	harlequinfish/red rasbora
Spicodiaptomus chilospinus	calanoid copepod (assumed nonresident)

Resident status of organisms for which only the genus and "sp." were provided as the scientific name (e.g., *Peltodytes* sp.) was based on the location where the organisms were collected.

This checklist was used to review the acceptability of results of aquatic toxicity tests on nonionic organic chemicals including all references that were obtained from AQUIRE (now ECOTOX) and passed the "Preliminary Review of Records from AQUIRE." Because this second review was performed on all test results regardless of whether the reference came from AQUIRE (now ECOTOX), all items on the AQUIRE (now ECOTOX) review were also included here. This review was performed using the original publication and sources of supplemental information; this review was not performed using only secondary sources.

This final review covered both the quality of the test result and whether it was the kind of result that had been specified for use in this document. A test result that was deemed unacceptable for use in this document might be acceptable for another use. A result that was deemed unacceptable was not necessarily an incorrect result; it just might have been too questionable to use. For example, an LC_{50} obtained using unacceptable methodology might have been the same as an LC_{50} using acceptable methodology. The LC_{50} from the test using the unacceptable methodology, however, was unacceptable because it was questionable. In many cases, some test results in a publication were acceptable, whereas others were unacceptable. Similarly, one result from a test (e.g., a 24-hr LC_{50}) might not have been acceptable although another (e.g., a 48-hr LC_{50}) was acceptable.

Each test result was placed in one of three categories for the purposes of this review:

1. A test result was assumed acceptable if the test was conducted at EPA laboratories in Corvallis (OR), Duluth (MN), Gulf Breeze (FL), or Narragansett (RI); was conducted at the U.S. Fish and Wildlife Service laboratory in La Crosse, Wisconsin; was contained in Mayer and Ellersieck (1986); was conducted at the U.S. Department of the Interior laboratory in Columbia, Missouri, after the period covered by the report published by Mayer and Ellersieck (1986); or was contained in the University of Wisconsin-Superior data summary volumes (Brooke et al.1984; Geiger et al.1985, 1986, 1988, 1990). Reports from these sources usually contained information concerning methodology, but the result was assumed acceptable even if little information was available concerning methodology. Results in this category were rejected only if a major problem was known to exist.

2. A test result was assumed acceptable if the test was reported to have been conducted according to procedures described by such American Society for Testing and Materials (ASTM) standards as:

   ASTM Standard E 729, Guide for Conducting Acute Toxicity Tests with Fishes, Macroinvertebrates, and Amphibians

   ASTM Standard E 1241, Guide for Conducting Early Life-Stage Toxicity Tests with Fishes

   ASTM Standard E 1193, Guide for Conducting Renewal Life-Cycle Tests with *Daphnia magna*

   ASTM Standard E 1295, Guide for Conducting Three-brood, Renewal Toxicity Tests with *Ceriodaphnia dubia*

Or procedures described by *Standard Methods*, the European Economic Community (EEC), the International Organization for Standardization, or the Organization for Economic Cooperation and Development (OECD), and if the description of the methodology at least mentioned such factors as acclimation, temperature control, controls, solvent and solvent control (if used), source of water, randomization, and duplication. Results in this category were, however, rejected if a single major problem was identified.

3. All other test results were in a third category. Whether they were accepted or rejected depended on the information available concerning the methodology and results. The result was rejected if insufficient information was available to evaluate the test. Identification of a single major problem, or at least three minor problems, were grounds for rejection of a test result, and most results with this number of identified problems were rejected. Best professional judgment was; however, applied to determine whether identified problems warranted rejection of the result.

The review of test results required judgments, starting with decisions about what items to include on the following list, and whether each one was major or minor. Applying the list also required judgment. For example, a test result was always rejected if a surfactant was used in the preparation of a stock solution or the test solutions, even if the test was conducted by Mount and Stephan (1967). If no information was given concerning the use of surfactants, test results in the first category above were deemed acceptable, but it was identified as a problem for other test results.

Reasons for Rejection (Asterisks indicate major problems; all others are minor problems.)

Report

___ * The test results were not available for public distribution in a dated and signed hard copy (e.g., publication, manuscript, letter, memorandum, etc.).

___ * The test results were from a secondary publication, except those results contained in the *Manual of Acute Toxicity: Interpretation and Data Base for 410 Chemicals and 66 Species of Freshwater Animals* (Mayer and Ellersieck 1986) were considered acceptable.

___ * Methodology and/or results were not adequately and clearly described, except for category 1. In some cases, other papers by the same or different authors provided the necessary information.

