UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
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OFFICE OF CHEMICAL SAFETY
AND POLLUTION PREVENTION

MEMORANDUM

SUBJECT: **Toxicity Testing and Ecological Risk Assessment Guidance for Benthic Invertebrates**

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Whole sediment toxicity testing is now being routinely required as part of pesticide registration actions (registration review, new pesticide registrations). To date, however, the Environmental Fate and Effects Division (EFED) has not established formal guidance on which specific sediment toxicity tests should be recommended and how results from these studies should be integrated into EFED ecological risk assessments.

Effective immediately, this memo provides guidance to EFED ecological risk assessors on **when to require whole sediment toxicity tests** and **how to integrate sediment toxicity tests results into EFED ecological risk assessments**. This guidance document was developed by the EFED sediment toxicity workgroup over the past several years and incorporates input from multiple EFED technical teams, senior scientists and management team briefings. Elements of this guidance have also been presented at international scientific meetings including the Society of Environmental Toxicology and Chemistry (SETAC) and the European Chemicals Agency (ECHA). Importantly, this guidance is intended to support interpretation of the sediment toxicity testing requirements set forth in 40 CFR Part 158 (Subpart G) and is not intended as a replacement or alteration of these regulations. A case study that implements elements of this guidance for assessing risk to benthic invertebrates is provided in **Attachment 1**.

This guidance memo provides further information and clarification on the following questions:

1. Why is sediment toxicity testing required?
2. When should sediment toxicity studies be requested?
3. Which benthic invertebrate species should be tested?
4. How should risks to benthic invertebrates be estimated?
5. Which levels of concern should be applied?
6. Which common assumptions and sources of uncertainties should be characterized in the risk assessment?

Guidance on addressing each of these questions is summarized in Sections 1 - 6 below.

1. Why Is Sediment Toxicity Testing Required?

As of October 26, 2007, sediment toxicity testing of benthic aquatic invertebrates has been conditionally required as part of the Office of Pesticide Program's (OPP) ecological effects data requirements contained in 40 CFR Part 158 Subpart G (USEPA 2007)[1]. Prior to this time, risk of benthic aquatic invertebrates was commonly evaluated in EFED using the Equilibrium Partitioning (EqP) approach in combination with water column toxicity data. The EqP approach involves comparing estimated environmental concentrations (EECs) of pesticides in sediment interstitial (pore) water to acute and chronic toxicity endpoints derived from water column-dwelling invertebrates toxicity tests (e.g., *Daphnia*, mysid shrimp).

While the EqP approach is still scientifically valid and broadly applicable for estimating risks to benthic invertebrates for non-ionic organic chemicals, sediment toxicity testing for pesticides offers several advantages over the EqP approach. First, sediment toxicity tests incorporate pesticide exposure from ingested food and sediment particles (in addition to respiration of pore water and overlying water through gills and integument), whereas the EqP approach generally excludes exposure via non-respiratory routes. Second, results from sediment toxicity tests can be used to directly interpret monitoring data of pesticides in benthic sediments. Third, sediment toxicity tests directly account for factors that affect chemical partitioning, bioavailability, and toxicity in the test system, such as the source and composition of sediment organic carbon. These and other sediment-specific factors are not readily addressed using current EqP methods. Furthermore, EqP is recognized as being limited to non-ionizable organic chemicals and is thus not readily applied to other types of chemicals such as metals, organometalics, and ionizable organic chemicals. Lastly, the current battery of sediment toxicity tests includes a benthic aquatic insect (midge) and two benthic crustacean amphipods which enable the effects of pesticides to be evaluated using species encompassing a broader taxonomic range compared to standard water column tests of aquatic invertebrates (*e.g., Daphnia*, mysid shrimp, oyster).

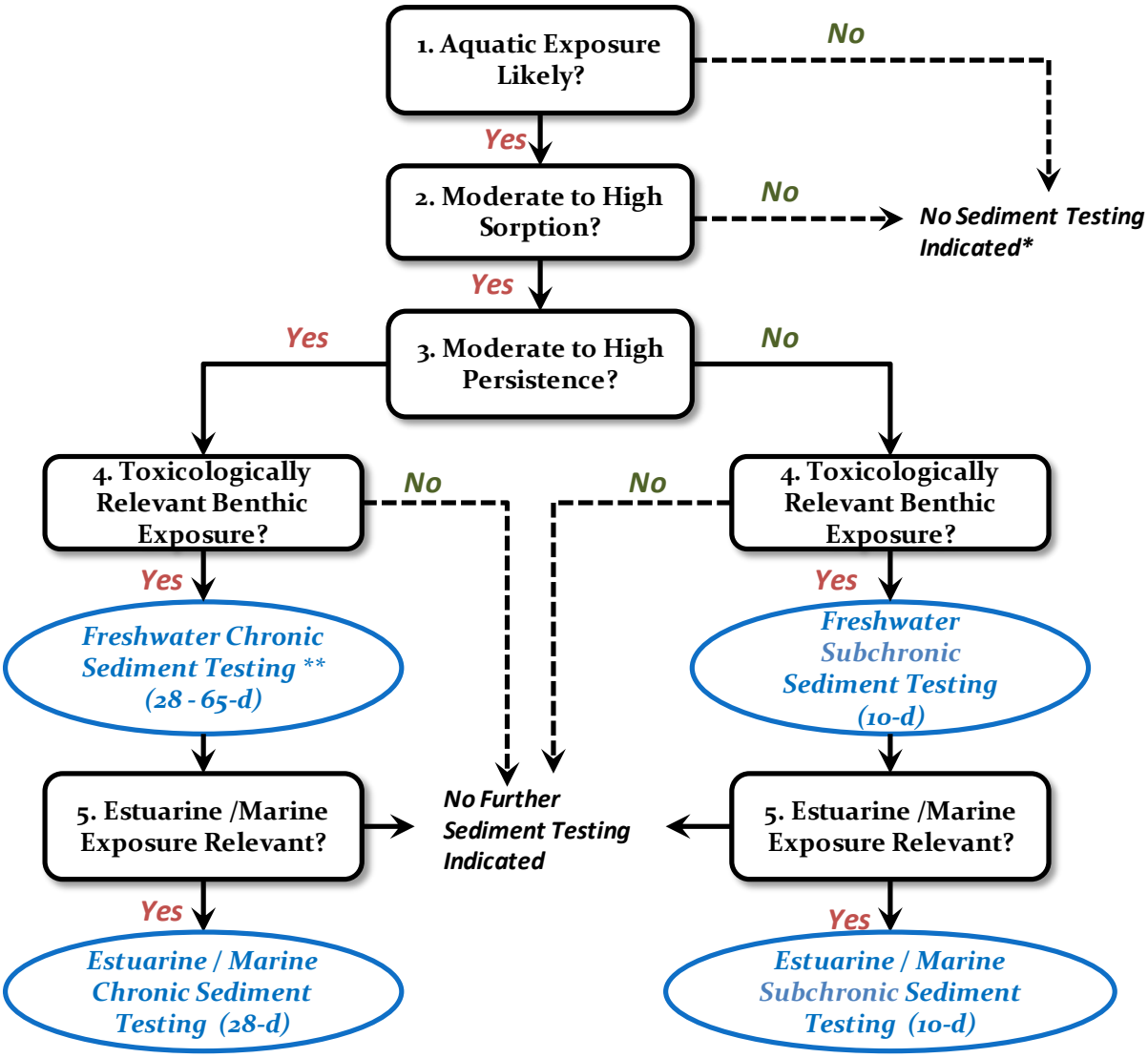
2. When Should Sediment Toxicity Testing Be Requested?

Whole sediment toxicity tests are conditionally required for a pesticide as specified in 40 CFR Part 158 Subpart G based on a series of toxicity testing 'triggers' that pertain to:

1. The likelihood of chemical exposure in aquatic ecosystems;
2. The extent the chemical partitions to sediment particles;
3. The persistence of the pesticide in the aquatic environment;
4. The toxicological relevance of predicted or monitored exposure concentrations; and
5. The likelihood of chemical exposure in estuarine/marine ecosystems.

[1] For Preamble language and Final Rulemaking, see: U.S. Environmental Protection Agency. 2007. Pesticides; Data Requirements for Conventional Chemicals, Technical Amendments, and Data Requirements for Biochemical and Microbial Pesticides; Final Rules *Federal Register* / Vol. 72, No. 207 / Friday, October 26, 2007.

A conceptual framework for evaluating the need for sediment toxicity testing is shown in **Figure 1.** Additional details on specific numeric triggers are provided **Sections 1.1 through 1.5.**



* Sediment testing may be required when evidence suggests available water column invertebrate test species are not adequate surrogates for risk assessment purposes (see Section 2.2).
** Chronic (life cycle) tests may be required as part of a tiered approach based on results of subchronic 10-d tests (see Section 3.2.1).

Figure 1. Conceptual Framework for Requesting for Sediment Toxicity Data (see Section number in parentheses for appropriate guidance) as interpreted from 40 CFR Part 158 Subpart G.

