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Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors

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GREAT LAKES WATER QUALITY INITIATIVE TECHNICAL SUPPORT DOCUMENT FOR THE PROCEDURE TO DETERMINE BIOACCUMULATION FACTORS

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I. INTRODUCTION

A. Purpose and Scope

The purpose of this document is to provide the technical information and rationale in support of the methods to determine bioaccumulation factors. Bioaccumulation factors, together with the quantity of aquatic organisms eaten and the percent lipid, determine the extent to which people and wildlife are exposed to chemicals through the consumption of aquatic organisms. The more bioaccumulative a pollutant is, the more important the consumption of aquatic organisms becomes as a potential source of contaminants to humans and wildlife.

Bioaccumulation factors are needed to determine both human health and wildlife Tier I water quality criteria and human health Tier II values. Also, they are used to define Bioaccumulative Chemicals of Concern among the Great Lakes Initiative universe of pollutants. Bioaccumulation factors range from less than one to several million.

B. Overview of Bioaccumulation and Bioconcentration

Aquatic organisms in nature absorb and retain some water-borne chemicals in their tissues at levels greater than the concentrations of these chemicals in the ambient water. This process is bioaccumulation. Bioaccumulation can be viewed simply as the result of competing rates of chemical uptake and depuration. However, bioaccumulation is a very dynamic process, affected by the physical and chemical properties of the chemical, the physiology and biology of the organism, environmental conditions, and the amount and source of the chemical. When uptake and depuration are equal, the ratio of the concentration of the chemical in the organism's tissue to the concentration of the chemical in the ambient water is the bioaccumulation factor (BAF). Thus:

$$\mathrm{BAF} = \frac{C_B}{C_w} \qquad \textbf{(1)}$$

where: C_B = concentration of chemical in the aquatic biota.
C_w = concentration of chemical in the ambient water.

The C_B is expressed on a mass per mass basis and the C_w is expressed in a mass per volume basis. For example, the C_B and C_w may be in mg/kg and mg/L respectively; the BAF is expressed in L/kg. Most C_w values available in the current literature are total concentrations. BAFs would be more useful if the C_w is limited to that portion of the total concentration that is available to the organism for uptake.

Bioaccumulation refers to uptake by aquatic organisms of a chemical from all sources such as diet and bottom sediments as well as the ambient water. Measured BAFs are based on field measurements of concentrations of the chemical in biota and water.

Bioconcentration refers to uptake of a chemical by aquatic organisms exposed only from the water. A bioconcentration factor (BCF) is, as is the BAF, the ratio between the concentration of the chemical in the aquatic biota and the concentration in the water. BCFs are measured in laboratory experiments and have the same units as BAFs. They are determined as follows:

$$BCF = \frac{C_B}{C_w} \tag{2}$$

where: C_B = concentration of chemical in the aquatic biota.
C_w = concentration of chemical in the water.

Reported BCFs, measured in the laboratory, are not always determined under steady-state conditions (i.e., conditions under which the concentrations in the biota and the surrounding water are stable over a period of time). Only steady-state BCFs, either measured directly or extrapolated based on the data, are useful for the determination of BAFs. The terms BAF and BCF are defined in this document to be steady-state BAF and steady-state BCF, respectively.

C. Outline of the Methods for Deriving Baseline BAFs

Baseline BAFs shall be derived using the following four methods, which are listed from most preferred to least preferred:

1. A measured baseline BAF for an organic or inorganic chemical derived from a field study of acceptable quality;

2. A predicted baseline BAF for an organic chemical derived using field-measured BSAFs of acceptable quality;

3. A predicted baseline BAF for an organic or inorganic chemical derived from a BCF measured in a laboratory study of acceptable quality and a FCM;

4. A predicted baseline BAF for an organic chemical derived from a K_{ow} of acceptable quality and a FCM.

D. GLI BAFs

The BAFs used by the GLI include the effects of all routes of chemical exposure, i.e, from water, sediment, and contaminated food, in the aquatic ecosystem. These BAFs by including all routes of exposure do not assume simple water-fish partitioning but rather are an overall expression of the total bioaccumulation using the concentration of the chemical in water column as a reference point. These BAFs do not ignore contaminated sediments.

Field-measured BAFs and BAFs derived using the BSAF methodology used in the final Guidance include all aspects of the environmental behavior of the chemicals including metabolism, disequilibrium, volatilization, predator-prey relationships, and include sources of the chemical from both the benthic and pelagic food webs. BAFs predicted using FCMs include many but not all of the environmental processes and interactions affecting bioaccumulative chemicals. The most notable process not accounted for in the predicted BAFs is metabolism and thus, when metabolism of the chemical is significant, the predicted BAFs will be larger than field derived BAFs. Thus, well field-measured BAFs are preferred.

The water column and sediment in any ecosystem are interconnected and in a subsequent chapter of this document, the interconnectedness between the sediment and water column concentrations of the chemicals is shown. This means that residues in fishes can also be predicted equally well using the concentration of the chemical in sediment as a reference point. In the methodology in the final Guidance, the concentration of the chemical in the water column has been selected as the reference point for bioaccumulation. The second method for deriving a baseline BAF uses the interconnectedness between the sediments and the water column to derive BAFs from field-measured BSAFs.

Sediment contamination in the Great Lakes is not localized except for small areas in tributaries and harbors which are slowly releasing contaminants to the open water systems. Most of the Great Lakes biomass is associated with the open waters which have concentrations of bioaccumulative chemicals that are strongly influenced by surface sediments in depositional basins which act as a source to benthic organisms and lake water through mixing. The BAFs used in the in the final Guidance are reflective of the open waters of the Great Lakes and include the effects of all routes of chemical exposure including contaminated the sediments.

E. Definitions

Baseline BAF (BAF_L^{fd}). For organic chemicals, a BAF that is based on the concentration of the freely dissolved chemical in the ambient water and takes into account the partitioning of the chemical within the organism; for inorganic chemicals, a BAF that is based on the wet weight of the tissue.

Baseline BCF (BCF_L^{fd}). For organic chemicals, a BCF that is based on the concentration of the freely dissolved chemical in the ambient water and takes into account the partitioning of the chemical within the organism; for inorganic chemicals, a BCF that is based on the wet weight of the tissue.

Bioaccumulation. The net accumulation of a substance by an organism as a result of uptake from all environmental sources.

Bioaccumulation factor (BAF). The ratio (in L/kg) of a substance's concentration in tissue of an aquatic organism to its concentration in the ambient water, in situations where both the organism and its food are exposed and the ratio does not change substantially over time.

Bioconcentration. The net accumulation of a substance by an aquatic organism as a result of uptake directly from the ambient water, through gill membranes or other external body surfaces.

Bioconcentration factor (BCF). The ratio (in L/kg) of a substance's concentration in tissue of an aquatic organism to its concentration in the ambient water, in situations where the organism is exposed through the water only and the ratio does not change substantially over time.

Biomagnification. The increase in tissue concentration of poorly depurated materials in organisms along a series of predator-prey associations, primarily through the mechanism of dietary accumulation.

Biota-sediment accumulation factor (BSAF). The ratio (in kg of organic carbon/kg of lipid) of a substance's lipid-normalized concentration in tissue of an aquatic organism to its organic carbon-normalized concentration in the surface sediment, in situations where the ratio does not change substantially over time, both the organism and its food are exposed, and the surface sediment is representative of average surface sediment in the vicinity of the organism.

Depuration. The loss of a substance from an organism as a result of any active or passive process.

Food-chain multiplier (FCM). The ratio of a BAF to an appropriate BCF.

Octanol-water partition coefficient (K_{OW}). The ratio of the concentration of a substance in the n-octanol phase to its concentration in the aqueous phase in an equilibrated two-phase octanol-water system. For log K_{OW}, the log of the octanol-water partition coefficient is a base 10 logarithm.

Uptake. Acquisition by an organism of a substance from the environment as a result of any active or passive process.

II. DATA REQUIREMENTS AND EVALUATION

Data used to calculate BAFs, BSAFs, and BCFs are obtained from EPA criteria documents, published papers, and other reliable sources. Data should be screened for acceptability using the criteria in The U.S. Environmental Protection Agency (EPA) guidelines for deriving aquatic life criteria (Stephan et al. 1985), and American Society for Testing and Materials guidance (practice E 1022-84) detailing methods for conducting a flow-through bioconcentration test (ASTM 1990).

In general, the Great Lakes Water Quality Initiative (GLWQI) BAF methods follow closely the EPA guidance (Stephan et al. 1985) with the addition of the BSAF methodology and the Food-Chain Multiplier (FCM) when a predicted BAF is calculated from a laboratory-measured or predicted BCF. The EPA published draft guidance on the control of bioaccumulative pollutants in surface waters which recommends the use of FCMs (USEPA 1991A).

No guidance can cover all the variations of experimental design and data presentation found in the literature concerning BAFs, BSAFs, BCFs and K_{OW}s. Professional judgment is needed throughout the BAF development process to select the best available information and use it appropriately.

III. DETERMINATION OF BAFs FOR ORGANIC CHEMICALS

A. Lipid Content of Fish Consumed By Humans and Wildlife

An important determinant of bioconcentration of non-polar organic chemicals in aquatic organisms is lipid content of the organism (see Barron, 1990 and the references cited by Barron, 1990). In the classic study by Reinert (1970), lipid normalization of DDT residues in fishes caused the differences between species and differences between size groups to become considerably less. It is now generally accepted that lipid normalization of chemical residues is essential in understanding and predicting the bioconcentration and bioaccumulation of bioaccumulative chemicals in aquatic organisms (Barron, 1990). Lipid normalization is now part of the EPA guidance on bioaccumulation (Stephan et al. 1985, USEPA 1991A), and is included in the BAF procedure in the final Guidance.

BAFs and BCFs are lipid-normalized by dividing the BAFs or BCFs by the fraction lipid of the tissue. Because BAFs and BCFs for organic chemicals are lipid-normalized, it does not make any difference whether the tissue sample is whole body or edible portion, but both the BAF (or BCF) and the percent lipid must be determined for the same tissue. The percent lipid of the tissue should be measured during the BAF or BCF study, but in some cases it can be reliably estimated from measurements on tissue from other organisms. If percent lipid is not reported for the test organisms in the original study, it may be obtained from the author; or, in the case of a laboratory study, lipid data for the same or a comparable laboratory population of test organisms that were used in the original study may be used.

A lipid-normalized BAF, of a chemical in tissue shall be calculated using the following equation:

$$BAF_R = \frac{BAF_T}{f_R} \qquad (3)$$

where: BAF_R = lipid-normalized BAF.
BAF_T = BAF based on the total concentration of the organic chemical in the tissue of biota (either whole organism or specified tissue) (µg/g).
f_R = fraction of the tissue that is lipid.

When deriving water quality criteria for human health and wildlife it is important to accurately characterize the potential exposure to a chemical. To do this, information is needed on several parameters including the quantity of aquatic biota consumed by humans and wildlife, the percent lipid in the aquatic biota, the trophic level of the aquatic biota and the BAF for that chemical. The quantity of aquatic biota consumed can be estimated using consumption surveys for humans and, where available, studies on the feeding habits of wildlife. To estimate BAFs that can be used in deriving human health and wildlife criteria, a standard percent lipid value is needed for both humans and wildlife. The standard percent lipid value used in the BAF derivation should, if possible, be a consumption-weighted percent lipid value. A consumption-weighted percent lipid value is preferred because it provides a more accurate characterization of the potential exposure to humans and wildlife than simply assuming humans and wildlife consume all or a subset of the species within the area of concern (in this case the area of concern is the Great Lakes Basin). To estimate a consumption-weighted percent lipid value for humans and wildlife the following information is needed: (1) a consumption survey that documents the type and quantity of aquatic biota consumed by humans and wildlife; (2) the percent lipid of the aquatic biota consumed by humans and wildlife; and (3) the trophic level of the aquatic biota consumed by humans and wildlife.

A consumption survey that documents the type and quantity of aquatic biota consumed by humans and/or wildlife in conjunction with the percent lipid values for those species will assist in accurately characterizing the potential exposure to humans and wildlife from consumption of contaminated aquatic biota. EPA has published the document "Consumption Surveys for Fish and Shellfish. A Review and Analysis of Survey Methods" (Feb. 1992, EPA 822/R-92-001) which may assist in conducting and analyzing the results of such surveys.

The second critical piece of information is the percent lipid values of aquatic biota consumed by humans and/or wildlife. The lipid values used for deriving human health BAFs should be from aquatic biota collected from the Great Lakes or their tributaries and be from the edible tissue (e.g., muscle). For wildlife, whole body lipid data should be used. Data on the edible tissue is available from the contaminant monitoring programs in the various Great Lakes States. Whole body lipid data are also available from the State monitoring programs, but is not as abundant.

Finally, the trophic level of the biota consumed should be determined. This is important when attempting to accurately characterize the potential exposure to humans and wildlife because humans and wildlife consume both trophic level 3 and trophic level 4 fish and the BAFs for trophic level 3 and trophic level 4 are different for many pollutants. If it is assumed that humans consume only trophic level 4 species, then the trophic level 4 BAFs used for deriving human health criteria could be overestimated or underestimated. The determination of the appropriate trophic level for a fish species will depend on the size and age of the fish being consumed. Some fish are in trophic level 3 when young, but in trophic level 4 as adults. Data on the size and age of fish consumed by humans and/or wildlife will, in most cases, not be included in a consumption survey. In these situations, best professional judgment will need to be exercised when determining the appropriate trophic level for a fish species.

For the Great Lakes Water Quality Initiative a consumption survey by West et al. (1993) was used to characterize the consumption patterns of sport anglers in the Great Lakes Basin (Table 5 of Appendix I). This study was selected because it represented the largest consumption survey of sport anglers in the Great Lakes Basin. In addition, it was possible to determine the type and quantity of each species consumed.

Percent lipid data from the fish contaminant monitoring programs in Michigan, Wisconsin, Ohio, Indiana, New York and Minnesota provided lipid data for edible tissues (e.g., muscle) of fish from each of the Great Lakes (Tables 1-3 of Appendix I). Most lipid data are for skin-on fillets because skin-on fillets are the accepted tissue sample used by most of the Great Lakes fish consumption advisory programs.

The report "Trophic Level and Exposure Analyses for Selected Piscivorous Birds and Mammals" (EPA, 1995) was used along with professional judgement to determine the trophic level of the fish species consumed by the sport anglers. Each consumed fish species was assigned to either trophic level 3 or trophic level 4 based on data from the report and/or professional judgement.

The data from the West survey (1993) in conjunction with the data from the fish monitoring programs and the report on trophic levels of various fish species were used to determine consumption weighted mean percent lipid values for use in deriving human health BAFs. The total grams per day of each species consumed by sport anglers was multiplied by the percent lipid value for that species to determine the grams of lipid consumed per day by sport anglers for that species. The grams of lipid consumed from all species were summed and divided by the total grams of fish consumed from trophic level 3 and trophic level 4 fish to arrive at a consumption weighted mean percent lipid value for each trophic level. These percent lipid values are used to derive BAFs which are then utilized in calculating human health criteria. The mean values for use in deriving human health BAFs are 1.82 for trophic level 3 fish consumed and 3.10 for trophic level 4 fish consumed (Table 6 of Appendix I). The values were not rounded to whole numbers because they are intermediate values that are used in the derivation of human health criteria.

For wildlife, an analysis of the most common prey species consumed by the five representative wildlife species used to derive wildlife criteria was conducted. The data allowed only a gross determination of the type of species consumed by the five representative species and the percent of prey species consumed from each trophic level. The analysis did not allow a quantitative determination of the quantity of the prey species consumed at each trophic level. Consequently, a consumption weighted percent lipid value similar to that derived for humans was not possible. Nonetheless, a percent lipid value for both trophic level 3 and trophic level 4 were estimated using whole fish lipid data from the U.S. Fish and Wildlife Service national contaminant biomonitoring program, the Canada Department of Fisheries and Oceans, the New York Department of Environmental Conservation, and the Michigan Department of Natural Resources (Table 4 of Appendix I). The trophic levels of the species consumed were determined using the data from the report "Trophic Level and Exposure Analyses for Selected Piscivorous Birds and Mammals" (EPA, 1995). The mean percent lipid values for wildlife for use in deriving wildlife BAFs are 6.46 for trophic level 3 prey species consumed and 10.31 for trophic level 4 prey species consumed (Table 7 of Appendix I). The values were not rounded to whole numbers because they are intermediate values that are used in the derivation of wildlife criteria.

B. Bioavailability

Baseline BAFs and BCFs for organic chemicals, whether measured or predicted, shall be based on the concentration of the chemical that is freely dissolved in the ambient water in order to account for bioavailability. For the purposes of this guidance, the relationship between the total concentration of the chemical in the water (i.e., that which is freely dissolved plus that which is sorbed to particulate organic carbon or to dissolved organic carbon) to the freely dissolved concentration of the chemical in the ambient water shall be calculated using the following equation:

$$C_w^{fd} = (f_{fd})(C_w^{t})$$

where: C_w^{fd} = freely dissolved concentration of the organic chemical in the ambient water.

C_w^t = total concentration of the organic chemical in the ambient water.

f_{fd} = fraction of the total chemical in the ambient water that is freely dissolved.

1. Determination of the Fraction of the Chemical that is Freely Dissolved in Water

The fraction of the chemical that is freely dissolved in the water, f_{fd}, can be determined using the following equation with the K_{OW} for the chemical and the DOC and POC of the water.

$$f_{fd} = \frac{1}{1 + \frac{(DOC)(K_{OW})}{10} + (POC)(K_{OW}} \qquad \textbf{(5)}$$

where: DOC = concentration of dissolved organic carbon, kg of organic carbon/L of water.

K_{OW} = octanol-water partition coefficient of the chemical.

POC = concentration of particulate organic carbon, kg of organic carbon/L of water.

2. Derivation of the Equation Defining f_{fd}

Experimental investigations have shown that hydrophobic organic chemicals exist in water in three phases, 1) the freely dissolved phase, 2) sorbed to suspended solids and 3) sorbed to dissolved organic matter (Hassett and Anderson (1979), Carter and Suffet (1982), Landrum et al. (1984), Gschwend and Wu (1985), McCarthy and Jimenez (1985), Eadie et al. (1990, 1992)). The total concentration of the chemical in water is the sum of the concentrations of the sorbed chemical and the freely dissolved chemical (Gschwend and Wu (1985) and Cook et al. (1993)):

$$C_w^t = C_w^{fd} + POC \cdot C_{poc} + DOC \cdot C_{doc} \qquad \textbf{(6)}$$

where: C_w^{fd} = concentration of freely dissolved chemical in the ambient water, kg of chemical/L of water.

C_w^t = total concentration of the chemical in the ambient water, kg of chemical/L of water.

C_{poc} = concentration of chemical sorbed to the particulate organic carbon. in the ambient water, kg of chemical/kg of organic carbon.

C_{doc} = concentration of chemical sorbed to the dissolved organic carbon

POC = concentration of particulate organic carbon in the ambient water, kg of organic carbon/L of water.
DOC = concentration of dissolved organic carbon in the ambient water, kg of organic carbon/L of water.

in the ambient water, kg of chemical/kg of organic carbon.

The above equation can also be expressed using partitioning relationships as:

$$C_w^t = C_w^{fd} \cdot (1 + POC \cdot K_{poc} + DOC \cdot K_{doc}) \qquad \textbf{(7)}$$

where:

$$K_{poc} = \frac{C_{poc}}{C_w^{fd}} \quad \text{and} \quad K_{doc} = \frac{C_{doc}}{C_w^{fd}} \qquad \textbf{(8)}$$

K_{poc} = equilibrium partition coefficient of the chemical between POC and the freely dissolved phase in the ambient water
K_{doc} = equilibrium partition coefficient of the chemical between DOC and the freely dissolved phase in the ambient water.

From equation 7, the fraction of the chemical which is freely dissolved in the water can be calculated using the following equations:

$$f_{fd} = \frac{C_w^{fd}}{C_t^w} \qquad \textbf{(9)}$$

$$f_{fd} = \frac{1}{1 + (DOC)(K_{doc}) + (POC)(K_{poc})} \qquad \textbf{(10)}$$

Experimental investigations by Eadie et al. (1990, 1992), Landrum et al. (1984), Yin and Hassett (1986, 1989), Chin and Gschwend (1992), and Herbert et al. (1993) have shown that K_{doc} is directly proportional to the K_{OW} of the chemical and is less than the K_{OW}. The K_{doc} can be estimated using the following equation:

$$K_{doc} \,.\, \frac{K_{OW}}{10} \tag{11}$$

The above equation is based upon the results of Yin and Hassett (1986, 1989), Chin and Gschwend (1992), and Herbert et al. (1993). These investigations were done using unbiased methods, such as the dynamic headspace gas-partitioning (sparging) and the fluorescence methods, for determining the K_{doc}.

Experimental investigations by Eadie at al. (1990, 1992) and Dean et al. (1993) have shown that K_{poc} is approximately equal to the K_{OW} of the chemical. The K_{poc} can be estimated using the following equation:

$$K_{poc} \,.\, K_{OW} \tag{12}$$

By substituting equations 11 and 12 into equation 10 , the following equation is obtained:

$$fd \;' \; \frac{1}{1 \;\%\; \frac{(DOC)(K_{OW})}{10} \;\%\; (POC)(K_{OW}} \tag{13}$$

C. Bioconcentration and Octanol-Water Partitioning

Numerous investigations have demonstrated a linear relationship between the logarithm of the bioconcentration factor (BCF) and the logarithm of the octanol-water partition coefficient (K_{OW}) for organic chemicals for fish and other aquatic organisms. Isnard and Lambert (1988) listed various regression equations that illustrate this linear relationship. The underlying assumption for the linear relationship between the BCF and K_{OW} is that the bioconcentration process can be viewed as a partitioning of a chemical between the lipids of the aquatic organisms and water and that the K_{OW} is an useful surrogate for this partitioning process (Mackay (1982)).

The regression equations demonstrating the linear relationship between the logarithms of the BCF and K_{OW} have been developed using organic chemicals which are slowly, if at all, metabolized by fishes or other aquatic organisms. For metabolizable chemicals, the regression equations developed between BCF and K_{OW} for non-metabolizable chemicals in most cases predict BCFs which are larger than the laboratory-measured BCFs. The losses of the chemicals due to metabolism are not accounted for in the simple partitioning model (Baron (1990), de Wolf et al. (1992)).

Mackay (1982) presented a thermodynamic basis for the partitioning process for bioconcentration and in essence, the BCF on a lipid-normalized basis (and freely dissolved concentration of the chemical in the water) should be similar if not equal to the K_{OW} for organic chemicals. Unfortunately, almost all of the reported regression equations have used BCFs reported on a wet weight basis instead of lipid-normalized. When regression equations are constructed using BCFs reported on a lipid-normalized basis, regression equations are obtained which have slopes and intercepts which are not significantly different from one and zero, respectively. For example, de Wolf et al. (1992) adjusted the relationship reported by Mackay (1982) to a 100 percent lipid basis (lipid normalized basis) and obtained the following relationship:

$$\log BCF \ ' \ 1.00 \log K_{OW} \ \& \ 0.08 \qquad \textbf{(14)}$$

For chemicals with large log K_{OW}s (i.e., greater than 6.0), reported BCFs are often not equal to the K_{OW} for non-metabolizable chemicals. As discussed by Gobas et al. (1989), this non-equality between the BCF and K_{OW} is not caused by a breakdown of the BCF-K_{OW} relationship but rather is caused by (1) not accounting for growth dilution which occurred during the BCF determination, (2) using the total concentration of the chemical in the water instead of the bioavailable (freely dissolved) concentration of the chemical in calculating the BCF, (3) not allowing sufficient time in the exposure to achieve steady-state conditions, and (4) not correcting for elimination of the chemical into the feces. BCFs for non-metabolizable chemicals are equal to the K_{OW} when the BCFs are reported on lipid-normalized basis, determined using the freely dissolved concentration of the chemical in the exposure water, corrected for growth dilution, determined from steady-state conditions or determined from accurate measurements of the chemical's uptake (k_1) and elimination (k_2) rate constants from and to the water, respectively, and determined using no solvent carriers in the exposure.

In the final Guidance, predicted BCFs are estimated using the following approximation:

$$BCF_R^{fd} \ . \ K_{OW} \qquad \textbf{(15)}$$

where: BCF_R^{fd} = BCF reported on lipid-normalized basis using the freely dissolved concentration of the chemical in the water.

This relationship is applicable to organic chemicals which are either slowly or not metabolized by aquatic organisms and have K_{OW}s greater than a 1000. For chemical with K_{OW}s less than a 1000, a slightly different relationship is applicable for organic chemicals because the portion of the chemical in the organism that is not associated with lipid becomes significant relative to the associated with the lipid. Appendix C contains a complete derivation of this relationship.

Equation 15 implicitly assumes that n-octanol is an appropriate surrogate for lipids in aquatic organisms. If n-octanol is not an appropriate surrogate for lipids, the slope and intercept of equation 14 will not be 1.0 and 0.0, respectively. The theoretical basis and the experimental data presented by Mackay (1982) suggest that n-octanol is a very reasonable surrogate for lipids.

Equation 15 is also supported by and consistent with the food-chain model of Gobas (1993). For the Gobas model, the BCF_R^{fd} is equal to K_{OW} when the growth rate of the organisms and metabolism rate of the chemical by the organisms are set equal to zero. It should be noted that the model does not use the partitioning process described by Mackay (1982) for bioconcentration. Instead the food-chain model predicts the k_1 and k_2 rate constants for the fishes and the bioconcentration factor is determined by dividing the uptake rate constant from water (k_1) by the elimination rate constant to water (k_2).

The above equation is also supported by and consistent with the equilibrium partitioning theory being developed by EPA for the derivation of sediment quality criteria (Di Toro et al. 1991). Both the sediment organic carbon-water equilibrium partition coefficient (µg of chemical/Kg of organic carbon in the sediment)/(µg of freely dissolved chemical/L of sediment pore water) (K_{soc} or K_{oc}) and the lipid/water equilibrium partition coefficient (µg of chemical/Kg of lipid)/(µg of freely dissolved chemical/L of sediment pore water) (K_L) have been demonstrated to be approximately equal to K_{OW} for organic chemicals in sediments and benthic organisms, respectively.

D. Food-Chain Biomagnification

The importance of uptake of chemicals through the diet and the potential for a stepwise increase in bioaccumulation from one trophic level to the next in natural systems has been recognized for many years (Hamelink et al. 1971). This pathway, involving transfer of a chemical in food through successive trophic levels, is called biomagnification. Many researchers have noted that the BAFs of some chemicals in nature exceed the bioconcentration factors measured in the laboratory or estimated by log K_{OW} models (e.g., Oliver and Niimi 1983, Oliver and Niimi 1988, Niimi 1985, Swackhammer and Hites 1988). Chemicals exhibiting this phenomenon are typically highly lipophilic, have low water solubilities, and are resistant to being metabolized by aquatic organisms (Metcalf et al. 1975).

1. Food-Chain Multiplier

FCMs for organic chemicals were determined using the model of Gobas (1993). This model includes both benthic and pelagic food chains thereby incorporating exposures of organisms to chemicals from both the sediment and the water column. With the model of Gobas (1993), disequilibrium between the concentrations of the chemicals in sediment and the water column are included in the predicted BAFs and the FCM derived from the predicted BAFs. The disequilibrium is accounted for by inputting the concentrations of the chemical in the sediment and water column to the model. Subsequently, the disequilibrium is incorporated into the pelagic and benthic food web pathways because the model predicts the chemical residues in benthic invertebrates by using equilibrium partitioning and in zooplankton by assuming that the BCF for zooplankton is equal to the K_{OW} of chemical after correction for lipid content. Chemical residues for all other organisms (e.g., fishes) are determined from the rates of (1) chemical uptake from food and water, (2) depuration and excretion of the chemical, (3) dilution due to growth of the organism, and (4) metabolism. This model requires the specification of the food chain structure, feeding preferences, temperature of the ecosystem, organic carbon content of the sediments, organism weights and lipid contents, and the rate of metabolism of the chemical. Because rates of metabolism for bioaccumulative chemicals are not known, the rate of metabolism used in determining the FCMs was zero (i.e., no metabolism).

The model of Gobas (1993) does not predict FCMs but rather it predicts the BAF for each species in the food chain. FCMs can be calculated from the predicted BAFs using the following equation:

$$FCM = \frac{BAF_{R}^{fd}}{K_{OW}} \tag{16}$$

where: K_{OW} = octanol-water partition coefficient.

BAF_{R}^{fd} = BAF reported on a lipid-normalized basis using the freely dissolved concentration of the chemical in water.

a. Data for the Model

The data of Oliver and Niimi (1988) and Flint (1986) for Lake Ontario were used for the feeding preferences, weights, and lipid contents for each species in the food chain (Table 1). The mean water temperature of Lake Ontario was set to 8°C and the organic carbon content of sediment was set to 2.7% as reported by Oliver and Niimi (1988) (Table 1). Values for the densities of the lipid and organic carbon were taken from Gobas (1993) (Table 1). The metabolic transformation rate constant was set equal to zero. The organic carbon content of the water column was set to 0.0 kg/L (see b. Calculation of the FCMs).

With the values specified in Table 1, the remaining data needed for the model of Gobas (1993) are the concentrations of the chemical in the sediment and water column, and the K_{OW} of the chemical. The K_{OW} of the chemical is used as the independent variable in deriving the FCMs and thus only the two chemical concentrations need to be defined for the model.

To determine the relationship between the total concentration of the chemical in the sediment and the freely dissolved concentration of the chemical in the water column, the following sediment-water column chemical concentration quotient (A_{soc}) was calculated for each chemical reported by Oliver and Niimi (1988):

$$\frac{\text{f total chemical/Kg of organic carbon (in}}{\text{reely dissolved chemical/L of water (in wa}}$$

The freely dissolved concentrations of the chemicals in the water column were calculated from the data of Oliver and Niimi (1988) using the equations of Gschwend and Wu (1985) and Cook et al. (1993). These equations are:

$$_{fd} \; ' \; \frac{1}{1 \; \% \; (DOC)(K_{doc}) \; \% \; (POC)(K_{poc}} \qquad \textbf{(17)}$$

$$C_w^{fd} \; ' \; C_w^{t} \; @ \; f_{fd} \qquad \textbf{(18)}$$

where: f_{fd} = fraction of the chemical which is freely dissolved in the water;
DOC = concentration of dissolved organic carbon;
K_{doc} = partition coefficient for the chemical between the DOC and the freely dissolved phase in the water;
POC = concentration of particulate organic carbon;
K_{poc} = partition coefficient for the chemical between the POC phase and the freely dissolved phase in the water;
C_w^{fd} = freely dissolved concentration of the chemical in the water;
C_w^{t} = total concentration of the chemical in the water.

The concentrations in the water reported by Oliver and Niimi (1988) were obtained by liquid-liquid extraction of aliquots of Lake Ontario water which had passed through a continuous-flow centrifuge to remove POC. Therefore, the concentrations in the water reported by Oliver and Niimi (1988) include both the freely dissolved chemical and the chemical associated with the DOC in the water sample. The above equations were used to derive the freely dissolved concentrations of the chemicals in the water by setting the POC = 0.0 mg/L, DOC = 2 mg/L, and $K_{doc} = K_{OW}/10$. K_{OW}s used to derive the freely dissolved concentrations are listed in Appendix B of this document. The relationship for determining K_{doc} from K_{OW} was developed from the results reported by Yin and Hassett

(1986, 1989), Eadie et al. (1990, 1992), Landrum et al. (1984), and Herbert et al. (1993) for partitioning to DOC.

In Figure 1, the ratios of A_{socw} to K_{OW} are plotted against the log K_{OW} for each chemical reported by Oliver and Niimi (1988). Visual inspection of Figure 1 suggest that the ratio of A_{socw} to K_{OW} is not strongly dependent upon the K_{OW}. Correlation coefficients of the ratio (of A_{socw} to K_{OW}) against log K_{OW} of 0.02, -0.34, and -0.55 were obtained for the pesticides, PCB congeners, and the group of chemicals consisting of the chlorinated benzenes, toluenes, and butadienes, respectively. The average (standard deviation & number of values) ratios for the A_{socw} to K_{OW} for pesticides, PCB congeners, pesticides and PCBs combined, and the group of chemicals consisting of the chlorinated benzenes, toluenes, and butadienes were 11.8 (8.4 & 9), 25.9 (26.8 & 46), 23.6 (25.3 & 55), and 294 (1188 & 12), respectively.

