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Development of National Bioaccumulation Factors:  
Supplemental Information for  
EPA's 2015 Human Health Criteria Update

U.S. Environmental Protection Agency  
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Office of Science and Technology  
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## 1. Purpose

This document describes the procedures and calculations EPA used to compute the national bioaccumulation factors (BAFs) that were, in turn, used to calculate the Agency's updated national recommended water quality criteria for human health for 94 chemicals (USEPA 2015). For a scientific discussion of and rationale for using these methods, see EPA's 2000 *Methodology for Deriving Ambient Water Quality Criteria for the Protection of Human Health* (2000 Methodology), *Technical Support Document Volume 2: Development of National Support Factors* (TSD), and EPA's final 94 criteria documents that describe the development of each chemical-specific bioaccumulation factor included in the 2015 update on the *National Recommended Water Quality Criteria – Human Health Criteria Table* webpage (USEPA 2000; USEPA 2003a; USEPA 2015).

## 2. Summary

EPA searched peer-reviewed journal articles, federal and state reports, and databases to obtain input variables—including species-level lipid content, trophic level (TL), degree of ionization and metabolism of the chemical, and chemical-specific octanol-water coefficient ( $K_{ow}$ )—to calculate BAFs used to update 94 national recommended human health criteria. EPA used data from the searches to classify each chemical, using the decision framework presented in Figure 3-1 of EPA's TSD (reproduced as Figure 1 in this document) to derive the most appropriate BAFs according to EPA's 2000 Methodology and its TSD (USEPA 2000; USEPA 2003a).

EPA documented source information and reviewed and confirmed the derivation of each value. In addition, quality control checks of data calculations and data entries were performed and any errors found were corrected before BAF values were finalized. BAFs were rounded in accordance with EPA's 2000 Methodology and quality control checks were performed to ensure that the significant digits for each result were correct (USEPA 2000). The procedures followed for calculating national BAF values were documented in each of the 94 criteria documents.

The remainder of this document is organized into sections 3 through 7 and a list of references. Section 3, Chemical Procedure Classification, provides details about the procedure decision framework used to classify each chemical. Section 4, Baseline BAFs, presents the basic equations used for computing baseline BAFs. Section 5, National BAFs, provides the basic equations used for computing national BAFs as a function of final baseline BAFs. The basic equations in sections 4 and 5 are supported by additional methods and steps for establishing the  $K_{ow}$ , food chain multiplier (FCM), fraction freely dissolved ( $f_{fd}$ ), lipid content, and trophic levels (TLs), which are summarized in section 6, Supporting Procedures. Section 7, Examples, provides numerical examples that demonstrate the approach to estimate baseline and national BAFs for the chemicals endrin and fluorene.