2.1 Likelihood of Aquatic Exposure

The first step in determining the need for sediment toxicity testing involves evaluating the likelihood that aquatic organisms would be exposed to the pesticide in question. According to 40 CFR Part 158, Subpart G, the likelihood of aquatic exposure is determined based on the use pattern of the pesticide. Specifically, whole sediment toxicity testing is **conditionally required** for all four outdoor use categories including:

- terrestrial uses (terrestrial food crop, terrestrial feed crop, and terrestrial nonfood crop);
- aquatic uses (aquatic food crop and aquatic nonfood);
- forestry uses; and
- residential outdoor uses.

Generally, whole sediment toxicity testing would **not** be considered for indoor uses or greenhouse uses, unless other lines of evidence (*e.g.,* pesticide monitoring data in sediments) clearly indicate that these pesticide use patterns are likely to result in pesticide exposure of benthic invertebrates. Other exceptions to this general guide may include uses that result in substantial pesticide release 'down the drain' (*e.g.,* pet shampoos, fabric treatments) and where these products may then appear in sludge from Publically Owned Treatment Works (POTW) facilities.

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2.2 Moderate to High Sorption Potential

The second step in deciding whether or not to request sediment toxicity testing involves evaluating the extent to which the pesticide is likely to sorb onto sediment particles. This sediment sorption potential is evaluated using pesticide fate property data including the solid-water distribution coefficient (K_d)[2], the organic carbon normalized solid-water distribution coefficient (K_{OC}), and the octanol-water partition coefficient (K_{OW}). The greater the value of each of these parameters, the greater the extent to which the pesticide is expected to sorb onto sediment particles. All else being equal, pesticides with higher sorption (partitioning) values are expected to result in greater exposure of benthic-dwelling invertebrates compared to pesticides with lower sorption values.

According to 40 CFR Part 158 Subpart G, pesticide sorption onto sediment particles is considered a trigger for sediment toxicity testing (*i.e.,* moderate to high sorption as specified in **Figure 1**) if **any** of the following conditions exist:

1. The K_d is ≥ 50 L/kg-solid
2. The K_{OC} is ≥1000 L/kg-organic carbon
3. The log K_{OW} is ≥ 3

[2] "Solid" may refer to soil or sediment.

As indicated in the preamble to 40 CFR Part 158 (p. 60944), values used for K_d and K_{OC} reflect **mean values** from the appropriate soil batch equilibrium studies.[3] If reliable sediment-based K_{OC} values are available, these may also be considered separately for comparison to the partitioning trigger. Although not explicitly discussed in the Part 158 regulations, it is also reasonable to consider a mean of appropriate K_{OW} values when multiple values are available to compare against the K_{OW} trigger above. As further discussed in the preamble of the Part 158 regulations, the K_d trigger of 50 was chosen to represent 80% sorption of the chemical to sediments with an organic carbon (OC) content of 2%. It is important to note that exposure to benthic invertebrates would still be expected to some extent for chemicals with K_d, K_{OC}, and K_{OW} values below the numeric triggers indicated above. However, in these circumstances, the predominant exposure route would be through the water column not benthic sediment. Therefore, addressing risks to water column dwelling invertebrates would be expected to encompass risk concerns to benthic dwelling invertebrates, taxonomic differences in species sensitivity notwithstanding. In situations where available data indicates standard water column invertebrate test species are not adequate surrogates for assessing risks to benthic invertebrates, sediment testing may be considered even when the partitioning triggers described previously are not exceeded. An example includes the much greater acute sensitivity of chironomids to neonicotinoid insecticides compared to *Daphnia*. Notably, water column tests can currently be conducted with some benthic invertebrate species on an acute basis (*e.g., C. dilutus*, *H. azteca*). However, chronic testing with these species currently requires the use of sediment toxicity test methods.

2.3 Moderate to High Persistence[4]

Information on the pesticide's environmental persistence is used primarily for determining whether the subchronic[5] (10-d) **or** chronic (28 to 60-day) whole sediment toxicity tests are considered more appropriate. Specifically, if **aerobic soil or aerobic aquatic metabolism half life is ≤10 days**, the subchronic (10-d) sediment toxicity test is generally considered more appropriate. Conversely, if the half life from the aerobic soil or aerobic aquatic metabolism studies is >10 days, the chronic (28 to 65-d) sediment toxicity test is generally considered more appropriate. If multiple values of aerobic soil or aerobic aquatic metabolism half lives are available and considered of equal reliability, the risk assessor should select the highest measured half life value for comparison with the 10-d half life trigger.

The basis for these persistence triggers pertains to selecting the most appropriate design of the sediment toxicity test rather than type of endpoints available from the tests. For example, unlike most standard water column toxicity tests, sediment toxicity tests are spiked once and prior to test initiation.

[3] Values of K_d and K_{OC} are measured under OPPTS Guideline 835.1230. Desorption coefficients measured in the guideline are not used for this evaluation.

[4] Note: the term "moderate to high persistence' is being used here qualitatively to distinguish chemicals with half lives greater than 10 days only for the purpose of sediment toxicity testing. Its use here does not imply applicability outside of the context of this guidance.

[5] Although the 40 CFR Part 158 rulemaking refers to the 10-d sediment toxicity tests as "acute," analysis of their duration relative to species life history and associated toxicity endpoints indicates the 10-d tests are more representative of subchronic tests, such as the fish early life stage test. When finalized, the 850.1735 and 850.1740 will refer to the 10-d sediment tests as subchronic tests. Therefore, they are referred to here as "subchronic (10-d) tests" for reasons of clarity.

Therefore, concentrations of short-lived pesticides (*e.g.,* half life ≤10-d) will decline substantially over the duration of the test such that a subchronic (10-d) test would more appropriate for quantifying the necessary dose-response information compared to a much longer chronic (28-65-d) toxicity test.

2.4 Toxicological Relevance of Benthic Exposure

Evaluating the toxicological relevance of benthic exposure to the pesticide of concern is the final step in determining the need for sediment toxicity test data. In this step, the likelihood that estimated or measured pesticide concentrations (*e.g.,* EECs) in sediment would lead to risk concerns for benthic invertebrates is specifically considered. The evaluation process essentially involves comparing pesticide EECs in sediment (modeled or monitored concentrations) to toxicity test endpoints for benthic invertebrates or water column invertebrates (as a surrogate for benthic invertebrates). In addition, the uncertainty associated with each type of EEC vs. toxicity comparison should be considered.

With respect to evaluating toxicological relevance of sediment exposure concentrations, 40 CFR Part 158 contains the following "sediment toxicity trigger" in considering the need for chronic (life cycle) sediment toxicity testing:

EEC in sediment > 0.1 • acute LC_{50}/EC_{50} value

However, no additional guidance is provided in the 40 CFR Part 158 rule regarding which EEC duration and which LC_{50}/EC_{50} value should be used in this comparison. Furthermore, no analogous sediment toxicity triggers are specified in the 40 CFR Part 158 rule regarding the need for subchronic (10-d) sediment toxicity tests.

Based on other information directly related to the 40 CFR Part 158 rule, it is apparent that the Agency intended to consider the toxicity of a pesticide in its determination of the need for chronic **and** subchronic (10-d) sediment toxicity testing. Specifically, in the Preamble to the Part 158 rulemaking, the Agency states:

> *"Once the Agency determines or extrapolates that the use pattern has the likelihood for chemical exposure to an aquatic system the triggers for persistence and adsorption are reviewed.* ***Toxicity will be taken into consideration relative to potential exposure."*** [emphasis added].

Furthermore, in response to numerous public comments on the sediment toxicity testing triggers proposed in the 2005 Part 158 proposed rule[6], the Agency states:

> *"The Agency must determine if the proposed use pattern will result in the compound reaching an aquatic system via drift and/or runoff at levels that could result in risk to aquatic organisms. This*

[6] USEPA. 2007. Response to Comments to Part 158 Rule Proposed March 11, 2005 Docket ID: OPP-2004-0387, p. 57. (available at: http://www.regulations.gov/#!documentDetail;D=EPA-HQ-OPP-2004-0387-0178)

potential for exposure to an aquatic system is determined through appropriate modeling or monitoring data. Once the Agency determines or extrapolates that the use pattern has the likelihood for chemical exposure to an aquatic system the triggers for persistence and adsorption are reviewed (previously discussed). ***Toxicity will be taken into consideration relative to potential exposure."*** [emphasis added]

Given the limited information in the 40 CFR Part 158 rule on the sediment toxicity comparison issue, additional guidance is provided below to assist risk assessors in evaluating a pesticide's toxicity as part of determining the need for sediment toxicity testing. It is recommended that risk assessors consider multiple lines of evidence in assessing the toxicological relevance of benthic sediment EECs for deciding when to recommend sediment toxicity testing.

2.4.1. Toxicity Evaluation for Chronic Sediment Testing

As stated in the 40 CFR Part 158 rule, the need for chronic (28 to 65-d) sediment toxicity tests is indicated when the "**EEC in sediment is greater than 0.1 • acute LC_{50}/EC_{50} value**." Given the lack of specificity in the 40 CFR Part 158 rule as to which EEC and which LC_{50}/EC_{50} value should be used in this comparison, it is recommended that risk assessors consider multiple lines of evidence for evaluating the toxicological relevance of sediment exposures with respect to the need for chronic toxicity testing of benthic invertebrates. Examples of such lines of evidence are presented in a series of comparisons below.