Test chambers

___ All test chambers and any compartments within the chambers were not identical.

___ * The test result was from a microcosm or model ecosystem study.

___ * The test chambers were made from or lined with PVC, except that the presence of PVC in chambers was acceptable if the test material was miscible with or very soluble in water or concentrations of the test material in solutions were measured.

Test material

___ The test material was not adequately described.

___ * The organisms were exposed to the test material via food, sediment, injection, gavage, etc.; exposure was not via only the test solutions.

___ * The test material was a component of a drilling mud, effluent, fly ash, mixture, formulation, sediment, or sludge.

___ The purity of the test material was less than 80 percent (e.g., the test material contained less than 80 percent active ingredient); analytical-grade, reagent-grade, or technical-grade materials were considered acceptable unless known to be unacceptable.

Exception: The test material could contain less active ingredient if data were available to show that tests on the material produced the same results as tests on material that was at least 80 percent pure.

___ * The test material was an emulsifiable concentrate, a wettable powder, or a specially prepared mixture that contained a surfactant and/or an organic solvent that was not miscible with water.

___ * A surfactant or an organic solvent that was not miscible with water was used in the preparation of a stock solution or the test solutions.

___ If a water-miscible solvent was used to prepare the stock solution and/or test solutions, its concentration exceeded 0.5 mL/L in the test solutions.

___ * The test material was introduced into the test chamber by evaporating it onto the test chamber and adding dilution water.

Exception: This procedure was acceptable if the concentrations of test material in the test solutions were measured.

___ * Concentrations of test material in the test solutions were not measured for chronic toxicity tests (measurement was not necessary for acute tests).

___ Measured concentrations of test material during a flow-through test varied too much.

___ * For highly volatile, hydrolyzable, or degradable materials, the test was static or renewal (i.e., not flow-through) and/or concentrations of test material were not measured often enough using acceptable analytical methods.

___ * Exposure to the test material was intermittent, not continuous.

Test organisms

___ * The test species was not an aquatic animal.

___ * The test species was a single-celled organism.

___ * The test species was not a resident North American species.

___ * The test species was *Wyeomyia smithii* (i.e., the pitcher plant mosquito) or was in the genus *Artemia* (i.e., it was a brine shrimp).

___ * The test was not conducted using "whole" organisms; for example, the test was conducted using tissues or cell cultures.

___ * The test result was calculated for a mixture of species, especially if the species were in different genera.

___ * At least some of the test organisms were in a life stage that is not aquatic for at least part of the test.

___ * The test organisms were cladocerans that were obtained from a stock culture in which ephippia were being produced.

___ The test organisms showed signs of stress or disease before the test.

___ * The test was begun with organisms within 10 days after they were treated to cure or prevent disease and/or the organisms were treated during the test.

___ * Test organisms were previously exposed to substantial concentrations of the test material or other contaminants and were not held in clean water for at least 10 days before the beginning of the test.

___ * The test organisms were not acclimated to or were not maintained in the dilution water at the test temperature for at least 48 hours before the beginning of the test.

___ The test organisms were mishandled or excessively disturbed before or during the test.

___ * The test organisms were fed during an acute toxicity test.

Exceptions:

1. Saltwater annelids and mysids could be fed during acute tests.
2. The test material does not sorb or complex readily with food.
3. Data were available to show that the presence of food probably would not affect the results of the test.

___ There were fewer than 10 test organisms per treatment.

___ There were not two or more replicates (groups of individuals of a species) tested for each concentration for chronic tests.

___ The test organisms were crowded in the test chambers.

___ * The test organisms reproduced during the test and all of the new organisms could not be distinguished from the initial organisms at the end of the test. (This has been a problem in some tests with rotifers.)

Controls

___ * There was no control treatment.

___ * There was a control treatment, but it was not comparable to the other treatments.

___ No data were reported for the controls.

___ * More than 10 percent of the control organisms died or showed signs of stress or disease or were otherwise adversely affected, except that a higher percentage was acceptable for a few species.

___ * Survival, growth, or reproduction in the control treatment for chronic tests were unacceptably low. (The limits of acceptability depended on the species.)

Dilution water

___ * Distilled or deionized water was used without addition of appropriate salts.

___ * Chlorinated water was used without adequate dechlorination.

___ * River water was used as the dilution water without appropriate treatment.

___ * The concentration of total organic carbon (TOC) or particulate matter (PM) in the dilution water exceeded 5 mg/L.

Exceptions:

1. TOC or PM could exceed 5 mg/L if a relationship was developed between toxicity and TOC or PM.
2. Data were available to show that TOC or PM probably would not affect the results of the test.