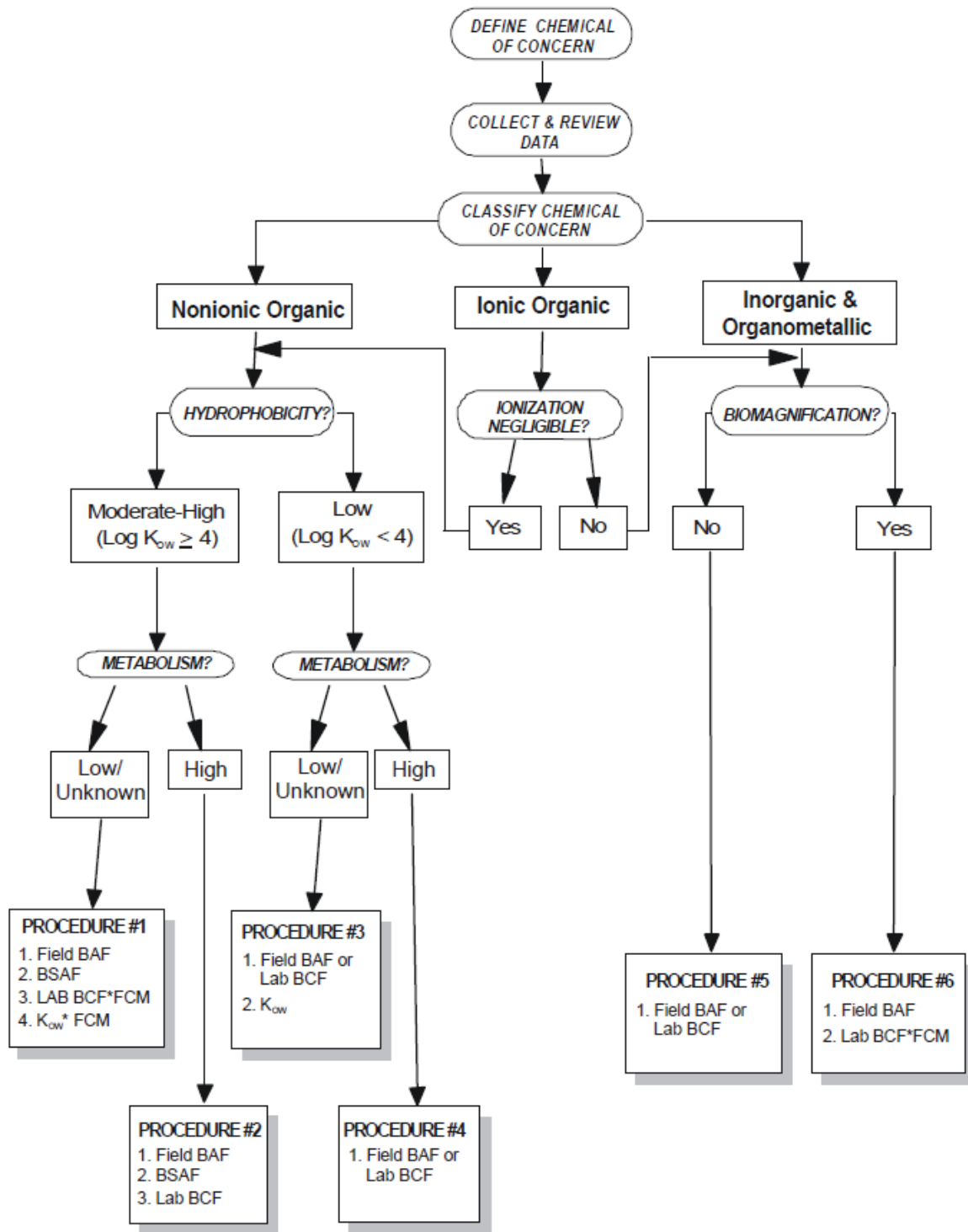


Figure 1. Framework for Selecting Methods for Deriving National BAFs (Source: USEPA 2003a, Figure 3-1, p. 3-2)

### 3. Chemical Procedure Classification

As explained in each of the updated 94 criteria documents (USEPA 2015), EPA used the decision framework presented in its TSD to identify procedures to derive national TL-specific BAFs for each chemical based on that chemical's properties (e.g., ionization and hydrophobicity), metabolism, and biomagnification potential (see Figure 1) (USEPA 2003a).

EPA followed the guidelines provided in section 5.5 of the TSD to assess the occurrence of cationic and anionic forms of the chemicals at typical environmental pH ranges. As explained in section 5.5, when a significant fraction of the total chemical concentration is expected to be present as the ionized species in water, procedures for deriving the national BAF rely on empirical (measured) methods (i.e., procedures #5 and #6 in Figure 1) (USEPA 2003a).

When an insignificant fraction of the total chemical is expected to be present as the ionized species (i.e., the chemical exists essentially in the neutral form), the national BAF is derived following procedures established for nonionic organic chemicals (e.g., procedures #1 through #4 in Figure 1) (USEPA 2003a). To evaluate whether ionization was negligible, EPA reviewed dissociation constant ( $pK_a$ ) information provided in Hazardous Substances Data Bank (HSDB) sources referenced in the individual criteria documents (USEPA 2015).