Comparison 1. Sediment EEC vs. Subchronic (10-d) Sediment NOAEC:

Compare the 21-d EEC in sediment (pore water or bulk sediment) to the lowest NOAEC from a subchronic (10-d) sediment toxicity test (pore water or bulk sediment[7]). ***If the 21-d EEC ≥ 0.1 • subchronic (10-d) sediment, chronic sediment toxicity testing is indicated.***

Comparison 1 presumes that NOAEC values from subchronic (10-d) sediment toxicity tests will be available for making such comparisons. It is based on the NOAEC from the subchronic sediment toxicity test since the NOAEC provides the toxicological basis for assessing subchronic and chronic risks of pesticides to benthic invertebrates (see Section 4). Notably, subchronic (10-d) sediment tests do not involve life cycle exposures, nor do they consider effects on reproduction. Therefore, NOAECs from chronic sediment tests may be considerably lower than NOAECs from subchronic (10-d) tests. To account for the expected differences in species sensitivity measured using a subchronic (10-d) and chronic (full life cycle) sediment toxicity test, a value of 0.1 is applied to the NOAEC from the subchronic (10-d) NOAEC[8]. In cases where the subchronic (10-d)

[7] Bulk sediment comparisons should be done on an organic carbon basis, where appropriate for the pesticide of interest. See organic carbon normalization section of this memo for additional guidance.

[8] A comparison of sediment toxicity data generated by the USGS Columbia, MO Research Laboratory suggest that a value of 0.1 would account for observed differences in NOAECs from subchronic (10-d) and chronic (life cycle) sediment toxicity tests. As additional sediment toxicity data are generated, re-evaluation of the 0.1 factor is appropriate to ensure it is adequately

sediment toxicity test results are not available, the risk assessor should consider other types of comparisons, such as those specified below, when evaluating the need for chronic sediment toxicity testing.

Comparison 2. Pore water EEC vs. Water Column NOAEC:

Compare the 21-d average sediment EEC in pore water to the lowest NOAEC from a chronic water column toxicity test with the most sensitive invertebrate species. **If the 21-d pore water EEC ≥ 1.0 • chronic water column NOAEC, the need for chronic sediment toxicity testing is indicated.**

This comparison is particularly useful when toxicity endpoints are unavailable from subchronic (10-d) sediment toxicity tests. Comparison 3 assumes that the chronic sensitivity of invertebrates on a water column basis provides a reasonable representation of their chronic sensitivity on a sediment pore water basis. The assumption of similar sensitivity of a given invertebrate species on the basis of water column and pore water exposure is supported by evaluations conducted for deriving USEPA EqP sediment toxicity benchmarks[9]. If the 21-d pore water EEC/chronic water column NOAEC >1, the need for chronic sediment toxicity testing is clearly indicated. It should be noted, however, that in some cases sediment test species (*e.g., Hyalella, Chironomus*) may be significantly more sensitive compared to standard OPP invertebrate test species (*e.g., Daphnia*). This is the case for pyrethroids and neonicotinoids, where *H. azteca* and *C. riparius, respectively,* are much more acutely sensitive compared to *D. magna*. Furthermore, sediment toxicity tests consider other routes of exposure (*e.g.,* ingestion of contaminated sediment and food) that are not fully considered in water column tests. **Therefore, risk assessors should not necessarily dismiss the need for sediment toxicity testing when ratios of the 21-d pore water EEC/water column invertebrate chronic NOAEC are less than 1, particularly as the ratio value approaches unity (*e.g.,* 0.1 -1) and when information suggests tested water column invertebrates may not adequately represent benthic invertebrate sensitivity.**

Comparison 3. Pore water EEC vs. Acute LC_{50}/EC_{50}

Compare the peak sediment EEC (pore water or bulk sediment) to the lowest LC_{50}/EC_{50} from an acute water column toxicity test with the most sensitive invertebrate species. ***If the peak pore water EEC >0.05 • acute water column invertebrate LC_{50}/EC_{50}, need for chronic sediment toxicity testing is indicated.***

Similar to comparison #2 above, comparison #3 assumes that the acute sensitivity of aquatic invertebrates on a water column basis provides a reasonable representation of their sensitivity on a sediment pore water basis. If the peak pore water EEC/water column invertebrate LC_{50}/EC_{50}

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[9] For example, see: USEPA. 2003. Procedures for the Derivation of Equilibrium Partitioning Sediment Benchmarks (ESBs) for the Protection of Benthic Organisms: Dieldrin. EPA/600/R-02/010. Office of Research and Development, Washington, DC 20460.

>0.05, the need for chronic sediment toxicity testing is indicated. The 0.05 cutoff was selected because it corresponds to the Federally threatened/endangered species LOC for aquatic animals. Risk assessors should consider the aforementioned uncertainty regarding potential species sensitivity differences among commonly tested organisms in water column vs. those tested in sediment. **Therefore, risk assessors should not necessarily dismiss the need for chronic sediment testing when the ratio of the peak pore water EEC/ water column LC_{50}/EC_{50} is less than 0.05, particularly as the ratio begins to approach the 0.05 value and when information suggests tested water column invertebrates may not adequately represent benthic invertebrate sensitivity.**

The previous comparisons assume that the sediment EEC is derived using appropriate aquatic exposure models of pesticide use (*e.g.,* PRZM/EXAMS). In the near future, sediment EECs (pore water and dry weight) will be readily obtained from the implementation of the Surface Water Calculator model. In the interim, guidance on obtaining sediment EECs from PRZM/EXAMs (PE5) is provided in **Attachment 2** based on output files described in **Attachment 3**. In situations where sediment EECs are not available from past assessments (e.g., for new chemical/new use assessments) high end estimates of sediment EECs may be obtained using the MS Cotton scenario.

In addition to model-based EECs, risk assessors should also consider available sediment monitoring data for the pesticide of concern in relation to its toxicity to aquatic invertebrates as an additional line of evidence. It is noted, however, that available sediment monitoring data for pesticides may not capture temporal or spatial variability associated with short-term exposure events and thus, may underestimate high end exposures that may actually occur in the aquatic environment.

2.4.2. Toxicity Evaluation for subchronic (10-d) Sediment Testing

As indicated previously, the 40 CFR Part 158 rule does not contain explicit toxicity-based triggers for evaluating the need for subchronic (10-d) sediment toxicity tests. However, the Agency is on record as indicating it will consider toxicity relative to exposure when requiring sediment toxicity testing. Furthermore, the targeting of testing requirements away from situations where results are not likely to inform risk management decisions is consistent with the OPP's Integrated Approaches for Testing and Assessment (IATA)[10] and the National Research Council's (NRC) recommendations on toxicity testing in the 21st century.[11] In this regard, it is recommended that risk assessors consider the following comparisons in evaluating the need for subchronic (10-d) sediment toxicity testing.

Comparison 4. Pore water EEC vs. Water Column NOAEC:

Compare the 21-d average sediment EEC in pore water to the lowest NOAEC from a chronic water column toxicity test with the most sensitive invertebrate species. ***If the 21-d pore water EEC > 1.0 • chronic water column invertebrate NOAEC, the need for subchronic (10-d) sediment toxicity testing is indicated.***

[10] http://www.epa.gov/pesticides/science/testing-assessment.html
[11] http://www.nap.edu/openbook.php?record_id=11970 .

The evaluation of toxicological relevance of sediment exposure for determining whether subchronic (10-d) sediment toxicity tests are needed can also be assessed using water column chronic toxicity endpoints and sediment EECs. Comparison #4 is identical to comparison #2 described previously, except that it is used to trigger subchronic testing here. Due to uncertainties regarding sensitivity differences between water column and benthic test species and the consideration of additional exposure routes in sediment tests, **risk assessors should not necessarily dismiss the need for sediment toxicity testing when ratios of the 21-d pore water EEC/water column invertebrate chronic NOAEC are less than 1, particularly as the ratio value approaches unity (*e.g.,* 0.1 -1).**

Comparison 5. Pore water EEC vs. Acute LC_{50}/EC_{50}:

Compare the peak sediment EEC (pore water or bulk sediment) to the lowest LC_{50}/EC_{50} from an acute water column toxicity test with the most sensitive invertebrate species. **If the peak pore water EEC > 0.05 • acute water column invertebrate LC_{50}/EC_{50}, the need for subchronic (10-d) sediment toxicity testing is indicated.**

Similar to comparison #3 above, comparison #5 assumes that the acute sensitivity of invertebrates on a water column basis provides a reasonable representation of their sensitivity on a sediment pore water basis. If the peak pore water EEC/water column invertebrate LC_{50}/EC_{50} > 0.05, the need for subchronic (10-d) sediment toxicity testing is indicated. The 0.05 cutoff is used because it corresponds to the Federally threatened/endangered species LOC for aquatic animals. Risk assessors should consider the aforementioned uncertainty regarding potential species sensitivity differences among commonly tested organisms in water column and sediment toxicity tests should be considered. **Therefore, risk assessors should not necessarily dismiss the need for subchronic (10-d) sediment testing when the ratio of the peak pore water EEC/ water column LC_{50}/EC_{50} is less than 0.05, particularly as it approaches the 0.05 value and when information suggests tested water column invertebrates may not adequately represent benthic invertebrate sensitivity.**

As described previously in Section 2.4.1, risk assessors should also consider available sediment monitoring data for the pesticide of concern in relation to its toxicity to aquatic invertebrates as an additional line of evidence in determining the need for sediment toxicity testing.