Based upon the independence of the ratios of A_{socw} to K_{OW} on K_{OW} for the pesticides and PCBs (the chemicals of primary concern in the derivation of food chain multipliers), a value of 25 was selected for this ratio, the average of the pesticides and PCBs combined. The resulting relationship between the concentration of the chemical in the sediment on an organic carbon basis (C_{soc}) and the freely dissolved concentration of the chemical in the water column (C_w^{fd}) is:

$$C_{soc} = 25 \cdot K_{OW} \cdot C_w^{fd} \qquad \textbf{(19)}$$

b. Calculation of the FCMs

The model of Gobas (1993) (MS-DOS version) was used to determine the FCMs. A listing of the source code in FORTRAN is provided in Appendix J for the food web model of Gobas (1993).

The model was run using the data listed in Table 1 with the above relationship (equation 19) between the C_{soc} and C_w^{fd} for K_{OW}s 3.5, 3.6, 3.7, 3.8, ..., and 9.0. The freely dissolved concentration of the chemical in the water was set to 1 ng/L and the concentration of the chemical in the sediment was calculated using the above sediment-water concentration relationship. The model of Gobas (1993) does not include solubility controls or limitations, and thus, the concentration of the chemical in the water used with the model is arbitrary for determining the BAFs (i.e., the BAF obtained using a 1 ng/L concentration of the chemical will be equal to that obtained using a 150 µg/L concentration of the chemical for a specified K_{OW}).

In using the model of Gobas (1993), we have not used his method for accounting for bioavailability. In section B of chapter III in this document, the procedure for determining the freely dissolved concentration of the chemical in the ambient water is presented. To not use or override the method of Gobas for accounting for bioavailability, we have set the concentration of the DOC in the model to an extremely small number, 1.0e-30 L/L. The model of Gobas (1993) takes the inputted total concentration of the chemical in the water and before doing any predictions, corrects for bioavailability by calculating the freely dissolved concentration of the chemical in the water. The freely dissolved concentration of the chemical in the water is then used *in all subsequent calculations by the model*. By setting the concentration of the DOC to 1.0e-30 L/L, the total concentration of the chemical inputted to the model becomes equal to the freely dissolved concentration of the chemical in the water because the correction for bioavailability using the bioavailability method of Gobas is extremely small.

For each value of K_{OW} inputted to the model, BAF_R^{fd}s are reported by the model for each organism in the food web. Using equation 16, FCMs were calculated for each organism using the reported BAF_R^{fd}s. Listed in Table 3 are the FCMs for trophic level 2 (zooplankton), trophic level 3 (forage fish), and trophic level 4 (piscivorous fish). The FCMs for the forage fish, trophic level 3, were determined by taking the geometric mean of the FCMs for sculpin and alewife. The FCMs for the smelt were not used in determining the mean FCMs for the forage fish because the diet of this organism includes small sculpin. This diet causes smelt to be at a trophic level slightly higher than 3 but less than trophic level 4. In contrast, the diets of the sculpin and alewife were solely trophic level 2 organisms (i.e., zooplankton and *Diporeia sp*).

c. Application of FCMs

In the absence of a field-measured BAF or a predicted BAF derived from the BSAF methodology, a FCM shall be used to calculate the baseline BAF for trophic levels 3 and 4 from a laboratory-measured or predicted BCF. For an organic chemical, the FCM used shall be derived from Table 3 using the chemical's log K_{OW} and linear interpolation. A FCM greater than 1.0 applies to most organic chemicals with a log K_{OW} of four or more. The trophic level used shall take into account the age or size of the fish species consumed by the human, avian or mammalian predator because, for some species of fish, the young are in trophic level 3 whereas the adults are in trophic level 4.

The FCMs were developed assuming no metabolism of the chemical by any of the organisms in the food web. Thus, for chemicals where metabolism is significant, the predicted BAFs will be larger than a field-measured BAF or BAF determined using the BSAF methodology. BAFs predicted using laboratory-measured BCFs (i.e., the product of the FCM and the laboratory-measured BCF), might be in closer agreement with the field derived BAFs than the BAFs predicted using predicted BCFs because laboratory-measured BCFs might include some metabolism in their determination. In general, for highly persistent chemicals, the effects of all metabolic processes can not be easily included in the BCF determination.

The FCMs were determined using a disequilibrium factor of 25 from K_{OW} (equation 16) between the concentrations of the chemical in the sediment on an organic carbon normalized basis and the freely dissolved concentration of the chemical in water column. This disequilibrium is incorporated into the pelagic and benthic food web pathways in the model of Gobas (1993) and is subsequently reflected in the BAFs predicted by the model and the resulting FCMs.

d. Evaluation of FCMs

Baseline BAFs were predicted using the model of Gobas (1993) for each chemical reported by Oliver and Niimi (1988). The predicted BAFs are equal to the product of the K_{OW} and the FCM determined for that organism. Baseline BAFs also were derived from the data of Oliver and Niimi (1988) by dividing the lipid-normalized concentration of the chemical in the fish by the freely dissolved concentration of the chemical in the water column. The freely dissolved concentration of the chemical in the water was determined as described above. These results are summarized in Tables 3 through 8 and Figures 2 through 7.

Measured chemical residues in fishes assigned to trophic level 3 can be higher than those in trophic level 4 from the same food chain. Potential causes of the higher concentrations (on a lipid basis) in the trophic level 3 fish include (1) growth rates which are much slower than the predator fishes, and (2) differing rates of depuration and elimination of the chemical by the predator fishes.

The average differences between the predicted and measured log BAFs were -0.61, 0.01, -0.17, -0.04, -0.10, and -0.12 for zooplankton, sculpin, alewives, small smelt, large smelt, and piscivorous fish, respectively.

Table 1. Environmental Parameters and Species Characteristics Used with the Model of Gobas (1993) for Deriving the Food Chain Multipliers

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Environmental parameters:

Mean water temperature: 8EC
Organic carbon content of the sediment: 2.7%
Organic carbon content of the water column: 1.0e-30 kg/L
Density of lipids: 0.9 kg/L
Density of organic carbon: 0.9 kg/L
Metabolic transformation rate constant: 0.0 day^{1}

Species characteristics:

Phytoplankton
Lipid content: 0.5%

Zooplankton: Mysids (*Mysis relicta*)
Lipid content: 5.0%

Diporeia sp.
Lipid content: 3.0%

Sculpin (*Cottus cognatus*)
Lipid content: 8.0%
Weight: 5.4 g
Diet: 18% zooplankton, 82% *Diporeia* sp.

Alewives (*Alosa pseudoharengus*)
Lipid content: 7.0%
Weight: 32 g
Diet: 60% zooplankton, 40% *Diporeia* sp.

Smelt (*Osmerus mordax*)
Lipid content: 4.0%
Weight: 16 g
Diet: 54% zooplankton, 21% *Diporeia* sp., 25% sculpin

Salmonids (*Salvelinus namaycush, Oncorhynchus mykiss, Oncorhynchus velinus namaycush*)
Lipid content: 11.0%
Weight: 2410 g
Diet: 10% sculpin, 50% alewives, 40% smelt

Table 2. Food-Chain Multipliers for Trophic Levels 2, 3 & 4.

Log K_{OW}	Trophic Level 2	Trophic[a] Level 3	Trophic Level 4
2.0	1.000	1.005	1.000
2.5	1.000	1.010	1.002
3.0	1.000	1.028	1.007
3.1	1.000	1.034	1.007
3.2	1.000	1.042	1.009
3.3	1.000	1.053	1.012
3.4	1.000	1.067	1.014
3.5	1.000	1.083	1.019
3.6	1.000	1.103	1.023
3.7	1.000	1.128	1.033
3.8	1.000	1.161	1.042
3.9	1.000	1.202	1.054
4.0	1.000	1.253	1.072
4.1	1.000	1.315	1.096
4.2	1.000	1.380	1.130
4.3	1.000	1.491	1.178
4.4	1.000	1.614	1.242
4.5	1.000	1.766	1.334
4.6	1.000	1.950	1.459
4.7	1.000	2.175	1.633
4.8	1.000	2.452	1.871
4.9	1.000	2.780	2.193
5.0	1.000	3.181	2.612
5.1	1.000	3.643	3.162
5.2	1.000	4.188	3.873
5.3	1.000	4.803	4.742
5.4	1.000	5.502	5.821
5.5	1.000	6.266	7.079
5.6	1.000	7.096	8.551
5.7	1.000	7.962	10.209
5.8	1.000	8.841	12.050
5.9	1.000	9.716	13.964
6.0	1.000	10.556	15.996
6.1	1.000	11.337	17.783
6.2	1.000	12.064	19.907
6.3	1.000	12.691	21.677
6.4	1.000	13.228	23.281

6.5	1.000	13.662	24.604

Table 2. Continued.

Log K_{OW}	Trophic Level 2	Trophic Level 3	Trophic Level 4
6.6	1.000	13.980	25.645
6.7	1.000	14.223	26.363
6.8	1.000	14.355	26.669
6.9	1.000	14.388	26.669
7.0	1.000	14.305	26.242
7.1	1.000	14.142	25.468
7.2	1.000	13.852	24.322
7.3	1.000	13.474	22.856
7.4	1.000	12.987	21.038
7.5	1.000	12.517	18.967
7.6	1.000	11.708	16.749
7.7	1.000	10.914	14.388
7.8	1.000	10.069	12.050
7.9	1.000	9.162	9.840
8.0	1.000	8.222	7.798
8.1	1.000	7.278	6.012
8.2	1.000	6.361	4.519
8.3	1.000	5.489	3.311
8.4	1.000	4.683	2.371
8.5	1.000	3.949	1.663
8.6	1.000	3.296	1.146
8.7	1.000	2.732	0.778
8.8	1.000	2.246	0.521
8.9	1.000	1.837	0.345
9.0	1.000	1.493	0.226

[a] The FCMs for trophic level 3 are the geometric mean of the FCMs for sculpin and alewife.

Table 3. Measured and Predicted BAFs for Zooplankton. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water (i.e., (µg of chemical/Kg of lipid)/(µg of freely dissolved chemical/L of water)).

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
1	ppDDT	6.45	6.45	6.95
2	ppDDE	6.76	6.76	7.66
3	ppDDD	6.06	6.06	6.34
4	mirex	6.89	6.89	7.12
5	photomirex	6.89	6.89	7.35
6	g-chlordane	6.00	6.00	5.93
7	alpha-BHC	3.78	3.78	4.90
8	gamma-BHC	3.67	3.67	5.08
9	HCBD	4.84	4.84	5.05
10	OCS	6.29	6.29	6.73
11	HCB	5.60	5.60	5.76
12	QCB	5.11	5.11	6.38
13	1,2,3,5-TeCB	4.65	4.65	5.35
14	1,2,4,5-TeCB	4.56	4.56	5.14
15	1,2,3,4-TeCB	4.59	4.59	5.33
16	1,3,5-TCB	4.17	4.17	4.71
17	1,2,4-TCB	3.99	3.99	4.90
18	1,2,3-TCB	4.10	4.10	4.07
19	2,4,5-TCT	4.93	4.93	
20	2,3,6-TCT	4.93	4.93	5.71
21	PCT	6.36	6.36	
31	8	5.07	5.07	
32	6	5.06	5.06	
33	5	4.97	4.97	
34	12	5.22	5.22	
35	13	5.29	5.29	
36	28+31	5.67	5.67	6.48
37	18	5.24	5.24	5.69
38	22	5.58	5.58	6.21
39	26	5.66	5.66	
40	16	5.16	5.16	
41	33	5.60	5.60	5.79
42	17	5.25	5.25	5.69
43	25	5.67	5.67	
44	24+27	5.40	5.40	
45	32	5.44	5.44	

46	66		6.20	6.20	7.11

Table 3. Continued.

	Chemical[a]	LogK_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
47	70+76	6.17	6.17	7.06
48	56+60+81	6.19	6.19	7.47
49	52	5.84	5.84	6.10
50	47+48	5.82	5.82	5.97
51	44	5.75	5.75	6.27
52	74	6.20	6.20	7.02
53	49	5.85	5.85	6.34
54	64	5.95	5.95	6.96
55	42	5.76	5.76	7.01
56	53	5.62	5.62	
57	40	5.66	5.66	
58	41+71	5.84	5.84	
59	46	5.53	5.53	
60	45	5.53	5.53	
61	101	6.38	6.38	6.61
62	84	6.04	6.04	7.53
63	118	6.74	6.74	7.37
64	110	6.48	6.48	7.11
65	87+97	6.29	6.29	7.38
66	105	6.65	6.65	7.36
67	95	6.13	6.13	6.14
68	85	6.30	6.30	7.12
69	92	6.35	6.35	
70	82	6.20	6.20	7.50
71	91	6.13	6.13	6.33
72	99	6.39	6.39	6.51
73	153	6.92	6.92	7.50
74	138	6.83	6.83	7.43
75	149	6.67	6.67	7.31
76	146	6.89	6.89	7.93
77	141	6.82	6.82	7.46
78	128	6.74	6.74	
79	151	6.64	6.64	6.62
80	132	6.58	6.58	7.08
81	156	7.18	7.18	
82	136	6.22	6.22	6.34
83	129	6.73	6.73	

84	180		7.36	7.36	7.66

Table 3. Continued.

	Chemical[a]	LogK_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
85	187+182	7.19	7.19	7.60
86	170+190	7.37	7.37	8.20
87	183	7.20	7.20	8.16
88	177	7.08	7.08	8.07
89	174	7.11	7.11	7.88
90	178	7.14	7.14	
91	171	7.11	7.11	
92	185	7.11	7.11	
93	173	7.02	7.02	
94	203+196	7.65	7.65	8.26
95	201	7.62	7.62	
96	194	7.80	7.80	7.69
97	195	7.56	7.56	
98	198	7.62	7.62	
99	205	8.00	8.00	
100	206	8.09	8.09	
101	207	7.74	7.74	
102	209	8.18	8.18	
	Average difference		-0.61	
	Standard deviation		0.39	
	Number of values		61	

[a] Chemical abbreviations taken from Oliver and Niimi(1988).

[b] Predicted BAFs were obtained by taking the product of the FCM and K_{OW} for each chemical. Because the FCM is set to 1.0 for zooplankton, the predicted log BAF equals log K_{OW}.

[c] Field-measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms (µg of chemical/Kg of lipid) by the freely dissolved concentration of thechemical in water (µg of freely dissolved chemical/L of water).

Table 4. Measured and Predicted BAFs for Sculpin. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water (i.e., (µg of chemical/Kg of lipid)/(µg of freely dissolved chemical/L of water)).

	Chemical[a]	Predicted[b] Log K_{OW}	Measured[c] Log BAF	Log BAF
1	ppDDT	6.45	7.67	7.47
2	ppDDE	6.76	8.01	7.83
3	ppDDD	6.06	7.18	6.89
4	mirex	6.89	8.14	7.77
5	photomirex	6.89	8.14	7.69
6	g-chlordane	6.00	7.10	7.12
7	alpha-BHC	3.78	3.83	4.69
8	gamma-BHC	3.67	3.72	5.05
9	HCBD	4.84	5.29	5.55
10	OCS	6.29	7.48	7.77
11	HCB	5.60	6.51	6.53
12	QCB	5.11	5.71	5.67
13	1,2,3,5-TeCB	4.65	5.00	
14	1,2,4,5-TeCB	4.56	4.85	
15	1,2,3,4-TeCB	4.59	4.90	4.91
16	1,3,5-TCB	4.17	4.31	
17	1,2,4-TCB	3.99	4.08	4.57
18	1,2,3-TCB	4.10	4.20	
19	2,4,5-TCT	4.93	5.43	
20	2,3,6-TCT	4.93	5.43	
21	PCT	6.36	7.56	6.41
31	8	5.07	5.67	
32	6	5.06	5.66	
33	5	4.97	5.51	
34	12	5.22	5.89	
35	13	5.29	6.02	
36	28+31	5.67	6.63	6.37
37	18	5.24	5.91	5.97
38	22	5.58	6.49	
39	26	5.66	6.62	
40	16	5.16	5.83	
41	33	5.60	6.51	
42	17	5.25	5.98	
43	25	5.67	6.63	
44	24+27	5.40	6.19	

45	32		5.44	6.23

Table 4. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
46	66	6.20	7.36	7.45
47	70+76	6.17	7.33	7.06
48	56+60+81	6.19	7.35	7.48
47	70+76	6.17	7.33	7.06
48	56+60+81	6.19	7.35	7.48
49	52	5.84	6.86	6.80
50	47+48	5.82	6.84	6.15
51	44	5.75	6.77	6.65
52	74	6.20	7.36	7.30
53	49	5.85	6.91	6.77
54	64	5.95	7.05	7.16
55	42	5.76	6.78	7.07
56	53	5.62	6.53	
57	40	5.66	6.62	
58	41+71	5.84	6.86	
59	46	5.53	6.38	
60	45	5.53	6.38	
61	101	6.38	7.59	7.30
62	84	6.04	7.14	8.05
63	118	6.74	7.99	7.86
64	110	6.48	7.71	7.44
65	87+97	6.29	7.48	7.54
66	105	6.65	7.90	7.82
67	95	6.13	7.26	6.98
68	85	6.30	7.49	7.50
69	92	6.35	7.56	7.70
70	82	6.20	7.36	7.60
71	91	6.13	7.26	6.44
72	99	6.39	7.60	
73	153	6.92	8.17	8.05
74	138	6.83	8.08	8.06
75	149	6.67	7.92	7.28
76	146	6.89	8.14	8.49
77	141	6.82	8.07	8.11
78	128	6.74	7.99	
79	151	6.64	7.88	8.34
80	132	6.58	7.82	7.41

81	156		7.18	8.42

Table 4. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
82	136	6.22	7.38	7.13
83	129	6.73	7.98	
84	180	7.36	8.57	8.45
85	187+182	7.19	8.43	8.07
86	170+190	7.37	8.58	9.15
87	183	7.20	8.44	8.81
88	177	7.08	8.33	8.63
89	174	7.11	8.36	8.24
90	178	7.14	8.39	
91	171	7.11	8.36	
92	185	7.11	8.36	
93	173	7.02	8.27	
94	203+196	7.65	8.78	9.14
95	201	7.62	8.78	
96	194	7.80	8.90	8.52
97	195	7.56	8.72	
98	198	7.62	8.78	
99	205	8.00	9.01	
100	206	8.09	9.04	
101	207	7.74	8.87	
102	209	8.18	9.08	
	Average difference		0.01	
	Standard deviation		0.42	
	Number of values		54	

[a] Chemical abbreviations taken from Oliver and Niimi (1988).

[b] Predicted BAFs were obtained by taking the product of the FCM and K_{OW} for each chemical.

[c] Field-measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms (µg of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water (µg of freely dissolved chemical/L of water).

Table 5. Measured and Predicted BAFs for Alewives. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water (i.e., (µg of chemical/Kg of lipid)/(µg of freely dissolved chemical/L of water)).

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
1	ppDDT	6.45	7.49	7.61
2	ppDDE	6.76	7.82	7.86
3	ppDDD	6.06	7.02	6.78
4	mirex	6.89	7.95	7.72
5	photomirex	6.89	7.95	7.63
6	g-chlordane	6.00	6.95	6.68
7	alpha-BHC	3.78	3.82	4.82
8	gamma-BHC	3.67	3.71	5.00
9	HCBD	4.84	5.22	
10	OCS	6.29	7.31	7.77
11	HCB	5.60	6.39	6.31
12	QCB	5.11	5.63	
13	1,2,3,5-TeCB	4.65	4.94	
14	1,2,4,5-TeCB	4.56	4.81	
15	1,2,3,4-TeCB	4.59	4.85	
16	1,3,5-TCB	4.17	4.29	
17	1,2,4-TCB	3.99	4.06	
18	1,2,3-TCB	4.10	4.18	
19	2,4,5-TCT	4.93	5.36	
20	2,3,6-TCT	4.93	5.36	
21	PCT	6.36	7.39	6.53
31	8	5.07	5.59	
32	6	5.06	5.58	
33	5	4.97	5.43	
34	12	5.22	5.80	
35	13	5.29	5.92	
36	28+31	5.67	6.51	6.68
37	18	5.24	5.82	6.39
38	22	5.58	6.37	
39	26	5.66	6.50	
40	16	5.16	5.74	
41	33	5.60	6.39	
42	17	5.25	5.88	
43	25	5.67	6.51	
44	24+27	5.40	6.09	

45	32	5.44	6.13

Table 5. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
46	66	6.20	7.20	7.57
47	70+76	6.17	7.17	7.31
48	56+60+81	6.19	7.19	7.79
49	52	5.84	6.72	6.84
50	47+48	5.82	6.70	6.85
51	44	5.75	6.63	6.86
52	74	6.20	7.20	7.35
53	49	5.85	6.76	6.98
54	64	5.95	6.90	7.30
55	42	5.76	6.64	7.38
56	53	5.62	6.41	
57	40	5.66	6.50	
58	41+71	5.84	6.72	
59	46	5.53	6.27	
60	45	5.53	6.27	
61	101	6.38	7.41	7.25
62	84	6.04	6.99	7.90
63	118	6.74	7.80	7.71
64	110	6.48	7.53	7.51
65	87+97	6.29	7.31	7.89
66	105	6.65	7.71	7.72
67	95	6.13	7.10	7.14
68	85	6.30	7.32	7.67
69	92	6.35	7.38	7.93
70	82	6.20	7.20	7.86
71	91	6.13	7.10	6.74
72	99	6.39	7.42	7.37
73	153	6.92	7.98	7.82
74	138	6.83	7.89	7.89
75	149	6.67	7.73	7.75
76	146	6.89	7.95	8.30
77	141	6.82	7.88	7.96
78	128	6.74	7.80	
79	151	6.64	7.69	8.17
80	132	6.58	7.63	7.45
81	156	7.18	8.23	
82	136	6.22	7.22	7.25

83	129	6.73	7.79

Table 5. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
84	180	7.36	8.38	8.15
85	187+182	7.19	8.24	7.99
86	170+190	7.37	8.39	8.84
87	183	7.20	8.25	8.46
88	177	7.08	8.13	8.54
89	174	7.11	8.16	8.51
90	178	7.14	8.19	
91	171	7.11	8.16	
92	185	7.11	8.16	
93	173	7.02	8.08	
94	203+196	7.65	8.59	8.82
95	201	7.62	8.59	
96	194	7.80	8.71	8.22
97	195	7.56	8.53	
98	198	7.62	8.59	
99	205	8.00	8.82	
100	206	8.09	8.86	
101	207	7.74	8.68	
102	209	8.18	8.89	
	Average difference		-0.17	
	Standard deviation		0.40	
	Number of values		51	

[a] Chemical abbreviations taken from Oliver and Niimi (1988).

[b] Predicted BAFs were obtained by taking the product of the FCM and K_{OW} for each chemical.

[c] Field-measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms (µg of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water (µg of freely dissolved chemical/L of water).

Table 6. Measured and Predicted BAFs for Small Smelt. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water (i.e., (µg of chemical/Kg of lipid)/(µg of freely dissolved chemical/L of water)).

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
1	ppDDT	6.45	7.49	7.43
2	ppDDE	6.76	7.82	8.11
3	ppDDD	6.06	7.02	6.80
4	mirex	6.89	7.95	7.73
5	photomirex	6.89	7.95	7.75
6	g-chlordane	6.00	6.95	6.44
7	alpha-BHC	3.78	3.82	4.56
8	gamma-BHC	3.67	3.71	4.77
9	HCBD	4.84	5.22	
10	OCS	6.29	7.31	7.61
11	HCB	5.60	6.39	6.14
12	QCB	5.11	5.63	
13	1,2,3,5-TeCB	4.65	4.94	
14	1,2,4,5-TeCB	4.56	4.81	
15	1,2,3,4-TeCB	4.59	4.85	
16	1,3,5-TCB	4.17	4.29	
17	1,2,4-TCB	3.99	4.06	
18	1,2,3-TCB	4.10	4.18	
19	2,4,5-TCT	4.93	5.36	
20	2,3,6-TCT	4.93	5.36	
21	PCT	6.36	7.39	
31	8	5.07	5.59	
32	6	5.06	5.58	
33	5	4.97	5.43	
34	12	5.22	5.80	
35	13	5.29	5.92	
36	28+31	5.67	6.51	6.57
37	18	5.24	5.82	
38	22	5.58	6.37	
39	26	5.66	6.50	
40	16	5.16	5.74	
41	33	5.60	6.39	
42	17	5.25	5.88	
43	25	5.67	6.51	
44	24+27	5.40	6.09	

45	32		5.44	6.13

Table 6. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
46	66	6.20	7.20	7.46
47	70+76	6.17	7.17	7.32
48	56+60+81	6.19	7.19	7.73
49	52	5.84	6.72	6.54
50	47+48	5.82	6.70	6.73
51	44	5.75	6.63	6.40
52	74	6.20	7.20	7.31
53	49	5.85	6.76	6.46
54	64	5.95	6.90	7.14
55	42	5.76	6.64	7.18
56	53	5.62	6.41	
57	40	5.66	6.50	
58	41+71	5.84	6.72	
59	46	5.53	6.27	
60	45	5.53	6.27	
61	101	6.38	7.41	7.05
62	84	6.04	6.99	7.90
63	118	6.74	7.80	7.76
64	110	6.48	7.53	7.41
65	87+97	6.29	7.31	7.79
66	105	6.65	7.71	7.71
67	95	6.13	7.10	6.83
68	85	6.30	7.32	7.41
69	92	6.35	7.38	7.17
70	82	6.20	7.20	7.77
71	91	6.13	7.10	6.40
72	99	6.39	7.42	6.43
73	153	6.92	7.98	7.93
74	138	6.83	7.89	7.87
75	149	6.67	7.73	7.63
76	146	6.89	7.95	8.30
77	141	6.82	7.88	7.84
78	128	6.74	7.80	
79	151	6.64	7.69	7.74
80	132	6.58	7.63	7.06
81	156	7.18	8.23	
82	136	6.22	7.22	

83	129		6.73	7.79

Table 6. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
84	180	7.36	8.38	8.18
85	187+182	7.19	8.24	8.01
86	170+190	7.37	8.39	8.86
87	183	7.20	8.25	8.59
88	177	7.08	8.13	8.54
89	174	7.11	8.16	8.31
90	178	7.14	8.19	
91	171	7.11	8.16	
92	185	7.11	8.16	
93	173	7.02	8.08	
94	203+196	7.65	8.59	8.79
95	201	7.62	8.59	
96	194	7.80	8.71	8.24
97	195	7.56	8.53	
98	198	7.62	8.59	
99	205	8.00	8.82	
100	206	8.09	8.86	
101	207	7.74	8.68	
102	209	8.18	8.89	
	Average difference		-0.04	
	Standard deviation		0.40	
	Number of values		48	

[a] Chemical abbreviations taken from Oliver and Niimi (1988).

[b] FCMs for alewives were used for the small smelt. Predicted BAFs were obtained by taking the product of the FCM and K_{OW} for each chemical.

[c] Field-measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms (µg of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water (µg of freely dissolved chemical/L of water).

Table 7. Measured and Predicted BAFs for Large Smelt. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water (i.e., (µg of chemical/Kg of lipid)/(µg of freely dissolved chemical/L of water)).

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
1	ppDDT	6.45	7.85	7.93
2	ppDDE	6.76	8.23	8.27
3	ppDDD	6.06	7.26	6.84
4	mirex	6.89	8.37	8.04
5	photomirex	6.89	8.37	7.97
6	g-chlordane	6.00	7.17	6.50
7	alpha-BHC	3.78	3.80	4.71
8	gamma-BHC	3.67	3.69	4.82
9	HCBD	4.84	5.13	
10	OCS	6.29	7.62	7.85
11	HCB	5.60	6.45	6.40
12	QCB	5.11	5.55	5.87
13	1,2,3,5-TeCB	4.65	4.85	
14	1,2,4,5-TeCB	4.56	4.72	
15	1,2,3,4-TeCB	4.59	4.77	
16	1,3,5-TCB	4.17	4.24	
17	1,2,4-TCB	3.99	4.03	
18	1,2,3-TCB	4.10	4.15	
19	2,4,5-TCT	4.93	5.26	
20	2,3,6-TCT	4.93	5.26	
21	PCT	6.36	7.72	
31	8	5.07	5.52	
32	6	5.06	5.51	
33	5	4.97	5.35	
34	12	5.22	5.74	
35	13	5.29	5.88	
36	28+31	5.67	6.60	6.92
37	18	5.24	5.76	
38	22	5.58	6.43	
39	26	5.66	6.59	
40	16	5.16	5.68	
41	33	5.60	6.45	
42	17	5.25	5.84	
43	25	5.67	6.60	
44	24+27	5.40	6.07	

45	32	5.44	6.11

Table 7. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
46	66	6.20	7.49	7.88
47	70+76	6.17	7.46	7.71
48	56+60+81	6.19	7.48	8.12
49	52	5.84	6.86	6.91
50	47+48	5.82	6.84	7.22
51	44	5.75	6.77	6.92
52	74	6.20	7.49	7.66
53	49	5.85	6.94	7.03
54	64	5.95	7.11	7.54
55	42	5.76	6.78	7.63
56	53	5.62	6.47	
57	40	5.66	6.59	
58	41+71	5.84	6.86	
59	46	5.53	6.29	
60	45	5.53	6.29	
61	101	6.38	7.76	7.35
62	84	6.04	7.20	8.29
63	118	6.74	8.20	8.13
64	110	6.48	7.89	7.81
65	87+97	6.29	7.63	8.06
66	105	6.65	8.11	8.11
67	95	6.13	7.36	7.17
68	85	6.30	7.64	7.85
69	92	6.35	7.73	7.80
70	82	6.20	7.49	8.14
71	91	6.13	7.36	6.90
72	99	6.39	7.77	7.40
73	153	6.92	8.40	8.24
74	138	6.83	8.31	8.22
75	149	6.67	8.13	7.99
76	146	6.89	8.37	8.66
77	141	6.82	8.30	8.17
78	128	6.74	8.20	
79	151	6.64	8.08	8.28
80	132	6.58	8.02	7.67
81	156	7.18	8.65	
82	136	6.22	7.51	

83	129	6.73	8.19

Table 7. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
84	180	7.36	8.79	8.45
85	187+182	7.19	8.66	8.34
86	170+190	7.37	8.80	9.02
87	183	7.20	8.67	8.85
88	177	7.08	8.56	8.78
89	174	7.11	8.59	8.71
90	178	7.14	8.62	
91	171	7.11	8.59	
92	185	7.11	8.59	
93	173	7.02	8.50	
94	203+196	7.65	8.96	9.13
95	201	7.62	8.98	
96	194	7.80	9.06	8.50
97	195	7.56	8.92	
98	198	7.62	8.98	
99	205	8.00	9.12	
100	206	8.09	9.13	
101	207	7.74	9.05	
102	209	8.18	9.13	
	Average difference		-0.10	
	Standard deviation		0.41	
	Number of values		49	

[a] Chemical abbreviations taken from Oliver and Niimi (1988).

[b] Predicted BAFs were obtained by taking the product of the FCM and K_{OW} for each chemical.

[c] Field-measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms (µg of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water (µg of freely dissolved chemical/L of water).

Table 8. Measured and Predicted BAFs for Piscivorous Fish. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water (i.e., (µg of chemical/Kg of lipid)/(µg of freely dissolved chemical/L of water)).

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
1	ppDDT	6.45	7.83	7.78
2	ppDDE	6.76	8.19	8.35
3	ppDDD	6.06	7.29	7.00
4	mirex	6.89	8.32	8.13
5	photomirex	6.89	8.32	8.07
6	g-chlordane	6.00	7.20	6.79
7	alpha-BHC	3.78	3.79	4.69
8	gamma-BHC	3.67	3.68	4.93
9	HCBD	4.84	5.14	
10	OCS	6.29	7.62	8.07
11	HCB	5.60	6.53	6.40
12	QCB	5.11	5.61	5.81
13	1,2,3,5-TeCB	4.65	4.85	
14	1,2,4,5-TeCB	4.56	4.70	
15	1,2,3,4-TeCB	4.59	4.75	5.07
16	1,3,5-TCB	4.17	4.22	
17	1,2,4-TCB	3.99	4.01	
18	1,2,3-TCB	4.10	4.13	
19	2,4,5-TCT	4.93	5.30	
20	2,3,6-TCT	4.93	5.30	
21	PCT	6.36	7.71	
31	8	5.07	5.58	
32	6	5.06	5.57	
33	5	4.97	5.38	
34	12	5.22	5.81	
35	13	5.29	5.96	
36	28+31	5.67	6.68	6.89
37	18	5.24	5.83	5.75
38	22	5.58	6.51	6.39
39	26	5.66	6.67	
40	16	5.16	5.75	5.92
41	33	5.60	6.53	5.32
42	17	5.25	5.92	5.52
43	25	5.67	6.68	
44	24+27	5.40	6.16	

Table 8. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
45	32	5.44	6.20	6.76
46	66	6.20	7.50	7.79
47	70+76	6.17	7.47	7.56
48	56+60+81	6.19	7.49	7.96
49	52	5.84	6.92	7.01
50	47+48	5.82	6.90	7.18
51	44	5.75	6.83	6.96
52	74	6.20	7.50	7.66
53	49	5.85	7.00	7.13
54	64	5.95	7.15	7.51
55	42	5.76	6.84	7.49
56	53	5.62	6.55	6.51
57	40	5.66	6.67	6.55
58	41+71	5.84	6.92	
59	46	5.53	6.38	
60	45	5.53	6.38	
61	101	6.38	7.75	7.45
62	84	6.04	7.24	8.28
63	118	6.74	8.16	8.15
64	110	6.48	7.87	7.79
65	87+97	6.29	7.63	8.08
66	105	6.65	8.07	8.13
67	95	6.13	7.38	7.25
68	85	6.30	7.64	7.89
69	92	6.35	7.72	8.11
70	82	6.20	7.50	8.13
71	91	6.13	7.38	6.92
72	99	6.39	7.76	7.39
73	153	6.92	8.35	8.32
74	138	6.83	8.26	8.30
75	149	6.67	8.09	7.99
76	146	6.89	8.32	8.73
77	141	6.82	8.25	8.32
78	128	6.74	8.16	
79	151	6.64	8.05	8.51
80	132	6.58	7.99	7.56
81	156	7.18	8.57	

82	136		6.22	7.52	7.37

Table 8. Continued.