For chemicals for which ionization was determined to be negligible at typical environmental pH ranges, EPA followed the steps in section 3.2.3 of the TSD to determine the procedures for deriving the national BAFs for nonionic organic chemicals (USEPA 2003a). EPA evaluated the  $\log K_{ow}$  values provided in the Agency for Toxic Substances and Disease Registry (ATSDR) and HSDB sources referenced in the individual criteria documents to determine whether chemicals should be classified as moderate-high hydrophobic (i.e.,  $\log K_{ow} \geq 4$ ) or low hydrophobic (i.e.,  $\log K_{ow} < 4$ ). Those chemicals were further evaluated to determine whether metabolism was low/unknown or high; sources of information found on the metabolism of the chemicals are referenced in the individual criteria documents.

For organic chemicals for which ionization was determined not to be negligible at typical environmental pH ranges and for the inorganic chemical included in the 2015 criteria update (i.e., cyanide), EPA followed the guidelines in section 3.2.1 of the TSD to evaluate the biomagnification potential of the chemicals (USEPA 2003a). The ATSDR, HSDB, and EPA sources used for the evaluations are referenced in the individual criteria documents.

The characteristics of each chemical used to derive national TL-specific BAFs are documented in section 4.4.2 of each criteria document.

Following this decision framework, EPA selected the method that provided BAF estimates for all three TLs (TL2–TL4) in the following priority:

1. BAF estimates using the BAF method (i.e., based on field-measured BAFs), if possible.
2. BAF estimates using the bioconcentration factor (BCF) method if (a) the BAF method did not produce estimates for all three TLs, and (b) the BCF method produced national-level BAF estimates for all three TLs.
3. BAF estimates using the  $K_{ow}$  method if (a) procedure #1 or #3 was applicable (see Figure 1), and (b) the BAF and BCF methods did not produce BAF estimates for all three TLs.

If the procedure called for the BAF method but there were fewer than three TL estimates and the  $K_{ow}$  method did not apply, EPA estimated the BAF for the reported TLs by using a geometric mean when there were two BAFs and using the single estimate when only one was available. EPA did not mix values from the BAF and BCF methods. If the BAF method did not have sufficient reliable data for any TLs, EPA used the BCF method estimates in the same manner. If none of these methods provided sufficient data or were appropriate for the procedure, EPA used the BCF from the previously recommended 2002/2003 criteria (USEPA 2002a; USEPA 2003b).

## 4. Baseline BAFs

Three methods for computing baseline BAFs ((Baseline BAF)<sub>TL,n</sub>) are described in this section:  $K_{ow}$ , BAF, and BCF methods. Refer to section 3 to determine the applicability of each method to a particular chemical. In particular, note that the  $K_{ow}$  method applies to chemicals that fall under procedure #1 or procedure #3 and does not apply to chemicals that are highly metabolized or have significant ionization. Also, including an FCM in the equations is applicable to chemicals that fall under procedure #1 using the  $K_{ow}$  and BCF methods, or procedure #6 using the BCF method. For other chemicals, the FCM can be dropped from the equations in this section (or equivalently set to 1.0).

EPA used field-measured BAFs and laboratory-measured BCFs available from peer-reviewed, publicly available databases to develop baseline BAFs (Arnot and Gobas 2006; Environment Canada 2006). BAF and BCF values from additional peer-reviewed sources also were collected and evaluated. If measurement units were not provided, the data from those sources were considered “unverified.” Those values were recorded but, ultimately, not used to calculate BAFs for use in revising the 94 criteria. The chemicals for which additional sources were used to calculate baseline BAFs are listed below:

- 1,4-Dichlorobenzene (Calamari et al. 1982)
- 2,4,5-TP (Kenaga 1980; USEPA 1995)
- 2,4-D (Wang et al. 1994)
- Benzo(a)anthracene, benzo(b)fluoranthene, benzo(k)fluoranthene, chrysene, dibenzo(a,h)anthracene, indeno(1,2,3-cd)pyrene—Field-measured BAF for benzo(a)pyrene, an index polycyclic aromatic hydrocarbon (PAH), was used as a surrogate for estimating BAFs for other PAHs. This approach is consistent with conclusions of Neff (2002) that benzo(a)pyrene is a good indicator of the presence of pyrogenic PAHs in the environment and that these types of PAHs are expected to concentrate in organisms such as fish and shellfish as does benzo(a)pyrene.
- Cyanide (USEPA 2003b)
- Dinitrophenols (USEPA 2002b)