3. Which Benthic Invertebrate Species Should Be Tested?

3.1 Recommend Species for the Subchronic (10-d) Tests

For the subchronic (10-d) freshwater sediment toxicity tests, procedures are described for two species in the current public draft OPPTS 850.1735 guideline: the amphipod, *Hyalella azteca*, and the midge,

Chironomus dilutus. The midge and amphipod have different life histories, occupy different taxonomic groups (amphipods are crustaceans, while midges are insects) and generally interact with sediments in different ways. Chironomid larvae are more infaunal (submerged in the sediment) whereas amphipods are more epibenthic (moving in and out of the surficial sediment layer). As a result, the amphipod and midge may experience differences in chemical uptake relative to different exposure routes (pore water respiration, sediment ingestion, food ingestion, dermal uptake, respiration of overlying water). Furthermore, physiological and taxonomic differences between midges (Class: Insecta; Order: Diptera) and amphipods (Class: Malacostraca; Order: Amphipoda) may result in substantial sensitivity differences between these taxa, especially with the highly-specific modes of action of many pesticides. For example, substantial differences in sensitivity have been observed for some pyrethroid insecticides, with *Hyalella* generally being more sensitive than *Chironomus*. On the contrary, the midge has been shown to be highly sensitive relative to other crustaceans to some neonicotinoid insecticides. Therefore, given that pesticides subject to sediment toxicity testing are expected to partition extensively to sediments in aquatic systems, it is recommended that both the amphipod and midge tests be requested for either the subchronic (10-d) or chronic sediment assays.

For the subchronic (10-d) estuarine/marine sediment toxicity test, procedures for multiple species of estuarine/marine amphipods are described in the public draft OPPTS 850.1740 guideline including: *Ampelisca abdita*, *Eohaustorius estuarius*, *Rhepoxynius abronius*, and *Leptocheirus plumulosus*. If the chemical is applied directly to estuarine/marine water bodies or is expected to enter these areas in environmentally-relevant concentrations, then the estuarine/marine sediment tests should be solicited, assuming the other aforementioned conditions for sediment toxicity requests are met. Only one species of estuarine/marine amphipod is typically requested and the most commonly tested species to date for pesticide registration has been *L. plumulosus*.

3.2 Recommend Species for the Chronic (Life Cycle) Tests

For chronic sediment toxicity testing, the same rationale described for selection of species for subchronic (10-d) toxicity testing applies. That is, chronic freshwater sediment toxicity tests should include both an amphipod and midge species and one estuarine/marine species should be tested if environmentally-relevant concentrations are expected (or in cases where the pesticide is applied directly to estuarine/marine water bodies). Currently, the 850 guidelines for chronic sediment toxicity testing are being finalized. However, Agency-wide guidelines are available for chronic testing of freshwater[12] and estuarine/marine organisms[13]. Therefore, as indicated in 40 CFR Part 158, the registrant is required to submit a protocol for approval prior to initiating the study until such time as the OCSPP 850 chronic sediment testing guidelines are published.

[12] USEPA 2000. Methods for Measuring the Toxicity and Bioaccumulation of Sediment-associated Contaminants with Freshwater Invertebrates. EPA 600/R-99/064. March.

[13] USEPA 2001. Methods for Assessing the Chronic Toxicity of Marine and Estuarine Sediment-associated Contaminants with the Amphipod *Leptocheirus plumulosus.* EPA 600/R-01/020. March.

3.2.1 Optional Tiered Testing Strategy for Chronic Sediment Testing

If following the previous evaluation of a pesticides aquatic exposure potential (Section 2.1), sorption potential (Section 2.2), persistence (Section 2.3), and toxicological relevance (Section 2.4) chronic sediment toxicity testing is indicated, **a tiered testing strategy** may be considered for implementing the necessary Data Call-In requirements. In this approach, sediment toxicity testing would first be conducted with the aforementioned species using the subchronic (10-d) sediment toxicity test guidelines (OSCPP 850.1735 and 850.1740). Then, pending a comparison of estimated environmental concentrations (EEC) in sediment and pore water with toxicity results from the 10-d sediment toxicity studies, the need for one or more chronic sediment toxicity studies would be determined (*e.g.,* per comparison #1). This tiered testing approach has the potential advantage of reducing the number of chronic (life cycle) studies that would be needed when results of the 10-d (subchronic) tests in conjunction with sediment EECs indicate chronic testing is not likely to alter risk assessment conclusions. In some cases, however, this tiered testing approach may result in the conduct of both a 10-d (subchronic) and a chronic (life cycle) study.

Appendix A provides generic examples of Data Call-in Justifications for both acute and chronic sediment toxicity studies. These should be modified to fit the specific circumstances of each pesticide.

4. How Should Risk To Benthic Invertebrates Be Estimated?

A variety of approaches are available for deriving risk quotients (RQs) for benthic invertebrates. These approaches differ according to:

- the environmental medium chosen for expressing the EEC (pore water, sediment);
- the environmental medium chosen for expressing toxicity (pore water, sediment, water column); and
- the source of the EEC (PRZM/EXAMS, sediment monitoring data).

Following considerable review, it is apparent that each approach for deriving a benthic invertebrate RQ has different strengths and limitations that depend on the quantity and quality of data available for the pesticide of concern. For example, sediment pore water is often a dominant route of exposure for infaunal benthic invertebrates and thus is considered appropriate for expressing the EEC and toxicity (NOAEC). For some highly hydrophobic chemicals (*e.g.,* Log K_{OW} >5), however, measured concentrations in pore water from sediment toxicity tests can be highly uncertain due to analytical error and factors that affect chemical bioavailability (see **Appendix B** for a discussion of bioavailability). Furthermore, some benthic invertebrates may be exposed to a greater extent via ventilation of overlying water or through ingestion of contaminated sediment. Although measurement of chemical concentrations in bulk sediment may be subject to less analytical error compared to their measurement in pore water for some pesticides, estimating the bioavailability of pesticide in bulk sediment can be uncertain due to factors that affect chemical sorption (*e.g.,* differences in organic carbon quality and composition). From a toxicological perspective, choosing to express the NOAEC for benthic invertebrates on results from a sediment toxicity test is reasonable. However, sediment toxicity testing is commonly available for a

limited number of species (2 or 3) whereas for some pesticides that have been registered for one or more decades, many more water column toxicity tests of invertebrates may be available. In these situations, the range in species sensitivity represented by invertebrates tested in the water column may better reflect the sensitivity of benthic invertebrates (on a pore water basis) compared to that defined by 2 or 3 sediment toxicity studies. Monitoring data can provide an important line of evidence in characterizing risk as part of the "Risk Description."

Given the chemical-specific nature of the strengths and limitations of each approach for deriving benthic invertebrate RQ values, **multiple approaches are recommended for deriving RQ values in estimating risk to benthic invertebrates**. This recommendation is somewhat analogous to using multiple types of RQ values for birds and mammals to estimate risk (*e.g.,* dose- and diet-based RQs). A depiction of the various types of RQ values that could be derived with a full complement of sediment and water column toxicity data is shown in **Table 1**. Details of each of these four RQ derivation approaches are discussed below.

Table 1. Recommended Approaches for Deriving RQ values for Benthic Invertebrates

Exposure Basis	Toxicity Basis	Freshwater RQ		Saltwater RQ	
		Acute	*Chronic*	*Acute*	*Chronic*
1. Modeled Pore Water EEC	**Measured Pore Water NOAEC**	**n.a.**	✓	**n.a.**	✓
2. Modeled Sediment EEC[1]	**Measured sediment NOAEC[1]**	**n.a.**	✓	**n.a.**	✓
3. Modeled pore water EEC	**Measured water column acute LC_{50}/EC_{50} or chronic NOAEC**	✓	✓	✓	✓
4. Monitored sediment concentration[1, 2]	**Measured sediment NOAEC[1]**	**n.a.**	✓	**n.a.**	✓

[1] Where appropriate, sediment EEC and toxicity values should be normalized on an organic carbon basis (*e.g.,* nonionic organic chemicals); normalization with other ligands or sediment dry weight may be appropriate for other classes of pesticides (*e.g.,* metals, ionizable organic chemicals)

[2] Comparisons based on monitoring data should be conducted as part of "Risk Description"

n.a. = not applicable because sediment toxicity tests typically reflect subchronic or chronic exposures rather than acute exposures.

4.1 Derivation of Chronic RQ Values

Derivation of chronic RQ values for benthic invertebrate can, in theory, be derived using all four approaches illustrated in **Table 1**.

Approach 1: Chronic Pore Water RQ (Using Sediment Toxicity Data). Approach 1 involves dividing the modeled EEC in sediment pore water by the sediment toxicity-based NOAEC measured in pore water:

$$\frac{\textit{21-d Average EEC in Pore Water (µg a.i./L-pw)}}{\textit{Chronic or Subchronic Pore Water NOAEC (µg a.i./L-pw)}}$$

The recommended 21-d average EEC reflects a 1-in-10 year return frequency analogous to that used to estimate chronic RQ values for water column invertebrates. The 21-d average EEC is also representative of the overall range in exposure durations that are typical of chronic and subchronic sediment toxicity studies conducted under OCSPP 850 Guidelines (generally 10-65 days). The sediment pore water NOAEC used for the denominator of this RQ should reflect the most sensitive NOAEC within freshwater and estuarine/marine taxa that is considered appropriate for quantitative use in risk assessment.