	Chemical[a]	Log K_{OW}	Predicted[b] Log BAF	Measured[c] Log BAF
83	129	6.73	8.15	
84	180	7.36	8.68	8.58
85	187+182	7.19	8.58	8.43
86	170+190	7.37	8.69	9.20
87	183	7.20	8.59	9.03
88	177	7.08	8.49	9.01
89	174	7.11	8.52	8.74
90	178	7.14	8.55	
91	171	7.11	8.52	
92	185	7.11	8.52	
93	173	7.02	8.44	
94	203+196	7.65	8.81	9.26
95	201	7.62	8.84	
96	194	7.80	8.88	8.56
97	195	7.56	8.78	
98	198	7.62	8.84	
99	205	8.00	8.89	
100	206	8.09	8.87	
101	207	7.74	8.90	
102	209	8.18	8.83	
	Average difference		-0.12	
	Standard deviation		0.40	
	Number of values		59	

[a] Chemical abbreviations taken from Oliver and Niimi (1988).

[b] Predicted BAFs were obtained by taking the product of the FCM and K_{OW} for each chemical.

[c] Field-measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms (µg of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water (µg of freely dissolved chemical/L of water).

E. Prediction of BAFs from Biota-Sediment Accumulation Factor (BSAF) Measurements

BSAFs may be used for measuring and predicting bioaccumulation directly from concentrations of chemicals in surface sediment. They may also be used to estimate BAF_{ℓ}^{fd}s (Cook et al., 1993; 1995). Since BSAFs are based on field data and incorporate effects of metabolism, biomagnification, growth, etc., BAF_{ℓ}^{fd}s estimated from BSAFs will incorporate the net effect of all these factors. The BSAF approach is particularly beneficial for developing water quality criteria for chemicals such as polychlorinated dibenzo-p-dioxins, dibenzofurans and certain biphenyl congeners which are difficult to measure in water and have reduced bioaccumulation potential due to metabolism. The calculation of BAF_{ℓ}^{fd} from BSAFs also provides a method for validation of all measured or predicted BAF_{ℓ}^{fd}s for organic chemicals.

1. Biota-Sediment Accumulation Factors BSAFs

BSAFs are measured by relating lipid-normalized concentrations of chemicals in an organism to organic carbon-normalized concentrations of the chemicals in surface sediment samples associated with the average exposure environment of the organism. The BSAF equation is:

$$BSAF = \frac{C_{\ell}}{C_{soc}} \qquad (20)$$

where: C_{ℓ} = lipid-normalized concentration of the chemical in tissues of the biota (μg/g lipid).
C_{soc} = organic carbon-normalized concentration of the chemical in the surface sediment (μg/g sediment organic carbon).

Since BSAFs are rarely measured for ecosystems which are at equilibrium, the BSAF inherently includes a measure of the disequilibrium of the ecosystem. This disequilibrium can be assessed for chemicals with log $K_{OW} > 3$ with the following relationship:

$$BSAF \approx \frac{C_b^{fd} \cdot K_{\ell}}{C_s^{fd} \cdot K_{soc}} = D_{bs} \cdot \frac{K_{\ell}}{K_{soc}} \approx D_{bs} \cdot 2 \qquad (21)$$

where: C_b^{fd} = concentration of freely dissolved chemical (associated with water) in the tissues of biota (μg/g wet tissue).
C_s^{fd} = concentration of freely dissolved chemical (associated with pore water) in the sediment (μg/g sediment organic carbon).
K_{ℓ} = lipid-water equilibrium partition coefficient = C_{ℓ}/C_b^{fd}.

K_{soc} = the sediment organic carbon-water equilibrium partition coefficient = C_{soc}/C_s^{fd}.

D_{bs} = the disequilibrium (fugacity) ratio between biota and sediment (C_b^{fd}/C_s^{fd}).

Measured BSAFs may range widely for different chemicals depending on K_R, K_{soc}, and the actual ratio of C_b^{fd} to C_s^{fd}. At equilibrium, which rarely exists between sediment and pelagic organisms such as fish, the BSAF would be expected to equal the ratio of K_R/K_{soc} which is thought to range from 1-4. When chemical equilibrium between sediment and biota does not exist, the BSAF will equal the disequilibrium (fugacity) ratio between biota and sediment ($D_{bs} = C_b^{fd}/C_s^{fd}$) times the ratio of the equilibrium partition coefficients (approximately 2).

The deviation of D_{bs} from the equilibrium value of 1.0 is determined by the net effect of all factors which contribute to the disequilibrium between sediment and aquatic organisms. $D_{bs} > 1$ can occur due to biomagnification or when surface sediment has not reached steady-state with water. $D_{bs} < 1$ can occur as a result of kinetic limitations for chemical transfer from sediment to water or water to food chain, and biological processes, such as growth or biotransformation of the chemical in the animal and its food chain. BSAFs are most useful when measured under steady-state conditions or pseudo-steady-state conditions in which chemical concentrations in water are linked to slowly changing concentrations in sediment. BSAFs measured for systems with new chemical loadings or rapid increases in loading may be unreliable due to underestimation of steady-state C_{soc}s.

2. Relationship of BAFs to BSAFs

Differences between BSAFs for different organic chemicals are good measures of the relative bioaccumulation potentials of the chemicals. When calculated from a common organism/sediment sample set, chemical-specific differences in BSAFs reflect primarily the net effect of biomagnification, metabolism, and bioenergetic and bioavailability factors on each chemical's D_{bs}. Ratios of BSAFs of PCDDs and PCDFs to a BSAF for TCDD (bioaccumulation equivalency factors, BEFs) have been proposed in the GLWQI for evaluation of TCDD toxic equivalency associated with complex mixtures of these chemicals (see 58 FR 20802). The same approach is applicable to calculation of BAFs for other organic chemicals. The approach requires data for a steady-state or near steady-state condition between sediment and water for both a reference chemical (r) with a field-measured BAF_R^{fd} and other chemicals (n=i) for which BAF_R^{fd}s are to be determined. BAF_R^{fd} for a chemical "i" is defined as:

$$(BAF_R^{fd})_i = \frac{(C_R)_i}{(C_w^{fd})_i} \qquad (22)$$

where: C_R = lipid-normalized concentration of the chemical in tissues of the biota (Fg/g lipid).

C_w^{fd} = concentration of freely dissolved chemical in water (Fg/FL water).

Substitution of C_R from equation 20 into C_R of equation 22 for the chemical i gives:

$$(BAF_R^{fd})_i \; ' \; (BSAF)_i \; @ \; \frac{(C_{soc})_i}{(C_w^{fd})_i} \tag{23}$$

In order to avoid confusion with the equilibrium partition coefficients K_{soc}, K_{poc} or K_{doc}, the chemical concentration quotient between sediment organic carbon and a freely dissolved state in overlying water is symbolized by A_{soc}:

$$(A_{soc})_i \; ' \; \frac{(C_{soc})_i}{(C_w^{fd})_i} \tag{24}$$

Thus the ratio of BAF_R^{fd} for chemical i and a reference chemical r is:

$$\frac{(BAF_R^{fd})_i}{(BAF_R^{fd})_r} \; , \; \frac{(BSAF)_i (A_{soc})_i}{(BSAF)_r (A_{soc})_r} \tag{25}$$

If both chemicals have similar fugacity ratios between water and sediment, as is the case for many chemicals in the open waters of the Great Lakes:

$$\frac{(A_{soc})_i}{(A_{soc})_r} \; , \; \frac{(K_{OW})_i}{(K_{OW})_r} \tag{26}$$

therefore:

$$(BAF_R^{fd})_i \; ' \; (BAF_R^{fd})_r \cdot \frac{(BSAF)_i (K_{OW})_i}{(BSAF)_r (K_{OW})_r} \tag{27}$$

The assumption of equal or similar fugacity ratios between water and sediment for each chemical is equivalent to assuming that for all chemicals used in BAF_R^{fd} calculations: (1) the concentration ratios between sediment and suspended solids in the water and (2) the degree of equilibrium between suspended solids and C_w^{fd} are the same. Thus, errors could be introduced by inclusion of chemicals with non-steady-state external loading rates or chemicals with strongly reduced C_w^{fd} due to rapid volatilization from the water. Note that

BAF$_R^{fd}$s calculated from BSAFs will incorporate any errors associated with measurement of the BAF$_R^{fd}$ for the reference chemical and the K$_{OW}$s for both the reference and unknown chemicals. Such errors can be minimized by comparing results from several reference chemicals, including those with similar K$_{OW}$s to those of the unknown chemicals, and by assuring consistent use of C_W^{fd} values which are adjusted for dissolved organic carbon binding effects on the fraction of each chemical that is freely dissolved (f_{fd}) in unfiltered, filtered or centrifuged water samples. BAF$_R$s based on total chemical concentration in water (BAF$_R^t$) can be calculated on the basis of f_{fd} for the dissolved and particulate organic carbon concentrations in the water (POC and DOC):

$$BAF_R^t = BAF_R^{fd} \cdot f_{fd} \qquad \textbf{(28)}$$

where:

$$= \frac{1}{1 + DOC \cdot K_{doc} + POC \cdot K_{poc}} \cdot \frac{1}{1 + \frac{DOC \cdot K_{OW}}{10} + POC} \qquad \textbf{(29)}$$

Further information on calculation of concentrations of freely dissolved chemicals in water may be found in section III.B of this document titled "Bioavailability".

3. Calculation of BAF$_R^{fd}$s from Lake Ontario Data

Two data sets are available to EPA for calculating BAF$_R^{fd}$s from BSAFs for fish in Lake Ontario. The Oliver and Niimi (1988) data set, which has been used extensively for construction of food chain models of bioaccumulation and calculation of FCMs, biomagnification factors and BAF$_R^{fd}$s from chemical concentrations determined in organisms and water, also contains surface sediment data which allows calculation of lakewide average BSAFs. The second data set is provided by an extensive sampling of fish and sediments in 1987 for EPA's Lake Ontario TCDD Bioaccumulation Study (U.S. EPA, 1990) for the purpose of determining BSAFs. These samples were later analyzed for PCDD, PCDF, PCB congeners and some organochlorine pesticides at ERL-Duluth. Although these data should be submitted for publication within this year, they are needed here to provide a unique data set for checking BAF$_R^{fd}$s calculated from Oliver and Niimi data from samples collected between 1981-1984 and calculating BAF$_R^{fd}$s for organic chemicals not measured by Oliver and Niimi.

BAF$_R^{fd}$s for salmonids were calculated for this demonstration of the BSAF ratio method using PCB congeners 52, 105 and 118 and DDT as reference chemicals. Several reference chemicals were used in order to examine the variability introduced by choice of reference chemical. The water analyses of Oliver and Niimi (1988) were adjusted for an estimated 2 mg/L residual dissolved organic carbon concentration in the centrifuged water (assumed no residual POC) and an estimated $K_{doc} = K_{OW}/10$ in order to calculate C_W^{fd} from f_{fd} (equation 30). Log K$_{OW}$s for PCBs are those reported by Hawker and Connell (1988).

Log K_{OW}s for PCDDs and PCDFs are those estimated by Burkhard and Kuehl (1986) except for the penta, hexa, and hepta chlorinated dibenzofurans which were estimated on the basis of assumed similarity to the trends reported for the PCDDs by Burkhard and Kuehl (1986). Log K_{OW}s for other chemicals are either as cited in the Appendix B of this document or noted in Table 9. Table 9 contains the measured and predicted log BAF_R^{fd}s from the two data sets.

4. Validity of BAF_R^{fd}s Calculated from BSAFs

Figures 8, 9, and 10 show the relationship of log BAF_R^{fd}s to log K_{OW}s for (1) Oliver and Niimi (1988) BAF_R^{fd}s determined from measured concentrations of freely dissolved chemicals in Lake Ontario water in 1984; (2) BAF_R^{fd}s calculated from BSAFs derived from Oliver and Niimi data; and (3) BAF_R^{fd}s calculated from EPA BSAFs for lake trout in Lake Ontario in 1987 (Cook et al., 1995). The diagonal lines represent a 1:1 ratio of log BAF to log K_{OW}. The PCB congener BAF_R^{fd}s in all three sets of data appear quite similar. The EPA BAF_R^{fd}s predictions (figure 3) include a number of chemicals not in the Oliver and Niimi data set. These are the PCDDs, PCDFs, chlordanes, nonachlors and dieldrin. Only the dieldrin BAF_R^{fd} has been measured elsewhere. The BAF_R^{fd}s for five of six chlordanes and nonachlors are much greater than those for PCBs with the same estimated log K_{OW}. Therefore, the log K_{OW} values chosen here for the chlordanes and nonachlors may be significantly underestimated. The bioaccumulative PCDDs and PCDFs (2,3,7,8-chlorinated), as expected due to metabolism in fish, have BAF_R^{fd}s 10-1000 fold less than PCBs with similar K_{OW}s. Thus, the BSAF method for measuring BAF_R^{fd}s appears to work well for Lake Ontario.

Accuracy of the BSAF method can be best judged on the basis of comparison of the BAF_R^{fd}s calculated from BSAFs to field-measured BAF_R^{fd}s. Figure 11 illustrates the agreement between log BAF_R^{fd}s calculated from the Oliver and Niimi water data and those calculated from the sediment data. The BAF_R^{fd}s for chlorinated benzenes and toluenes may tend to be underestimated with BSAFs because the water-sediment fugacity gradient is altered in comparison to PCBs in response to rapid volatilization losses from water. Use of EPA BSAFs measured from a different set of fish and sediment samples collected several years after the Oliver and Niimi samples gives BAF_R^{fd}s that correlate equally well with the BAF_R^{fd}s calculated from Oliver and Niimi data (figure 12).

All of the above correlations were based on the BSAF method using the Oliver and Niimi measured Lake Ontario salmonid BAF_R^{fd} for PCB congener 52 as the reference. Very similar correlations result for comparisons of data in Table 9 for PCB congeners 105, 118 or DDT as reference chemicals. The BSAF method is strengthened through use of several reference chemicals with a range of K_{OW}s and greatest likelihood for accuracy in measurements of concentrations in water. The two data sets and four reference chemicals resulted in either four or eight determinations of BAF_R^{fd} for each chemical listed in Table 9. Mean log BAF_R^{fd}s (geometric means of BAF_R^{fd}s) for the 4-8 determinations from Lake

Ontario data are reported in Table 10. The BAF_{R}^{fd} for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) at 7.85×10^6 compares well to 3.03×10^6 estimated by a different method for TCDD log $K_{OW} = 7$ by Cook et al. (1993). The small difference in the two estimates may be attributable to an underestimate of the sediment-disequilibrium between sediment and water by Cook et al. (1993) that resulted in an overestimate of C_{w}^{fd}.

The greatest test for robustness of the BSAF method for predicting BAF_{R}^{fd}s that are applicable throughout the Great Lakes would be a comparison of two totally independent data sets based on different ecosystems and conditions. Such a comparison can be made for bioaccumulation of PCBs in Lake Ontario fish and Green Bay fish. The EPA Green Bay/Fox River Mass Balance Study involved extensive sampling of water, sediment and fish in 1989. Green Bay is a shallower, smaller, and more eutrophic body of water than Lake Ontario. Measurement of bioaccumulation in Green Bay is complicated by the movement and interaction of biota through gradients of decreasing PCBs, nutrients and suspended organic carbon which extend from the Fox River to the outer bay and Lake Michigan. Table 9 contains brown trout BAF_{R}^{fd}s calculated from PCB BSAFs measured in the mid-bay region using PCB congeners 52 and 118 as reference chemicals. The reference chemical BAF_{R}^{fd}s were determined with water and brown trout data from the same region. Concentrations of freely dissolved PCBs were calculated, as for Lake Ontario, on the basis of dissolved organic carbon in the water samples and an assumed $K_{doc} = K_{OW}/10$. Despite the complex exposures of Green Bay fish, figures 13 and 14 illustrate log BAF_{R}^{fd} - log K_{OW} relationships found in Green Bay which are similar to those from the Oliver and Niimi and EPA Lake Ontario data sets. The correlations between the PCB BAF_{R}^{fd}s for Green Bay brown trout and BAF_{R}^{fd}s based on Oliver-Niimi salmonid and water measurements and EPA lake trout BSAFs are shown in figures 15-18 for reference chemicals PCB 52 and PCB 118, respectively. Good agreement exists between Green Bay brown trout predictions and Lake Ontario measured and BSAF-predicted BAF_{R}^{fd}s for both reference chemicals.

The means of log BAF_{R}^{fd}s calculated for each chemical from two sets of BSAFs and four reference chemicals for 124 chemicals measured in Lake Ontario trout (Table 10) are plotted against log K_{OW} in figure 19. Only 59 of these chemicals have field-measured BAF_{R}^{fd}s. Correlations between the mean Lake Ontario trout and Green Bay brown trout BAF_{R}^{fd}s (figures 20 and 21) indicate that the Green Bay brown trout may be slightly larger. This may be a sample set artifact associated with the complex Green Bay fish-water-sediment relationships in Green Bay rather than an actual site/species/food chain-specific difference in bioaccumulation. The agreement of the Green Bay and Lake Ontario results demonstrates the general applicability of BAF_{R}^{fd}s calculated from BSAFs in predicting bioaccumulation in Great Lakes fish from estimated C_{w}^{fd}s.

5. How to Apply the BSAF Method for Predicting BAF_{R}^{fd}s

If high quality data are not available for calculating BAF_{R}^{fd}s for organic chemicals that are expected to bioaccumulate, the mean BAF_R^{fd}s reported in Table 10 may be used. To apply the method for additional chemicals, site-specific determinations, or biota from different trophic levels than salmonids, the following steps and data requirements must be completed:

a. Reliable BAF_R^{fd}s which have been measured for several reference chemicals in biota in the ecosystem must be chosen. The water sample analyses should approximate the average exposure of the organism and its food chain over a time period that is most appropriate for the chemical, organism and ecosystem. Each C_w^{fd} used to calculate a BAF_R^{fd} should be based on a consistent adjustment of the concentration of total chemical in water for DOC and POC using equation 30. It is preferable to choose at least some reference chemicals on the basis of log K_{OW} and chemical class similarity with the test chemicals.

b. Measured (slow-stir method or equivalent preferred) or estimated Log K_{OW} values are chosen for each chemical.

c. Obtain chemical residue and % lipid data for representative samples of the tissues of the organisms. Migration patterns, food chain movement and hydrodynamic factors should be considered. For highly bioaccumulative chemicals variation of chemical residues in adult fish in the open waters of the Great Lakes within an annual cycle is usually slight.

d. Obtain chemical concentrations and % organic carbon data for surface sediment samples. Sediment sampling sites should be selected to allow prediction of ratios of freely dissolved chemical concentrations in the overlying water of the ecosystem region of interest. A 1 cm layer of surface sediment is ideal but 3 cm samples will work if sedimentation rates are large and periodic scouring events are not likely. Although desirable, sediment samples do not have to represent the average surface sediment condition in the area of the ecosystem affecting the exposure of the organisms for which bioaccumulation is to measured. Since this is a ratio method, the concentrations of each chemical in sediment need only be predictive of the ratios of concentrations of the chemicals in the ecosystem water.

e. With the data from steps 3 and 4, calculate BSAFs for chemicals of interest and reference chemicals (equation 21).

f. With BSAFs and K_{OW}s for each chemical, plus BAF_R^{fd}s for reference chemicals, calculate BAF_R^{fd}s using equation 27.

g. Use the BAF_R^{fd}s to predict chemical residues in fish and other biota or to establish unsafe concentrations of chemicals in water only on the basis of chemical concentration expressions for water and organisms that are consistent with the BAF_R^{fd}

definition and measurement.

6. Summary

BAF_R^{fd}s calculated from two different BSAF data sets for Lake Ontario salmonids are similar and agree well with field-measured BAF_R^{fd}s of Oliver and Niimi (1988). The BSAF method allows calculation of BAF_R^{fd}s for chemicals which have not been measured in Great Lakes water but are detectable in fish tissues and sediments. BAF_R^{fd}s can also be calculated for other fish species and biota at lower trophic levels in the food web. BAF_R^{fd}s calculated for PCBs in Green Bay brown trout agree well with the Lake Ontario salmonid/lake trout values despite differences in ecosystem, food chain and exposure conditions. Mean log BAF_R^{fd}s (geometric mean of BAF_R^{fd}s) from 4-8 determinations from Lake Ontario data are summarized in Table 10.

Table 9. Great Lakes Trout BAF$^{d}_{RR}$s Calculated from Measured BSAFs/BAFs.

Chemical	log K_{ow}	BSAF Ol.&Niimi[a] measured	log BAF Ol.&Niimi[a] measured	BSAF EPA[b] measured	log BAF Ol.&Niimi[a] ref PCB 52	log BAF EPA[b] ref PCB 52	log BAF Ol.&Niimi[a] ref PCB 105	log BAF EPA[b] ref PCB 105
dieldrin	5.3			6.65		7.67		6.95
ddt	6.45	1.09	7.78	1.67	7.87	8.22	7.54	7.50
dde	6.76	4.14	8.35	7.7	8.76	9.19	8.43	8.47
ddd	6.06	0.28	7.00		6.90		6.56	
mirex	6.89	1.43	8.13	1.31	8.43	8.55	8.09	7.84
photomirex	6.89	5.48	8.07		9.01		8.68	
g-chlordane	6.0	2.22	6.79		7.73		7.40	
t-chlordane	6.0			2.00		7.85		7.13
c-chlordane	6.0			4.77		8.23		7.51
t-nonachlor	6.0			10.5		8.57		7.85
c-nonachlor	6.0			0.51		7.25		6.54
alpha-hch	3.78	2.45	4.69		5.55		5.22	
gamma-hch	3.67	0.69	4.93		4.89		4.56	
hcbd	4.84							
ocs	6.29	0.98	8.07		7.67		7.33	
hcb	5.6	0.09	6.40		5.95		5.62	
pcb	5.11	0.04	5.81		5.07		4.73	
1235tcb	4.56							
1245tcb	4.56							
1234tcb	4.59	0.01	5.07		4.11		3.78	
135tcb	4.17							
124tcb	3.99							
123tcb	4.1							
245tct	4.93							
236tct	4.93							
pct	6.36							
total-PCB	6.14	1.85	7.81		7.79		7.46	
PCBs								
5	4.97							
6	5.06			0.36		6.16		5.44
8	5.07							

12	5.22			0.44		6.41		5.69
13	5.29							
16	5.16		5.92					
17	5.25	0.15	5.52	0.99	5.80	6.79	5.47	6.07

Table 9. Great Lakes Trout $\text{BAF}^{d}_{\mathbb{R}}$s Calculated from Measured BSAFs/BAFs.

Chemical	log K_{ow}	BSAF Ol.&Niimi[a] measured	log BAF Ol.&Niimi[a] measured	BSAF EPA[b] measured	log BAF Ol.&Niimi[a] ref PCB 52	log BAF EPA[b] ref PCB 52	log BAF Ol.&Niimi[a] ref PCB 105	log BAF EPA[b] ref PCB 105
18	5.24	0.26	5.75	0.1	6.05	5.79	5.71	5.07
22	5.58	0.21	6.39	0.27	6.28	6.56	5.95	5.84
25	5.67	0.25		0.33	6.44	6.74	6.11	6.02
26	5.66	1.72		0.44	7.28	6.85	6.94	6.13
32	5.44	0.18	6.76		6.09		5.75	
33	5.60	0.15	5.32	0.49	6.15	6.84	5.82	6.12
40	5.66	0.10	6.55	0.18	6.06	6.46	5.72	5.74
42	5.76	0.52	7.49		6.86		6.53	
44	5.75	0.48	6.96	0.4	6.82	6.90	6.48	6.18
45	5.53			0.22		6.42		5.70
46	5.53	0.57		0.02	6.67	5.38	6.34	4.66
49	5.85	0.69	7.13		7.07		6.74	
52	5.84	0.61	7.01	0.42	7.01	7.01	6.67	6.29
53	5.62	1.84	6.51		7.27		6.93	
63	6.17			0.82		7.63		6.91
64	5.95	0.73	7.51		7.20		6.86	
66	6.20	0.85	7.79		7.52		7.18	
74	6.20	3.45	7.66	0.61	8.12	7.53	7.79	6.81
77	6.36			0.29		7.37		6.65
81	6.36			0.67		7.73		7.01
82	6.20	2.45	8.13	0.18	7.97	7.00	7.64	6.28
83	6.26			1.33		7.93		7.21
84	6.04	3.04	8.28		7.91		7.57	
85	6.30	1.45	7.89	1.29	7.85	7.96	7.51	7.24
87	6.29			1.37		7.97		7.25
91	6.13	1.25	6.92	0.64	7.61	7.48	7.28	6.76
92	6.35	1.43	8.11		7.89		7.55	
95	6.13	1.40	7.25		7.66		7.33	
97	6.29			0.28		7.28		6.56
99	6.39	0.68	7.39	1.51	7.61	8.12	7.27	7.40
100	6.23			1.78		8.03		7.31
101	6.38	2.45	7.45	1.06	8.15	7.95	7.82	7.23

105	6.65	2.70	8.13	4.49	8.47	8.85	8.13	8.13
110	6.48	1.53	7.79	0.82	8.05	7.94	7.71	7.22
118	6.74	4.09	8.15	1.72	8.74	8.52	8.40	7.80
119	6.58			3.83		8.71		7.99

Table 9. Great Lakes Trout BAF$^{d}_{R}$s Calculated from Measured BSAFs/BAFs.

Chemical	log K_{ow}	BSAF Ol.&Niimi[a] measured	log BAF Ol.&Niimi[a] measured	BSAF EPA[b] measured	log BAF Ol.&Niimi[a] ref PCB 52	log BAF EPA[b] ref PCB 52	log BAF Ol.&Niimi[a] ref PCB 105	log BAF EPA[b] ref PCB 105
126	6.89			3.21		8.94		8.22
128	6.74	3.61		2.78	8.68	8.73	8.35	8.01
129	6.73	1.75		1.13	8.36	8.33	8.02	7.61
130	6.8			2.15		8.68		7.96
132	6.58	0.87	7.56		7.90		7.57	
PCB 136	6.22	10.87	7.37		8.64		8.30	
138	6.83	4.25	8.30		8.84		8.51	
141	6.82	2.75	8.32	1.74	8.64	8.61	8.31	7.89
146	6.89	3.22	8.73	1.25	8.78	8.53	8.45	7.81
149	6.67	2.33	7.99	0.93	8.42	8.19	8.09	7.47
151	6.64	3.38	8.51	1.65	8.55	8.40	8.22	7.69
153	6.92	4.22	8.32	1.91	8.93	8.75	8.59	8.03
156	7.18	3.97			9.16		8.83	
158	7.02			1.52		8.75		8.03
167	7.27			0.69		8.66		7.94
171	7.11	2.71			8.93		8.59	
172	7.33			1.36		9.01		8.29
174	7.11	1.54	8.74	1.25	8.68	8.75	8.35	8.03
177	7.08	3.53	9.01	1.91	9.01	8.91	8.68	8.19
178	7.14	4.48		2.76	9.18	9.13	8.84	8.41
180	7.36	3.78	8.58	3.26	9.32	9.42	8.99	8.70
183	7.20	5.62	9.03	2.68	9.33	9.17	9.00	8.46
185	7.11	1.55		2.24	8.68	9.01	8.35	8.29
189	7.71			0.71		9.11		8.39
194	7.80	1.53	8.56	2.47	9.37	9.74	9.03	9.02
195	7.56	1.90			9.22		8.89	
197	7.3			1.1		8.89		8.17
198	7.62			6.55		9.98		9.26
201	7.62	1.53		1.13	9.19	9.22	8.85	8.50
205	8.00	0.34		0.48	8.91	9.23	8.58	8.51
206	8.09	0.47		0.34	9.15	9.17	8.81	8.45
207	7.74	0.66		0.89	8.95	9.24	8.61	8.52

209	8.18	0.14		0.03	8.70	8.20	8.36	7.48
24+27	5.40	0.25		0.12	6.17	6.02	5.83	5.30
28+31	5.67	0.52	6.89	0.19	6.77	6.50	6.43	5.78
37+42	5.8			0.62		7.14		6.42

Table 9. Great Lakes Trout BAF^{d}_{R}s Calculated from Measured BSAFs/BAFs

Chemical	log K_{ow}	BSAF Ol.&Niimi[a] measured	log BAF Ol.&Niimi[a] measured	BSAF EPA[b] measured	log BAF Ol.&Niimi[a] ref PCB 52	log BAF EPA[b] ref PCB 52	log BAF Ol.&Niimi[a] ref PCB 105	log BAF EPA[b] ref PCB 105
47+48	5.82	1.23	7.18	0.65	7.29	7.17	6.95	6.46
41+64+71	5.87			0.46		7.08		6.36
56+60	6.11			0.31		7.15		6.43
70+76	6.17	1.49	7.56	0.61	7.72	7.50	7.39	6.78
66+95	6.17			0.53		7.44		6.72
56+60+81	6.19	0.55	7.96		7.32		6.98	
84+92	6.2			1.22		7.83		7.11
87+97	6.29	2.45	8.08		8.06		7.73	
PCB 137+176	6.8			1.16		8.41		7.69
138+163	6.91			2.23		8.81		8.09
156+171+202	7.18			1.25		8.82		8.10
182+187	7.19	3.80	8.43		9.15		8.81	
157+200	7.23			1.56		8.97		8.25
170+190	7.37	2.06	9.20	4.17	9.06	9.53	8.73	8.81
195+208	7.64			0.72		9.04		8.33
196+203	7.65	1.56	9.26	1.12	9.23	9.25	8.89	8.53
2378-TCDD	7.02			0.059		7.34		6.62
12378-PeCDD	7.5			0.054		7.78		7.06
123478-HxCDD	7.8			0.018		7.60		6.88
123678-HxCDD	7.8			0.0073		7.21		6.49
123789-HxCDD	7.8			0.0081		7.26		6.54
1234678-HpCDD	8.2			0.0031		7.24		6.52
OCDD	8.6			0.00074		7.02		6.30
2378-TCDF	6.5			0.047		6.72		6.00
12378-PeCDF	7.0			0.013		6.66		5.94
23478-PeCDF	7.0			0.095		7.52		6.81
123478-HxCDF	7.5			0.0045		6.70		5.98
123678-HxCDF	7.5			0.011		7.09		6.37
123789-HxCDF	7.5			0.037		7.61		6.90

234678-HxCDF	7.5	0.04	7.65	6.93
1234678-HpCDD	8.0	0.00065	6.36	5.64
1234789-HpCDD	8.0	0.023	7.91	7.19
OCDF	8.8	0.00099	7.34	6.62

Table 9. Great Lakes Trout BAF$^{d}_{RR}$s Calculated from Measured BSAFs/BAFs

Chemical	log K_{ow}	log BAF Ol.&Niimi[a] ref DDT	log BAF EPA[b] ref DDT	log BAF Ol.&Niimi[a] ref PCB 118	log BAF EPA[b] ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB 118
dieldrin	5.3		7.23		7.30			
ddt	6.45	7.78	7.78	7.29	7.85			
dde	6.76	8.67	8.75	8.18	8.82			
ddd	6.06	6.80		6.31				
mirex	6.89	8.33	8.11	7.84	8.18			
photomirex	6.89	8.92		8.43				
g-chlordane	6	7.64		7.14				
t-chlordane	6		7.41		7.48			
c-chlordane	6		7.78		7.85			
t-nonachlor	6		8.13		8.20			
c-nonachlor	6		6.81		6.88			
alpha-hch	3.78	5.46		4.97				
gamma-hch	3.67	4.80		4.31				
hcbd	4.84							
ocs	6.29	7.57		7.08				
hcb	5.6	5.86		5.37				
pcb	5.11	4.97		4.48				
1235tcb	4.56							
1245tcb	4.56							
1234tcb	4.59	4.02		3.53				
135tcb	4.17							
124tcb	3.99							
123tcb	4.1							
245tct	4.93							
236tct	4.93							
pct	6.36							
total-PCB	6.14	7.70		7.21				