___ The dilution water contained unusual amounts or ratios of inorganic ions.

Test conditions

___ Turbulence in the test chamber, resulting from aeration, stirring, or design (of flow-through chambers), was excessive.

___ The temperature, pH, etc., of the test solutions were not adequately controlled.

___ * The pH of the dilution water was below 6.5 or above 9.0.

___ * The concentration of dissolved oxygen in a renewal or flow-through test was less than 60 percent of saturation.

___ * The concentration of dissolved oxygen during a static test was less than 60 percent saturation during the first 48 hours, or less than 40 percent of saturation from 48 to 96 hours.

___ Treatments, test organisms, and experimental units were not appropriately randomized.

___ * The dilution factor was greater than 9.

The toxicity tests that were not rejected were next evaluated to determine whether they provided the kinds of acute and chronic results that were to be used, as described in the next two sections.

A.2 Compilation of Acute Values

The following kinds of results of acute toxicity tests were used:

1. For midges, phantom midges, daphnids, and other cladocerans, the result used was the 48-hr EC_{50} based on percentage of organisms immobilized plus percentage of organisms killed. If such an EC_{50} was not available from a test, the 48-hr LC_{50} was used in place of the desired 48-hr EC_{50}. An EC_{50} or LC_{50} of longer

than 48 hours was used as long as the animals were not fed and the control animals were acceptable at the end of the test. Tests with daphnids and other cladocerans should have been started with organisms less than 24 hours old, and tests with midges and phantom midges should have been started with second- or third-instar larvae.

2. For embryos and larvae of barnacles, bivalve molluscs (clams, mussels, oysters, and scallops), sea urchins, lobsters, crabs, shrimp, and abalones, the result used was the 96-hr EC_{50} based on the percentage of organisms with incompletely developed shells plus the percentage of organisms killed. If such an EC_{50} was not available from a test, the lower of the 96-hr EC_{50} based on percentage of organisms with incompletely developed shells and the 96-hr LC_{50} was used in place of the desired 96-hr EC_{50}. If the duration of the test was between 48 and 96 hours, the EC_{50} or LC_{50} at the end of the test was used.

3. For all other freshwater and saltwater animal species and older life stages of barnacles, bivalve molluscs, sea urchins, lobsters, crabs, shrimp, and abalones, the result used was the 96-hr EC_{50} based on the percentage of organisms exhibiting loss of equilibrium plus the percentage of organisms immobilized plus the percentage of organisms killed. If such an EC_{50} was not available from a test, the 96-hr LC_{50} was used in place of the desired 96-hr EC_{50}.

Acceptable freshwater acute test results were entered in taxonomic order. If the tests were conducted properly, acute values reported as "greater than" values and those that were above the solubility of the test material were entered because rejection of such acute values would unnecessarily lower the Final Acute Value (FAV) by eliminating acute values for resistant species. Reported results were not rounded off to fewer than four significant digits.

In the case of a species for which at least one acceptable acute value was available, the species mean acute value (SMAV) was calculated as the geometric mean of the results of all flow-through tests in which the concentrations of test material were measured. In the case of a species for which no such result was available, the SMAV was calculated as the geometric mean of all available acute values (i.e., results of flow-through tests in which the concentrations were not measured and results of static and renewal tests based on initial concentrations of test material). (Nominal concentrations were acceptable for most test materials if measured concentrations were not available.) If only one acceptable acute value was available for a species, the SMAV was that value. The following information was also considered:

1. If the available data indicated that one or more life stages were more resistant than one or more other life stages of the same species by at least a factor of 2, the data for the more resistant life stages were not used in the calculation of the SMAV. This procedure was followed because a species can be considered protected from acute toxicity only if all life stages are protected.

2. The agreement of the data within and between species was considered. Acute values that appeared to be questionable in comparison with other acute and chronic data for the same species and for other species in the same genus usually were not used in the calculation of a SMAV. For example, if the acute values available for a species or genus differed by more than a factor of 10, some or all of the values usually were not used in calculations.

SMAVs were not rounded off to fewer than four significant digits.

The geometric mean of N numbers was calculated as the Nth root of the product of the N numbers. Alternatively, the geometric mean was calculated by adding the logarithms of the N numbers, dividing the sum by N, and taking the antilog of the quotient. Either natural (base e) or common (base 10) logarithms were used to calculate geometric means as long as they were used consistently within each set of data (i.e., the antilog used matched the logarithm used). The geometric mean of two numbers was usually calculated as the square root of the product of the two numbers. The geometric mean of one number was that number.