Approach 2: Chronic Sediment RQ (Using Sediment Toxicity Data). Approach 2 consists of dividing the modeled EEC in bulk sediment by the sediment toxicity-based NOAEC measured in bulk sediment.

$$\frac{\textit{21-d Average Sediment EEC (µg a.i./kg-dry wt.[or kg-OC])}}{\textit{Chronic or Subchronic Sediment NOAEC (µg a.i./ kg-dry wt. [or Kg-OC])}}$$

When appropriate, bulk sediment-based RQ values should be determined on a sediment organic carbon basis in order to account for the influence of sediment organic carbon on the bioavailability of the pesticide. The organic carbon content in sediment is referred to as total organic carbon (TOC) and does not include mineralized carbon present as carbonates or bicarbonates. For many hydrophobic organic chemicals, partitioning and toxicity are commonly influenced by the amount of organic carbon present on the solid phase in addition to the type of organic carbon present (*e.g.,* humic acid, fulvic acid, soot carbon). The following equation can be used to convert the bulk sediment EECs and toxicity endpoints expressed on a sediment dry weight basis to EECs and endpoints on an OC-normalized basis. Notably, this equation accounts for the amount of organic carbon present but not the type of organic carbon present.

$$\mu\text{g a.i./kg-OC} = \frac{\mu\text{g a.i./kg sediment dry weight}}{\text{kg TOC/kg sediment dry weight}}$$

where:

µg a.i. /kg dry weight is the toxicity endpoint (NOAEC) or EEC expressed in terms of bulk sediment dry weight, and

kg TOC/kg dry weight is the mass total organic carbon per mass of dry sediment.[14]

As with RQ values derived using approach #1, the sediment-based NOAEC used for the denominator of this RQ should reflect the most sensitive NOAEC within freshwater and estuarine/marine taxa that is

[14] kg TOC/kg sediment dry weight is usually reported as % TOC. The default %TOC used in the standard EXAMS pond is 4% while the % TOC in sediment toxicity studies varies (typically from 2% to 10%).

considered appropriate for quantitative use in risk assessment.

Approach 3: Chronic Pore Water RQ (Using Water Column Toxicity Data). Approach 3 consists of dividing the modeled EEC in sediment pore water by the water column toxicity-based NOAEC measured from chronic invertebrate toxicity tests:

$$\frac{\text{21-d Average EEC in Pore Water (µg a.i./L-pw)}}{\text{Chronic Water Column NOAEC (µg a.i./ L)}}$$

The sediment pore water EEC is the same as that described earlier for deriving RQ values using approach #1. However, the chronic invertebrate NOAEC is based on results from chronic water column tests with aquatic invertebrates (the most sensitive values within freshwater and estuarine/marine taxa). This approach is referred to as the equilibrium partitioning (EqP) sediment method and is considered appropriate for organic chemicals whose partitioning is governed by organic carbon. The EqP approach is based on the Agency Equilibrium Partitioning Sediment Benchmarks (USEPA, 2002[15]). This extrapolation method is useful for estimating potential sediment exposure values, as well as sediment toxicity values that can be used in a screening level risk assessment. The EqP theory holds that a nonionic organic chemical in sediment partitions between sediment organic carbon, interstitial (pore) water and lipid phases of benthic organisms. At equilibrium, if the concentration in any phase is known, then the concentration in the other phases can be predicted through the K_{oc}. Therefore, EECs can be calculated from the pore water concentration (an output from PRZM/ EXAMS) and compared to the toxicity endpoints from the appropriate water column invertebrate toxicity tests. EqP theory assumes that all organic carbon contained in the TOC measurement have equal sorption capacities for chemicals and that partitioning to sediments is described by TOC alone (not other materials such as mineral-coated clays). Detailed discussion of EqP can be found in USEPA 2002.

Approach 4: Chronic Sediment RQ (Using Monitored Sediment Concentrations). Approach 4 consists of dividing the monitored concentration of a pesticide in bulk sediment by the sediment toxicity-based NOAEC measured in bulk sediment.

$$\frac{\text{Monitoring-Based Sediment Exposure Concentration (µg a.i./kg-dry wt. [or Kg-OC])}}{\text{Chronic or Subchronic Sediment NOAEC (µg a.i./ kg-dry wt. [or Kg-OC])}}$$

The choice of the value for the sediment exposure concentration depends largely on the quantity and representativeness of sediment monitoring data. Ideally, the monitored sediment concentration should reflect an exposure concentration analogous to the model-based sediment EEC. In practice, however, such data will not be available to compute an analogous 21-d average EEC with a 1-in-10 year return frequency. Therefore, risk assessors should use best professional judgment in selecting the appropriate monitored sediment concentration. In many cases, this may be the maximum value or upper 95th or 99th

[15] USEPA 2002. Technical Basis for the Derivation of Equilibrium Partitioning Sediment Guidelines (ESGs) for the Protection of Benthic Organisms: Nonionic Organics [Draft]. EPA 822-R-02-041.October.

percentile of the detected concentrations in sediment. As described previously, monitoring-based RQ values should be described in the Risk Description section as an additional line of evidence to support the risk assessment conclusions.

4.2 Derivation of Acute RQ Values

The current battery of sediment toxicity studies outlined in the OSCPP 850 and OECD sediment toxicity studies do not represent exposures typical of acute toxicity tests with aquatic animals (e.g., 48-96 hours). Therefore, acute toxicity endpoints will not likely be available from sediment toxicity studies. In these cases, the acute RQ value can be estimated using water column toxicity data as described in approach #3 above:

$$\frac{\text{Peak EEC in Pore Water (µg a.i./L-pw)}}{\text{Acute Water Column } LC_{50} \text{ or } EC_{50} \text{ (µg a.i./ L)}}$$

Instead of the 21-d average EEC as described for the chronic RQ derivation, the peak 1-in-10 year EEC in pore water is used. In addition, the acute LC_{50} or EC_{50} is used instead of the chronic NOAEC. As described previously, RQ values should be derived separately for freshwater and estuarine/marine benthic invertebrates, understanding that the numerator (EEC) would be identical.

5. Which Levels Of Concern Should Be Applied?

The same LOCs for other aquatic organisms should be applied for evaluation of risk to sediment-dwelling invertebrates.

Acute risk, non-listed species LOC: 0.5
Acute risk, restricted use LOC: 0.1
Acute risk, listed species LOC: 0.05
Chronic risk, non-listed and listed LOC: 1.0

6. What Common Assumptions And Sources Of Uncertainties Should Be Discussed In The Risk Assessment?

Many of the standard assumptions and sources of uncertainty associated with assessing risks to water column organisms apply to sediment dwelling organisms (*e.g.,* use of limited number of surrogate test species, PRZM/EXAMS modeling assumptions, use of maximum pesticide application rates, *etc.*). However, there are other key assumptions and sources of uncertainty that are more specific to the aforementioned procedures for assessing risk to benthic invertebrates. For **approach #1** (pore water RQs), one key uncertainty that should be discussed is the bioavailability of pesticide measured in pore water from the sediment toxicity test. For nonionic organic chemicals with log K_{OW} >5, dissolved organic carbon in pore water can substantially reduce chemical bioavailability and toxicity. In such cases, it may be desirable to estimate the freely dissolved concentration of chemical in the pore water based on

sediment concentrations, TOC in sediment and K_{OC} since measured concentrations in pore water may grossly underestimate toxicity. An illustration of the effect of organic carbon (dissolved and particulate) on the bioavailable (freely dissolved) fraction of a pesticide is shown in **Figure 2** for different values of log K_{OW}. An additional consideration for benthic invertebrate RQ values derived using **approach #1** is analytical error and uncertainty in pore water measurements, particularly with concentrations that approach the limit of quantification.

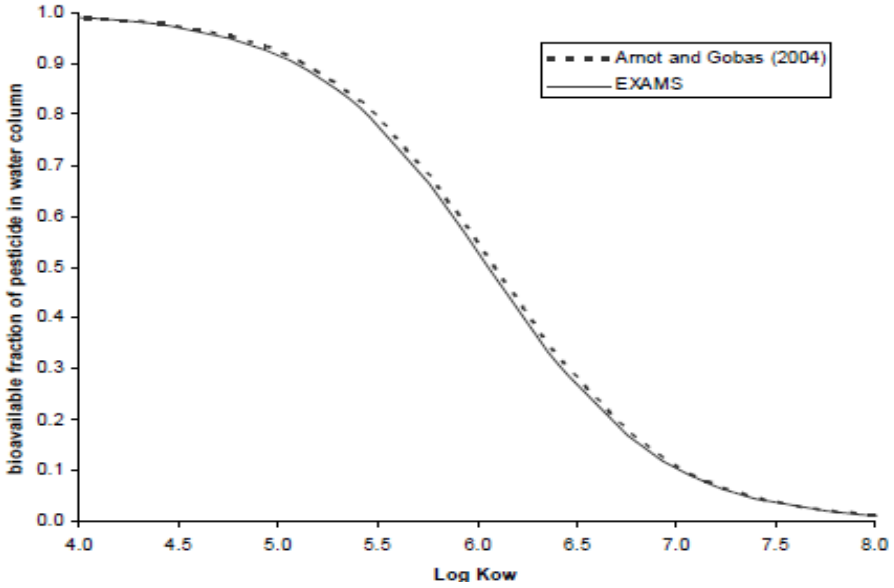

Figure 2. Estimated freely dissolved (bioavailable) fraction of a pesticide in water column according to the EXAMS and Arnot and Gobas (2004) models parameterized according to the OPP standard pond (Source: OPP KABAM Users Guide, USEPA 2009).