### 4.1 $K_{ow}$ Method

The  $K_{ow}$  method of computing baseline BAFs is applicable to chemicals that fall under procedures #1 and #3. It is a function of  $K_{ow}$  and an appropriate FCM. One baseline BAF can be calculated for each combination of chemical and TL to which the  $K_{ow}$  method applies. As described in section 5.4 of the TSD, this method is used for each nonionic, moderate-to-highly hydrophobic chemical with metabolism that is considered negligible or is unknown (USEPA



2003a). In this method, the  $K_{ow}$  is assumed to be equal to the baseline BCF, and thus the organic carbon and lipid normalization procedures are not needed. To account for biomagnification, the  $K_{ow}$  value is multiplied by an appropriate FCM. The  $K_{ow}$  method baseline BAF equation is shown below (USEPA 2003a, p. 5-23):

$$(\text{Baseline BAF})_{TL\ n} = K_{ow} \cdot (\text{FCM})_{TL\ n}$$

where:

$(\text{Baseline BAF})_{TL\ n}$	=	baseline BAF for TL “n” (L/kg-lipid)
FCM	=	FCM for TL “n”
$K_{ow}$	=	n-octanol-water partition coefficient

For chemicals that fall under procedure #3 ( $\log K_{ow} < 4$ ), the FCM can be dropped from the equation (or equivalently set to 1.0). See section 6.1,  $K_{ow}$ , and section 6.2, Food Chain Multiplier, for information on how the  $K_{ow}$  and FCM were determined. See section 7.1,  $K_{ow}$  Method: Endrin, for an example of how to apply the  $K_{ow}$  method for computing both baseline and national BAFs for endrin.

## 4.2 BAF Method

The BAF method is applicable to all chemicals. In the BAF method, a baseline BAF is calculated for each field sample BAF as shown in the equation below (USEPA 2003a, p. 5-1):

$$(\text{Baseline BAF})_i = \left[ \frac{\text{BAF}_T^t}{f_{fd}} - 1 \right] \cdot \frac{1}{f_l}$$

where:

$(\text{Baseline BAF})_i$	=	baseline BAF for field sample i (L/kg-lipid)
$\text{BAF}_T^t$	=	total BAF from field sample (i.e., total concentration of chemical in tissue / total concentration of chemical in water [L/kg-tissue])
$f_{fd}$	=	fraction of the total concentration of chemical in water that is freely dissolved
$f_l$	=	fraction of tissue that is lipid

Multiple  $(\text{Baseline BAF})_i$  are averaged to a  $(\text{Baseline BAF})_{TL\ n}$  by using the following procedure:

1. Compute the geometric mean across each chemical, computation method, TL, and species to compute a set of “species-mean baseline BAFs.”
2. Compute the geometric mean across each chemical, computation method, and TL to compute a set of “trophic level-mean baseline BAFs” using the results from the previous step.

See section 6.3, Fraction Freely Dissolved, for information on computing the fraction of the total concentration of chemical in water that is freely dissolved, and section 6.4, Lipid Content, for information on estimating the fraction of tissue that is lipid. See section 7.2.1, BAF Method, for an example of how to apply the BAF method to fluorene.

### 4.3 BCF Method

The BCF method is applicable to all chemicals. In the BCF method, a baseline BAF is calculated for each laboratory-measured BCF as shown in the equation below (USEPA 2003a, p. 5-19):

$$(\text{Baseline BAF})_i = (\text{FCM})_{\text{TL } n} \cdot \left[ \frac{\text{BCF}_T^t}{f_{fd}} - 1 \right] \cdot \frac{1}{f_\ell}$$

where:

(Baseline BAF) <sub>i</sub>	=	baseline BAF for laboratory sample i (L/kg-lipid)
FCM	=	FCM for TL associated with species from laboratory measurement
BCF <sub>T</sub> <sup>t</sup>	=	total BCF from laboratory measure (i.e., total concentration of chemical in tissue / total concentration of chemical in water [L/kg-tissue])
f <sub>fd</sub>	=	fraction of the total concentration of chemical in water that is freely dissolved
f <sub>ℓ</sub>	=	fraction of tissue that is lipid

For chemicals that fall under procedures #1 and #6 and when the log K<sub>ow</sub> is greater than or equal to 4, the species must be assigned to a particular TL (i.e., 2, 3, or 4) and the appropriate FCM selected. For other cases, the FCM can be dropped from the equation (or equivalently set to 1.0).