A.3 Compilation of Chronic Values

Results of three kinds of chronic toxicity tests were used:

1. *Life-cycle toxicity tests*. These tests consist of exposures of each of two or more groups of individuals of a species to a different concentration of the test material throughout a life cycle. To ensure that all life stages and life processes are exposed, tests with fish begin with embryos or newly hatched young less than 48 hours old, continue through maturation and reproduction, and end not less than 24 days (90 days for salmonids) after the hatching of the next generation. Tests with daphnids begin with young less than 24 hours old and continue until 7 days past the median time of first brood release in the controls.

For fish, data are obtained and analyzed on survival and growth of adults and young, maturation of males and females, eggs spawned per female, embryo viability (salmonids only), and hatchability. For daphnids, data are obtained and analyzed on survival and young per female. For mysids, data are obtained and analyzed on survival, growth, and young per female.

2. *Partial life-cycle toxicity tests*. These tests consist of exposures of each of two or more groups of individuals of a species of fish to different concentrations of the test material through most portions of a life cycle. Partial life-cycle tests are allowed with fish species that require more than a year to reach sexual maturity, so that all major life stages are exposed to the test material in less than 15 months (i.e., the tests begin with immature juveniles at least 2 months prior to active gonad development and end not less than 24 days (90 days for salmonids) after hatching of the next generation).

Data are obtained and analyzed on survival and growth of adults and young, maturation of males and females, eggs spawned per female, embryo viability (salmonids only), and hatchability.

3. *Early life-stage toxicity tests*. These tests consist of 28- to 32-day (60-days post hatch for salmonids) exposures of the early life stages of a species of fish from shortly after fertilization through embryonic, larval, and early juvenile development. Results of early life-stage tests in which the incidence of mortalities or abnormalities increased substantially near the end of the test are not used because the results of such tests are probably not good predictions of the results of comparable life-cycle or partial life-cycle tests.

Data are obtained and analyzed on survival and growth. Results of early life-stage tests were used as predictions of results of life-cycle and partial life-cycle tests with the same species. Therefore, when results of a life-cycle or partial life-cycle test were available, results of an early life-stage test with the same species were not used.

Acceptable freshwater and saltwater chronic test results were sorted by taxonomic order. Reported results were not rounded off to fewer than four significant digits.

A chronic value was obtained either by calculating the geometric mean of the lower and upper chronic limits from a chronic test or by analyzing chronic data using regression analysis. A lower chronic limit was the highest tested concentration (a) in an acceptable chronic test, (b) that did not cause an unacceptable amount of adverse effect on any of the specified biological measurements, and (c) below which no tested concentration caused an unacceptable effect. An upper chronic limit was the lowest tested concentration (a) in an acceptable chronic test, (b) that did cause an unacceptable amount of adverse effect on one or more of the specified biological measurements, and (c) above which all tested concentrations also caused such an effect.

Because various authors have used a variety of terms and definitions to interpret and report results of chronic tests, reported results were reviewed carefully. The amount of effect that was considered unacceptable was based on a statistical hypothesis test and/or the percent reduction from the controls. For example, a small percent reduction (e.g., 3 percent) was considered acceptable even if it was statistically significantly different from the control, whereas a large percent reduction (e.g., 30 percent) was considered unacceptable even if it was not statistically significant.

A.4 Compilation of Acute-Chronic Ratios

Acceptable freshwater and saltwater ACRs and the test results on which they were based were recorded.

1. For each chronic value for which at least one corresponding appropriate acute value was available, an ACR was calculated, using for the numerator the geometric mean of the results of all acceptable flow-through acute tests in the same dilution water and in which the concentrations were measured. Static and renewal tests were acceptable for daphnids. Acute tests with fish should have been started with juveniles, whereas acute tests with daphnids should have been started with organisms less than 24 hr old.
2. Acute test(s) that were part of the same study as the chronic test were used if available. If acute tests were not conducted as part of the same study, acute tests conducted in the same laboratory and dilution water, but in a different study, were used. If no such acute tests were available, results of acute tests conducted in the same dilution water in a different laboratory were used. If no such acute tests were available, an ACR was not calculated.
3. For fish, if chronic test data for life-cycle or partial life-cycle tests were available for a species, they were used for the denominator instead of an early life-stage test for the same species.

For each species, the species mean acute-chronic ratio (SMACR) was calculated as the geometric mean of all ACRs available for that species.