With **approach #2**, concentrations of pesticide measured in sediment from toxicity tests are relatively high compared to those of pore water (**approach #1**). However, risk assessors should verify that analytical methods were sufficient to extract adequate amounts of chemical from test sediments. In addition, previously discussed assumptions regarding normalizing to organic carbon should be briefly described. In some cases for highly hydrophobic pesticides, the risk assessor may wish to evaluate the sensitivity of risk estimates to assumptions regarding 'burial' of pesticide by deposited sediments. Methods for estimating the impact of sediment burial have been incorporated into the most recent version of the EXAMS model.

For **approach #3**, the appropriateness of water column toxicity tests as surrogates of benthic organism sensitivity should be discussed. For some pesticides with highly-specific modes of action, considerable variability may occur among aquatic invertebrates in different taxonomic groups.

For **approach #4**, the primary concern is the adequacy of monitoring data for representing 'high end' exposures expected of aquatic ecosystems which are highly vulnerable to pesticide use. Importantly, most aquatic monitoring studies lack sufficient temporal and spatial resolution to capture truly high end

exposures that are comparable to model-derived EECs. Therefore, a lack of risk as indicated by comparisons with sediment monitoring data does not necessarily preclude risk.

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Appendix A. Generic Language on Justification of Sediment Toxicity Data Requests

Guideline Numbers: 850.1735 and 850.1740 **Study Titles: Whole Sediment: Subchronic Freshwater Invertebrates** **Whole Sediment: Subchronic Marine Invertebrates**
Rationale for Requiring the Data
No subchronic sediment toxicity tests for freshwater or marine invertebrates have been submitted to satisfy the Agency's updated data requirements for outdoor uses in 40 CFR Part 158 (October 26, 2007). Benthic organisms may be exposed to run-off or spray drift from applications used in [terrestrial, aquatic, forestry and/or residential outdoor uses], based on the fate properties of [chemical X]. The following lines of evidence suggest the potential for ecologically significant exposure of benthic-dwelling organisms to pesticide X [INSERT RATIONALE BASED ON SEDIMENT TRIGGERS, MONITORING DATA AND OTHER LINES OF EVIDENCE]. For freshwater sediment testing, tests on an amphipod (*e.g., Hyalella azteca)* and a midge (*e.g., Chironomus dilutus)* are requested. Both freshwater species, *Hyalella* and *Chironomus* differ substantially in their ecological niche (*i.e.,* epibenthic vs. infaunal species), life history and phylogeny. For estuarine/marine sediment testing, tests on one amphipod species is requested (*e.g., Leptocheirus plumulosus*).
Practical Utility of the Data
How will the data be used? Data from sediment toxicity studies will be used to estimate potential risks to benthic organisms associated with uses of [chemical X]. The data will reduce uncertainties associated with the current risk assessment for benthic species and will improve our understanding of the potential effects of [chemical X] on aquatic ecosystems. **How could the data impact the Agency's future decision-making?** If the data indicates that registered [chemical X] uses may pose a risk of adverse effects to non-target benthic organisms above the Agency Level of Concern, the Agency may explore decision options to mitigate this risk. The lack of these data will limit the flexibility the Agency and registrants have in coming into compliance with the Endangered Species Act, and could result in use restrictions for [chemical X] which may otherwise be avoided, or which are unnecessarily severe.

Guideline Number: None (Agency-Wide Guidelines found in USEPA 2000 and 2001) **Study Title: Whole sediment: Chronic invertebrates freshwater and marine**
Rationale for Requiring the Data
No chronic sediment toxicity tests for freshwater or marine invertebrates have been submitted to satisfy the Agency's updated data requirements for outdoor uses in 40 CFR Part 158 (October 26, 2007). Benthic organisms may be exposed to run-off or spray drift from applications used in [terrestrial, aquatic, forestry and/or residential outdoor uses], based on the fate properties of [chemical X]. The following lines of evidence suggest the potential for ecologically significant exposure of benthic-dwelling organisms to pesticide X [INSERT RATIONALE BASED ON SEDIMENT TRIGGERS, MONITORING DATA AND OTHER LINES OF EVIDENCE]. For freshwater sediment testing, tests on an amphipod (*e.g., Hyalella azteca)* and a midge (e.g., *Chironomus dilutus)* are requested. Both freshwater species, *Hyalella* and *Chironomus* differ substantially in their ecological niche (*i.e.,* epibenthic vs. infaunal species), life history and phylogeny. For estuarine/marine sediment testing, tests on one amphipod species is requested (*e.g., Leptocheirus plumulosus*). In some situations, a tiered testing strategy may be considered for requesting chronic sediment toxicity testing.. In this approach, sediment toxicity testing would first be conducted with the aforementioned species using the subchronic (10-d) sediment toxicity test guidelines (OSCPP 850.1735 and 850.1740). Then, pending a comparison of estimated environmental concentrations (EEC) in sediment and pore water with toxicity results from the 10-d

sediment toxicity studies, the need for one or more chronic sediment toxicity studies would be determined. This tiered testing approach has the potential advantage of reducing the number of chronic (life cycle) studies that would be needed when results of the 10-d (subchronic) tests in conjunction with sediment EECs indicate chronic testing is not likely to alter risk assessment conclusions. In some cases, however, this tiered testing approach may result in the conduct of both a 10-d (subchronic) and a chronic (life cycle) study.

Practical Utility of the Data

How will the data be used?

Data from sediment toxicity studies will be used to estimate potential risks to benthic organisms associated with uses of [chemical X]. The data will reduce uncertainties associated with the current risk assessment for benthic species and will improve our understanding of the potential effects of chemical X on aquatic ecosystems.

How could the data impact the Agency's future decision-making?

If the data indicates that registered [chemical X] uses may pose a risk of adverse effects to non-target benthic organisms above the Agency Level of Concern, the Agency may explore decision options to mitigate this risk. The lack of these data will limit the flexibility the Agency and registrants have in coming into compliance with the Endangered Species Act, and could result in use restrictions for [chemical X] which may otherwise be avoided, or which are unnecessarily severe.

Appendix B. Bioavailability, Estimating Exposure, and Evaluating Toxicity in Sediment

1. What is bioavailability? Why is it important?

The question of what concentration of a contaminant is safe is not straight forward, as the total concentration in a media is not always equal to the amount that an organism is exposed to, especially in soils and sediment. The bioavailable portion is the portion that has the potential or tendency to enter and interact physiologically with an organism. It is this portion that is relevant in evaluating the toxicity of contaminants in soils and sediments. It is important to evaluate what the bioavailable fraction is in a toxicity test because if the total concentration in a test is considered rather than the bioavailable fraction, toxicity may be underestimated and thus, the potential for risk underestimated. Additionally, toxicity tests that consider only total concentrations will not reliably predict whether toxicity is likely to occur and the endpoints will be highly variable (*e.g.*, the results from different soils or sediments will be very different).

2. How do we currently predict exposure in risk assessments and how does that relate to the bioavailable fraction?

A. Estimating Exposure

Exposure Analysis Modeling System (EXAMS) provides freely dissolved pesticide concentrations in surface water and pore water[16]. Additionally, the pesticide concentration in sediment on a dry weight basis is normalized to the fraction organic carbon in sediment (4%) and is used as an estimated environmental concentration (EEC) in sediment risk assessments. The Environmental Fate and Effects Division's (EFED's) current risk assessment methodologies and EECs are considering the bioavailable fraction in the risk assessment.

B. Water Column Toxicity Testing

For water column toxicity tests, OPPTS Guideline 850.1000 requires that 1) water have a total organic carbon of less than 2 mg/L, 2) water be centrifuged or filtered prior to measuring the chemical concentration, and 3) that the chemical concentration be measured for all chemicals with a poor water solubility. Filtering with a 0.45 µm filter will remove any particulate organic matter in the water but may leave some dissolved organic carbon, which may make up most of the organic material in the water. As the concentration of dissolved organic carbon is low, for most chemicals this measured concentration will be within 20% of the dissolved concentration. The bioavailable fraction or dissolved concentration will only be considerably different from the total water concentration when the dissolved organic carbon concentration is high or the log K_{OW} of the compound is greater than six[17].

[16] Pore water is defined as the water occupying the spaces between sediment particles.

[17] Assuming a DOC concentration of 2 mg/L, for a chemical with a log K_{OW} of 6, 86% of the compound is in the freely dissolved form in a water column toxicity test.