Multiple (Baseline BAF)<sub>i</sub> are averaged to a (Baseline BAF)<sub>TL n</sub> by using the same procedure as described in section 4.2, BAF Method. See section 6.3, Fraction Freely Dissolved, for information on computing the fraction of the total concentration of chemical in water that is freely dissolved, and section 6.4, Lipid Content, for information on estimating the fraction of tissue that is lipid. See section 7.2.2, BCF Method, for an example of how to apply the BCF method to fluorene.

## 5. National BAFs

Final baseline BAFs are used to compute national BAFs. EPA's TSD presents the formula for computing national TL-specific BAFs as follows (USEPA 2003a, p. 6-1):

$$\text{National BAF}_{(\text{TL } n)} = [(\text{Final Baseline BAF})_{\text{TL } n} \cdot (f_\ell)_{\text{TL } n} + 1] \cdot (f_{fd})$$

where:

National BAF	=	national BAF (L/kg-tissue)
(Final Baseline BAF) <sub>TL n</sub>	=	mean baseline BAF for TL "n" (L/kg-lipid)
f <sub>ℓ(TL n)</sub>	=	fraction of tissue that is lipid in aquatic organisms at TL "n"
f <sub>fd</sub>	=	fraction of the total concentration of chemical in water that is freely dissolved

To derive national BAFs, EPA uses national default values of lipid fraction (f<sub>ℓ</sub>) that are specific to each TL. The national default values of lipid fraction for TLs 2, 3, and 4 are:

$$\begin{aligned}
 f_{l(TL\ 2)} &= 0.019 \\
 f_{l(TL\ 3)} &= 0.026 \\
 f_{l(TL\ 4)} &= 0.030
 \end{aligned}$$

These values reflect consumption-weighted mean values of the lipid fraction of aquatic organisms that are commonly consumed throughout the United States. See section 6.2 of EPA's TSD for a description of the technical basis of EPA's national default values for lipid fraction (USEPA 2003a).

See section 6.3, Fraction Freely Dissolved, for information on computing the fraction of the total concentration of chemical in water that is freely dissolved. See section 7, Examples, for examples of calculated national BAFs.

## 6. Supporting Procedures

This section discusses selected supporting procedures used to calculate baseline and national BAFs, including  $K_{ow}$ , FCM,  $f_{fd}$ , lipid content, and species TL.

### 6.1 $K_{ow}$

$K_{ow}$  values were selected from ATSDR or HSDB sources with preference given to ATSDR. An average log  $K_{ow}$  was computed if a range or multiple values was reported from the selected source. The  $K_{ow}$  values that were used are provided in the BAF Calculation Table.xlsx spreadsheet, on the Chemical-Level Reference tab.

### 6.2 Food Chain Multiplier

For chemicals that fall under procedure #1 and either the  $K_{ow}$  method or the BCF method is being applied, or that fall under procedure #6 and the BCF method is being used, the FCM is selected from Table 4-6 in the TSD (reproduced as Table 1 in this document) using the chemical's Log  $K_{ow}$  and linear interpolation (USEPA 2003a, p. 4-39). Chemicals with a Log  $K_{ow}$  less than 4 have an FCM equal to 1.0. The calculated FCMs for each chemical are provided in the BAF Calculation Table.xlsx spreadsheet, on the Chemical-Level Reference tab.