PCBs								
5	4.97					0.14	4.88	5.12
6	5.06		5.72		5.79	1.7	6.05	6.29
8	5.07					0.14	4.98	5.22
12	5.22		5.97		6.04			
13	5.29							
16	5.16							
17	5.25	5.71	6.35	5.22	6.42	0.75	5.89	6.13

Table 9. Great Lakes Trout BAF$^{d}_{R}$s Calculated from Measured BSAFs/BAFs

Chemical	log K_{ow}	log BAF Ol.&Niimi[a] ref DDT	log BAF EPA[b] ref DDT	log BAF Ol.&Niimi[a] ref PCB 118	log BAF EPA[b] ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB 118
18	5.24	5.95	5.34	5.46	5.41	0.64	5.81	6.05
22	5.58	6.19	6.12	5.70	6.19	0.39	5.94	6.18
25	5.67	6.35	6.29	5.86	6.36	0.73	6.30	6.54
26	5.66	7.18	6.41	6.69	6.48	0.95	6.40	6.64
32	5.44	5.99		5.50				
33	5.60	6.06	6.39	5.57	6.46	0.29	5.83	6.07
40	5.66	5.96	6.02	5.47	6.09	0.69	6.26	6.50
42	5.76	6.77		6.28				
44	5.75	6.72	6.46	6.23	6.53			
45	5.53		5.98		6.05	1.16	6.36	6.60
46	5.53	6.58	4.94	6.09	5.01	0.61	6.08	6.32
49	5.85	6.98		6.49		3.34	7.14	7.38
52	5.84	6.91	6.57	6.42	6.64	4.74	7.28	7.52
53	5.62	7.17		6.68		2.12	6.71	6.95
63	6.17		7.19		7.26	4.37	7.57	7.81
64	5.95	7.10		6.61				
66	6.20	7.42		6.93		3.1	7.46	7.70
74	6.20	8.03	7.09	7.54	7.16	2.46	7.36	7.60
77	6.36		6.93		7.00	4.12	7.74	7.98
81	6.36		7.29		7.36	11.6	8.19	8.43
82	6.20	7.88	6.56	7.39	6.63	4.05	7.57	7.81
83	6.26		7.49		7.56	5.67	7.78	8.02
84	6.04	7.81		7.32		7.2	7.66	7.90
85	6.30	7.75	7.51	7.26	7.59	7.25	7.92	8.16
87	6.29		7.53		7.60	6.13	7.84	8.08
91	6.13	7.52	7.04	7.02	7.11	8.44	7.82	8.06
92	6.35	7.79		7.30				
95	6.13	7.57		7.08				
97	6.29		6.84		6.91	6.42	7.86	8.10
99	6.39	7.51	7.67	7.02	7.74	7.18	8.01	8.25
100	6.23		7.58		7.65	1.71	7.23	7.47
101	6.38	8.06	7.51	7.57	7.58	10.01	8.14	8.38
105	6.65	8.37	8.41	7.88	8.48	5.35	8.14	8.38

110	6.48	7.95	7.50	7.46	7.57	4.15	7.86	8.10
118	6.74	8.64	8.08	8.15	8.15	4.96	8.20	8.44
119	6.58		8.27		8.34	3.03	7.83	8.07

Table 9. Great Lakes Trout BAF$^{d}_{R}$s Calculated from Measured BSAFs/BAFs

Chemical	log K_{ow}	log BAF Ol.&Niimi[a] ref DDT	log BAF EPA[b] ref DDT	log BAF Ol.&Niimi[a] ref PCB 118	log BAF EPA[b] ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB 118
126	6.89		8.50		8.57			
128	6.74	8.59	8.29	8.10	8.36	10.21	8.51	8.75
129	6.73	8.26	7.89	7.77	7.96			
130	6.8		8.24		8.31	11.21	8.61	8.85
132	6.58	7.81		7.32				
136	6.22	8.55		8.05				
138	6.83	8.75		8.26				
141	6.82	8.55	8.16	8.06	8.24	9.30	8.55	8.79
146	6.89	8.69	8.09	8.20	8.16	10.0	8.66	8.90
149	6.67	8.33	7.74	7.84	7.81	8.7	8.37	8.61
151	6.64	8.46	7.96	7.97	8.03	9.7	8.39	8.63
153	6.92	8.84	8.31	8.34	8.38	5.35	8.41	8.65
156	7.18	9.07		8.58				
158	7.02		8.31		8.38			
167	7.27		8.21		8.28	16.0	9.24	9.48
171	7.11	8.83		8.34				
172	7.33		8.57		8.64			
174	7.11	8.59	8.31	8.10	8.38	4.46	8.52	8.76
177	7.08	8.92	8.47	8.43	8.54	8.04	8.75	8.99
178	7.14	9.08	8.69	8.59	8.76			
180	7.36	9.23	8.98	8.74	9.05	10.96	9.16	9.40
183	7.20	9.24	8.73	8.75	8.80	6.5	8.78	9.02
185	7.11	8.59	8.56	8.10	8.63	3.23	8.38	8.62
189	7.71		8.67		8.74	3.45	9.01	9.25
194	7.80	9.27	9.30	8.78	9.37	3.29	9.08	9.32
195	7.56	9.13		8.64				
197	7.3		8.45		8.52			
198	7.62		9.54		9.61	0.46	8.05	8.29
201	7.62	9.10	8.78	8.60	8.85	4.79	9.06	9.30

205	8.00	8.82	8.79	8.33	8.86	3.09	9.25	9.49
206	8.09	9.05	8.73	8.56	8.80	0.95	8.83	9.07
207	7.74	8.85	8.79	8.36	8.86	1.3	8.62	8.86
209	8.18	8.60	7.76	8.11	7.83	0.19	8.22	8.46
24+27	5.40	6.07	5.58	5.58	5.65	1.55	6.35	6.59
28+31	5.67	6.68	6.05	6.18	6.12	0.67	6.26	6.50
37+42	5.8		6.70		6.77	6.75	7.39	7.63

Table 9. Great Lakes Trout BAF$^{d}_{\ell}$s Calculated from Measured BSAFs/BAFs

Chemical	log K_{ow}	log BAF Ol.&Niimi[a] ref DDT	log BAF EPA[b] ref DDT	log BAF Ol.&Niimi[a] ref PCB 118	log BAF EPA[b] ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB 118
47+48	5.82	7.19	6.73	6.70	6.80	7.86	7.47	7.71
41+64+71	5.87		6.64		6.71	2.55	7.04	7.28
56+60	6.11		6.71		6.78	1.14	6.93	7.17
70+76	6.17	7.63	7.05	7.14	7.12	1.2	7.01	7.25
66+95	6.17		7.00		7.07	3.1	7.43	7.67
56+60+81	6.19	7.22		6.73		1.15	7.02	7.26
84+92	6.2		7.39		7.46	7.25	7.82	8.06
87+97	6.29	7.97		7.48		6.3	7.85	8.09
137+176	6.8		7.97		8.04	1.43	7.72	7.96
138+163	6.91		8.36		8.43	11.94	8.75	8.99
156+171+202	7.18		8.38		8.45	10.70	8.97	9.21
182+187	7.19	9.05		8.56		9.38	8.92	9.16
157+200	7.23		8.53		8.60	8.66	8.93	9.17
170+190	7.37	8.97	9.09	8.48	9.16	4.10	8.74	8.98
195+208	7.64		8.60		8.67	1.01	8.41	8.65
196+203	7.65	9.13	8.80	8.64	8.87	4.24	9.04	9.28
2378-TCDD	7.02		6.90		6.97			
12378-PeCDD	7.5		7.34		7.41			
123478-HxCDD	7.8		7.16		7.23			
123678-HxCDD	7.8		6.77		6.84			
123789-HxCDD	7.8		6.81		6.88			
123334678-Hp	8.2		6.80		6.87			

OCDD	8.6	6.57	6.64
2378-TCDF	6.5	6.28	6.35
12378-PeCDF	7.0	6.22	6.29
23478-PeCDF	7.0	7.08	7.15
123478-HxCDF	7.5	6.26	6.33
123678-HxCDF	7.5	6.65	6.72
123789-HxCDF	7.5	7.17	7.24
234678-HxCDF	7.5	7.21	7.28
1234678-HpCD	8.0	5.92	5.99
1234789-HpCD	8.0	7.47	7.54
OCDF	8.8	6.90	6.97

Table 10. Mean BAF_{R}^{fd}s from Lake Ontario BSAFs for Salmonids

Chemical	log K_{OW}	Number BAFs	Mean log BAF_{R}^{fd}	Mean BAF_{R}^{fd}
dieldrin	5.30	4	7.29	1.93e+07
ddt	6.45	8	7.73	5.33e+07
dde	6.76	8	8.66	4.56e+08
ddd	6.06	4	6.64	4.39e+06
mirex	6.89	8	8.17	1.49e+08
photomirex	6.89	4	8.76	5.74e+08
g-chlordane	6.00	4	7.48	3.00e+07
t-chlordane	6.00	4	7.46	2.91e+07
c-chlordane	6.00	4	7.84	6.95e+07
t-nonachlor	6.00	4	8.18	1.53e+08
c-nonachlor	6.00	4	6.87	7.43e+06
alpha-hch	3.78	4	5.30	2.00e+05
gamma-hch	3.67	4	4.64	4.34e+04
hcbd	4.84			
ocs	6.29	4	7.41	2.58e+07
hcb	5.60	4	5.70	5.01e+05
pcb	5.11	4	4.81	6.47e+04
1235tcb	4.56			
1245tcb	4.50			
1234tcb	4.59	4	3.86	7.25e+03
135tcb	4.17			
124tcb	3.99			
123tcb	4.10			
245tct	4.93			
236tct	4.93			
pct	6.36			
PCBs				
5	4.97			
6	5.06	4	5.78	6.02e+05
8	5.07			
12	5.22	4	6.03	1.06e+06
13	5.29			
16	5.16			
17	5.25	8	5.98	9.52e+05
18	5.24	8	5.60	3.96e+05
22	5.58	8	6.10	1.27e+06
25	5.67	8	6.27	1.87e+06

26	5.66	8	6.75	5.57e+06

Table 10. Mean BAF_{ℓ}^{fd}s from Lake Ontario BSAFs for Salmonids (continued)

Chemical	log K_{OW}	Number BAFs	Mean log BAF_{ℓ}^{fd}	Mean log BAF_{ℓ}^{fd}
PCBs				
32	5.44	4	5.84	6.84e+05
33	5.60	8	6.18	1.50e+06
40	5.66	8	5.94	8.72e+05
42	5.76	4	6.61	4.06e+06
44	5.75	8	6.54	3.46e+06
45	5.53	4	6.04	1.09e+06
46	5.53	8	5.71	5.08e+05
49	5.85	4	6.82	6.61e+06
52	5.84	8	6.69	4.90e+06
53	5.62	4	7.02	1.04e+07
63	6.17	4	7.25	1.77e+07
64	5.95	4	6.94	8.80e+06
66	6.20	4	7.26	1.83e+07
74	6.20	8	7.51	3.23e+07
77	6.36	4	6.99	9.68e+06
81	6.36	4	7.35	2.24e+07
82	6.20	8	7.17	1.48e+07
83	6.26	4	7.55	3.53e+07
84	6.04	4	7.65	4.50e+07
85	6.30	8	7.58	3.83e+07
87	6.29	4	7.59	3.89e+07
91	6.13	8	7.23	1.69e+07
92	6.35	4	7.64	4.32e+07
95	6.13	4	7.41	2.55e+07
97	6.29	4	6.90	7.95e+06
99	6.39	8	7.54	3.49e+07
100	6.23	4	7.64	4.40e+07
101	6.38	8	7.73	5.43e+07
105	6.65	8	8.34	2.18e+08
110	6.48	8	7.68	4.74e+07
118	6.74	8	8.31	2.04e+08
119	6.58	4	8.33	2.12e+08
126	6.89	4	8.56	3.63e+08
128	6.74	8	8.39	2.44e+08
129	6.73	8	8.03	1.06e+07
130	6.80	4	8.30	1.98e+08

132	6.58	4	7.65	4.47e+07

Table 10. Mean BAF^{d}_{R}s from Lake Ontario BSAFs for Salmonids (continued)

Chemical	log K_{ow}	Number BAFs	Mean log BAF^{d}_{R}	Mean BAF^{d}_{R}
PCBs				
136	6.22	4	8.39	2.44e+08
138	6.83	4	8.59	3.88e+08
141	6.82	8	8.31	2.03e+08
146	6.89	8	8.34	2.18e+08
149	6.67	8	7.98	9.66e+07
151	6.64	8	8.16	1.45e+08
153	6.92	8	8.52	3.31e+08
156	7.18	4	8.91	8.12e+08
158	7.02	4	8.37	2.32e+08
167	7.27	4	8.27	1.87e+08
171	7.11	4	8.67	4.72e+08
172	7.33	4	8.63	4.24e+08
174	7.11	8	8.40	2.51e+08
177	7.08	8	8.64	4.38e+08
178	7.14	8	8.83	6.80e+08
180	7.36	8	9.05	1.13e+09
183	7.20	8	8.94	8.63e+08
185	7.11	8	8.53	3.36e+08
189	7.71	4	8.72	5.30e+08
194	7.80	8	9.23	1.72e+09
195	7.56	4	8.97	9.32e+08
197	7.30	4	8.50	3.20e+08
198	7.62	4	9.60	3.98e+09
201	7.62	8	8.89	7.70e+08
205	8.00	8	8.75	5.64e+08
206	8.09	8	8.84	6.90e+08
207	7.74	8	8.77	5.92e+08
209	8.18	8	8.13	1.35e+08
24+27	5.40	8	5.78	5.98e+07
28+31	5.67	8	6.31	2.06e+06
37+42	5.80	4	6.76	5.70e+06
47+48	5.82	8	6.91	8.18e+06
41+64+71	5.87	4	6.70	4.97e+06
56+60	6.11	4	6.76	5.82e+06
70+76	6.17	8	7.29	1.96e+07
66+95	6.17	4	7.06	1.14e+07

56+60+81	6.19	4	7.06	1.16e+07
84+92	6.20	4	7.45	2.82e+07

Table 10. Mean BAF^{d}_{R}s from Lake Ontario BSAFs for Salmonids (continued)

Chemical	log K_{OW}	Number BAFs	Mean log BAF^{d}_{R}	Mean BAF^{d}_{R}
PCBs				
87+97	6.29	4	7.81	6.46e+07
137+176	6.80	4	8.03	1.07e+08
138+163	6.91	4	8.42	2.64e+08
156+171+202	7.18	4	8.44	2.76e+08
182+187	7.19	4	8.89	7.85e+08
157+200	7.23	4	8.59	3.86e+08
170+190	7.37	8	8.98	9.53e+08
195+208	7.64	4	8.66	4.58e+08
196+203	7.65	8	8.92	8.27e+08
PCDDs				
2378-TCDD	7.02	4	6.95	9.00e+06
12378-PeCDD	7.50	4	7.40	2.49e+07
123478-HxCDD	7.80	4	7.22	1.65e+07
123678-HxCDD	7.80	4	6.83	6.71e+06
123789-HxCDD	7.80	4	6.87	7.44e+06
1234678-HpCDD	8.20	4	6.85	7.16e+06
OCDD	8.60	4	6.63	4.29e+06
PCDFs				
2378-TCDF	6.50	4	6.34	2.16e+06
12378-PeCDF	7.00	4	6.28	1.89e+06
23478-PeCDF	7.00	4	7.14	1.38e+07
123478-HxCDF	7.50	4	6.32	2.07e+06
123678-HxCDF	7.50	4	6.70	5.07e+06
123789-HxCDF	7.50	4	7.23	1.70e+07
234678-HxCDF	7.50	4	7.27	1.84e+07
1234678-HpCDF	8.00	4	5.98	9.47e+05
1234789-HpCDF	8.00	4	7.53	3.35e+07
OCDF	8.80	4	6.96	9.10e+06

F. Bioaccumulation Equivalency Factors (BEFs)

The use of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) toxicity equivalency factors (TEFs) for assessing the total TCDD toxicity risk from complex mixtures of polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) in aquatic environments is complicated by the wide range of bioaccumulation potentials associated with these chemicals. Human and wildlife exposures are related to residues of each chemical in fish and other aquatic organisms ingested as food. Each congener's TCDD equivalent risk is proportional to the product of the congener's TEF times the concentration of the chemical in the food. The sum of all the products provides a TCDD equivalence concentration (TEC) for the food exposure. When it is necessary to relate water or effluent concentrations of PCDDs and PCDFs to risk estimates for food exposure, the TEC equals the sum of the products of the water concentration, BAF and TEF for each congener present. Note that the BAFs and water concentrations have to be based either on freely dissolved chemical (C_w^{fd}) or on total chemical (C_w^t) in water (i.e., consistent definition).

$$\sum_i [(C_w^t)_i \, (BAF^t)_i \, (TEF)_i] = \sum_i [(C_w^{fd})_i \, (BAF^{fd}) \qquad \textbf{(30)}$$

BAFs for PCDDs and PCDFs have not been measured due to the very small water concentrations present in contaminated ecosystems. Concentrations of these chemicals can be measured in surface sediments to provide a measure of the relative amounts of each chemical present in association with organic carbon of the ecosystem. Furthermore, the relative activities of each chemical and TCDD should be similar for both sediment organic carbon and organic carbon suspended in water. The fugacity gradients of each chemical between sediment and water may or may not be similar, depending on differences in chemical loading to the water which are not near steady-state with surface sediment. The biota-sediment accumulation factor (BSAF) is a direct measure of each chemical's distribution between sediment organic carbon and lipid of associated aquatic organisms. When PCDDs and PCDFs have similar sources and distribution patterns between water and sediment, the BSAFs at a site will provide good measures of the bioaccumulation potentials relative to TCDD or any other chemical for which a BAF has been estimated (Cook et al., 1995). Systems with steady-state distributions of the chemicals between sediment and water are most appropriate for these measurements of relative bioaccumulation potential.

Definitions/Symbols

The following bioaccumulation terms and symbols are used to derive and apply TCDD bioaccumulation equivalency factors (BEFs). "C" is used for concentration and "f" for fraction. Subscripts are used to indicate the mass basis for "C" or "f" (w = water, ℓ = lipid in tissue, t = whole tissue wet weight, s = dry sediment, soc = sediment organic carbon, and ssoc = suspended solids organic carbon); superscripts are used to indicate the water phase of the chemical (fd = freely dissolved, b = bound to organic carbon in water, and t =

total chemical = fd+b; and subscripts following parentheses indicate the chemical (tcdd = 2,3,7,8-TCDD and i = the ith chemical).

bioaccumulation factors

$$BAF_{R}^{t} \text{ ' } C_{R}/C_{w}^{t}\,, \qquad BAF_{t}^{t} \text{ ' } C_{t}/C_{w}^{t} \text{ ' } f_{R}(BAF_{R}^{t} \tag{31}$$

$$3AF_{R}^{fd} \text{ ' } C_{R}/C_{w}^{fd}\,, \qquad BAF_{t}^{fd} \text{ ' } C_{t}/C_{w}^{fd} \text{ ' } f_{R}(BAF_{R}^{fc} \tag{32}$$

$$BAF_{R}^{b} \text{ ' } C_{R}/C_{w}^{b}\,, \qquad BAF_{t}^{b} \text{ ' } C_{t}/C_{w}^{b} \text{ ' } f_{R}(BAF_{R}^{b} \tag{33}$$

biota-sediment accumulation factor

$$BSAF \text{ ' } C_{R}\,/C_{soc} \text{ ' } \frac{C_{t}(f_{soc}}{C_{s}(f_{R}} \tag{34}$$

organic carbon - water partitioning

$$f_{fd} \text{ ' } (1\%DOC(K_{OW}/10 \,\%\, POC(K_{OW})^{\&1} \tag{35}$$

fraction dissolved

fraction bound to oc in water $\qquad f_b = 1\text{-}f_{fd}$

TCDD bioaccumulation equivalency factor

$$(BEF)_{i} \text{ ' } \frac{(BSAF\,)_{i}}{(BSAF\,)_{tcdd}} - \frac{(BAF_{R}^{b})_{i}}{(BAF_{R}^{b})_{tcdd}} \tag{36}$$

Calculation of BAFs and TEC from BEFs

The ratio (equation 36) between each PCDD and PCDF congener's BSAF to that of TCDD will be called the TCDD bioaccumulation equivalency factor (BEF). Because BAFs based on freely dissolved chemical in water (BAF^{fd}) are directly proportional to K_{OW} which varies among PCDDs and PCDFs, the BEF describes only the BAF relative to TCDD on the basis of organic carbon bound chemical concentration in water (BAF^{b}). This assumes that the relative amounts of each PCDD and PCDF congener in the organic carbon of surface sediments are the same as in suspended organic carbon. The relationship between particulate organic carbon (POC), dissolved organic carbon (DOC), K_{OW} and f_{fd}

is presented in equation 36. the importance of each chemical's K_{OW} should be evident. The BEF can be used to calculate $(BAF^{t}_{R})_i$ and $(BAF^{fd})_i$. $(BAF^{t}_{R})_i$s estimated from BEFs, under the condition of similar sediment/water fugacity ratios for each chemical, may be used to predict bioaccumulation by pelagic fish from estimated C_{w}^{fd}s regardless of site-specific differences in chemical distribution between sediment and water.

$$BAF_{R}^{\,b} \text{ ' } BAF_{R}^{\,t}/f_b \tag{37}$$

$$(BEF)_i \text{ ' } \frac{(BAF_{R}^{\,b})_i}{(BAF_{R}^{\,b})_{tcdd}} \text{ ' } \frac{(BAF_{R}^{\,t})_i\,(f_b)_{tcdd}}{(BAF_{R}^{\,t})_{tcdd}\,(f_b)_i} \tag{38}$$

so,

$$(BAF_{R}^{\,t})_i \text{ ' } \frac{(BEF)_i\,(BAF_{R}^{\,t})_{tcdd}\,(f_b)_i}{(f_b)_{tcdd}} \tag{39}$$

and,

$$)_i \text{ ' } \frac{(BAF_{R}^{\,t}\,)_i}{(f_{fd})_i} \text{ ' } \frac{(BEF\,)_i\,(BAF_{R}^{\,fd})_{tcdd}\,(f_b)_i\,(}{(f_{fd})_i\,(f_b)_{tcdd}} \tag{40}$$

because $(f_b)_i(f_{fd})_{tcdd}/(f_{fd})_i(f_b)_{tcdd} = (K_{OW})_i/(K_{OW})_{tcdd}$:

$$(BAF_{R}^{\,fd})_i \text{ ' } \frac{(BEF)_i\,(BAF_{R}^{\,fd})_{tcdd}\,(K_{OW})_i}{(K_{OW})_{tcdd}} \tag{41}$$

A TCDD TEC can be calculated on the basis of wet tissue residue $(TEC_t)_{tcdd}$ or lipid normalized residue $(TEC_R)_{tcdd}$; water concentration of total chemical $(TEC_{w}^{t})_{tcdd}$ or freely dissolved chemical $(TEC_{w}^{fd})_{tcdd}$. When bioaccumulation is to be predicted on the basis of freely dissolved chemical (C_{w}^{fd}), the relative differences in BAF^{fd}s for PCDD and PCDF congeners will be less than for their BAF^{t}s. This is because f_{fd}s for the higher chlorinated, more hydrophobic congeners are less than f_{fd} for TCDD. When the TEC is based on concentration of chemicals in tissue, $TEC_{t}^{t} = TEC_{t}^{fd}$ and $TEC_{R}^{t} = TEC_{R}^{fd}$. Thus if $(BAF_{R}^{fd})_{tcdd}$ is the reference bioaccumulation factor:

$$:cdd \text{ ' } \mathbf{j}_{\,i} \left[\frac{(C_{w}^{fd})_i\,(BEF)_i\,(BAF_{t}^{fd})_{tcdd}\,(K_{OW})_i\,(}{(K_{OW})_{tcdd}} \right. \tag{42}$$

$$ {}_{cdd} \;\;' \;\; \mathbf{j}_{\,i} \left[\frac{(C_w^{fd})_i \,(BEF)_i \,(BAF_{R}^{fd})_{tcdd} \,(K_{ow})_i \,(}{(K_{OW})_{tcdd}} \right. \qquad \mathbf{(43)} $$

$$ (TEC_t)_{tcdd} \;\; ' \;\; (TEC_{R})_{tcdd} \;(\; f_{R} \qquad \mathbf{(44)} $$

Great Lakes BEFs

Lake Ontario sediment and fish residue data (Lodge et al., 1994) provide a basis for calculation of BEFs. However, very few PCDDs and PCDFs measured as sediment contaminants are detectable in fish tissue. Table 11 below provides estimated BEFs calculated from lake-wide average concentrations of toxicologically important PCDDs and PCDFs in surface sediment and lake trout samples collected in 1987 for the EPA Region II Lake Ontario TCDD Bioaccumulation Study. Lake Ontario conditions in 1987 involve sediment as the principal source of these chemicals to the water and food chain. The BSAFs if measured under conditions of steady-state between external chemical loading, water, food chain and surface sediment would be somewhat larger but BEFs should be similar. Lake Ontario sediment cores also demonstrate that all PCDD and PCDF congener concentrations have similar temporal trends during the past four decades and all have water column concentrations that are strongly controlled by sediment resuspension due to large declines in loading from sources external to the lake. Limited comparison to BEFs calculated from data obtained for other ecosystems confirms these bioaccumulation potential differences and suggests that this BEF set would be predictive of bioaccumulation differences for PCDDs and PCDFs for fish in ecosystems outside the Great Lakes. Similar results are likely for other persistent bioaccumulative organic chemicals such as PCBs and chlorinated pesticides.

BEFs for Calculation of TCDD Toxicity Equivalence Concentrations in Water in Relation to a GLWQI TCDD Criterion to Protect Human Health

BEFs are measures of bioaccumulation differences between chemicals but do not incorporate differences in bioavailability attributable to partitioning in water. Use of BAF^{fd}s and C_w^{fd}s eliminates bioavailability variation due to partitioning of chemicals with different hydrophobicities to organic carbon in water. When BAFs, based on the concentration of total TCDD in water (BAF_{R}^{t}s) are used, site-specific bioavailability differences are incorporated into the BAF_{R}^{t}. The final Guidance utilizes TCDD BAF_{R}^{t}s for protection of human health. Trophic levels three and four, each with a different fraction lipid, are considered for human exposure. The TCDD BEFs presented in Table 11 are based on lake trout (trophic level four). TCDD BEFs for trophic level 3 fish such as smelt are not likely to be significantly different, however they could be calculated and used in the same manner as the trophic level four TCDD BEFs. The choice of specific dissolved (DOC) and particulate (POC) organic carbon concentrations in water for calculation of TCDD BAF^t_ℓs for human health must be considered when applying BEFs to calculate TCDD toxicity equivalence concentrations in water on the basis of concentrations of total chemical in water, $(TEC^t_w)_{tcdd}$, from concentrations of each PCDD and PCDF congener:

$$EC_w^t)_{tcdd} = \sum (C_w^t)_x \, (TEF)_x \, (BEF)_x \left[\frac{(1-f_{fd})_x}{(1-f_{fd})_{tcd}} \right. \qquad \textbf{(45)}$$

The human health BAF^t_ℓs for TCDD were calculated for default conditions of DOC = 2.0 mg/L and POC = 0.04 mg/L. If the product of $(BEF)_x$ times $(1-f_{fd})_x/(1-f_{fd})_{tcdd}$ is defined as the BEF for health criteria based on total chemical concentration (BEF^t_w), equation 46 can be simplified to equation 47. Table 11 contains TEFs and BEF^t_ws for calculating human health $(TEC^t_w)_{tcdd}$s from C^t_ws, either measured or estimated for the default DOC and POC conditions. TCDD BEF^t_ws differ only slightly from TCDD BEFs in proportion to differences in hydrophobicity.

$$(TEC_w^t)_x = (C_w^t)_x \, (TEF)_x \, (BEF_w^t)_x \qquad \textbf{(46)}$$

Table 11. TCDD Bioaccumulation equivalency factors (BEFs) and TCDD bioaccumulation equivalency factors for human health criteria for total chemical concentration in water (BEF^t_ws). The BEFs and BEF^t_ws are derived for toxicologically important PCDDs and PCDFs from lakewide averages of concentrations in Lake Ontario lake trout and surface sediment in depositional areas.

Congener	**log K_{OW}[a]**	**BSAF**	**TCDD BEF**	**TCDD BEF^t_w**
2,3,7,8-TCDD	7.02	0.059	1.0	1.0
1,2,3,7,8-PeCDD	7.50	0.054	0.92	1.13
1,2,3,4,7,8-HxCDD	7.80	0.018	0.31	0.40
1,2,3,6,7,8-HxCDD	7.80	0.0073	0.12	0.16
1,2,3,7,8,9-HxCDD	7.80	0.0081	0.14	0.18
1,2,3,4,6,7,8-HpCDD	8.20	0.0031	0.051	0.072
OCDD	8.60	0.00074	0.012	0.017
2,3,7,8-TCDF	6.5[b]	0.047	0.80	0.48
1,2,3,7,8-PeCDF	7.0[b]	0.013	0.22	0.22

2,3,4,7,8-PeCDF	7.0[b]	0.095	1.6	1.59
1,2,3,4,7,8-HxCDF	7.5[b]	0.0045	0.076	0.094
1,2,3,6,7,8-HxCDF	7.5[b]	0.011	0.19	0.23
2,3,4,6,7,8-HxCDF	7.5[b]	0.040	0.67	0.84
1,2,3,7,8,9-HxCDF	7.5[b]	0.037	0.63	0.78
1,2,3,4,6,7,8-HpCDF	8.0[b]	0.00065	0.011	0.015
1,2,3,4,7,8,9-HpCDF	8.0[b]	0.023	0.39	0.52
OCDF	8.80	0.001	0.016	0.023

[a] Burkhard and Kuehl, 1987.
[b] Estimated based on degree of chlorination and Burkhard and Kuehl, 1987.

Example of a $(TEC)_{tcdd}$ Calculation Using the BEF Method

Projected PCDD and PCDF loadings to a Great Lake result in estimated water concentrations (C_w^t) of 0.0001, 0.0008, 0.0002, 0.0008 and 0.02 pg/ml for 2,3,7,8-TCDD, 2,3,7,8-TCDF, 1,2,3,7,8-PeCDD, 2,3,4,7,8-PeCDF and 1,2,3,4,6,7,8-HpCDD, respectively. The concentration of POC is 0.2 mg/L, DOC is 2.0 mg/L, so the C_w^{fd}s for each congener are 0.00002, 0.0006, 0.000015, 0.00016, and 0.0003 pg/L, respectively. The BAF_R^{fd} for TCDD is estimated to be 7.85×10^6 and TEFs are 1.0, 0.1, 0.5 0.5 and 0.01 for each congener, respectively. At 9% lipid (f_R=0.09), the 2,3,7,8-TCDD $BAF_{.09R}^{fd}$ = 7.07×10^5. From equation 46 the TCDD toxicity equivalency concentration for fish with f_R=0.09, $(TEC_{.09R})_{tcdd}$, is calculated to be:

$(TEC_{.09R})_{tcdd} = (7.07 \times 10^5)[(0.00002)(1.0)(10.5 \times 10^6)(1.0)/10.5 \times 10^6 + (0.0006)(0.8)(0.63 \times 10^6)(0.1)/10.5 \times 10^6 + (0.000015)(0.92)(31.6 \times 10^6)(0.5)/10.5 \times 10^6 + (0.00016)(1.6)(10 \times 10^6)(0.5)/10.5 \times 10^6 + (0.0003)(0.05)(158 \times 10^6)(0.01)/10.5 \times 10^6] = 14.4 + 20.4 + 1.5 + 0.86 + 1.6 = 38.8$ pg TCDD eq./g wet fish.

In this hypothetical example 2,3,7,8-TCDD contributes 37% of the TEC. Without use of the BEF approach (all $BAF_{.09R}^{fd}$s = 7.07×10^5), the TEC is calculated to be 14.4 + 42.4 + 0.5 + 5.7 + 21.2 = 84.2 pg TCDD eq./g wet fish with TCDD contributing only 17%. The overestimation of bioaccumulation for TCDF, PeCDF and HpCDD leads to a greater TEC estimate. Since there appears to be an association between TEFs and BEFs (i.e., the more toxic congeners are the most bioaccumulative, primarily due to slower rates of biotransformation), additional data suitable for validating the BSAFs used to calculate the BEFs are needed.