3. How do we address bioavailability when evaluating the potential risk to sediment dwelling organisms?

A. Background on the Equilibrium Partitioning Model and Sediment Quality Guidelines

In the 1990s, sediment quality guidelines were developed based on research showing that organic matter was the primary sorbent of organic contaminants and that toxicity was better predicted by NOC concentrations in pore water and NOC concentrations in bulk sediment normalized to organic carbon rather than total sediment NOC concentrations (DiToro *et al.*, 1991b). In other words, the freely dissolved NOC concentration strongly correlated with uptake and can be thought of as a measure of bioavailability (DiToro *et al.*, 1991b). Equilibrium partitioning theory provided a means to predict chemical concentrations in pore water from chemical concentration in total sediment using sorption coefficients (DiToro *et al.*, 1991b). It predicts that organic contaminants will primarily distribute between organism lipid and sediment organic carbon (OC) and will achieve equilibrium, so that concentrations in different media may be predicted from the concentration in another media using sorption coefficients.

$$K_d = \frac{C_{sed}}{C_{pw\text{-}fd}} = K_{OC} f_{OC} \qquad \text{(Equation 1)}$$

where,

K_d is the sediment - water distribution coefficient,
C_{sed} is the sorbed NOC concentration in sediment,
$C_{pw\text{-}fd}$ is the freely dissolved NOC concentration in pore water,
K_{OC} is the organic carbon (OC) – water normalized distribution coefficient, and
f_{OC} is the fraction OC in sediment.

Equilibrium partitioning sediment guidelines (ESGs) estimate an NOC concentration in water, below which effects are not expected to occur, NOC concentrations in sediment are then expressed in terms of the principle binding phase (*e.g.*, total organic carbon for NOCs and acid volatile sulfides for metals) and compared to the ESG to determine whether effects are likely to occur (Budzinski *et al.*, 1997; USEPA, 2000).

In order to evaluate whether toxicity in a particular sediment is likely to occur, a freely dissolved NOC concentration in pore water may be estimated from total NOC concentrations in sediments. That estimated NOC concentration in pore-water is compared to the water column toxicity endpoint (which may be corrected for dissolved organic carbon) or freely dissolved NOC concentration in pore water toxicity endpoint from a sediment toxicity study. Alternatively, a NOC concentration in bulk sediment on a dry weight basis, normalized to the fraction organic carbon may be compared to the toxicity endpoint from a sediment toxicity test expressed in the same manner. **Table B-1** summarizes the possible exposure estimates and toxicity endpoints that may be used in order to evaluate whether there is a

potential for risk to occur in soils and sediments. The main assumption in the equilibrium partitioning model is that the dominant sorbent is organic carbon, thus, expression of toxicity on a pore water basis or on a basis of the fraction of organic carbon in sediment will reduce the variability in toxicity endpoints between soils and sediments. A water column toxicity test and the assumption that the pore water is the only route of exposure neglect the potential for exposure through ingestion. Organisms do ingest detritus and organic materials in sediment toxicity tests, so when an endpoint from a sediment toxicity test is used and compared to a pesticide concentration in bulk sediment expressed on an OC normalized basis, the potential for ingestion is not neglected in the risk assessment.

Table B-1. Summary of exposure estimates and the possible toxicity endpoints that may be compared to evaluate the potential for risk in soils and sediments.

1. **Exposure Estimates**	2. **Toxicity Endpoints**	3. **Assumptions**	4. **Limitations**
Dissolved NOC concentration in pore water	Measured or Estimated NOC concentration in pore water from a sediment toxicity test	Dissolved concentration is a good estimate of exposure. Organic carbon is the dominant sorbent.	Neglects the potential for exposure through the diet. Sorption has been shown to be influenced by many factors other than organic carbon.
	NOC concentration in water from a water column toxicity test	Dissolved concentration is good estimate of exposure. Sensitivity of water column aquatic invertebrates are representative of benthic aquatic invertebrates	
NOC concentration in sediment on a dry weight basis, normalized to the fraction organic carbon	NOC concentration in sediment on a dry weight basis, normalized to organic carbon	Organic carbon is the dominant sorbent for NOCs.	Sorption has been shown to be influenced by many factors other than organic carbon.

B. Total vs. freely dissolved concentrations in pore water

Total chemical concentrations in pore water will overestimate the dissolved chemical concentration in pore water, especially for chemicals with a high K_{OW} or K_{OC}. The fraction of NOC that is freely dissolved in the water column can be calculated using the following equation:

$$f_{fd} = \frac{1}{(1 + [DOC]K_{DOC} + [POC]K_{POC})} \qquad \text{(equation 2)}$$

where,

f_{fd} is the fraction NOC freely dissolved,

[POC] is the concentration of particulate organic carbon in kg POC/L water,

[DOC] is the concentration of dissolved organic carbon in kg DOC/L water, and
K_{DOC} is the dissolved organic-carbon water distribution coefficient in L water/kg DOC, and the
K_{POC} is the particulate organic-carbon water distribution coefficient in L water/kg POC.

For highly soluble chemicals, the difference in the dissolved versus the total concentration will be minor. **Figure B-1** shows the fraction freely dissolved over a range of log K_{OW}. The graph was created using equation 2 and assuming a DOC concentration of 0.1, 1.0, and 10 mg/L, that no particulate organic carbon was present, and the following relationship between the K_{DOC} and *n*-octanol-water partition coefficient (K_{OW}) (Burkhard, 2000).

$$K_{DOC} = 0.08\, K_{OW} \qquad \text{(equation 3)}$$

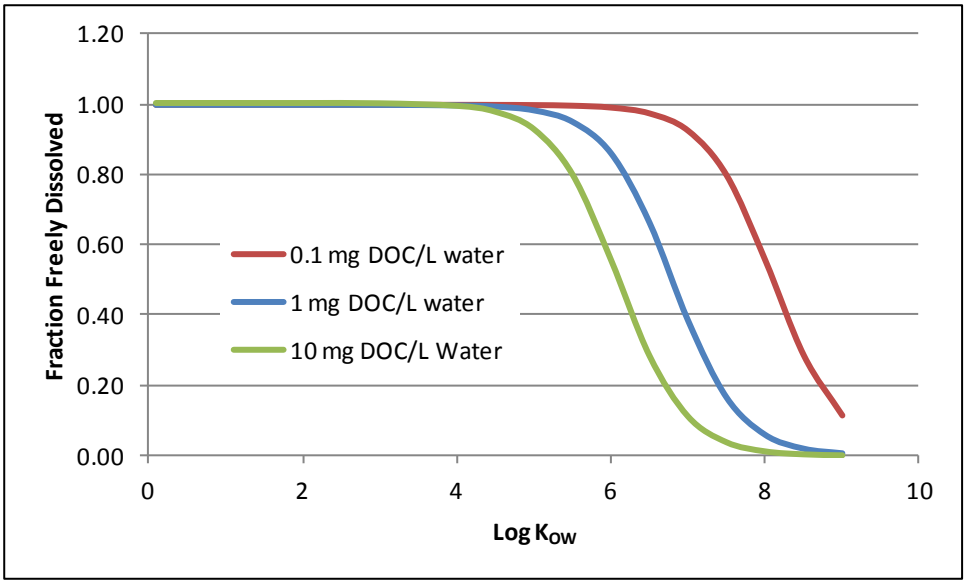

Figure B-1. Fraction of freely dissolved chemical as a function of the log K_{OW}

These results show that for chemicals with a log K_{OW} less than four, the fraction freely dissolved will range from 0.9 to 1.0 the total chemical concentration for DOC concentrations up to 100 mg DOC/L water. For chemicals with a log K_{OW} greater than four, the fraction freely dissolved can be much less than the total concentration in water or pore water. At 10 mg/L, the freely dissolved concentration remains above 0.90 for compounds with a log K_{OW} up to five and drops down to 55 percent for a log K_{OW} of six. For chemicals with a log K_{OW} less than four, it is typically feasible to reliably measure the chemical concentration in pore water as the DOC left in pore water will not significantly alter the bioavailability of the compound.

C. Estimating freely dissolved pore water concentration for sediment toxicity tests for chemicals with a log K_{OW} greater than four.

For chemicals with a log K_{OW} greater than four, it may not be possible to directly measure the concentration in pore water and if pore water concentrations are measured, some correction of the pore water concentration may be needed because the concentration of DOC in pore water can be high and the bioavailable fraction can be much lower than the total concentration. There are a few different methods that may be used in this situation. The first is to estimate the chemical concentration in pore water using equation four:

$$C_{pw\text{-}fd} = \frac{C_{sed\text{-}dw}}{K_{OC}\, f_{OC}} \qquad \text{(equation 4)}$$

where,

$C_{pw\text{-}fd}$ is the freely dissolved chemical concentration in pore water in µg/L,
$C_{sed\text{-}dw}$ is the chemical concentration in sediment on a dry weight basis in µg chemical/kg-sediment dry weight,
K_{OC} is the organic-carbon normalized sediment-water distribution coefficient in L/kg-organic carbon, and
f_{OC} is the fraction organic carbon in sediment.

Ideally, the K_{OC} used in the equation would be measured in the sediment that the toxicity test is conducted in. Additionally, the range of equilibrium chemical concentrations in pore water that the K_{OC} was measured in should overlap with the range of chemical concentrations used for toxicity testing. When these data are not available for the specific test, a K_{OC} may be estimated using submitted fate data. Sorption coefficient data are typically submitted on four soils and one sediment. While sediment K_{OC} values tend to be higher than soil K_{OC} values (Allen-King *et al.*, 2002), data are only available for a few soils and sediments. Therefore, selection of the K_{OC} value(s) for use in this equation should be based on those considered the most representative of chemical partitioning in test sediments.