A.5 Calculation Procedures

For each genus for which one or more SMAVs were available, the genus mean acute value (GMAV) was calculated as the geometric mean of the SMAVs available for the genus. The GMAVs were ranked from highest to lowest, with the lowest GMAV assigned rank 1. The associated SMAVs and freshwater SMACRs were also entered.

To derive a freshwater FAV (Stephan et al., 1985), it was necessary to have results of acceptable acute toxicity tests with at least one species of freshwater animal in eight different families, such that all of the following requirements were satisfied:

1. The family Salmonidae in the Class Osteichthyes.
2. A second family in the Class Osteichthyes, preferably a commercially or recreationally important warm-water species (e.g., bluegill, channel catfish).
3. A third family in the phylum Chordata (may be in the class Osteichthyes or may be an amphibian, etc.).
4. A planktonic crustacean (e.g., cladoceran, copepod).
5. A benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).
6. An insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).
7. A family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).
8. A family in any order of insect or any phylum not already represented.

If all eight of the minimum data requirements (MDRs) were satisfied, the FAV was calculated using the computer program given on page 98 of Stephan et al. (1985), using the total number of GMAVs and the four lowest. The calculated FAV was compared with the low SMAVs to determine whether the FAV should be lowered to protect a commercially or recreationally important species.

If all eight of the acute freshwater MDRs were not met, a freshwater secondary acute value (SAV) was calculated. To derive a freshwater SAV, it was necessary to have at least one acceptable acute toxicity test with a species in one of three genera (*Daphnia, Ceriodaphnia*, or *Simocephalus*) in the Family Daphnidae.

The SAV was calculated using the lowest GMAV and the secondary acute factor (SAF) corresponding to the number of minimum data requirements that were satisfied:

$$\textbf{SAV} = \frac{\text{lowest Genus Mean Acute Value}}{\text{Secondary Acute Factor}}$$

The SAFs from GLI (1995):

Number of MDRs Satisfied	SAF
1	21.9
2	13.0
3	8.0
4	7.0
5	6.1
6	5.2
7	4.3

If sufficient data are available, chronic values can be calculated in the same manner as acute values, without the use of an ACR. Genus mean chronic values (GMCVs) were then calculated as the geometric mean of available chronic values. If the necessary data were available, the chronic value was calculated using the computer program used to calculate the FAV. (This option is rarely used because the chronic MDRs are rarely satisfied.)

If the data were not available to allow use of the computer program (e.g., Stephan et al. 1985), a final acute-chronic ratio (FACR) was calculated if acceptable ACRs were available for at least one species of aquatic animal in at least three different families, and of the three species:

1. At least one was a fish.
2. At least one was an invertebrate.
3. At least one was an acutely sensitive freshwater species. (The other two could be saltwater species.)

If the MDRs for calculation of an FACR were satisfied, an FACR was calculated; otherwise an SACR was derived.

For some materials, the ACR seems to be the same for all species, but for other materials the ratio seems to increase or decrease as the SMAV increases. The FACR was obtained in one of four ways, depending on the data available:

1. If the SMACR seemed to increase or decrease as the SMAVs increased, the FACR was calculated as the geometric mean of the ACRs for species whose SMAVs were close to the FAV or SAV.
2. If no major trend was apparent and the ACRs for a number of species were within a factor of 10, the FACR was calculated as the geometric mean of the SMACRs that were within a factor of 10.
3. For acute tests conducted on metals and possibly other substances with embryos and larvae of barnacles, bivalve molluscs, sea urchins, lobsters, crabs, shrimp, and abalones, the ACR was usually assumed to be 2. Chronic tests are very difficult to conduct with most such species, but it is likely that the sensitivities of embryos and larvae would determine the results of life-cycle tests. Thus, if the lowest available SMAVs were obtained with embryos and larvae of such species, the FACR was assumed to be 2.
4. If the most appropriate SMACRs were less than 2.0, and especially if they were less than 1.0, acclimation had probably occurred during the chronic test. Because continuous exposure and acclimation cannot be assured to provide adequate protection in field situations, the FACR was assumed to be 2.

If the available SMACRs did not fit one of the above cases, an FACR could not be obtained and an SACR was derived if possible.

If the available ACRs did not satisfy the minimum data requirements for derivation of an FACR, sufficient ACRs of 18 were assumed so that the MDRs were satisfied. The SACR was then calculated as the geometric mean of the measured and assumed ACRs. If no experimentally determined ACRs were available, the SACR was 18 (GLI 1995).

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