IV. DETERMINATION OF BAFs FOR INORGANIC CHEMICALS

The lipid-BAF relationship does not apply to the determination of BAFs for inorganic chemicals. BAF and BCF data for inorganics are not as transferable from one species, or one tissue, to another as organic data. Bioaccumulation of some trace metals is substantially greater in internal organs than muscle tissue. For example, BCFs for rainbow trout liver, kidney, gut and skin, and muscle exposed to cadmium for 178 days were about 325, 75, 7, and 1 respectively (Giles 1988). Merlini and Pozzi (1977) reported that lead bioconcentrated 30 times more in bluegill liver than in bluegill muscle tissue after eight days. They reported a BCF for muscle tissue of 0.46.

Because bioaccumulation can differ dramatically between tissues, BAFs or BCFs for edible tissue of fish should be used for BAFs to calculate human health criteria. Similarly, BAFs or BCFs for whole body of fish should be used for the BAFs used to calculate wildlife criteria.

BAFs or BCFs for inorganic chemicals measured in plants or invertebrate animals might be one or more orders of magnitude greater than BAFs or BCFs for the edible tissue of fish (see Table 5 in the EPA criteria documents for cadmium, copper, lead and nickel; USEPA 1985A, USEPA 1985B, USEPA 1985C, and USEPA 1986). For this reason plant or invertebrate BAFs and BCFs should not be used to calculate human health criteria and values. If site-specific conditions warrant, and the resulting criteria are more stringent, plant or invertebrate BAFs or BCFs could be used to calculate wildlife criteria.

Mercury and certain other metals are subject to methylation through microbial action in nature. The organo-metallic form of the metal, especially methyl mercury, is highly bioaccumulative in the muscle tissue of fish (Grieb et al. 1990).

V. CALCULATION OF BASELINE BAFs FOR ORGANIC CHEMICALS

A. Baseline BAF from a Field-Measured BAF

A baseline BAF shall be calculated from a field-measured BAF of acceptable quality using the following equation:

$$\text{Baseline BAF} = \left(\frac{\text{Measured BAF}_T^t}{f_{fd}} - 1 \right) \left(\frac{1}{f_R} \right)$$

where: BAF_T^t = BAF based on total concentration in tissue and ambient water.

f_R = fraction of the tissue that is lipid.

f_{fd} = fraction of the total chemical that is freely dissolved in the ambient water.

The trophic level to which the baseline BAF applies is the same as the trophic level of the organisms used in the determination of the field-measured BAF. For each trophic level, a species mean baseline BAF shall be calculated as the geometric mean if more than one measured baseline BAF is available for a given species. For each trophic level, the geometric mean of the species mean baseline BAFs shall be calculated.

If a baseline BAF based on a field-measured BAF is available for either trophic level 3 or 4, but not both, the baseline BAF for the other trophic level shall be calculated using the ratio of the FCMs that are obtained by linear interpolation from Table B-1 for the chemical.

B. Baseline BAF from Field-Measured BSAF Methodology

A baseline BAF for organic chemical "i" shall be calculated from a field-measured BSAF of acceptable quality using the following equation:

$$(\text{Baseline BAF})_i = (\text{BAF}_R^{fd})_r \cdot \frac{(\text{BSAF})_i \cdot (K_{OW})_i}{(\text{BSAF})_r \cdot (K_{OW})_r}$$

where: $(\text{BAF}_R^{fd})_r$ = BAF based on the measurement of freely dissolved reference chemical in the water column.
$(\text{BSAF})_i$ = BSAF for chemical "i".
$(\text{BSAF})_r$ = BSAF for the reference chemical "r".
$(K_{OW})_i$ = octanol-water partition coefficient for chemical "i".
$(K_{OW})_r$ = octanol-water partition coefficient for the reference chemical "r".

The trophic level to which the baseline BAF applies is the same as the trophic level of the organisms used in the determination of the BSAF. For each trophic level, a species mean baseline BAF shall be calculated as the geometric mean if more than one baseline BAF is predicted from BSAFs for a given species. For each trophic level, the geometric mean of the species mean baseline BAFs shall be calculated.

If a baseline BAF based on a measured BSAF is available for either trophic level 3 or 4, but not both, the baseline BAF for the other trophic level shall be calculated using the ratio of the FCMs that are obtained by linear interpolation from Table 3 for the chemical.

C. Baseline BAF from a Laboratory-Measured BCF

A baseline BAF for trophic level 3 and a baseline BAF for trophic level 4 shall be calculated from a laboratory-measured BCF of acceptable quality and a FCM using the following equation:

$$\text{Baseline BAF} = (\text{FCM})\,(\text{Measured baseline BCF})$$

$$\text{Baseline BAF ' (FCM)}\left[\frac{\text{Measured BCF}_T^t}{f_{fd}} \text{ \& } 1\right]\left(\frac{1}{f_R}\right)$$

where: BCF_T^t = BCF based on total concentration in tissue and water.
f_R = fraction of the tissue that is lipid.
f_{fd} = fraction of the total chemical that is freely dissolved in the ambient water.
FCM = the food-chain multiplier obtained from Table 3 by linear. interpolation for trophic level 3 or 4, as necessary.

For each trophic level, a species mean baseline BAF shall be calculated as the geometric mean if more than one baseline BAF is predicted from laboratory-measured BCFs for a given species. For each trophic level, the geometric mean of the species mean baseline BAFs shall be calculated.

D. Baseline BAF from a Octanol-Water Partition Coefficient

A baseline BAF for trophic level 3 and a baseline BAF for trophic level 4 shall be calculated from a K_{OW} of acceptable quality and a FCM using the following equation:

$$\text{Baseline BAF ' (FCM)(predicted baseline BCF) ' (FCM)}(K_{OW})$$

where: FCM = the food-chain multiplier obtained from Table 3 by linear interpolation for trophic level 3 or 4, as necessary.
K_{OW} = octanol-water partition coefficient.

VI. CALCULATION OF BASELINE BAFs FOR INORGANIC CHEMICALS

For most inorganic chemicals, the baseline BAFs for trophic levels 3 and 4 are both assumed to equal the BCF determined for the chemical with fish (i.e., the FCM is assumed to be 1 for both trophic levels 3 and 4). However, a FCM greater than 1 might be applicable to some metals, such as mercury, if, for example, an organometallic form of the metal biomagnifies.

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Appendix A. Procedure for Deriving Recommended Values for Log K_{OW}

Measured values of K_{OW} have been obtained using the slow-stir, generator-column, and shake-flask techniques. The shake-flask technique has been reported to be acceptable only for chemicals whose log K_{OW}s are less than 4 (Karickhoff et al. 1979; Konemann et al. 1979; Braumann and Grimme 1981; Harnisch et al. 1983; Brooke et al. 1990). Brooke et al. (1986) reported that the shake-flask technique is acceptable for chemicals whose log K_{OW}s are less than 5, whereas Chessells et al. (1991) stated that this technique is acceptable for values of log K_{OW} up to about 5.5. Although the three techniques seem to give about the same values on the average up to at least a log K_{OW} of 4.5, the slow-stir and generator-column techniques are given preference in the final Guidance for chemicals whose log K_{OW}s are greater than 4; because phase separation is always a potential problem with the shake-flask technique, it is possible that the slow-stir and generator-column techniques should also be given preference for chemicals whose log K_{OW}s are less than 4.

Predicted values of K_{OW} have been based on reverse-phase high performance liquid chromatography (RPLC) and thin-layer chromatography (TLC). Generally, results obtained using the RPLC technique should be used in the final Guidance if the calibration curve is based on measured values of K_{OW}, but not if the calibration curve is based on values calculated on a basis such as fragment or substituent constants; the actual values used in the calibration curve are more important, however, than the source of the values. Because it is based on more measurements and seems to have a better scientific basis, the version of RPLC that includes extrapolation to zero percent solvent is given preference over the version that does not include extrapolation to zero percent solvent. Values based on TLC are not considered because this technique has not been adequately investigated.

Calculated values of K_{OW} have been obtained using a variety of methods, but the most widely used is the computer program CLOGP. Calculated values of K_{OW} should be used only as a last resort.

Because of potential interference due to radioactivity associated with impurities, values of K_{OW} that are determined by measuring radioactivity in water and/or octanol are less reliable and should be used only as a last resort.

Thus, values of K_{OW} are given priority based on the technique used as follows:

Log $K_{OW} < 4$:	Priority	Technique
	1	Slow-stir.
	1	Generator-column.
	1	Shake-flask.
	2	Reverse-phase liquid chromatography on C18 with extrapolation to zero percent solvent (RPLC-E).
	3	Reverse-phase liquid chromatography on C18 without extrapolation to zero percent solvent (RPLC).
	4	Calculated by the CLOGP program.

Log $K_{OW} > 4$:	Priority	Technique
	1	Slow-stir.
	1	Generator-column.
	2	Reverse-phase liquid chromatography on C18 with extrapolation to zero percent solvent (RPLC-E).
	3	Reverse-phase liquid chromatography on C18 without extrapolation to zero percent solvent (RPLC).
	4	Shake-flask.
	5	Calculated by the CLOGP program.

Values that seem to be different from the rest should be considered outliers and not used.

For each chemical the available value of log K_{OW} with the highest priority should be the recommended value, except that if more than one such value is available, the arithmetic mean of log K_{OW}s or the geometric mean of K_{OW}s should be the recommended value. In some cases, another value may be the recommended value if adequately justified.

A K_{OW} can describe the partitioning of an individual chemical more usefully than it can describe the partitioning of a mixture, such as toxaphene, PCBs, or chlordane. When a measured value is not available for a mixture, a recommended value may be derived by using the value for a major component or by calculating a weighted or unweighted average of the values for various components. If an unweighted average is used, the arithmetic average of values of log K_{OW} may be used or the geometric mean of values of K_{OW} may be used.

Measured and predicted values should be taken from the original publications. Values may be referenced to Medchem in some cases, preferably only if Medchem associates the value with Hansch, Leo, and/or Pamona College; all such values are assumed to have been determined by the shake-flask technique.

Recommended values for log K_{OW} should be given to three decimal digits (e.g., 4.321) because these are intermediate values in the calculation of BAFs, criteria, and permit limits.

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Appendix B. Derivation of Recommended Values of Log K_{OW}

Appendix A describes the procedure for deriving recommended values of log K_{OW} that are used for chemicals in the final Guidance. Various techniques that can be used to measure, predict, and calculate the log K_{OW} of a chemical are given priorities in Appendix A. This Appendix B presents the application of the procedure to various chemicals and gives the recommended value of log K_{OW} that is used in the final Guidance for each of the chemicals.

It was inconvenient to repeatedly acknowledge duplicate publication of two sets of values below; only the original investigators are cited in both cases. Banerjee et al. (1980) is cited for values that are also reported by Veith et al. (1980). Similarly, de Bruijn et al. (1990) is cited for values that are also reported by Brooke et al. (1990).

Except as noted, all calculated values of log K_{OW} were obtained using version 3.4 of CLOGP.

The notation "(R)" indicates that the value was based on measurement of radioactivity.

Benzene [CAS#: 71-43-2]

The values that have the highest priorities are:

2.186	Slow-stir	de Bruijn et al. 1989
2.13	Generator-column	Miller et al. 1985
2.114	Shake-flask	Karickhoff et al. 1979
2.13	Shake-flask	Medchem
2.130	Shake-flask	Watari et al. 1982
2.20	RPLC-E	Hammers et al. 1982
2.23	RPLC-E	Harnisch et al. 1983
2.18	RPLC	Miyake and Terada 1982
2.48	RPLC	Swann et al. 1983
2.25	RPLC	Rapaport and Eisenreich 1984
2.39	RPLC	Veith et al. 1979a
2.13	RPLC	Veith et al. 1980
2.26	RPLC	de Kock and Lord 1987
2.121	Shake-flask (R)	Banerjee et al. 1980
2.1	Consensus	Klein et al. 1988

The value used in the final Guidance is 2.138, which is the average of the top five values.

Chlordane [CAS#: see below]

There are several relevant CAS numbers:

CAS#:	57-74-9	Chlordane, mixture of cis and trans
CAS#:	5103-71-9	alpha-chlordane; cis-chlordane

CAS#:	5103-74-2	beta-chlordane; trans-chlordane
CAS#:	5566-34-7	gamma-chlordane
CAS#:	12789-03-6	Chlordane, technical

All of these, and all of their mixtures, are expected to have similar values for log K_{OW}, BCF, and BAF.

The value that has the highest priority is:

6.00	RPLC	Veith et al. 1979b

The value used in the final Guidance is 6.00.

Chlorobenzene [CAS#: 108-90-7]

The values that have the highest priorities are:

2.784	Slow-stir	Brooke et al. 1990
2.898	Slow-stir	de Bruijn et al. 1989
2.98	Generator-column	Miller et al. 1985
2.80	Shake-flask	Voice et al. 1983
2.89	Shake-flask	Medchem
2.840	Shake-flask	Watari et al. 1982
2.83	RPLC-E	Hammers et al. 1982
2.94	RPLC	Miyake and Terada 1982
3.00	RPLC	de Kock and Lord 1987
2.8	Consensus	Klein et al. 1988

The value used in the final Guidance is 2.865, which is the average of the top six values.

Cyanide [CAS#: 57-12-5]

A value of log K_{OW} is not used for cyanide.

DDD [CAS#: see below]

There are several relevant CAS numbers:

CAS#:	72-54-8	p,p'-DDD; 4,4'-DDD
CAS#:	53-19-0	o,p'-DDD; 2,4'-DDD
CAS#:	4329-12-8	m,p'-DDD; 3,4'-DDD

All of these, and all of their mixtures, are expected to have similar values for log K_{OW}, BCF, and BAF.

The values that have the highest priorities are:

5.90	Slow-stir	Stancil 1994
6.217	Slow-stir	de Bruijn et al. 1989
4.73	RPLC	McDuffie 1981
5.00	RPLC	de Kock and Lord 1987

The value used in the final Guidance is 6.058, which is the average of the top two values.

DDE [CAS#: see below]

There are several relevant CAS numbers:

CAS#:	72-55-9	p,p'-DDE; 4,4'-DDE
CAS#:	3424-82-6	o,p'-DDE; 4,4'-DDE

All of these, and all of their mixtures, are expected to have similar values for log K_{OW}, BCF, and BAF.

The values that have the highest priorities are:

6.57	Slow-stir	Stancil 1994
6.956	Slow-stir	de Bruijn et al. 1989
5.89	RPLC	Burkhard et al. 1985
5.83	RPLC	Veith et al. 1979a
5.69	RPLC	Veith et al. 1979b
5.63	RPLC	Swann et al. 1983
5.89	RPLC	McDuffie 1981
6.09	RPLC	de Kock and Lord 1987

The value used in the final Guidance is 6.763, which is the average of the top two values.

DDT [CAS#: see below]

There are several relevant CAS numbers:

CAS#:	50-29-3	p,p'-DDT; 4,4'-DDT
CAS#:	789-02-6	o,p'-DDT; 2,4'-DDT
CAS#:	33086-18-9	DDT

All of these, and all of their mixtures, are expected to have similar values for log K_{OW}, BCF, and BAF.

The values that have the highest priorities are:

6.198	Slow-stir	Brooke et al. 1986
6.307	Slow-stir	Brooke et al. 1990
6.38	Slow-stir	Stancil 1994
6.914	Slow-stir	de Bruijn et al. 1989
6.38	RPLC-E	Hammers et al. 1982
6.06	RPLC-E	Harnisch et al. 1983
5.84	RPLC-E	Harnisch et al. 1983
6.4	RPLC-E	Brooke et al. 1986
5.44	RPLC	Burkhard et al. 1985
5.13	RPLC	Rapaport and Eisenreich 1984
5.75	RPLC	Veith et al. 1979b
5.63	RPLC	de Kock and Lord 1987
6.36	Shake-flask	Chiou et al. 1982
5.1	Shake-flask (R)	Platford et al. 1982
6.2	Consensus	Klein et al. 1988

The value used in the is 6.450, which is the average of the top four values.

Dieldrin [CAS#: 60-57-1]

The values that have the highest priorities are:

5.335	Slow-stir	Stancil 1994; U.S. EPA 1991a
5.401	Slow-stir	de Bruijn et al. 1989
4.538	Slow-stir	Brooke et al. 1986
5.16	Generator-column	U.S. EPA 1991a
5.11	RPLC-E	Hammers et al. 1982
4.65	RPLC	de Kock and Lord 1987
5.01	Shake-flask	U.S. EPA 1991a

The value of 4.54 is considered an outlier. The value used in the final Guidance is 5.299, which is the average of the first, second, and fourth values.

2,4-Dimethylphenol [CAS#: 105-67-9]

The values that have the highest priority are:

2.30	Shake-flask	Medchem
1.99	RPLC	Veith et al. 1980
2.07	RPLC	Haky and Young 1984
2.420	Shake-flask (R)	Banerjee et al. 1980

The value used in the final Guidance is 2.30.

2,4-Dinitrophenol [CAS#: 51-28-5]

The value that has the highest priority is:

1.51	Shake-flask	Medchem
1.67	Shake-flask	Medchem
1.54	Shake-flask	Medchem
1.56	Shake-flask	Medchem
1.59	Shake-flask	Medchem
1.55	Shake-flask	Medchem
1.50	Consensus	Klein et al. 1988

The value used in the final Guidance is 1.570, which is the average of the top six values.

Hexachlorobenzene [CAS#: 118-74-1]

The values that have the highest priorities are:

5.47	Generator-column	Miller et al. 1985
5.731	Slow-stir	de Bruijn et al. 1989
5.9	RPLC-E	Brooke et al. 1986
5.66	RPLC-E	Hammers et al. 1982
5.46	RPLC-E	Harnisch et al. 1983
5.26	RPLC-E	Harnisch et al. 1983
6.71	RPLC	Rapaport and Eisenreich 1984

6.86	RPLC	Burkhard et al. 1985
7.42	RPLC	Veith et al. 1979a
5.23	RPLC	Veith et al. 1979b
6.92	RPLC	de Kock and Lord 1987
5.47	Shake-flask	Harnisch et al. 1983
5.50	Shake-flask	Chiou et al. 1982
5.00	Shake-flask	Konemann et al. 1979
5.2	Shake-flask	Platford et al. 1982
5.44	Shake-flask	Briggs 1981
5.312	Shake-flask	Watari et al. 1982

The value used in the final Guidance is 5.600, which is the average of the top two values.

Hexachlorobutadiene [CAS#: 87-68-3]

The values with the highest priorities are:

4.785	Shake-flask	Banerjee et al. 1980
4.90	Shake-flask	Chiou 1985

The value used in the final Guidance is 4.842.

Hexachlorocyclohexane (HCCH) [CAS#: 608-73-1]

alpha-HCCH	[CAS#: 319-84-6]
beta-HCCH	[CAS#: 319-85-7]
delta-HCCH	[CAS#: 319-86-8]
gamma-HCCH	[see lindane]

The most useful values that were found are:

alpha:	3.776	Slow-stir	de Bruijn et al. 1989
beta:	3.842	Slow-stir	de Bruijn et al. 1989

The values used in the final Guidance are:

HCCH: 3.769
alpha: 3.776
beta: 3.842
delta: 3.769

The value used for HCCH and for delta is the average of the values obtained by de Bruijn et al. (1989) for alpha, beta, and gamma.

Hexachloroethane [CAS#: 67-72-1]

The values that have the highest priorities are:

4.04	RPLC	McDuffie 1981
4.05	RPLC	Veith et al. 1980
4.14	Shake-flask	Chiou 1985
3.93	Shake-flask	Veith et al. 1980

These values are close to 4, and the range of the four values is small. The value used in the final Guidance is 4.040, which is the average of the four values.

Lindane (gamma-HCCH) [CAS#: 58-89-9]

The values that have the highest priorities are:

3.688	Slow-stir	de Bruijn et al. 1989
3.61	Shake-flask	Medchem
3.72	Shake-flask	Medchem
3.32	Shake-flask	Platford 1981,1982
3.89	RPLC	Veith et al. 1979b
3.66	RPLC	Saito et al. 1993
3.00	RPLC	de Kock and Lord 1987

The value of 3.32 is considered an outlier. The value used in the is 3.673, which is the average of the top three values.

Mercury [CAS#: 7439-97-6]

A value for log K_{OW} is not used for mercury.

Methylene chloride [CAS#: 75-09-2]

The value that has the highest priority is:

1.25	Shake-flask	Medchem

The value used in the final Guidance is 1.25.

Mirex [CAS#: 2385-85-5]

The value that has the highest priority is:

6.89	RPLC	Veith et al. 1979b
5.28	Shake-flask	Medchem
4.650	Calculated	CLOGP

The value used in the final Guidance is 6.89.

Nonachlor [CAS#: see below]

There are several relevant CAS numbers:

CAS#:	3734-49-4	Nonachlor
CAS#:	5103-73-1	cis-nonachlor
CAS#:	39765-80-5	trans-nonachlor

The value that has the highest priority is:

5.655	Calculated	CLOGP

The value used in the final Guidance is 6.0, which is the value used for the structurally similar chlordane and is considered to be a better value for nonachlor than 5.655; this value is used only in connection with the BSAF methodology.

Octachlorostyrene [CAS#: 29082-74-4]

The value that has the highest priority is:

6.29	RPLC	Veith et al. 1979b

The value used in the final Guidance is 6.29.

PCBs

See Appendix F of this document.

Pentachlorobenzene [CAS#: 608-93-5]

The values that have the highest priorities are:

5.183	Slow-stir	de Bruijn et al. 1989
5.03	Generator-column	Miller et al. 1985
5.06	RPLC-E	Hammers et al. 1982
5.29	RPLC	Veith et al. 1980
6.12	RPLC	de Kock and Lord 1987
5.20	Shake-flask	Chiou 1985
4.88	Shake-flask	Konemann et al. 1979
5.167	Shake-flask	Watari et al. 1982
4.940	Shake-flask (R)	Banerjee et al. 1980

The value used in the final Guidance is 5.106, which is the average of the top two values.

2,3,4,5,6-Pentachlorotoluene [CAS#: 877-11-2]

The value that has the highest priority is:

6.356	Calculated	CLOGP

The only value available is 6.356; this value is used only in the study of the food-chain model.

Photomirex [CAS#: 39801-14-4]

The value that has the highest priority is:

4.537	Calculated	CLOGP

The value used in the final Guidance is 6.89, which is the value used for mirex and is considered to be a better value for photomirex than 4.537.

2,3,7,8-TCDD [CAS#: 1746-01-6]

The value that has the highest priority is:

6.42	Slow-stir	Sijm et al. 1989
6.63	Slow-Stir	Marple et al. 1986
7.02	RPLC	Burkhard and Kuehl 1986

As per pages 2-2, 2-3, and 3-9 of U.S. EPA (1993), the value used in the final Guidance is 7.02.

1,2,3,4-Tetrachlorobenzene [CAS#: 634-66-2]

The values that have the highest priorities are:

4.635	Slow-stir	de Bruijn et al. 1989
4.55	Generator-column	Miller et al. 1985
4.41	RPLC-E	Hammers et al. 1982
4.75	Shake-flask	Bruggeman et al. 1982

4.60	Shake-flask	Chiou 1985
4.46	Shake-flask	Konemann et al. 1979
4.375	Shake-flask	Watari et al. 1982

The value used in the final Guidance is 4.592, which is the average of the top two values.

1,2,3,5-Tetrachlorobenzene [CAS#: 634-90-2]

The values that have the highest priorities are:

4.658	Slow-stir	de Bruijn et al. 1989
4.65	Generator-column	Miller et al. 1985
4.35	RPLC-E	Hammers et al. 1982
4.59	Shake-flask	Chiou 1985
4.50	Shake-flask	Konemann et al. 1979
4.459	Shake-flask (R)	Banerjee et al. 1980

The average of the top two values is 4.654; this value is used only in the study of the food-chain model.

1,2,4,5-Tetrachlorobenzene [CAS#: 95-94-3]

The values that have the highest priorities are:

4.604	Slow-stir	de Bruijn et al. 1989
4.51	Generator-column	Miller et al. 1985
4.52	RPLC-E	Hammers et al. 1982
4.70	Shake-flask	Chiou 1985
4.52	Shake-flask	Konemann et al. 1979
4.555	Shake-flask	Watari et al. 1982

The value used in the final Guidance is 4.557, which is the average of the top two values.

Toluene [CAS#: 108-88-3]

The values that have the highest priorities are:

2.65	Generator-column	Miller et al. 1985
2.786	Slow-stir	de Bruijn et al. 1989
2.63	Slow-stir	Brooke et al. 1990
2.73	Shake-flask	Medchem
2.77	Shake-flask	Medchem
2.77	RPLC-E	Harnisch et al. 1983
2.78	RPLC-E	Hammers et al. 1982
2.78	RPLC	Burkhard et al. 1985
2.99	RPLC	Veith et al. 1980
2.89	RPLC	Rapaport and Eisenreich 1984
2.62	RPLC	Miyake and Terada 1982
3.00	RPLC	de Kock and Lord 1987
2.21	Shake-flask (R)	Banerjee et al. 1980

2.7	Consensus	Klein et al. 1988

The value used in the final Guidance is 2.713, which is the average of the top five values.

Toxaphene [CAS#: 8001-35-2]

The value that has the highest priority is:

4.330	Calculated	CLOGP

The value used in the final Guidance is 4.330.

1,2,3-Trichlorobenzene [CAS#: 87-61-6]

The values that have the highest priorities are:

4.139	Slow-stir	de Bruijn et al. 1989
4.04	Generator-column	Miller et al. 1985
4.11	Shake-flask	Konemann et al. 1979
4.14	Shake-flask	Chiou 1985
4.053	Shake-flask	Watari et al. 1982
3.88	RPLC-E	Hammers et al. 1982
4.02	RPLC	McDuffie 1981

The top five values are all close to 4 and the range is small. The average of the top five values is 4.096; this value is used only in the study of the food-chain model.

1,2,4-Trichlorobenzene [CAS#: 120-82-1]

The values that have the highest priorities are:

4.050	Slow-stir	de Bruijn et al. 1989
3.98	Generator-column	Miller et al. 1985
3.93	Shake-flask	Konemann et al. 1979
4.02	Shake-flask	Chiou et al. 1982; Chiou 1985
3.970	Shake-flask	Watari et al. 1982
3.96	RPLC-E	Hammers et al. 1982
4.23	RPLC	Veith et al. 1979b
4.22	RPLC	de Kock and Lord 1987
4.20	Consensus	Klein et al. 1988

The top five values are all close to 4 and the range is small. The value used in the final Guidance is 3.990, which is the average of the top five values; currently this value is only used in the study of the food-chain model.

1,3,5-Trichlorobenzene [CAS#: 108-70-3]

The values that have the highest priorities are:

4.189	Slow-stir	de Bruijn et al. 1989
4.02	Generator-column	Miller et al. 1985
4.15	Shake-flask	Konemann et al. 1979
4.31	Shake-flask	Chiou 1985
4.190	Shake-flask	Watari et al. 1982

4.17	RPLC-E	Hammers et al. 1982

The top five values are all close to 4 and the range is small. The average of the top five values is 4.172; this value is used only in the study of the food-chain model.

Trichloroethylene [CAS#: 79-01-6]

The values that have the highest priorities are:

2.53	Generator-column	Miller et al. 1985
3.14	Shake-flask	Harnisch et al. 1983
2.67	RPLC-E	Harnisch et al. 1983
2.56	RPLC-E	Harnisch et al. 1983
2.420	Shake-flask (R)	Banerjee et al. 1980
2.4	Consensus	Klein et al. 1988

The value used in the final Guidance is 2.53. The value of 3.14 is considered an outlier.

2,3,6-Trichlorotoluene [CAS#: 2077-46-5]

The value that has the highest priority is:

4.930	Calculated	CLOGP

The only value available is 4.930; this value is used only in the study of the food-chain model.

2,4,5-Trichlorotoluene [CAS#: 6639-30-1]

The value that has the highest priority is:

4.930	Calculated	CLOGP

The only value available is 4.930; this value is used only in the study of the food-chain model.

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Appendix C. Derivation of Basic Equations Concerning Bioconcentration and Bioaccumulation of Organic Chemicals

Introduction

Most work dealing with the bioconcentration and bioaccumulation of organic chemicals has concerned chemicals whose log K_{OW}s are greater than 3. The purpose of this appendix is to explain why modifications of the equations generally used with such chemicals are necessary so that the equations also are appropriate for chemicals whose K_{OW}s, BCFs, or BAFs are less than 1000, and to derive all of the appropriate equations that are used in the calculation of BAFs for the final Guidance.

Background

Bioconcentration factors were originally defined as:

$$BCF_T^t = \frac{C_B^t}{C_W^t} \qquad (1)$$

where:

BCF_T^t = a total bioconcentration factor (i.e., a BCF that is based on the total concentrations of the chemical in the water and in the aquatic biota).

C_B^t = the total concentration of the chemical in the aquatic biota, based on the wet weight of the aquatic biota.

C_W^t = the total concentration of the chemical in the water around the aquatic biota.

This is not the nomenclature that was used originally, but it is used here for clarity.

It was subsequently realized that extrapolation of BCFs for organic chemicals from one species to another would be more accurate if the BCFs were normalized on the basis of the amount of lipid in the aquatic biota. It was also realized that extrapolation of BCFs for organic chemicals from one water to another would be more accurate if the BCFs were calculated on the basis of the freely dissolved concentration of the organic chemical in the water around the aquatic biota. Thus two additional BCFs were defined and used:

$$BCF_R^t = \frac{C_R}{C_W^t} \qquad (2)$$

$$BCF_R^{fd} = \frac{C_R}{C_W^{fd}} \qquad (3)$$

where:

BCF_R^t = the lipid-normalized total bioconcentration factor (i.e., normalized to

100 percent lipid and based on the total concentration of the chemical in the water around the biota).

C_R = the lipid-normalized concentration of the chemical in the aquatic biota.

$BCF_R^{\tau\alpha}$ = the lipid-normalized, freely dissolved bioconcentration factor.

$C_W^{\tau\alpha}$ = the freely dissolved concentration of chemical in the water around the aquatic biota.

The experimental definition of C_R is:

$$C_R = \frac{\text{the total amount of chemical in the aquatic biota}}{\text{the amount of lipid in the aquatic biota}}$$

$$= \frac{(B)(C_B^t)}{L} = \frac{(B)(C_B^t)}{(f_R)(B)} = \frac{C_B^t}{f_R} \tag{4}$$

where:

B = the wet weight of the aquatic biota.

L = the weight of the lipid in the aquatic biota.

f_R = the fraction of the aquatic biota that is lipid = L/B.

Using equation 4 to substitute for C_R in equation 2 and then using equation 1:

$$BCF_R^t = \frac{C_B^t}{(C_W^t)(f_R)} = \frac{BCF_T^t}{f_R} \tag{5}$$

If f_{fd} = the fraction of the chemical in the water around the aquatic biota that is freely dissolved, then:

$$f_{fd} = \frac{C_W^{fd}}{C_W^t} \tag{6}$$

Using equations 4 and 6 to substitute for C_R and C_W^{fd} in equation 3 and then using equation 1:

$$BCF_R^{fd} = \frac{C_B^t}{(f_R)(C_W^t)(f_{fd})} = \frac{BCF_T^t}{(f_R)(f_{fd})} \tag{7}$$

Equations 1, 5, and 7 show the relationships between the three different bioconcentration factors.

Theoretical justification for use of both lipid-normalization and the freely dissolved concentration of the organic chemical in the ambient water is based on the concept of equilibrium partitioning, whereas practical justification is provided by the general similarity of the value of $\mathrm{BCF}_{R}^{\tau\alpha}$ for an organic chemical across both species and waters. It will be demonstrated, however, that a more complete application of equilibrium partition theory shows that $\mathrm{BCF}_{R}^{\tau\alpha}$ extrapolates well only for chemicals whose K_{OW}s are greater than 1000, whereas a different BCF extrapolates well for organic chemicals whose K_{OW}s are greater than 1000 as well as for chemicals whose K_{OW}s are less than 1000.

Partition Theory and Bioconcentration

Equilibrium partition theory provides the understanding necessary to ensure proper use of K_{OW}s, BCFs, and BAFs in the derivation of water quality criteria for organic chemicals. For the purpose of applying partition theory, aquatic biota can be modelled as consisting of water, lipid, and non-lipid organic matter (Barber et al. 1991). In this model, an organic chemical in aquatic biota exists in three forms:

1. Chemical that is freely dissolved in the water that is in the biota.
2. Chemical that is partitioned to the lipid that is in the biota.
3. Chemical that is partitioned to non-lipid organic matter in the biota. The total concentration of chemical in the water inside the biota includes chemical that is partitioned to lipid and non-lipid organic matter in the water.