Another option is to estimate the dissolved concentration using equation five:

$$C_{pw\text{-}fd} = \frac{C_{pw\text{-}tot}}{1+[DOC]K_{DOC}} \qquad \text{(equation 5)}$$

where,

C_{pw-tot} is the total chemical concentration measured in pore water,
[DOC] is the concentration of dissolved organic carbon (DOC) in the measured water, and
K_{DOC} is the DOC-water partition coefficient.

For this equation the K_{DOC} may be estimated using equation three. There may be other methods of estimating K_{DOC} that are more appropriate for the chemical of interest. Teams are encouraged to use the most reliable K_{DOC} available for the chemical of interest.

D. Considerations for NOC concentrations in bulk sediment normalized to the fraction organic carbon

The sediment concentrations measured in toxicity tests are the total NOC concentration in sediment. The concentration should be expressed on a dry weight basis and normalized to the fraction organic carbon in the sediment.

4. Limitations of the Equilibrium Partitioning Approach

A large body of data has been collected that supports the equilibrium partitioning model (DiToro *et al.*, 1991b; Ferraro *et al.*, 1990; Tracey and Hansen, 1996). However, over the past two decades several findings have suggested that this model is not adequate to predict the toxicity of sediment. Measured K_d values are often much greater than that predicted by organic matter alone (Bucheli and Gustafsson, 2000, 2001; Fletcher *et al.*, 1994; Gustafsson and Gschwend, 1999a; Gustafsson and Gschwend, 1997; Gustafsson and Gschwend, 1999b; Kraaij *et al.*, 2002; Mcgroddy *et al.*, 1996; Muller *et al.*, 2000) and uptake by organisms exposed to the same total NOC concentration in sediment is highly variable, even when normalized to f_{OC} and f_{lipid}. The presence of nonlinear sorption isotherms (Chiou *et al.*, 1998; Huang *et al.*, 1997; Karapanagioti *et al.*, 2000; Kleineidam *et al.*, 1999; Xia and Ball, 1999), fast and slow sorption domains (Pignatello and Xing, 1996; Shor *et al.*, 2003), competition (Zhao *et al.*, 2002), and a decreasing desorption and extractability with time (Alexander, 1995) indicate that a simple linear partitioning model is not adequate for modeling sorption in complex systems containing heterogeneous organic matter with varying sorptive properties. Finally, others have shown that the fast desorbing fraction is a good predictor of bioavailability and diet should also be considered as an exposure pathway (Gaskell *et al.*, 2007; Sormunen *et al.*, 2008). While it is acknowledged that many factors influence bioavailability of NOCs and there is much variability in measured K_{OC}s, for prospective risk assessments the equilibrium partitioning model is the best model available that reliably reduces the variation in estimated exposure across soils and sediments for organic compounds. For site specific and retrospective risk assessments, consideration of site specific parameters and sorption may be more appropriate and/or necessary.

A. Organic Carbon is the Dominant Sorbent for Nonionic Organic Chemicals

The paradigm that organic materials are the dominant sorbent for organic chemicals in soils and sediments gained wide acceptance in the 1990s and is still a widely accepted paradigm (Pignatello, 2011). However, it is important to understand that organic materials are not the only sorbents important in understanding sorption of NOCs. The simplest paradigm is that NOCs primarily sorb to amorphous organic materials via absorption which is sometimes called partitioning (*e.g.*, sorption into a 3-dimensional matrix) in the same way compounds partition into water and organic solvents (Cornelissen *et al.*, 2005). This type of sorption is linear, rapid, is not constrained by a limited number of sorption sites, and does not exhibit competition of solutes for sorption sites. However, it is known that nonlinear sorption (adsorption) isotherms are commonly observed. Nonlinear sorption or adsorption is viewed as sorption onto a two dimensional surface where the solute condenses onto the surface. In

adsorption, a nonlinear isotherm is observed due to the nature of the sorbent changing with loading, due to a limited surface area for sorption, or due to a heterogeneous sorbent. For adsorption, competition between solutes for sorption sites and saturation of sorption sites may occur. The variation in sorption coefficients across concentrations may be as high as three orders of magnitude and thus the nonlinearity of the sorption isotherm can have a profound effect on bioavailability (Pignatello, 2011). One theory on the source of nonlinear sorption is the presence of high surface area carbon materials (*e.g.*, black carbon, soot carbon, *etc.*) which have a very high surface area and high sorption coefficients (10 to 100 times the values observed for amorphous organic matter) (Cornelissen *et al.*, 2005).

While the dominant paradigm has been that organic materials account for the majority of sorption in soils and sediments, research has also shown that sorption to clay materials can be substantial. It has been demonstrated that, "for several classes of important NOCs and pesticides, smectite clays are equally or more effective adsorbents than SOM (compared as isolated components)" (Boyd *et al.*, 2011). Sorption coefficients for an individual compound will vary widely for different types of organic materials and for different types of clays (Allen-King *et al.*, 2002; Tracey and Hansen, 1996). Methods have been developed to estimate sorption in systems with clay and organic materials using a mineral phase availability factor. However, these models are too complex for use with the limited data sets available for most pesticides and are specific to an individual soil or sediment system.

The many factors affecting sorption and the quality and amount of information available for most pesticides is not adequate to fully determine the drivers of sorption of many pesticides. In one system, both absorption and adsorption will be occurring, and adsorption may be to hard carbon materials or clays. While sorption to clays can be important for some compounds and in some systems, sorption to clays in a different soil may not be dominant for that same compound in a different soil system. The limited sorption data available for pesticides does not allow for a sufficient analysis to consider sorption in this type of detail. For most pesticides, data are only available on four soils and one sediment and sorption coefficients tend to be higher in sediment versus soil. The properties of those soils and sediments are not held constant with varying one type of clay or type of organic carbon across soils and sediments. Data on sorption for relatively pure black carbon or clay materials may not be environmentally relevant as organic materials and biofilms can block surfaces and pores, resulting in less than additive sorption. Additionally, aggregation and composite particles may occur. Finally, organic materials can change the swelling and shrinking of clay materials and block access to interlayers. Sorption coefficients measured on pure materials may not be used to predict sorption in complex systems. Measurement of organic carbon may be indirectly determined (using the Walkley-Black method of oxidation with $K_2Cr_2O_7$ followed by titration of excess dichromate with $FeSO_4$) rather than the preferred method of removal of inorganic carbon by acid digestion, combustion of dry sediment, followed by infra-red determination of CO_2 using a CHN analyzer (USEPA, 1999). Methods of identifying specific types of carbon require additional analyses. Available data are not sufficient to identify the types of clay or carbon in the various systems tested. The high solids to water ratio may not be appropriate for characterization sorption of compounds with a high sorption coefficient (USEPA, 1999). Finally, reliable methods of predicting sorption across types of clays are not available. Therefore, given the body of evidence supporting the importance of organic materials on sorption of NOC, it is not

possible to conclude that organic carbon does not at least play a role in sorption. This issue was addressed in a 1999 Scientific Advisory Panel examining Sediment Toxicity and Fate of Synthetic Pyrethroids and they concluded the following on page eight of the final report.

"*Kd values are obtained under a given set of conditions for a given soil type. The use of Kd in place of K_{OC} limits the Agency to the use of a value which is operationally defined and which cannot be extrapolated beyond the experiment that generated the value. The advantage of using OC as a normalizing basis is that it allows one to estimate partitioning across a wide variety of soil/sediment types. This approach is central to the risk assessment of non-ionic chemicals sorbed to sediments*."

Normalization of total sediment concentrations to OC should be performed for all sediment toxicity tests for NOC compounds.

Abbreviations and Nomenclature

C_{sed}	Sorbed NOC concentration in sediment
C_{sed-dw}	NOC concentration in sediment on a dry weight basis
$C_{sed-toc}$	NOC concentration in sediment on a dry weight basis normalized to the fraction organic carbon
C_{pw-fd}	Freely dissolved NOC concentration in pore water
C_{pw-tot}	Total NOC concentration in pore water (e.g., included NOC in DOC and in water)
DOC	Dissolved organic carbon
[DOC]	Concentration of dissolved organic carbon
dw	Dry weight
EEC	Estimated environmental concentration
EFED	Environmental Fate and Effects Division
ESG	Equilibrium partitioning sediment guidelines
EXAMS	Exposure Analysis Modeling System
f_{fd}	Fraction freely dissolved
f_{OC}	Fraction organic carbon
K_{DOC}	Dissolved organic carbon-water partition coefficient
K_{OC}	Organic-carbon water normalized sediment or soil water distribution coefficient
K_{OW}	n-octanol-water partition coefficient
K_{POC}	Particulate organic carbon-water partition coefficient
L	liter
mg	milligram
NOC	Nonionic organic chemical
OC	Organic carbon
OCSPP	Office of Chemical Safety and Pollution Prevention
POC	Particulate organic carbon
[POC]	Concentration of particulate organic carbon
PRZM	Pesticide root zone model

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