### 6.3 Fraction Freely Dissolved

The fraction of the total concentration of chemical in water that is freely dissolved ( $f_{fd}$ ) is included in both the BCF method and the national BAF equations. The equation used to compute  $f_{fd}$  is shown below (USEPA 2003a, p. 4-7):

$$f_{fd} = \frac{1}{1 + POC \cdot K_{ow} + DOC \cdot 0.08 \cdot K_{ow}}$$

where:

- POC = concentration of particulate organic carbon (POC) in water (kilograms of particulate organic carbon per liter of water) (kg/L)
- DOC = concentration of dissolved organic carbon (DOC) in water (kilograms of dissolved organic carbon per liter of water) (kg/L)
- $K_{ow}$  = n-octanol-water partition coefficient

Table 1. Food Chain Multipliers for Trophic Levels 2, 3, and 4 (Source: USEPA 2003a, Table 4-6, p. 4-39)

Log K <sub>ow</sub>	Trophic Level 2	Trophic Level 3	Trophic Level 4	Log K <sub>ow</sub>	Trophic Level 2	Trophic Level 3	Trophic Level 4	Log K <sub>ow</sub>	Trophic Level 2	Trophic Level 3	Trophic Level 4
4.0	1	1.23	1.07	5.7	1	7.40	9.54	7.4	1	12.0	19.5
4.1	1	1.29	1.09	5.8	1	8.21	11.2	7.5	1	11.5	17.6
4.2	1	1.36	1.13	5.9	1	9.01	13.0	7.6	1	10.8	15.5
4.3	1	1.45	1.17	6.0	1	9.79	14.9	7.7	1	10.1	13.3
4.4	1	1.56	1.23	6.1	1	10.5	16.7	7.8	1	9.31	11.2
4.5	1	1.70	1.32	6.2	1	11.2	18.5	7.9	1	8.46	9.11
4.6	1	1.87	1.44	6.3	1	11.7	20.1	8.0	1	7.60	7.23
4.7	1	2.08	1.60	6.4	1	12.2	21.6	8.1	1	6.73	5.58
4.8	1	2.33	1.82	6.5	1	12.6	22.8	8.2	1	5.88	4.19
4.9	1	2.64	2.12	6.6	1	12.9	23.8	8.3	1	5.07	3.07
5.0	1	3.00	2.51	6.7	1	13.2	24.4	8.4	1	4.33	2.20
5.1	1	3.43	3.02	6.8	1	13.3	24.7	8.5	1	3.65	1.54
5.2	1	3.93	3.68	6.9	1	13.3	24.7	8.6	1	3.05	1.06
5.3	1	4.50	4.49	7.0	1	13.2	24.3	8.7	1	2.52	0.721
5.4	1	5.14	5.48	7.1	1	13.1	23.6	8.8	1	2.08	0.483
5.5	1	5.85	6.65	7.2	1	12.8	22.5	8.9	1	1.70	0.320
5.6	1	6.60	8.01	7.3	1	12.5	21.2	9.0	1	1.38	0.210

For deriving the national BAF  $f_{fd}$  term, EPA uses national default DOC and POC values for estimating a representative fraction of chemical that is freely dissolved in U.S. surface waters. The national default values of DOC and POC are (USEPA 2003a, p. 6-2):

$$\begin{aligned} \text{DOC} &= 2.9 \times 10^{-6} \text{ kg/L [= 2.9 mg/L]} \\ \text{POC} &= 0.5 \times 10^{-6} \text{ kg/L [= 0.5 mg/L]} \end{aligned}$$

See section 6.3 of EPA's TSD for a description of the technical basis of EPA's national default values for DOC and POC (USEPA 2003a).

The calculated  $f_{fd}$  for each chemical is provided in the BAF Calculation Table.xlsx spreadsheet, on the Chemical-Level Reference tab.

#### 6.4 Lipid Content

The following hierarchical steps were used to select lipid content for baseline BAF calculation:

1. Use measured values if provided.
2. Select a lipid content based on species from Tables 4-5 and 6-3 in the TSD (USEPA 2003a, p. 4-37, 6-18).
3. Use an average species value from all studies in database with reported values.
4. Apply national lipid fractions based on assigned trophic level, as listed below:

$$\begin{aligned} f_{l(TL\ 2)} &= 0.019 \\ f_{l(TL\ 3)} &= 0.026 \\ f_{l(TL\ 4)} &= 0.030 \end{aligned}$$

Measured values, values in Tables 6-3 and 4-5 in the TSD, and database average species values all were reported as lipid content (USEPA 2003a). To convert to a lipid fraction, the values were multiplied by 0.01. No conversion was needed for national TL lipid fractions.