According to this model:

$$C_{B}^{t} = (f_{W})(C_{WB}^{fd}) + (f_{R})(C_{L}) + (f_{N})(C_{N}) \qquad (8)$$

where:

f_W = the fraction of the aquatic biota that is water.
$C_{WB}^{\tau\alpha}$ = the freely dissolved concentration of the organic chemical in the water in the aquatic biota.
f_R = the fraction of the aquatic biota that is lipid.
C_L = the concentration of the organic chemical in the lipid.
f_N = the fraction of the aquatic biota that is non-lipid organic matter.
C_N = the concentration of the organic chemical in the non-lipid organic matter in the aquatic biota.

The most important partitioning of the organic chemical within the aquatic biota is between the lipid and the water, which is described by the following equation:

$$K_{LW} = \frac{C_{L}}{C_{WB}^{fd}} \qquad (9)$$

where:

K_{LW} = the lipid-water partition coefficient.

"K_{LW}" (Gobas 1993) is used herein because it is more descriptive than "K_L", which is used by DiToro et al. (1991). This partition coefficient is central to the equilibrium partition approach that is used to derive sediment quality criteria (DiToro et al. 1991), the Gobas model that is used to derive Food-Chain Multipliers for the final Guidance, and the equations given here that are used to derive BCFs and BAFs for the final Guidance.

In order for equations 8 and 9 to be correct, partition theory requires that the concentration of the organic chemical in the lipid, C_L, be defined as:

$$\frac{\text{amount of chemical partitioned to lipid in aquat}}{\text{the amount of lipid in the aquatic biota}}$$

It is difficult to determine C_L experimentally because it is not easy to measure only the chemical that is partitioned to the lipid (i.e., it is not easy to separate the three different kinds of chemical that, according to the model, exist in aquatic biota). Because all of the organic chemical in the biota is measured when C_R is determined, C_R can be determined easily, and C_R is higher than C_L.

It is useful to define another bioconcentration factor as:

$$BCF_L^{fd} \ ' \ \frac{C_L}{C_W^{fd}} \qquad (10)$$

Because C_L is lower than C_R, $BCF_L^{fd} < BCF_R^{fd}$.

The only difference between K_{LW} and BCF_L^{fd} is that the denominator in K_{LW} is C_{WB}^{fd}, whereas the denominator in BCF_L^{fd} is C_W^{fd}. When partition theory applies, however, all phases are in equilibrium and so:

$$C_W^{fd} \ ' \ C_{WB}^{fd} \qquad (11)$$

Therefore, when the organic chemical is not metabolized by the aquatic biota and when growth dilution is negligible:

$$BCF_L^{fd} \ ' \ K_{LW} \qquad (12)$$

Because octanol is a useful surrogate for lipid, a reasonable approximation is that:

$$K_{LW} \ ' \ K_{OW} \qquad (13)$$

where:

K_{OW} = the octanol-water partition coefficient.

Thus:

$$\text{predicted } BCF_L^{fd} \text{ ' } K_{LW} \text{ ' } K_{OW} \tag{14}$$

By using equations 9 and 11 to substitute for C_L and C_{WB}^{fd} in equation 8:

$${}_B^{t} \text{ ' } (f_W)(C_W^{fd}) \ \% \ (f_R)(BCF_L^{fd})(C_W^{fd}) \ \% \ (f_N)(C_N \tag{15}$$

By using equation 6 to substitute for C_W^{fd} in equation 15:

$$(f_W)(f_{fd})(C_W^t) \ \% \ (f_R)(BCF_L^{fd})(f_{fd})(C_W^t) \ \% \ (f_N) \tag{16}$$

Dividing by C_W^t gives:

$$\frac{{}_B^{t}}{{}_W^{t}} \text{ ' } (f_W)(f_{fd}) \ \% \ (f_R)(BCF_L^{fd})(f_{fd}) \ \% \ \frac{(f_N)(C_N}{C_W^t} \tag{17}$$

Using equation 1 and rearranging gives:

$$CF_T^t \text{ ' } (f_{fd})[\ f_W \ \% \ (f_R)(BCF_L^{fd}) \ \% \ \frac{(f_N)(C_N)}{(f_{fd})(C_W^t)}\ ] \tag{18}$$

Using equation 6:

$$BCF_T^t \text{ ' } (f_{fd})[\ f_W \ \% \ (f_R)(BCF_L^{fd}) \ \% \ \frac{(f_N)(C_N)}{C_W^{fd}}\ ] \tag{19}$$

Substituting $x \text{ ' } f_W \ \% \ (f_N)(\frac{C_N}{C_W^{fd}})$ and rearranging gives:

$$BCF_T^t \text{ ' } (f_{fd})[\ x \ \% \ (f_R)(BCF_L^{fd})\ ] \tag{20}$$

The term "$(f_R)(BCF_L^{fd})$" accounts for the amount of organic chemical that is partitioned to the lipid in the biota, whereas in "x", the term "f_W" accounts for the amount of organic chemical that is freely dissolved in the water in the biota and the term "$(f_N)(\frac{C_N}{C_W^{fd}})$"

accounts for the amount of organic chemical that is partitioned to non-lipid organic matter in the biota. The relative magnitudes of these three terms depend on the following:

a. Because of bones and other inorganic matter, the sum of $f_W + f_R + f_N$ must be less than 1.
b. f_W is usually about 0.7 to 0.9.
c. Because f_R must be measured if the BAF or BCF is to be useful, f_R is known for the aquatic biota; it is usually between 0.03 and 0.15.
d. The term " $\left(\frac{C_N}{C_W^{fd}}\right)$ " is similar to BCF_L^{fd} (see equation 10) and is therefore probably related to K_{OW} (see equation 14), although the affinity of the chemical for non-lipid organic matter is probably much less than its affinity for lipid.

Although such considerations aid in understanding "x", the magnitude of "x" in equation 20 is important only for chemicals whose log K_{OW}s are in the range of 1 to 3. For organic chemicals whose log K_{OW}s are about 1, f_{fd} is about 1. In addition, such chemicals distribute themselves so as to have similar concentrations in water and in the different organic phases in the aquatic biota, which means that BCF_T^t will be approximately 1 if both metabolism and growth dilution are negligible. An organic chemical whose log K_{OW} is less than 1 will also have a BCF_T^t on the order of 1 because water is the predominant component in aquatic biota. Setting "x" equal to 1 is about right in the range of log K_{OW}s in which it is not negligible (see also McCarty et al. 1992).

Substituting x = 1 into equation 20:

$$BCF_T^t = (f_{fd})[1 + (f_R)(BCF_L^{fd})] \tag{21}$$

Rearranging gives:

$$BCF_L^{fd} = \left(\frac{BCF_T^t}{f_{fd}} - 1\right)\left(\frac{1}{f_R}\right) \tag{22}$$

BCF_L^{fd} can be called the "baseline BCF" because it is the most useful BCF for extrapolating from one species to another and from one water to another for organic chemicals with both high and low K_{OW}s. The baseline BCF is intended to reference bioconcentration of organic chemicals to partioning between lipid and water.

Equations 12, 13, and 22 demonstrate that both K_{OW} and

$$\left(\frac{BCF_T^t}{f_{fd}} - 1 \right)\left(\frac{1}{f_R} \right)$$

are useful approximations of the baseline BCFs. It will probably be possible to improve both approximations within a few years, but such improvements might not affect the BCFs substantially and probably will not require changes in the rest of the equations or the terminology.

When BCF_T^t is greater than 1000, the "-1" in equation 22 is negligible and so this equation becomes equivalent to equation 7 (i.e., when BCF_T^t is large, BCF_R^{fd} is a useful approximation of the baseline BCF).

Bioaccumulation

By analogy with equations 21 and 22:

$$BAF_T^t = (f_{fd})\left[1 + (f_R)(BAF_L^{fd}) \right] \tag{23}$$

$$BAF_L^{fd} = \left(\frac{BAF_T^t}{f_{fd}} - 1 \right)\left(\frac{1}{f_R} \right) \tag{24}$$

BAF_L^{fd} can be called the "baseline BAF" because it is the most useful BAF for extrapolating from one species to another and from one water to another for chemicals with both high and low K_{OW}s.

It is convenient to define a food-chain multiplier (FCM) as:

$$FCM = \frac{\text{baseline BAF}}{\text{baseline BCF}} \equiv \frac{BAF_L^{fd}}{BCF_L^{fd}} \tag{25}$$

Some of the consequences of equation 25 are:

1. Substituting equations 22 and 24 into equation 25:

$$FCM = \frac{BAF_T^t - f_{fd}}{BCF_T^t - f_{fd}} \tag{26}$$

Therefore, $BAF_T^t = (FCM)(BCF_T^t)$ only when f_{fd} is much less than BAF_T^t and

BCF_T^t.

2. When FCM = 1 (as for trophic level 2 in the Gobas model):

$$\text{baseline BAF ' baseline BCF} \qquad (27)$$

3. Predicted baseline BAFs can be obtained using FCMs and the following rearrangement of equation 25:

predicted baseline BAF = (FCM)(baseline BCF) (28)

   a. Using a laboratory-measured BCF in equation 22:

$$\text{predicted baseline BAF} \quad ' \; (FCM)(\text{measured } BCF_L^{fd}) \qquad (29)$$

$$' \; (FCM)\left(\frac{BCF_T^t}{f_{fd}} \;\&\; 1\right)\left(\frac{1}{f_R}\right) \qquad (30)$$

   b. Using a predicted BCF in equation 14:

$$\text{predicted baseline BAF} \quad ' \; (FCM)(\text{ predicted } BCF_L^{fd}) \qquad (31)$$

$$' \; (FCM)(K_{OW}) \qquad (32)$$

The FCMs used to calculate predicted baseline BAFs must be appropriate for the trophic level of the aquatic biota for which the predicted baseline BAF is intended to apply.

Although BAFs can be related to BCFs using FCMs, BAFs and BCFs can also be related using Biomagnification Factors (BMFs). The tow systems are entirely compatible, but confusion can result if the terms are not used consistently and clearly. Because both systems are used in the final Guidance and elsewhere, it is appropriate to explain the relation between the two here. The basic difference is that FCMs always relate back to trophic level one, whereas BMFs always relate back to the next trophic level. In the FCM system:

BAF_{TL1} = BCF

BAF_{TL2} = $(FCM_{TL2})(BAF_{TL1})$

BAF_{TL3} = $(FCM_{TL3})(BAF_{TL1})$

$BAF_{TL4} = (FCM_{TL4})(BAF_{TL1})$

In the BMF system:

$BAF_{TL1} = BCF$

$BAF_{TL2} = (BMF_{TL2})(BAF_{TL1})$

$BAF_{TL3} = (BMF_{TL3})(BAF_{TL2})$

$BAF_{TL4} = (BMF_{TL4})(BAF_{TL3})$

Therefore:

$BMF_{TL2} = FCM_{TL2}$

$BMF_{TL3} = (FCM_{TL3})/(FCM_{TL2})$

$BMF_{TL4} = (FCM_{TL4})/(FCM_{TL3})$

Both metabolism and growth dilution can cause BMFs to be less than 1.

Calculation of Criteria

Baseline BCFs and BAFs can be extrapolated between species and waters, but they cannot be used directly in the calculation of criteria that are based on the total concentration of the chemical in the water. The BCFs and BAFs that are needed to calculate such criteria can be calculated from measured and predicted baseline BCFs and BAFs using the following equations, which are derived from equations 21 and 23:

$$BCF_T^t = [1 + (\text{baseline BCF})(f_R)](f_{fd}) \qquad (33)$$

$$BAF_T^t = [1 + (\text{baseline BAF})(f_R)](f_{fd}) \qquad (34)$$

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Appendix D. Derivation of Baseline BAFs from Field-Measured BAFs and Laboratory-Measured BCFs

Some of the more important restrictions on use of field-measured BAFs and laboratory-measured BCFs in the final Guidance are:

1. A laboratory-measured BCF is not used if it is based on the measurement of radioactivity unless the BCF is intended to include metabolites or when there is confidence that there is no interference due to metabolites.

2. For a chemical for which log K_{OW} is greater than 4, a laboratory-measured BCF or a field-measured BAF is not used unless the concentrations of POC and DOC were measured or can be reliably estimated in the ambient water because:
   a. The higher the K_{OW}, the more the calculated baseline BAF will depend on the concentrations of POC and DOC.
   b. If log K_{OW} is very large and there is fast equilibrium with POC and DOC, uptake via ingestion of food particles in a bioconcentration test might be substantial, thereby giving a high estimate of the bioconcentration factor.

   If reliable values for POC and DOC are not available and if log K_{OW} is less than 4, the fraction of the toxicant that is not freely dissolved is negligible.

3. BCFs and BAFs are used only if the percent lipid was measured or could be reliably estimated.

Baseline BAFs were not calculated in this appendix from field data reported by Oliver and Niimi (1988) because baseline BAFs were calculated from these data in Tables 4, 5 and 8. The equation presented here is equivalent to that used for Tables 4, 5, and 8, as demonstrated below with DDE.

The following equation from Section III.B is used to calculate the fraction of the chemical that is freely dissolved in the ambient water:

$$133f_{fd} = \frac{1}{1 + \frac{(DOC)(K_{OW})}{10} + (POC)(K_{OW})}$$

where:

f_{fd} = fraction that is freely dissolved.
DOC = concentration of dissolved organic carbon (kg/L).
POC = concentration of particulate organic carbon (kg/L).
K_{OW} = octanol-water partition coefficient.

The following equation from Appendix C is used to calculate a measured baseline BAF from a field-measured BAF:

$$\text{measured baseline BAF} = \left(\frac{BAF_T^t}{f_{fd}} - 1\right)\left(\frac{1}{f_R}\right)$$

where:

BAF_T^t = BAF based on total concentrations of the organic chemical in the tissue and in the ambient water.

f_R = fraction lipid in the tissue.

The trophic level to which the baseline BAF applies depends on the organisms used in the determination of the field-measured BAF.

The following equation from Appendix C is used to calculate a measured baseline BAF from a laboratory-measured BCF:

$$\text{predicted baseline BAF} = (FCM)\left(\frac{BCF_T^t}{f_{fd}} - 1\right)\left(\frac{1}{f_R}\right)$$

where:

BCF_T^t = BCF based on total concentrations of the organic chemical in the tissue and in the ambient water.

FCM = Food-Chain Multiplier.

The trophic level to which the predicted baseline BAF applies depends on the trophic level to which the FCM applies.

Benzene

Based on a predicted BCF and a FCM. See Appendix H.

Chlorobenzene

Based on a predicted BCF and a FCM. See Appendix H.

Chlordane

The following field-measured BAFs are available for alpha and gamma chlordane:

BAF	% L	Species	Reference
1,400,000	7.592	R. trout	Oliver and Niimi 1985
76,000	7.592	R. trout	Oliver and Niimi 1985

Geometric mean BAF = 326,190

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for chlordane is 6.00. The resulting value of f_{fd} is 0.7843, and then:

$$\text{Measured baseline BAF}_{TL4} \text{ ' } \left(\frac{326,190}{0.7843} \text{ \& } 1\right)\left(\frac{1}{0.07592}\right) \text{ ' } 5,478,115$$

A measured baseline BAF of 6,166,000 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

Cyanides

No appropriate BAF or BCF exists for this chemical.

DDE

The following field-measured BAF is available:

BAF	% L	Species	Reference
18,000,000	7.592	R. trout	Oliver and Niimi 1985

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for DDE is 6.763. The resulting value of f_{fd} is 0.3856, and then:

$$\text{easured baseline BAF}_{TL4} \text{ ' } \left(\frac{18,000,000}{0.3856} \text{ \& } 1\right)\left(\frac{1}{0.07592}\right) \text{ ' } 614,864,29$$

A measured baseline BAF of 223,900,000 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

The following field-measured BAF is also available:

BAF	% L	Species	Reference
11,315,789	11.00	Salmonids	Oliver and Niimi 1988

Salmonids are expected to be in trophic level 4. These data were obtained from Lake Ontario, but the water sample was centrifuged before the concentration of DDE was measured. Thus the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.0 kg/L

The log K_{OW} derived in Appendix B for DDE is 6.763. The resulting value of f_{fd} is 0.4632, and then:

$$\text{Measured baseline BAF}_{TL4} = \left(\frac{11{,}315{,}789}{0.4632} - 1\right)\left(\frac{1}{0.11}\right) = 222{,}083{,}394$$

The log of this baseline BAF is 8.3465, which is very similar to the value of 8.35 that is derived in Table 8 for DDE from the same dataset. Thus the equation used here is equivalent to that used to calculate the fiel-measured BAFs given in Tables 4, 5, 6, 7 and 8 .

Dieldrin

Based on the BSAF methodology. See Section III.E and Appendix H.

2,4-Dimethylphenol

Based on a predicted BCF and a FCM. See Appendix H.

2,4-Dinitrophenol

Based on a predicted BCF and a FCM. See Appendix H.

Hexachlorobenzene

The following field-measured BAFs are available:

BAF	% L	Species	Reference

1,467,000	20.9	L. trout	Oliver and Nicol 1982
494,667	7.592	R. trout	Oliver and Niimi 1983

Geometric mean BAF = 851,866
Geometric mean % L = 12.60

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for hexachlorobenzene is 5.600. The resulting value of f_{fd} is 0.9013, and then:

$$\text{Measured baseline BAF}_{TL4} \;'\; \left(\frac{851{,}866}{0.9013} \;\&\; 1\right)\left(\frac{1}{0.1260}\right) \;'\; 7{,}501{,}150$$

A measured baseline BAF of 2,512,000 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

Hexachlorobutadiene

A field-measured baseline BAF of 354,813 is given in Table 4 for sculpin, which is at trophic level 3. For this chemical, the log K_{OW} is 4.842, and so the FCM for trophic level 3 is 2.59 and the FCM for trophic level 4 is 2.00. This results in a baseline BAF of (354,813)(2.00)/(2.59) = 273,987 for trophic level 4.

The following field-measured BAF is available:

BAF	% L	Species	Reference
3,274	7.592	R. trout	Oliver and Niimi 1983

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for hexachlorobutadiene is 4.842. The resulting value of f_{fd} is 0.9812, and then:

$$\text{Measured baseline BAF}_{TL4} = \left(\frac{3,274}{0.9812} - 1\right)\left(\frac{1}{0.07592}\right) = 43,937$$

This measured baseline BAF of 43,937 is considered a better value for trophic level 4 because it is based on concentrations in fish at trophic level 4.

alpha-Hexachlorocyclohexane (alpha-HCCH)

The following laboratory-measured BCFs are available:

BCF	% L	Baseline BCF	Reference
140	3.1	4484	Canton et al. 1975,1978
124	3.1	3968	Canton et al. 1975,1978
1600	7.19	22239	Oliver and Niimi 1985
2400	7.38	32507	Oliver and Niimi 1985

Because the log K_{OW} derived in Appendix B for alpha-HCCH is 3.776, which is less than 4, f_{fd} is assumed to be 1.0. The baseline BCFs are calculated using the equation given above.

Geometric mean baseline BCF = 10650

The FCM for trophic level 4 for log K_{OW} = 3.776 is 1.04, which gives:

Predicted baseline BAF_{TL4} = (10650)(1.04) = 11076.

The following field-measured BAF is available:

BAF	% L	Species	Reference
700	7.592	R. trout	Oliver and Niimi 1985

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for alpha-HCCH is 3.776. The resulting value of f_{fd} is 0.9984, and then:

$$\text{Measured baseline BAF}_{TL4} \; ' \; \left(\frac{700}{0.9984} \; \& \; 1\right)\left(\frac{1}{0.07592}\right) \; ' \; 9,222$$

A measured baseline BAF of 48,980 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

Hexachloroethane

The following laboratory-measured BCFs are available:

BCF	% L	Species	Reference
510	8.2	R. trout	Oliver and Niimi 1983
1200	8.7	R. trout	Oliver and Niimi 1983

Geometric mean BCF = 782
Geometric mean % Lipid = 8.45

Because the log K_{OW} derived in Appendix B for hexachloroethane is 4.040, f_{fd} is assumed to be 1.0. Therefore:

$$\text{Measured baseline BCF} \; ' \; \left(\frac{782}{1} \; \& \; 1\right)\left(\frac{1}{0.0845}\right) \; ' \; 9243$$

The FCM for trophic level 4 for log K_{OW} = 4.040 is 1.08, which gives:

Predicted baseline BAF_{TL4} = (9243)(1.08) = 9982.

The following field-measured BAF is available:

BAF	% L	Species	Reference
1,302	7.592	R. trout	Oliver and Niimi 1983

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for hexachloroethane is 4.040. The resulting value of f_{fd} is 0.9970, and then:

$$\text{Measured baseline BAF}_{TL4} = \left(\frac{1,302}{0.9970} - 1\right)\left(\frac{1}{0.07592}\right) = 17,188$$

Lindane

The following laboratory-measured BCFs are available:

BCF	% L	Baseline BCF	Reference
180	7.6	2355	Veith et al. 1979
420	2.65	15811	Rogers et al. 1983
1200	7.19	16676	Oliver and Niimi 1985
2000	7.38	27087	Oliver and Niimi 1985

Because the log K_{OW} derived in Appendix B for lindane is 3.673, which is less than 4, f_{fd} is assumed to be 1.0. The baseline BCFs are calculated using the equation given above.

Geometric mean baseline BCF = 11388

The FCM for trophic level 4 for log K_{OW} = 3.673 is 1.03, which gives:

Predicted baseline BAF_{TL4} = (11388)(1.03) = 11730.

The following field-measured BAF is available:

BAF	% L	Species	Reference
1000	7.592	R. trout	Oliver and Niimi 1985

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for lindane is 3.673. The resulting value of f_{fd} is 0.9987, and then:

$$\text{Measured baseline BAF}_{TL4} = \left(\frac{1,000}{0.9987} - 1\right)\left(\frac{1}{0.07592}\right) = 13,176$$

A measured baseline BAF of 85,110 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data..

Mercury

See Appendix E.

Methylene Chloride

Based on a predicted BCF and a FCM. See Appendix H.

Mirex

The following field-measured BAF is available:

BAF	% L	Species	Reference
15,000,000	7.592	R. trout	Oliver and Niimi 1985

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for mirex is 6.89. The resulting value of f_{fd} is 0.3190, and then:

$$\text{easured baseline } BAF_{TL4} \ ' \ \left(\frac{15,000,000}{0.3190} \ \& \ 1\right)\left(\frac{1}{0.07592}\right) \ ' \ 619,361,73$$

A measured baseline BAF of 134,900,000 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

Octachlorostyrene

The following field-measured BAF is available:

BAF	% L	Species	Reference
1,400,000	7.592	R. trout	Oliver and Niimi 1985

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for octachlorostyrene is 6.29. The resulting value of f_{fd} is 0.6510, and then:

$$\text{Measured baseline BAF}_{TL4} = \left(\frac{1{,}400{,}000}{0.6510} - 1\right)\left(\frac{1}{0.07592}\right) = 28{,}326{,}351$$

A measured baseline BAF of 117,500,000 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

PCBs

See Appendix F.

Pentachlorobenzene

The following field-measured BAFs are available:

BAF	% L	Species	Reference
56,570	20.9	L. trout	Oliver and Nicol 1982
16,150	7.592	R. trout	Oliver and Niimi 1983

Geometric mean BAF = 30,226
Geometric mean % L = 12.60

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for pentachlorobenzene is 5.106. The resulting value of f_{fd} is 0.9661, and then:

$$\text{Measured baseline BAF}_{TL4} = \left(\frac{30{,}226}{0.9661} - 1\right)\left(\frac{1}{0.1260}\right) = 248{,}299$$

A measured baseline BAF of 645,700 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

2,3,7,8-TCDD

Based on the BSAF methodology. See Section III.E and Appendix H.

1,2,3,4-Tetrachlorobenzene

The following field-measured BAFs are available:

BAF	% L	Species	Reference
69,280	20.9	L. trout	Oliver and Nicol 1982
8,769	7.592	R. trout	Oliver and Niimi 1983
7,700	7.592	R. trout	Oliver and Niimi 1985

Geometric mean BAF = 16,724
Geometric mean % L = 10.64

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for 1,2,3,4-tetrachlorobenzene is 4.592. The resulting value of f_{fd} is 0.9894, and then:

$$\text{Measured baseline BAF}_{TL4} = \left(\frac{16,724}{0.9894} - 1\right)\left(\frac{1}{0.1064}\right) = 158,855$$

A measured baseline BAF of 117,500 is derived in Table 8 based on Oliver and Niimi (1988); this is considered a better value and is used in the final Guidance because it is based on a more comprehensive set of data.

1,2,4,5-Tetrachlorobenzene

The following field-measured BAFs are available:

BAF	% L	Species	Reference

31,620	20.9	L. trout	Oliver and Nicol 1982
5,034	7.592	R. trout	Oliver and Niimi 1983

Geometric mean BAF = 12,616
Geometric mean % L = 12.60

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for 1,2,4,5-tetrachlorobenzene is 4.557. The resulting value of f_{fd} is 0.9902, and then:

$$\text{Measured baseline BAF}_{TL4}\ '\ \left(\frac{12,616}{0.9902}\ \&\ 1\right)\left(\frac{1}{0.1260}\right)\ '\ 101,110$$

Toluene

Based on a predicted BCF and a FCM. See Appendix H.

Toxaphene

The following field-measured BAF is available:

BAF	% L	Species	Reference
1,778,636	8.284	L. trout	Swain et al. 1986

Trout are expected to be at trophic level 4. These data were obtained from Siskiwit Lake, in which the concentrations of POC and DOC are expected to be similar to those in Lake Superior:

DOC = 0.000002 kg/L
POC = 0.00000004 kg/L

The log K_{OW} derived in Appendix B for toxaphene is 4.330. The resulting value of f_{fd} is 0.9949, and then:

$$\text{Measured baseline BAF}_{TL4}\ '\ \left(\frac{1,778,636}{0.9949}\ \&\ 1\right)\left(\frac{1}{0.08284}\right)\ '\ 21,580,789$$

1,2,4-Trichlorobenzene

The following laboratory-measured BCFs are available:

BCF	% L	Baseline BCF	Reference
2800	7.6	36829	Veith et al. 1979
1600	9.12	17533	Kosian et al. 1981
85	2.1(e)	4000	ssi and Calamari 1983
349	3.2(h)	10875	ssi and Calamari 1983
39	0.7(a)	5429	ssi and Calamari 1983
1300	8.2	15841	Oliver and Niimi 1983
3200	8.7	36770	Oliver and Niimi 1983
2300	7.19	31975	Oliver and Niimi 1985
3700	7.38	50122	Oliver and Niimi 1985
124	1.8	6833	Geyer et al. 1985
248	2.2	11227	Geyer et al. 1985
498	4.4	11295	Geyer et al. 1985
914	5.0	18260	Geyer et al. 1985
769	5.2	14769	Geyer et al. 1985
769	5.2	14769	Geyer et al. 1985
1127	5.7	19754	Geyer et al. 1985
1365	5.8	23517	Geyer et al. 1985
1442	7.7	18714	Geyer et al. 1985
991	8.2	12073	Geyer et al. 1985
410	3.79	10792	Carlson and Kosian 1987
2026	11.4	17763	Smith et al. 1990

Because the log K_{OW} derived in Appendix B for 1,2,4-trichlorobenzene is 3.990, which is less than 4, f_{fd} is assumed to be 1.0. The baseline BCFs are calculated using the equation given above.

Geometric mean baseline BCF = 15497

The FCM for trophic level 4 for log K_{OW} = 3.990 is 1.07, which gives:

Predicted baseline BAF_{TL4} = (15497)(1.07) = 16582

A field-measured baseline BAF of 37,154 is given in Table 2 of Section 3 for sculpin, which is at trophic level 3. For this chemical, the log K_{OW} is 3.990, and so the FCM for trophic level 3 is 1.24 and the FCM for trophic level 4 is 1.07. This results in a baseline BAF of (37,154)(1.07)/(1.24) = 32,060 for trophic level 4.

The following field-measured BAFs are available:

BAF	% L	Species	Reference
5,270	20.9	L. trout	Oliver and Nicol 1982
899.5	7.592	R. trout	Oliver and Niimi 1983
1,200	7.592	R. trout	Oliver and Niimi 1985

Geometric mean BAF = 1,785
Geometric mean % L = 10.64

Trout are expected to be in trophic level 4. These data were obtained from Lake Ontario, in which the concentrations of POC and DOC are expected to be:

DOC = 0.000002 kg/L
POC = 0.000000075 kg/L

The log K_{OW} derived in Appendix B for 1,2,4-trichlorobenzene is 3.990. The resulting value of f_{fd} is 0.9973, and then:

$$\text{Measured baseline } BAF_{TL4} = \left(\frac{1,785}{0.9973} - 1\right)\left(\frac{1}{0.1064}\right) = 16,812$$

This measured baseline BAF of 16,812 is considered a better value for trophic level 4 because it is based on concentrations in fish at trophic level 4.

Trichloroethylene

Based on a predicted BCF and a FCM. See Appendix H.

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Appendix E. Derivation of Baseline BAFs for Mercury

In the Gobas model, which is used in the derivation of BAFs and FCMs for organic chemicals, only bioconcentration applies to trophic levels 1 and 2, whereas biomagnification occurs between trophic levels 2 and 3 and between trophic levels 3 and 4. In their study with mercury, however, Watras and Bloom (1992) found that biomagnification occurred between trophic levels 1 and 2 and between trophic levels 2 and 3. Watras and Bloom (1992) only studied trophic levels 1, 2, and 3, but a substantial amount of data from other investigators show a biomagnification factor between fishes. Thus the model used here with mercury will provide for bioconcentration at trophic level 1, and biomagnification at trophic levels 2, 3, and 4.

The BCFs for inorganic mercury and methylmercury are 2,998 and 52,175 (U.S. EPA 1985). It is possible that the higher BCFs obtained in the tests with fathead minnows should not be used because they reflect some bioaccumulation, not just bioconcentration, due to the fact that this species is a grazer and therefore possibly ate food that contained mercury. Accumulation through food is considered negligible, however, because this species does not do well in chronic tests unless food is provided; it is unlikely that grazing would provide a substantial amount of food or mercury. It is, of course, also possible that the food provided for the fish might rapidly sorb mercury from the water; there is no reason to believe that such sorption is substantial or that it occurs more in bioconcentration tests with one species than with the other. Another possibility is that lower BCFs were obtained with salmonids than with fathead minnows because of growth dilution. Several investigators have determined BCFs for organic chemicals with small fish, such as guppies, to reduce or avoid the effects of growth dilution. If growth dilution occurs, bioconcentration tests with salmonids would produce BCFs that are too low unless calculation of the results accounts for growth dilution.

Based on the data of Gill and Bruland (1990), it will be assumed that, on the average, 17 percent of the total mercury in the Great Lakes is methylmercury and that 83 percent is inorganic mercury. Thus the weighted average BCF is: (0.17)(52,175) + (0.83)(2,998) = 11,358. Based on data for phytoplankton, Watras and Bloom (1992) obtained a BCF of about 25,000 for total mercury at a pH of 6.1. This pH is below 6.5 and therefore this BCF might not be appropriate for use in the derivation of water quality criteria.

The data of Watras and Bloom (1992) show an increase of about a factor of 2 from trophic level 1 to trophic level 2, and an increase of about a factor of 1.26 from trophic level 2 to trophic level 3.

A variety of studies have found that total mercury increases from prey fish to predator fish by factors ranging from 1.2 to 15, with a mean of about 5:

7.7 to 9.2	MacCrimmon et al. 1983
up to 8.4	Wren et al. 1983

up to 6 and 13	Skurdal et al. 1985
8 and 15	Mathers and Johansen 1985
2.9	Parks 1988
6.4	Cope et al. 1990

The BCF and BMFs derived above result in:

(11,358)(2.00) = 22,716
(22,716)(1.26) = 28,622
(28,622)(5.00) = 143,110

The corresponding FCMs are:

Trophic Level 2: FCM = 22,716/11,358 = 2.00
Trophic Level 3: FCM = 28,622/11,358 = (2.00)(1.26)
Trophic Level 4: FCM = 143,110/11,358 = (2.00)(1.26)(5.00)

Bloom (1992) concluded that "for all species studied, virtually all (>95%) of the mercury present is as CH_3Hg and that past reports of substantially lower CH_3Hg fractions may have been biased by analytical and homogeneity variability". Therefore, it will be assumed that 97.5 percent of the mercury in fish in the Great Lakes is methylmercury:

(28,622)(0.975) = 27,906
(143,110)(0.975) = 139,532

Although McKim et al. (1976) and Heiskary and Helwig (1983) found higher concentrations of mercury in the edible portion of fish than in the whole body, Huckabee et al. (1974) and Heisinger et al. (1979) found the same concentration in whole body and muscle tissue. Thus for a specific trophic level, the human health and wildlife BAFs will be the same.

This derivation indicates that for total mercury in the water column the baseline BAFs should be:

Trophic level	Baseline BAF
3	27,906
4	139,532

The difference between trophic levels 3 and 4 is important.

A. Comparison of field-measured BAFs for mercury with the BAFs derived above must properly identify the trophic level of the aquatic biota used in the determination of the field-measured BAF. If field-measured BAFs are compared to the BAF derived for trophic level 4, the field-measured BAFs must have been determined with aquatic biota that are in trophic level 4. Many of the field-measured BAFs for mercury have been determined with aquatic biota that is in trophic level 3. It might also be necessary to account for a different percent methylmercury in the water column. In addition, the age of the fish is probably important because the concentration of mercury in fish seems to increase consistently with age without showing signs of leveling off.

B. If the aquatic biota consumed by humans and wildlife is incorrectly assigned to too high a trophic level on the average, the resulting criteria will be unnecessarily low, but not because the derived BAFs for mercury are too high. For example, if all the consumed food is assumed to be trophic level 4, the BAF used to derive the criterion will be 139,532. If, however, the consumed food is actually a 1:1 combination of trophic levels 3 and 4, the BAF of 139,532 would be used with half of the consumed food, and a BAF of 27,906 would be used with the other half of the consumed food.

C. Identification of the trophic level of some species of fish must take into account the age and/or size of the specific organisms of concern. Some species of fish are in trophic level 3 when they are young, but are in trophic level 4 when they are older. The trophic level might also vary from one body of water to another, depending on the food chain. With both humans and wildlife, knowing the species consumed is not necessarily sufficient to allow an accurate identification of the trophic level of the consumed food.

EPA has completed a more comprehensive analysis of data concerning the bioaccumulation of mercury by fish, which is being peer reviewed at this time. The final Guidance had intended to use the baseline BAFs contained in the initial draft of the report but it was decided to wait until the report has been peer-reviewed and completed. The initial draft of the report contained higher baseline BAFs than those derived herein.

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Appendix F. Derivation of Baseline BAFs for PCBs

Although a K_{OW} can usefully describe the partitioning of a mixture between octanol and water, the relation between K_{OW}s and BAFs is more uncertain for mixtures than for individual chemicals. The additional uncertainty occurs because the composition of the mixture will differ from one phase to another, due to differential partitioning and to differences in metabolism by aquatic organisms. The uncertainty increases as the magnitudes of the differences between the properties of the individual components of the mixture increase.

Although Burkhard and Kuehl (1986), Burkhard et al. (1985), Chiou et al. (1977), de Bruijn et al. (1988), Karickhoff et al. (1979), Miller et al. (1985), Rapaport and Eisenreich (1984), Veith et al. (1979a), and Woodburn et al. (1984) have published measured values for the log K_{OW} of various PCB mixtures and congeners, the set of values published by Hawker and Connell (1988) is considered the best for use in the final Guidance. Similarly, laboratory-measured BCFs and BAFs have been reported in such publications as Bruggeman et al. (1981), Gobas and Schrap (1990), Gobas et al. (1989), Hansen et al. (1971), Oliver and Niimi (1984, 1985), Snarski and Puglisi (1976), Veith et al. (1979a,b), but the data reported by Oliver and Niimi (1988) are considered the best for use in the final Guidance.

Hawker and Connell (1988) and Oliver and Niimi (1988) contain K_{OW}s and BAFs, respectively, for individual PCB congeners and so mean values can be calculated for various of mixtures. Calculation of an arithmetic mean of the logarithms of the K_{OW}s or BAFs is equivalent to calculation of a geometric mean of the K_{OW}s or BAFs. A mean that is calculated by giving each value the same weight is often called an unweighted mean; alternatively a mean can be calculated by giving a weight of 1 to some values and giving a weight of 0 to all other values. Another alternative is to assign weights based on the relative amounts of the congeners in commercial mixtures or in organisms, water, and/or sediment, based on data reported in such publications as Schulz et al. (1989) and Oliver and Niimi (1988).

For the purpose of the final Guidance, it seems most appropriate to assign weights based on the concentrations in fish in the Great Lakes, because these represent the congeners that are ingested the most by eating aquatic life from the Great Lakes. Table F1 contains the relevant information and most of the necessary calculations. The results are:

$$\text{Mean log } K_{OW} = \frac{26{,}735.25}{4{,}057.3} = 6.589419$$

Weighted geometric mean K_{OW} = 3,885,000

$$\text{Mean log BAF}_{TL3} = \frac{31{,}413.95}{4{,}057.3} = 7.742575$$

Weighted geometric mean BAF_{TL3} = 55,281,000

$$\text{Mean log BAF}_{TL4} = \frac{32{,}728.31}{4{,}057.3} = 8.066525$$

Weighted geometric mean BAF_{TL4} = 116,553,000

These mean values are used when generic values are needed for PCBs in the final Guidance.

By using a log K_{OW} of 6.589, FCMs from Table 2, and equation 32 from Appendix C, the following results are obtained:

For trophic level 3:

FCM_{TL3} = 13.94
predicted BAF_{TL3} = 54,110,000

For trophic level 4:

FCM_{TL4} = 25.53
predicted BAF_{TL} = 99,090,000

The weighted geometric mean field-measured BAFs calculated above are higher than these predicted BAFs.

It is also possible to calculated a "mean" BAF_{TL4} for PCBs from the data given by Oliver and Niimi (1988) for total PCBs in water and salmonids:

$$BAF_{TL4} = \frac{(4300\ \text{ng/g})(1000\ \text{pg/ng})(1000\,\text{g/l})}{(1100\ \text{pg/L})(0.11)(0.4837)} = 73{,}470{,}000$$

where 0.11 is the fraction of the salmonids that was lipid and 0.4837 is the fraction dissolved that is calculated for a chemical with log K_{OW} = 6.589 in Lake Ontario. This value is lower that both of the above values for BAF_{TL4}.

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Table F.1. Log K_{OW}s and BAFs for PCB Congeners

Congener	**Weight**	**Log K_{OW}**	**Product**	**BAF**	**BAF**	**Product**	**BAF**	**Product**
			(Log K_{OW})	(Scul)	(Ale)	ave(Sc+Al)	(Salmon)	(Salmon)
28+31	36.	5.67	204.12	6.37	6.68	234.90	6.89	248.04
18	4.3	5.24	22.53	5.97	6.39	26.57	5.75	24.73
22 (1.7)	0.	5.58	0.00			0.00	6.39	0.00
16 (0.3)	0.	5.16	0.00			0.00	5.92	0.00
33 (0.3)	0.	5.60	0.00			0.00	5.32	0.00
17 (0.3)	0.	5.25	0.00			0.00	5.52	0.00
32 (0.3)	0.	5.44	0.00			0.00	6.76	0.00
66	160.	6.20	992.00	7.45	7.57	1,201.60	7.79	1,246.40
70+76	140.	6.17	863.80	7.06	7.31	1,005.90	7.56	1,058.40
56+60+81	74.	6.19	458.06	7.48	7.79	564.99	7.96	589.04
52	62.	5.84	362.08	6.80	6.84	422.84	7.01	434.62
47+48	60.	5.82	349.20	6.15	6.85	390.00	7.18	430.80
44	45.	5.75	258.75	6.65	6.86	303.98	6.96	313.20
74	38.	6.20	235.60	7.30	7.35	278.35	7.66	291.08
49	31.	5.85	181.35	6.77	6.98	213.13	7.13	221.03
64	28.	5.95	166.60	7.16	7.30	202.44	7.51	210.28
42	10.	5.76	57.60	7.07	7.38	72.25	7.49	74.90
53 (1.5)	0.	5.62	0.00			0.00	6.51	0.00
40 (1.3)	0.	5.66	0.00			0.00	6.55	0.00
101	270.	6.38	1,722.60	7.30	7.25	1,964.25	7.45	2,011.50
84	260.	6.04	1,570.40	8.05	7.90	2,073.50	8.28	2,152.80
118	250.	6.74	1,685.00	7.86	7.71	1,946.25	8.15	2,037.50
110	230.	6.48	1,490.40	7.44	7.51	1,719.25	7.79	1,791.70
87+97	200.	6.29	1,258.00	7.54	7.89	1,543.00	8.08	1,616.00
105	110.	6.65	731.50	7.82	7.72	854.70	8.13	894.30
95	80.	6.13	490.40	6.98	7.14	564.80	7.25	580.00
85	58.	6.30	365.40	7.50	7.67	439.93	7.89	457.62

Table F.1. (Continued). Log K_{OW}s and BAFs for PCB Congeners

Congener	**Weight**	**Log K_{OW}**	**Product**	**BAF**	**BAF**	**Product**	**BAF**	**Product**
			(Log K_{OW})	(Scul)	(Ale)	ave(Sc+Al)	(Salmon)	(Salmon)
92	53.	6.35	336.55	7.70	7.93	414.20	8.11	429.83
82	29.	6.20	179.80	7.60	7.86	224.17	8.13	235.77
91	29.	6.13	177.77	6.44	6.74	191.11	6.92	200.68

Table F.1. (Continued). Log K_{OW}s and BAFs for PCB Congeners

Congener	**Weight**	**Log K_{OW}**	**Product**	**BAF**	**BAF**	**Product**	**BAF**	**Product**
			(Log K_{ow})	(Scul)	(Ale)	ave(Sc+Al)	(Salmon)	(Salmon)
99 (20)	0.	6.39	0.00		7.37	0.00	7.39	0.00
153	430.	6.92	2,975.60	8.05	7.82	3,412.05	8.32	3,577.60
138	260.	6.83	1,775.80	8.06	7.89	2,073.50	8.30	2,158.00
149	190.	6.67	1,267.30	7.28	7.75	1,427.85	7.99	1,518.10
146	88.	6.89	606.32	8.49	8.30	738.76	8.73	768.24
141	83.	6.82	566.06	8.11	7.96	666.91	8.32	690.56
151	51.	6.64	338.64	8.34	8.17	421.01	8.51	434.01
132	39.	6.58	256.62	7.41	7.45	289.77	7.56	294.84
136	31.	6.22	192.82	7.13	7.25	222.89	7.37	228.47
180	200.	7.36	1,472.00	8.45	8.15	1,660.00	8.58	1,716.00
187+182	130.	7.19	934.70	8.07	7.99	1,043.90	8.43	1,095.90
170+190	84.	7.37	619.08	9.15	8.84	755.58	9.20	772.80
183	71.	7.20	511.20	8.81	8.46	613.09	9.03	641.13
177	36.	7.08	254.88	8.63	8.54	309.06	9.01	324.36
174	32.	7.11	227.52	8.24	8.51	268.00	8.74	279.68
203+196	52.	7.65	397.80	9.14	8.82	466.96	9.26	481.52
194	23.	7.80	179.40	8.52	8.22	192.51	8.56	196.88
SUM	4,057.3		26,735.25			31,413.95		32,728.31

The weights are those reported by Oliver and Niimi (1988) for salmonids. Oliver and Niimi (1988) did not report the concentrations of congeners 22, 16, 33, 17, 32, 53, 40, and 99 in sculpin and/or alewives. To avoid irregularities in the treatment of the data, these eight were all assigned weights of zero. The actual weights of the eight are given in parentheses in the first column. The total weight for the eight is 25.7, which means that the total weight of all congeners in salmonids was 4083; the eight constitute about 0.6 percent of the total for all congeners.

The log K_{OW}s and BAFs are from Tables 4, 5, and 8.

Appendix G. Baseline BAFs for Trophic Level Four by Four Methods

The purpose of this appendix is to identify how many of the four methods in the final Guidance have been used to derive baseline BAFs for 31 chemicals for:

1) Use in deriving human health criteria for chemicals in Table 3 of part 132
2) Use in deriving wildife criteria for chemicals on Table 4 of part 132
3) Use in determining the bioaccumulative chemicals of concern in Table 6a of part 132.

Baseline BAFs for the other 107 chemicals of initial focus will be available in a separate document, "Derivation of Human Health and Wildlife Bioaccumulation Factors for the Great Lakes Initiative." Because they are referenced to a standard set of conditions, baseline BAFs for trophic level 4 are used in this appendix, although those for trophic level 3 could have been used. For each chemical, baseline BAFs were derived by each of the four methods whose data requirements were satisfied.

For inorganic chemicals, the BAF based on the wet weight of muscle tissue of species consumed by humans is used as the baseline BAF.

The four baseline BAFs that can be derived for organic chemicals using the methods described in the final Guidance are:

1. A measured baseline BAF that is based on field data that includes the measured concentrations of the chemical in tissue of aquatic organisms and in the ambient water.

   A measured baseline BAF is calculated from a field-measured BAF_T^L by using the equation:

$$\text{Measured baseline BAF} = \left(\frac{\text{measured } BAF_T^t}{f_{fd}} \; \& \; 1\right)\left(\frac{1}{f_R}\right)$$

   Except as noted, the measured baseline BAFs are from Table 8 in Section III.D.

2. A predicted baseline BAF that is based on BSAF methodology.

   All the baseline BAFs predicted using BSAF methodology are from Table 10.

3. A predicted baseline BAF that is based on a laboratory-measured BCF and a Food-Chain Multiplier (FCM); the FCM is 1 for most inorganic chemicals and is derived from log K_{OW} for organic chemicals.

   A predicted baseline BAF is calculated from a measured BCF_T^L by using the equation:

$$\text{Predicted baseline BAF} = (\mathrm{FCM})\left(\frac{\text{measured BCF}_T^t}{f_{fd}} \,\&\, 1\right)\left(\frac{1}{f_R}\right)$$

Except as noted, baseline BAFs based on laboratory-measured BCFs and FCMs are derived in Appendix D.

4. A predicted baseline BAF that is based on a predicted BCF and a FCM, where the predicted baseline BCF equals K_{OW} and the FCM is derived from log K_{OW}.

   A predicted baseline BAF is calculated from a predicted BCF by using the equation:

$$\text{Predicted baseline BAF} = (\mathrm{FCM})(K_{OW})$$

   A predicted baseline BAF obtained using this equation will equal one obtained using the Gobas model.

Method 1 gives the most preferred baseline BAF, whereas method 4 gives the least preferred. Baseline BAFs may be derived using other methods if justified by good science. All four procedures can be used with organic chemicals, but only procedures 1 and 3 can be used with inorganic chemicals. Some measured and predicted BCFs and BAFs are geometric means.

BAFs less than 10 are rounded to one decimal digit; BAFs between 10 and 1000 are rounded to whole numbers; BAFs greater than 1000 are rounded to four significant digits; this does not imply anything about the precision or accuracy of the values. All BAFs are intermediate values in the calculation of permit limits and so critical rounding should be performed only at the permit limit. For a chemical with a low BAF, however, the criterion is controlled by intake via ingestion of water rather than by ingestion of tissue of aquatic life. Thus a low BAF does not need many digits.

Except as noted, the values given for log K_{OW} are derived in Appendix B using the procedure described in Appendix A.

The FCMs for organic chemicals are derived by linear interpolation of the values given in Table F.2.

Table G.1. Baseline BAFs for Trophic Level 4

Chemical	Measured BAF for T.L. 4	Predicted BAF for Trophic Level 4			Log K_{OW}	FCM_{TL4}	FCM_{TL3}
	(Method 1)	(Method 2)	(Method 3)	(Method 4)			
Benzene				137	2.138	1.00	1.00
Chlordane	6,166,000	34,290,000[a]		16,000,000	6.00	16.00	10.56[b]
Chlorobenzene				740	2.865	1.01	1.02
Cyanide							
DDD	10,000,000	4,390,000		19,460,000	6.058	17.03	11.01[b]
DDE	223,900,000	456,000,000		153,900,000	6.763	26.56	14.30[b]
DDT	60,260,000	53,300,000		67,470,000	6.450	23.94	13.44[b]
Dieldrin		19,300,000[f]		941,600	5.200	4.73	4.79
2,4-Dimethylphenol				200	2.30	1.00	1.01
2,4-Dinitrophenol				37	1.570	1.00	1.00
Hexachlorobenzene	2,512,000	501,000		3,404,000	5.600	8.55	7.10[b]
Hexachlorobutadiene	43,940[c]			139,000	4.842	2.00	2.59
Hexachlorocyclohexane	64,570[g]			6,111	3.769	1.04	1.15[b]
alpha-Hexachlorocyclohexane	48,980	200,000	11,076	6,209	3.776	1.04	1.15[b]
beta-Hexachlorocyclohexane	64,570[g]			7,229	3.842	1.04	1.18[b]
delta-Hexachlorocyclohexane	64,570[g]			6,111	3.769	1.04	1.15[b]
Hexachloroethane	17,190[c]		9,982	11,840	4.040	1.080	1.28
Lindane	85,110	43,400	11,730	4,851	3.673	1.03	1.12[b]
Mercury			140,000[d]			12.60	2.52

Chemical	**Measured BAF for T.L. 4**	**Predicted BAF for Trophic Level 4**			**Log K_{OW}**	**FCM_{TL4}**	**FCM_{TL3}**
	(Method 1)	**(Method 2)**	**(Method 3)**	**(Method 4)**			
Methylene chloride				18	1.25	1.00	1.00
Mirex	134,900,000	143,000,000		207,000,000	6.89	26.67	14.39[b]
Octachlorostyrene	117,500	25,800,000		41,920,000	6.29	21.50	12.63[b]
PCBs	116,600,000[e]			99,090,000	6,589[e]	25.53	13.94[b]
Pentachlorobenzene	645,700	64,700		408,500	5.106	3.20	3.67[b]
Photomirex	117,500,000	371,100,000		207,000,000	6,89	26.67	14.39[b]
2,3,7,8-TCDD		9,000,000		273,200,000	7.02	26.09	14.27[b]
1,2,3,4-Tetrachlorobenzene	117,500	7,250		56,670	4.592	1.45	1.94[b]
1,2,4,5-Tetrachlorobenzene	101,110[c]			50,480	4.557	1.40	1.87
Toluene				516	2.713	1.00	1.02
Toxaphene	21,580,000[c]			25,660	4.330	1.20	1.53
Trichloroethylene				339	2.53	1.00	1.01

[a] This is the geometric meanof the mean baseline BAFs for the g, t, and c isomer of chlordane in Table 10.

[b] Not used.

[c] See Appendix D.

[d] See Appendix E.

[e] See Appendix F.

[f] This is based on concentrations of dieldrin in sediment and fish. However, the concentration in fish is probably partially due to exposure of the fish to aldrin, which is converted to dieldrin. Thus this BAF is probably not appropriate where there is substantially more or less aldrin.

[g] This is the geometric mean of the measured baseline BAFs for alpha-HCCH and lindane (gamma-HCCH).

Appendix H. Recommended Baseline BAFs for Trophic Levels Three and Four

The BAFs given in the table are recommended for use in derivation of human health criteria. BAFs recommended for use in the derivation of wildlife criteria are given on the next page. All BAFs given for human health and for wildlife are based on wet weight of the tissue of the aquatic biota.

For an organic chemical, "Baseline BAFs" are based on 100% lipid and on the concentration of freely dissolved chemical in the water. All BAFs given for human health are for trophic levels 3 and 4. BAFs in the table that are not baseline BAFs are based on 1.82 percent lipid for trophic level 3 and 3.10 percent lipid for trophic level 4. The human health guidelines in the final Guidance currently specify that humans consume aquatic biota that are in trophic level 3 and 4 and that the applicable percent lipid is 1.82 and 3.10, respectively.

To calculate human health and wildlife BAFs for an organic chemical, the K_{OW} of the chemical shall be used with a POC concentration of 0.00000004 Kg/L and a DOC concentration of 0.000002 Kg/L from Lake Superior (Eadie et al.) to yield the fraction freely dissolved:

$$f_{fd} = \frac{1}{1 + \frac{(DOC)(K_{OW})}{10} + (POC)(K_{OW})}$$

$$= \frac{1}{1 + \frac{(0.000002\ kg/L)(K_{OW})}{10} + (0.00000004\ kg/L)(K_{OW})}$$

$$= \frac{1}{1 + (0.00000024\ kg/L)(K_{OW})}$$

The human health BAFs for an organic chemical shall be calculated using the following equations:

For trophic level 3:
Human Health BAF^{HH}_{TL3} = [(baseline BAF)(0.0182)+ 1](f_{fd})

For trophic level 4:
Human Health BAF^{HH}_{TL4} = [(baseline BAF)(0.0310)+ 1](f_{fd})

where:

0.0182 and 0.0310 are the standardized fraction lipid values for trophic levels 3 and 4, respectively, that are used to derive human health criteria and values for the final Guidance.

The wildlife BAFs for an organic chemical shall be calculated using the following equations:

For trophic level 3:

$$\text{Wildlife BAF}^{WL}_{TL3} = [(\text{baseline BAF})(0.0646)+1](f_{fd})$$

For trophic level 4:

$$\text{Wildlife BAF}^{WL}_{TL4} = [(\text{baseline BAF})(0.1031)+1](f_{fd})$$

where:

0.0646 and 0.1031 are the standardized fraction lipid values for trophic levels 3 and 4, respectively, that are used to derive wildlife criteria for the final Guidance.

Wildlife

Water quality criteria are currently being derived for wildlife for only four chemicals and so the BAFs are presented here. Although it is possible that wildlife consume some aquatic biota that are in trophic level 2, BAFs for the derivation of wildlife criteria are given here only for trophic levels 3 and 4. Note that the trophic level refers to an organism, not to a species, genus, or family, because individuals of some species are not in the same trophic level for their whole life span. For example, many species that are in trophic level 4 as adults are in trophic level 3 when they are young.

Wildlife BAFs are given for 6.46 and 10.31 percent lipid because the wildlife guidelines in the final Guidance currently specify 6.46 percent lipid for trophic level 3 and 10.31 percent lipid for trophic level 4.

Chemical	**Trophic Level 3**		**Trophic Level 4**		**Fraction Freely Dissolved**	**Method**[a]
	Baseline	**$BAF^t_{6.46\%l}$**	**Baseline**	**$BAF^t_{10.31\%l}$**		
DDT	34,670,000[b]	1,336,000	60,260,000	3,706,000	0.597	1
Mercury	27,900	27,900	140,000	140,000	–	3
PCBs (class)	55,280,000[l]	1,850,000	116,600,000[l]	6,224,000	0.518	1
2,3,7,8-TCDD	9,360,000[c]	172,100	9,000,000	264,100	0.258	2

Human Health

Human health BAFs are given for 1.82 and 3.10 percent lipid because the human health guidelines in the final Guidance currently specify 1.82 percent lipid for trophic level 3 and 3.10 percent lipid for trophic level 4.

Chemical	Trophic Level 3		Trophic Level 4		Fraction Freely Dissolved	Method[a]
	Baseline	$BAF^{t}_{1.82\%l}$	Baseline	$BAF^{t}_{3.10\%l}$		
Benzene	137	3	137	5	1.000	4
Chlordane	7,943,000[b]	116,600	6,166,000	154,200	0.806	1
Chlorobenzene	747	15	740	24	1.000	4
Cyanide	1	1	1	1	–	–
DDD	6,839,000[b]	97,680	10,000,000	243,300	0.785	1
DDE	69,980,00[b]	532,800	223,900,000	2,903,000	0.418	1
DDT	34,670,000[b]	376,400	60,260,000	1,114,000	0.597	1
Dieldrin	4,180,000[c,d]	72,610	19,300,000[d]	571,000	0.954	2
2,4-Dimethylphenol	202	5	200	7	1.000	4
2,4-Dinitrophenol	37	2	37	2	1.000	4
Hexachlorobenzene	2,630,000[b]	43,690	2,512,000	71,080	0.913	1
Hexachlorobutadiene	354,800[e]	6,352	43,940	1,341	0.984	1
Hexachlorocyclohexane	77,620[f]	1,412	64,570	2,000	0.999	1
alpha-Hexachlorocyclohexane	56,890[b]	1,035	48,980	1,517	0.999	1
beta-Hexachlorocyclohexane	77,620[f]	1,411	64,570	1,999	0.998	1
delta-Hexachlorocyclohexane	77,620[f]	1,412	64,570	2,000	0.999	1
Hexachloroethane	20,370[g]	371	17,190	532	0.997	1
Lindane	105,900[b]	1,926	85,110	2,636	0.999	1
Mercury	27,900[h]	27,900	140,000	140,000	–	3
Methylene Chloride	18	1	18	2	1.000	4
Mirex	55,590,000[b]	353,400	134,900,000	1,461,000	0.349	1
Octachlorostyrene	58,880,000[b]	730,000	117,500,000	2,481,000	0.681	1
PCBs (class)	55,280,000[i]	520,900	116,600,000[i]	1,871,000	0.518	1
Pentachlorobenzene	467,700[e]	8,248	645,700	19,420	0.970	1
Photomirex	45,710,000[b]	290,600	117,500,000	1,272,000	0.349	1
2,3,7,8-TCDD	9,360,000[c]	48,490	9,000,000	79,420	0.285	2
1,2,3,4-Tetrachlorobenzene	81,280[e]	1,467	117,500	3,610	0.991	1
1,2,3,5-Tetrachlorobenzene	135,100[g]	2,439	101,110	3,109	0.991	1
Toluene	527	11	516	17	1.000	4
Toxaphene	27,510,000[g]	498,100	21,580,000	665,600	0.995	1
Trichloroethylene	342	7	339	12	1.000	4

[a] The methods used to calculate the recommended baseline BAFs for trophic level 4 were:

1 = A measured baseline BAF was based on a field-measured BAF.
2 = A predicted baseline BAF was based on field-measured BSAF methodology.
3 = A predicted baseline BAF was based on a laboratory-measured BCF and a Food-Chain Multiplier (FCM).
4 = A predicted baseline BAF was based on a predicted BCF and a FCM.

[b] This is the geometric mean of measured baseline BAFs for sculpin and alewives (see Tables 4 and 5), both of which are in trophic level 3.

[c] Cook, P.M. 1995. Memorandum to C.E. Stephan. March 7.

[d] This is based on the concentrations of dieldrin in sediment and fish. However, the concentration in fish is probably partially due to exposure of the fish to aldrin, which is converted to dieldrin. Thus this BAF is probably not appropriate where there is substantially more or less aldrin.

[e] This is a measured baseline BAF for sculpin (see Table 4), which is in trophic level 3.

[f] This is the geometric mean of the measured baseline BAFs for alpha-HCCH and lindane (gamma-HCCH).

[g] This baseline BAF for trophic level 3 was calculated by using the following equation:

$$BAF_{TL3} = (BAF_{TL4})\left(\frac{FCM_{TL3}}{FCM_{TL4}}\right)$$

where:

BAF_{TL3} = Baseline BAF for trophic level 3
BAF_{TL4} = Baseline BAF for trophic level 4
FCM_{TL3} = Food-Chain Multiplier for trophic level 3
FCM_{TL4} = Food-Chain Multiplier for trophic level 4

The values needed for this calculation are given in Appendix G.

[h] See Appendix E.

[I] See Appendix F.

Appendix I. Derivation of Consumption Weighted Mean Percent Lipid for Human Health and Wildlife

TABLE 1
LIPID CONTENT OF EDIBLE PORTION OF FISH

LAKES/SPECIES	PERCENT LIPID Xg	Xa	N	PORTION	SOURCE
SUPERIOR					
Bloater Chub		10.27	3	F	WDNR
Brown Trout		6.40	11	F	WDNR
Carp		7.84	9	F	WDNR
Chinook		3.35	10	Fs	MDNR
Chinook		2.95	4	F	WDNR
Chinook		2.96	5	F	MPCA
Chinook		2.68	14	F	MPCA
Coho		7.50	3	F	WDNR
Coho		1.39	8	F	MPCA
Coho		1.56	5	F	MPCA
Herring		9.20	1	F	WDNR
Herring		4.58	6	D	MPCA
Lake Trout		11.42	44	F	WDNR
Lake Trout		10.46	71	F	MPCA
Lake Trout		9.21	28	F	MPCA
Lake Trout	11.34		71	F	MDNR
Rainbow Smelt		0.90	3	D	MPCA
Rainbow Trout		2.13	3	F	WDNR
Rainbow Trout		1.24	8	F	MPCA
Walleye		1.91	33	F	WDNR
Whitefish	7.85		10	F	MDNR
Whitefish		7.15	2	F	MPCA
Yellow Perch		0.92	8	F	WDNR
HURON					
Brown Trout	7.54		20	F	MDNR
Carp	11.37		9	Fs	MDNR
Channel Catfish	10.69		1	Fs	MDNR
Chinook	1.72		44	F	MDNR
Coho	3.96		8	F	MDNR
Lake Trout	14.12		80	F	MDNR
Walleye	1.62		10	F	MDNR

LAKES/SPECIES	PERCENT LIPID Xg	 Xa	N	PORTION	SOURCE
ERIE					
Carp	3.44		8	Fs	MDNR
Chinook		3.88	21	F	NYDEC
Channel Catfish	7.11		10	Fs	MDNR
Coho		4.50	22	F	NYDEC
Lake Trout		13.00	5	F	NYDEC
Smallmouth Bass		1.99	19	F	NYDEC
Walleye	2.56		40	F	MDNR
Walleye		1.98	9	Fs	OEPA
White Bass		4.42	8	Fs	OEPA
Whitefish		8.75	4	Fs	OEPA
ONTARIO					
Brown Trout		10.40	91	F	NYDEC
Channel Catfish Chinook		12.80	47	Fs	NYDEC
Coho		2.75	45	F	NYDEC
Lake Trout		3.38	98	F	NYDEC
Rainbow Trout		14.53	120	F	NYDEC
Smallmouth Bass		9.04	57	F	NYDEC
White Perch		1.85	161	F	NYDEC
		5.64	33	F	NYDEC
STATEWIDE (Wisconsin)					
Bass (largemouth)		0.70	107	F	WDNR
Bluegill		0.83	74	F	WDNR
Bowfin		0.40	1	F	WDNR
Buffalo (bigmouth)		8.66	115	F	WDNR
Burbot		0.86	39	F	WDNR
Cisco		6.09	14	F	WDNR
Crappie		0.92	135	F	WDNR
Muskie		1.53	11	F	WDNR
Redhorse Suckers		1.86	72	F	WDNR
Rockbass		0.44	85	F	WDNR

LAKES/SPECIES	PERCENT LIPID Xg	 Xa	N	PORTION	SOURCE
MICHIGAN (Green Bay)					
Black Bullhead		1.10	8	Fs	WDNR
Brook Trout		4.97	9	F	WDNR
Brown Trout		9.44	106	F	WDNR
Carp		8.17	48	F	WDNR
Channel Catfish		4.75	15	Fs	WDNR
Chinook		4.63	46	F	WDNR
Coho		7.70	1	F	WDNR
Lake Trout		11.88	28	F	WDNR
Rainbow Trout		6.39	45	F	WDNR
Smallmouth Bass		1.34	10	F	WDNR
Walleye		2.71	67	F	WDNR
White Bass		3.76	18	F	WDNR
Yellow Perch		0.76	26	F	WDNR
MICHIGAN					
Black Bullhead		1.80	1	Fs	WDNR
Bloater Chub		14.75	92	F	WDNR
Brook Trout		4.33	68	F	WDNR
Brown Trout		11.96	170	F	WDNR
Brown Trout	5.68		46	F	MDNR
Brown Trout		11.19	21	A	IDEM
Brown Trout		11.22	6	D	IDEM
Brown Trout		3.88	5	Fs	IDEM
Brown Trout		6.70	9	F	IDEM
Carp		20.43	2	F	IDEM
Carp	6.82		16	Fs	MDNR
Carp		10.68	47	F	WDNR
Channel Catfish		8.92	11	Fs	WDNR
Chinook		4.20	275	F	WDNR
Chinook		4.92	30	A	IDEM
Chinook		2.60	4	D	IDEM
Chinook		1.45	5	Fs	IDEM
Chinook		2.46	28	F	IDEM
Chinook	1.79		71	F	MDNR
Chinook-Trim	0.99		10	O	MDNR

LAKES/SPECIES	PERCENT LIPID Xg	Xa	N	PORTION	SOURCE
MICHIGAN (con't)					
Coho		5.96	19	A	IDEM
Coho		6.51	8	D	IDEM
Coho		1.95	2	Fs	IDEM
Coho		2.80	18	F	IDEM
Coho	2.42		36	F	MDNR
Coho		3.82	164	F	WDNR
Lake Trout		17.25	156	A	IDEM
Lake Trout		16.58	13	D	IDEM
Lake Trout		8.81	3	Fs	IDEM
Lake Trout		12.01	9	F	IDEM
Lake Trout	16.67		60	F	MDNR
Lake Trout		12.71	311	F	WDNR
Lake Trout-trim	9.19		10	O	MDNR
Longnose Sucker		5.45	2	A	IDEM
Longnose Sucker		4.95	3	F	IDEM
Longnose Sucker	5.59		10	F	MDNR
Northern Pike		3.00	2	A	IDEM
Northern Pike	0.57		10	Fs	MDNR
Rainbow Trout	3.76		25	F	MDNR
Steelhead		11.09	17	A	IDEM
Steelhead		7.10	3	D	IDEM
Steelhead		2.77	2	Fs	IDEM
Steelhead		5.62	6	F	IDEM
Walleye	1.63		11	F	MDNR
Walleye		1.45	9	Fs	MDNR
Walleye		2.19	9	F	WDNR
Whitefish		9.00	1	A	IDEM
White Sucker		2.45	2	A	IDEM
White Sucker	1.61		10	F	MDNR
Yellow Perch		3.00	1	A	IDEM
Yellow Perch		1.55	6	D	IDEM
Yellow Perch		1.06	9	F	IDEM
Yellow Perch	0.82		10	F	MDNR
Yellow Perch		0.95	24	F	WDNR

Key to Abbreviations

Percent Lipid:
Xg = geometric mean, contributing program (source) used geometric means to summarize data.
Xa = arithmetic mean, contributing program (source) used arithmetic means to summarize data.

N = Number of fish sampled

Portion:
F = filet, skin on
Fs = filet, skin off

A = Anterior section through fish
D = dressed (gutted, head removed)
0 = filet, skin off, visible fat removed (trimmed)

Source:

MDNR = Michigan Department of Natural Resources. Fish Contaminant Monitoring Program, Data for Lakes Erie, Huron, Michigan and Superior 1986-1989.

MPCA = Minnesota Pollution Contol Agency. Minnesota Fish Consumption Advisory Program, Data for Lake Superior.

IDEM = Indiana Department of Environmental Management, OWM-Biological Studies, Data for Lake Michigan.

OEPA = Ohio Environmental Protection Agency. Ohio Dept. of Natural Resources, Data for Lake Erie.

WDNR = Wisconsin Department of Natural Resources. Data for Lakes Michigan and Superior and State of Wisconsin.

NYDEC = New York Department of Environmental Conservation. Data for Lakes Erie and Ontario.

APPENDIX I: TABLE 2
LIPID CONTENT OF EDIBLE PORTION OF FISH

LAKES/SPECIES	N*	MEAN PERCENT LIPID
LAKE SUPERIOR		
Bloater chub	1	10.27
Brown trout	1	6.40
Carp	1	7.84
Chinook	4	2.99
Coho	3	3.48
Herring	2	6.89
Lake trout	4	10.61
Rainbow smelt	1	0.90
Rainbow trout	2	1.69
Walleye	1	1.91
Whitefish	2	7.50
Yellow perch	1	0.92
LAKE HURON		
Brown trout	1	7.54
Carp	1	11.37
Chinook	1	7.72
Channel catfish	1	10.69
Coho	1	3.96
Lake trout	1	14.12
Walleye	1	1.62
LAKES ST. CLAIR AND ERIE		
Carp	1	3.44
Channel catfish	1	7.11
Chinook	1	3.88
Coho	1	4.50
Lake trout	1	13.00
Smallmouth bass	1	1.99
Walleye	2	2.27
White bass	1	4.42
Whitefish	1	8.75

LAKES/SPECIES	N*	MEAN PERCENT LIPID
LAKE MICHIGAN (inc. Green Bay)		
Black bullhead	2	1.45
Bloater chub	1	14.75
Brook trout	2	4.65
Brown trout	7	8.58
Carp	4	11.53
Channel catfish	2	6.84
Chinook	7	3.15
Coho	7	4.45
Lake trout	7	13.70
Longnose sucker	3	5.33
Northern pike	2	1.79
Rainbow trout (steelhead)	6	6.12
Smallmouth bass	1	1.34
Walleye	4	2.00
White sucker	2	2.03
White bass	1	3.76
Whitefish	1	9.00
Yellow perch	6	1.36
LAKE ONTARIO		
Brown trout	1	10.40
Channel catfish	1	12.80
Chinook	1	2.75
Coho	1	3.38
Lake trout	1	14.53
Rainbow trout	1	9.04
Smallmouth bass	1	1.85
White perch	1	5.64
WISCONSIN (statewide)		
Bass (largemouth)	1	0.70
Bluegill	1	0.83
Bowfin	1	0.40
Buffalo (bigmouth)	1	8.66
Burbot	1	0.86
Cisco	1	6.09
Crappie	1	0.92
Muskie	1	1.53
Redhorse suckers	1	1.86
Rockbass	1	0.44

* Number of state programs reporting data for a species.

APPENDIX I: TABLE 3
LIPID CONTENT OF EDIBLE PORTION OF FISH

Species	Mean Percent Lipid
Black bullhead	1.45
Bloater chub	12.51
Bluegill	0.83
Bowfin	0.40
Brook trout	4.65
Brown tout	8.23
Buffalo	8.66
Burbot	0.86
Carp	8.55
Channel catfish	9.36
Chinook	2.90
Cisco	6.09
Coho	3.95
Crappie	0.92
Herring	6.89
Lake Trout	13.19
Largemouth bass	0.70
Longnose sucker	5.33
Musky	1.53
Northern pike	1.79
Rainbow smelt	0.90
Rainbow trout	5.62
Redhorse sucker	1.86
Rockbass	0.44
Smallmouth bass	1.73
Walleye	1.95
White perch	5.64
White bass	4.09
White sucker	2.03
Whitefish	8.42

Yellow perch	1.14

APPENDIX I: TABLE 4
LIPID CONTENT OF WHOLE FISH

Species	LAKE*						CDF&O**	MEAN
	Sup.	Mich.	Hur.	St.C.	Erie	Ont.		
Alewife							9.73	9.73
Bloater	13.1	22.3						17.70
Bluegill		1.55##						1.55
Bluntnose minnow						1.5#		1.50
Brown bullhead						6.1	3.58	4.84
Brown trout						12.2	15.44	13.82
Channel catfish			18.7			11.7		15.20
Coho salmon							8.45	8.45
Common carp			10.5	9.5	11.6	5.8	8.59	9.20
Emerald shiner					1.6#	2.7#		2.15
Freshwater drum					8.4			8.40
Lake trout	16.6	17.0	20.5			15.3#	17.25	17.33
Lake whitefish	10.5		10.0					10.25
Lake herring						6.0		6.00
Northern pike							2.17	2.17
Pink salmon							1.78	1.78
Rainbow smelt							4.78	4.78
Rainbow trout							7.59	7.59
Redhorse					6.4			6.40
Rock bass						4.8		4.80
Skipjack herring	9.8							9.80
Slimy sculpin							6.95	6.95
Smallmouth bass		1.32##						1.32
Spake							10.12	10.12
Spottail shiner					2.0#	1.8#		1.90
Sunfish		1.73##						1.73
Walleye				8.1	11.4		8.01	9.17
White bass				9.6	9.8		10.16	9.85
White perch						10.2#		10.20
White sucker		6.8	6.0		4.9		5.15	5.71

Yellow perch		7.4	4.1		4.2	5.6	5.95	5.50

Footnotes

* Data for the individual lakes from U.S. Fish and Wildlife Service National Contaminant Biomonitoring Program 1976-1984.

** CDF&O = Canada Department of Fisheries and Oceans. Percent lipid data for unspecified Great Lakes. These data are averaged together with the lake-specific data from the U.S. Fish and Wildlife Service.

Value includes data from the New York State Department of Environmental Conservation.

Values are from Michigan Department of Natural Resources

Data Sources:

Canada Department of Fisheries and Oceans, Great Lakes Contaminant Surveillance Program, 1977-1985.

New York Department of Environmental Conservation

Schmitt, C.J., J.L. Zajicek and P.H. Peterman. 1990. National contaminant biomonitoring program: residues of organochlorine chemicals in U.S. freshwater fish, 1976-1984. Arch. Environ. Contam. Toxicol. 19: 748-781.

Michigan Department of Natural Resources

APPENDIX I: TABLE 5
AVERAGE DAILY PER CAPITA ESTIMATES OF FISH CONSUMPTION BY SPECIES FROM THE 1991-1992 MICHIGAN SPORT ANGLERS FISH CONSUMPTION STUDY[1]

SPECIES	CONSUMPTION RATE (grams/person/day)	
	Mean	**Bias-adjusted Mean[2]**
Perch (Yellow)	3.03	2.63
Walleye	2.59	2.25
Bluegill	2.20	1.91
Pike (Northern)	0.97	0.84
Salmon	0.95	0.82
Bass (Largemouth)	0.73	0.63
Other[3]	0.75	0.65
Trout (Lake)	0.70	0.61
Trout (Rainbow)	0.69	0.60
Smelt	0.50	0.43
Crappie	0.49	0.43
Trout (Brown)	0.48	0.42
Trout (Brook)	0.31	0.27
Catfish (Channel)	0.29	0.25
Salmon (Coho)	0.29	0.25
Whitefish	0.21	0.18
Salmon (Chinook/King)	0.20	0.17
Sucker (White)	0.17	0.15
Bass (Smallmouth)	0.16	0.14
Bullhead	0.13	0.11
Perch/Bluegill	0.11	0.10
Rockbass	0.11	0.10
Whitebass	0.07	0.06
Sunfish	0.05	0.04
Bass/Bluegill	0.04	0.03

APPENDIX I: TABLE 5 (continued)
AVERAGE DAILY PER CAPITA ESTIMATES OF FISH CONSUMPTION BY SPECIES FROM THE 1991-1992 MICHIGAN SPORT ANGLERS FISH CONSUMPTION STUDY[1]

SPECIES	CONSUMPTION RATE (grams/person/day)	
	Mean	Bias-adjusted Mean[2]
Burbot	0.03	0.03
Carp	0.03	0.03
Muskie	0.02	0.02
Buffalo (Bigmouth)	0.02	0.02
Sucker (Longnose)	0.02	0.02
Cisco	0.01	0.01
Bowfin	0.01	0.01
Redhorse	0.01	0.01
Walley/Perch	0.01	0.01
Pike/Perch	0.01	0.01

[1] Source: Fish Consumption Estimates Based on the 1991-1992 Michigan Sport Anglers Fish Consumption Survey. February 21, 1995. USEPA. Submitted by SAIC to EPA under Contract No. 68-C4-0046.

[2] The bias-adjusted mean consumption rate is calculated by multiplying of the actual consumption rate times the nonresponse bias correction of 0.86834 (1.0 - 0.13174) from West et al. 1991-1992 Michigan Sport Anglers Fish Consumption Study - Final Report to the Michigan Great Lakes Protection Fund, Michigan Department of Natural Resources. University of Michigan, School of Natural Resources, Natural Resource Sociology Research Lab. Technical Report #6. May 1993.

[3] Other includes "other single species", "other combinations", and "species not recorded".

APPENDIX I: TABLE 6
CALCULATION OF A CONSUMPTION WEIGHTED MEAN PERCENT LIPID VALUE FOR TROPHIC LEVEL 3 FISH CONSUMED BY HUMANS

Species	Bias-Adjusted[1] Consumption (g/day)	Lipid (%)[3]	Size (cm)[6]	Trophic Level[6]	Assigned Trophic Level[8]	Product[9]
Bluegill	1.91	0.83	5-27	2.6 - 3.0	3	1.59
Crappie	0.43	0.92	13-42	3.0 - 3.4	3	0.40
Trout (Brook)	0.27	4.65	10-40	3.2	3	1.26
Whitefish	0.18	8.42	3-40	3.0 - 3.4	3	1.52
Other	0.16[2]	1.82[4]	---	---	3	0.29
Sucker (White)	0.15	2.03	5-60	2.7 - 2.9	3	0.30
Bullhead	0.11	1.45	> 10	2.7 - 3.2	3	0.16
Perch/Bluegills	0.10	1.01[5]	---	< 3.5[7]	3	0.10
Sunfish	0.04	0.83[5]	---	2.8 - 3.3	3	0.03
Carp	0.03	8.55	10-23	2.2 - 3.1	3	0.26
Buffalo (Bigmouth)	0.02	8.66	25-46	2.6 - 3.0	3	0.17
Sucker (Longnose)	0.02	5.33	35-60	2.4 - 3.0	3	0.11
Redhorse	0.01	1.86	> 6.5	2.9	3	0.02
Cisco	0.01	6.09	20-30	3.0 - 3.1	3	0.06
TOTAL	**3.44**					**6.27**

APPENDIX I: TABLE 6 (continued)
CALCULATION OF A CONSUMPTION WEIGHTED MEAN PERCENT LIPID VALUE FOR TROPHIC LEVEL 4 FISH CONSUMED BY HUMANS

Species	Bias-Adjusted[1] Consumption (g/day)	Lipid (%)[3]	Size (cm)[6]	Trophic Level[6]	Assigned Trophic Level[8]	Product[9]
Perch (Yellow)	2.63	1.14	20-30	3.1 - 3.8	4	3.00
Walleye	2.25	1.95	30-80	3.9 - 4.5	4	4.39
Pike (Northern)	0.84	1.79	> 10	4.0	4	1.50
Salmon	0.82	3.53[10]	---	4.0	4	2.90
Bass (Largemouth)	0.63	0.70	> 20	3.8	4	0.44
Trout (Lake)	0.61	13.19	> 40	4.0 - 4.5	4	8.05
Trout (Rainbow)	0.60	5.62	> 50	4.0	4	3.37
Other	0.49[2]	3.10[4]	---	> 3.5	4	1.52
Smelt	0.43	0.90	---	3.1 - 3.5	4	0.39
Trout (Brown)	0.42	8.23	---	> 3.5[11]	4	3.46
Catfish (Channel)	0.25	9.36	> 45	3.5 - 3.9	4	2.34
Salmon (Coho)	0.25	3.95	45-60	4.0 - 4.5	4	0.99
Salmon (Chinook)	0.17	2.90	---	> 3.5[12]	4	0.49
Bass (Smallmouth)	0.14	1.73	> 10	3.4 - 3.9	4	0.24
Rockbass	0.10	0.44	> 7.5	3.3 - 3.7	4	0.04
Whitebass	0.06	4.09	> 20	3.9	4	0.25
Bass/Bluegills	0.03	0.85[5]	---	> 3.5[13]	4	0.03
Burbot	0.03	0.86	> 50	4.0	4	0.03
Muskie	0.02	1.53	---	> 3.5[14]	4	0.03
Pike/Perch	0.01	1.30[5]	---	> 3.5[15]	4	0.01
Walleye/Perch	0.01	1.51[5]	---	> 3.5[16]	4	0.02
Bowfin	0.01	0.40	---	4.0	4	0.01
TOTAL	**10.80**					**33.50**

Consumption weighted mean percent lipid value for Trophic Level 3 (6.27/3.44) = 1.82
Consumption weighted mean percent lipid for Trophic Level 4 (33.50/10.80) = 3.10

Total grams of lipid consumed per day from Trophic Level 3 (6.27/100)= 0.0627
Total grams of lipid consumed per day from Trophic Level 4 (33.50/100) = 0.3349

24.16% of fish consumed are Trophic level 3
75.84% of fish consumed are Trophic level 4

[1] The bias-adjusted consumption rate comes from Table 5 of Appendix I.

[2] Consumption rate calculated by multiplying bias-adjusted consumption rate "other" category (0.65 g/day) in Table 5 of Appendix I by percent of fish consumed in trophic level 3 (24.16%) or trophic level 4 (75.84%).

[3] Percent lipid values are taken from Table 3 of Appendix I unless otherwise noted.

[4] Percent lipid is the overall consumption weighted mean lipid value for trophic level 3 or trophic level 4.

[5] Percent lipid is weighted average of Perch/Bluegill, Smallmouth Bass/Largemouth Bass/Bluegill, Pike/Perch, or Walleye/Perch. Lipid value for sunfish assumed to be the same as for bluegill.

[6] Size values and Trophic levels taken from: USEPA. 1995. Trophic Level and Exposure Analyses for Selected Piscivorous Birds and Mammals. Volume I: Analyses for Species on the Great Lakes Basin and of the Great Lakes Basin and Volume III: Appendices.

[7] Trophic level assumed to be less than 3.5 based on bluegill data.

[8] Species were placed in trophic level 4 if the highest value in the reported range was greater than or equal to 3.5. Species were placed in a trophic level 3 when the highest value in the reported range was less than 3.5.

[9] Product is equal to the bias-adjusted consumption rate for that species multiplied by the percent lipid for that species times 100.

[10] Percent lipid is weighted average of Coho and Chinook Salmon.

[11] Trophic level assumed to be greater than 3.5 based on other trout data.

[12] Trophic level assumed to be greater than 3.5 based on other salmon data.

[13] Trophic level assumed to be greater than 3.5 based on bass data.

[14] Trophic level assumed to be greater than 3.5 based on knowledge of Muskie feeding habits.

[15] Trophic level assumed to be greater than 3.5 based on Pike/Perch data.

[16] Trophic level assumed to be greater than 3.5 based on Walleye/Perch data.

APPENDIX I: TABLE 7
CALCULATION OF A PERCENT LIPID VALUE FOR TROPHIC LEVEL 3 FISH CONSUMED BY WILDLIFE

Species[1]	Lipid (%)[2]	Size (cm)[3]	Mean Trophic Level[3]	Assigned Trophic Level[4]
Longnose/White Sucker	5.71[5]	35-60	2.8	3
Whitefish	10.25	3-40	3.2	3
Alewife	9.73	5-23	3.2	3
Common Carp	9.20	> 23	2.4	3
Lake Herring	6.00	20-30	3.1	3
Yellow Perch	5.45	< 7	3.0	3
Smallmouth bass	1.32	< 7	3.4	3
Bluegill	1.55	< 7	2.8	3
Redhorse suckers	6.40	< 7	2.7	3
Trout (brown)	13.82	8-18	3.2	3
Trout (rainbow)	7.59	7-23	3.2	3
Sculpin	6.95	< 8	3.0	3
Sunfish	1.73	5-10	3.1	3
Rainbow smelt	4.78	2-17	3.1	3
AVERAGE	**6.46**			

APPENDIX I: TABLE 7 (continued)
CALCULATION OF A PERCENT LIPID VALUE FOR TROPHIC LEVEL 4 FISH CONSUMED BY WILDLIFE

SPECIES[1]	LIPID (%)[2]	SIZE (cm)[3]	MEAN TROPHIC LEVEL[3]	ASSIGNED TROPHIC LEVEL[4]
Lake trout	17.33	20-40	3.8	4
Walleye	9.17	15-30	3.5	4
Bloater chub	17.70	20-30	3.5	4
Pike (Northern)	2.17	25	4.0	4
Trout (Average of brown and rainbow trout)	10.71	7-23	3.5	4
Rock bass	4.80	10-22	3.5	4
AVERAGE	**10.31**			

[1] The species selected are those consumed by the 5 representative species used to derive wildlife criteria and those with available percent lipid data. Other species consumed by the 5 representative species but not included in the tables because of lack of lipid data include: trophic level 3 - burbot, pumpkinseed, blackstripe topminnow, darters, brook silverside, bullhead, blacknose dace, creek chub, mudminnow, stickleback, and brook trout. Source of data: USEPA. 1995. Trophic Level and Exposure Analyses for Selected Piscivorous Birds and Mammals. Volume I: Analyses for Species on the Great Lakes Basin and of the Great Lakes Basin and Volume III: Appendices.

[2] Percent lipid taken from Table 4 in Appendix I unless otherwise noted.

[3] Size values and trophic levels taken from source cited in footnote 1.

[4] Species were placed in a trophic level 3 if the mean value was less than 3.5. Species were placed in trophic level 4 if the mean value was greater than or equal to 3.5.

[5] Percent lipid data for white suckers were assumed to be similar for both longnose and white sucker.

Appendix J. FORTRAN Source Code for the Model of Gobas (1993)

This source code includes the feeding preferences, lipid content, and weight of the organisms; temperature; and sediment organic carbon content used in the final Guidance for deriving the FCMs. This code does not include the correction for bioavailability discussed in the journal article by Gobas.

```
      real lipid(6),weights(6)
      real residues(6),pref(5,4),Kow
      common Kow, VF, VL, cf, residues, pref, c_w, t, ink

c data
c for lipids, residues, and weights
c zoo, dip, scu, ale, sme, pf
      data lipid/0.05,0.03,0.08,0.07,0.04,0.11/
      data weights/0,0,0.0054,0.032,0.016,2.41/
      data residues/0,0,0,0,0,0/

c for pref columns: scu, ale, sme, pf
c for pref row: zoo, dip, scu, ale, sme
      data pref/0.18,0.82,0,0,0,0.60,0.40,0,0,0,
      x      0.54,0.21,0.25,0,0,0,0,0.10,0.50,0.40/

      density_oc=0.9
      density_dip=0.9
c  temperature and sediment organic carbon
      t=8
      soc=0.027

      write(6,*) '  Input log Kow'
      read(5,*) Kow
      Kow = 10**Kow
      c_w = 1
      c_sed = 25 * Kow * c_w * soc

c  zooplankton
      residues(1) = lipid(1)*Kow*c_w

c  diporeia
      residues(2) = c_sed*density_oc/soc*lipid(2)/density_dip

c  sculpin
      VF=weights(3)
      VL=lipid(3)
```

```
      ink=1
      call fish
      residues(3)=cf

c  alewives
      VF=weights(4)
      VL=lipid(4)
      ink=2
      call fish
      residues(4)=cf

c  smelt
      VF=weights(5)
      VL=lipid(5)
      ink=3
      call fish
      residues(5)=cf

c  piscivorous fish
      VF=weights(6)
      VL=lipid(6)
      ink=4
      call fish
      residues(6)=cf

      write(6,1215)
1215        format(t26,'Log BAF ',t46,'FCM'/
    ×  t22,'(lipid normalized',/,t22,'& freely dissolved)')
      write(6,1220) ((log10(residues(i)/c_w/lipid(i)),
    × residues(i)/c_w/lipid(i)/Kow),i=1,6)
1220        format(t5,'Zooplankton',t22,f10.3,t40,f10.3/
    × t5,'Diporeia',t22,f10.3,t40,f10.3/
    × t5,'Sculpin',t22,f10.3,t40,f10.3/
    × t5,'Alewives',t22,f10.3,t40,f10.3/
    × t5,'Smelt',t22,f10.3,t40,f10.3/
    × t5,'Piscivorous fish',t22,f10.3,t40,f10.3)

      stop
      end

      subroutine fish
      real residues(6),pref(5,4),Kow
      real k1, k2, km, kd, kg, ke
```

```
      common Kow, VF, VL, cf, residues, pref, c_w, t, ink

      QW = 88.3*VF**0.6
      QL = QW/100.0
      k1 = 1/(VF/QW + VF/QL/Kow)
      k2 = k1/(VL*Kow)
      ED = 1/(5.3e-8*Kow + 2.3)
      FD = 0.022*VF**0.85*EXP(0.06*t)
      kd = ED*FD/VF
      km = 0

c  Note the following errors in the manuscript.
c  ke is not 0.25*kd
      ke = 0.20*kd
c  temperature equations are different
      if(t.lt.17.5) then
      kg = 0.002*vf**-0.2
      else
      kg = 0.01*vf**-0.2
      endif

      cf=0
      do 10 i=1,5
      cf=cf+pref(i,ink)*residues(i)
10    continue
      cf = (k1*c_w + kd*cf)/(k2 + ke + km + kg)

      return
      end
```

Appendix K. Determination of BAFs for DDT and Metabolites and Biomagnification Factors for the Derivation of Wildlife Criteria

I. DETERMINATION OF A BAF FOR TOTAL DDT AND METABOLITES

In order to calculate an avian class-specific wildlife value for DDT, a BAF for a mixture of DDT, DDE and DDD representative of the Great Lakes had to be determined. This was necessary because the study from which the test dose was derived (Anderson et al., 1975) was based on exposure to pelicans from anchovies containing DDE, DDD and DDT.

A BAF for the total DDT mixture (DDTr) was calculated from the BAFs for DDE, DDE, and DDT derived for the Lake Ontario ecosystem by Oliver and Niimi (1988). There was no statistically significant difference between the distribution of these compounds for the total DDT mixture between the Lake Ontario ecosystem and the California coastal ecosystem, the location of the field study by Anderson et al. (1975). (In the report by Anderson et al. (1975), the average composition of the total DDT mixture in anchovies was 69.4% (8.3% standard deviation, n = 6, range 60.0 to 80.0%) for DDE and 30.6% for the sum of DDT and DDD. The distribution of the total DDT mixture in the Great Lakes for forage fish (i.e., sculpin, alewife, and smelt) taken from the report of Oliver and Niimi (1988) was 77.5% (6.4%, n = 4, range 71.4 to 84.9%) for DDE and 22.5% for the sum of the DDT and DDD.

Below is the analysis and calculations carried out to determine the appropriate BAF for the total DDT mixture in wildlife prey species in trophic levels three and four. The molecular weights for DDE, DDD, and DDT were used in these calculations and are 318.0, 320.1, and 354.5 g/mole for each compound, respectively. This analysis is consistent with Appendix B of 40 CFR Part 132, Great Lakes Water Quality Initiative Methodology for Deriving Bioaccumulation Factors. Chemical-specific, fish species-specific data obtained from or derived from the work of Oliver and Niimi (1988) are presented in Table K.1 and Table K.2 below.

Table K.1. Measured log BAF^{fd}_{R} and measured residues for DDE, DDD, and DDT in fish derived from a Lake Ontario ecosystem by Oliver and Niimi (1988).

	Measured Log BAF^{fd}_{R}			**Measured Residues (ng/g)**		
	DDE	**DDD**	**DDT**	**DDE**	**DDD**	**DDT**
Sculpin	7.83	6.89	7.47	190	47	29
Alewife	7.86	6.78	7.61	180	32	35
Large[1] Smelt	8.26	6.84	7.93	260	21	41
Small[2] Smelt	8.11	6.80	7.43	180	19	13
Pisc[3] fish	8.37	7.00	7.78	860	83	80

[1] large fish, [2] small fish, [3] piscivorous fish

Table K.2. Measured residues and the average composition of the DDE, DDD, and DDT derived from Oliver and Niimi (1988).

	Measured Residues (moles/g fish)				Average Composition of Congeners (% mole basis)		
	DDE	**DDD**	**DDT**	**Sum**	**DDE**	**DDD**	**DDT**
Sculpin	0.597	0.147	0.082	0.826	72.32	17.78	9.90
Alewife	0.566	0.100	0.099	0.765	74.01	13.08	12.91
Large[1] Smelt	0.818	0.066	0.116	0.999	81.85	6.57	11.58
Small[2] Smelt	0.566	0.059	0.037	0.662	85.49	8.97	5.54
Pisc[3] Fish	2.704	0.259	0.226	3.189	84.79	8.13	7.08

[1] large fish, [2] small fish, [3]piscivorous fish

To be consistent with the Gobas model (1993) which was used to derive Food Chain Multipliers for organic chemicals (as described in this parent document), the prey of trophic level 3 fish are considered to be sculpin and alewife and the prey of trophic level 4 fish are considered to be piscivorous fish. Using the data in Tables K.1 and K.2 above, and taking the geometric means to determine the average values for forage fish (i.e., sculpin and alewife) for DDE, DDD, and DDT, the average percent compositions are 73.2%, 15.4%, and 11.4%, respectively and the log BAF^{fd}_{R} values are 7.84, 6.83, and 7.54, respectively.

The composite log BAF^{fd}_{R} for each trophic level can then be determined as presented below:

The composite $BAF^{fd}_{R,3}$ (DDT mixture; trophic level 3) =

$BAF^{fd}_{R,3}$ = (.732)(10**7.84) + (.154)(10**6.83) + (.114)(10**7.54)

= 50,642,027 + 1,041,167 + 3,952,800 = 55,635,994

log $BAF^{fd}_{R,3}$ = 7.75

The composite $BAF^{fd}_{R,4}$ (DDT mixture; trophic level 4) =

$BAF^{fd}_{R,4}$ = (.848)(10**8.37) + (.081)(10**7.00) + (.071)(10**7.78)

= 198,327,759 + 813,197 + 4,263,920 = 203,404,876

log $BAF^{fd}_{R,4}$ = 8.31

The next step is to calculate the BAF based on the total DDT mixture using the appropriate percent lipids of Great Lakes fish for wildlife species. The lipid values for wildlife are 6.46% and 10.31% for trophic levels 3 and 4, respectively. The log K_{OW}s for DDE, DDD, and DDT are 6.76, 6.06, and 6.45, respectively.

The K_{OW} for the total DDT mixture for trophic level 3 is:

= (.732)(10**6.76) + (.154)(10**6.06) + (.114)(10**6.45)

= 4,210,299 + 177,117 + 321,497 = 4,708,913

log K_{OW} = 6.67

The K_{OW} mixture for the total DDT mixture for trophic level 4 is:

= (.848)(10**6.76) + (.081)(10**6.06) + (.071)(10**6.45)

= 4879252 + 93367 + 199439 = 5172058

log K_{OW} = 6.71

Applying the equation immediately below permits the determination of the fraction of the chemical which is freely dissolved:

$$f_{fd} = 1/(1 + DOC * K_{OW} / 10 + POC * K_{OW})$$

where:

DOC = 2.0e-6 kg of dissolved organic carbon per liter
POC = 0.04e-6 Kg of particulate organic carbon per liter
K_{OW} = n-octanol water partition coefficient.

The fraction of the chemical which is freely dissolved for trophic level 3 is:

$f_{fd,3}$ = 1/(1 + 2.0e-6*10**6.67/10 + 0.04e-6*10**6.67)

= 0.4695

The fraction of the chemical which is freely dissolved for trophic level 4 is:

$f_{fd,4}$ = 1/(1 + 2.0e-6*10**6.72/10 + 0.04e-6*10**6.71)
= 0.4462

The $BAF^{fd}_{6.46R,3}$ for the total DDT mixture for trophic level 3 (based on freely dissolved and 6.46% lipid) is:

= 6.46% * 55635994 = 3594085

log $BAF^{fd}_{6.46R,3}$ = 6.56

Adjusting this value for the total chemical in the water results in the following $BAF^{t}_{6.46\%R,3}$ for trophic level 3:

$BAF^{t}_{6.46\%R,3}$ = $f_{fd,3}$ * $BAF^{fd}_{6.46R,3}$
= 0.4695 * 3,594,084
= 1,687,000

The $BAF^{fd}_{10.31R,4}$ for the total DDT mixture for trophic level 4 (based on freely dissolved and 10.31% lipid) is:

= 10.31% * 203,404,876 = 20,971,043
log $BAF^{fd}_{10.31R,4}$ = 7.32

Adjusting this value for the total chemical in the water results in the following $BAF^{t}_{10.31\%R,4}$ for trophic level 4:

$BAF^{t}_{10.31\%R,4}$ = $f_{fd,4}$ * $BAF^{fd}_{10.31R,4}$
= 0.4462 * 20,971,043
= 9,357,000

Therefore, the final BAFs used to determine the avian wildlife values are 1,687,000 for trophic level 3 and 9, 357,000 for trophic level 4.

II. DETERMINATION OF BIOMAGNIFICATION FACTORS FOR THE DERIVATION OF WILDLIFE VALUES FOR THE BALD EAGLE

In the derivation of wildlife criteria for the Great Lakes Water Quality Initiative, five species were selected as representative of avian and mammalian species resident in the Great Lakes basin likely to experience the highest exposures to bioaccumulative contaminants through the aquatic food web. One of these representative species is the bald eagle. Estimates of prey species for the bald eagle indicate that approximately eight percent of a bald eagle's diet (on a wet weight basis) consists of piscivorous birds (i.e., gulls; EPA, 1995a,b). A Biomagnification Factor (BMF) is needed to quantify the contribution of contaminant to the eagle's diet from ingestion of gulls. The BMFs used for the derivation of wildlife criteria for the four chemicals for which wildlife criteria exist in the Great Lakes Water Quality Initiative are presented in Table K.3. These were derived from the work of Braune and Norstrom (1989), unless otherwise indicated, who measured the concentrations of various contaminants in both gulls from Lake Ontario and in the prey fish of the gulls. The BMFs presented in Table K.3 are the ratios of the concentration of a contaminant in the gulls to the concentration in their prey fish.

The BMF for the total DDT mixture (DDTr) is calculated by using the average percentages of the various DDT congeners in trophic level 3 fish presented in the section above.

$$\begin{aligned} \text{BMF (DDTr)} &= (0.732)(85) + (0.154)(3.2) + (0.114)(3.2) \\ &= 62.2 + .49 + .36 \\ &= 63 \end{aligned}$$

Table K.3. Biomagnification factors used to derive wildlife values for the bald eagle.

Chemical	**Biomagnification Factor**[1]
DDE	85
DDD	3.2[2]
DDT	3.2
DDTr	63
Mercury	10[3]
2,3,7,8-TCDD	30
PCBs	90

[1] All values derived from Braune and Norstrom (1989) unless otherwise indicated.

[2] Not reported by Braune and Norstrom and assumed to be similar to that for DDT.

[3] Derived by analysis of data in Noreheim and Forslie (1978), Wren et al. (1983), and Vermeer et al. (1973) and the application of best professional judgment.

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