The selected lipid fraction for each BAF or BCF value is provided in the BAF Calculation Table.xlsx spreadsheet, on the Baseline BAFs tab. To derive national BAFs, EPA uses national default values of lipid fraction ( $f_l$ ) that are specific to each TL (see section 5, National BAFs).

## 6.5 Species Trophic Level

TL assignment information was primarily obtained from the EPA 2014 NHANES Fish Consumption Rate Report and Fishbase.org and used to determine TLs for organisms in the BCF and BAF data sources (USEPA 2014; Froese and Pauly 2015). When no primary source was available, an expert fishery biologist and an expert invertebrate zoologist provided TL identifications. These experts checked all TL identifications for correctness and consistency. The following university websites were consulted to inform the experts' review:

- Central Michigan University Zooplankton of the Great Lakes (McNaught 2015)
- Encyclopedia of Life (Encyclopedia of Life 2015)
- The Murray-Darling Freshwater Research Centre Australian Freshwater Invertebrates Guide (Murray-Darling Freshwater Research Centre 2013)
- University of Maine School of Marine Science (University of Maine 2015)
- University of Michigan Animal Diversity Web (Myers et al. 2015)

The results of this analysis are provided in the BAF Calculation Table.xlsx spreadsheet, on the Species-Level Reference tab.

## 7. Examples

This section presents examples that collectively demonstrate the  $K_{ow}$ , BCF, and BAF methods of deriving baseline and national BAFs. The reader can compare these examples to the companion BAF Calculation Table.xlsx spreadsheet.

### 7.1 $K_{ow}$ Method: Endrin

The Log  $K_{ow}$  for endrin from ATSDR ranges from 5.34 to 5.6 (see BAF Calculation Table.xlsx, Chemical-Level Reference tab). Thus, an average Log  $K_{ow}$  value of 5.47 was used ( $K_{ow} = 10^{5.47}$ ). Based on the FCMs presented in Table 1, the FCMs for TLs 3 and 4 were interpolated to be 5.637 and 6.299, respectively. The FCM for TL 2 is 1.0. Multiplying the interpolated FCMs by  $K_{ow}$  yielded values of 295,120.92, 1,663,596.64, and 1,858,966.69 L/kg as the baseline BAFs for TLs 2, 3, and 4, respectively. The calculation of endrin's baseline BAF for TL 4 is shown below:

$$\begin{aligned}(\text{Baseline BAF})_{\text{TL } 4} &= K_{ow} \cdot (\text{FCM})_{\text{TL } 4} \\(\text{Baseline BAF})_{\text{TL } 4} &= 10^{5.47} \cdot 6.299 = 1,858,966.69 \text{ L/kg-lipid}\end{aligned}$$

Converting the baseline BAF expressed on a L/kg-lipid content to a national BAF expressed on a L/kg-tissue basis relies on the national default values of lipid fraction ( $f_l$ ) and fraction of the

total concentration of chemical in water that is freely dissolved ( $f_{fd}$ ). The calculation of  $f_{fd}$  for endrin is shown below:

$$f_{fd} = \frac{1}{1 + \text{POC} \cdot K_{ow} + \text{DOC} \cdot 0.08 \cdot K_{ow}}$$

$$f_{fd} = \frac{1}{1 + 0.5 \times 10^{-6} \cdot 10^{5.47} + 2.9 \times 10^{-6} \cdot 0.08 \cdot 10^{5.47}} = 0.8223$$

The  $f_{fd}$  value is substituted into the national BAF equation along with the trophic-specific value for  $f_l$ . Continuing with the endrin example and TL 4 ( $f_{l(TL\ 4)}=0.030$ ), the national BAF is calculated using the following equation:

$$\text{National BAF}_{(TL\ 4)} = [(\text{Final Baseline BAF})_{TL\ 4} \cdot (f_l)_{TL\ 4} + 1] \cdot (f_{fd})$$

$$\text{National BAF}_{(TL\ 4)} = [1,858,966.69 \cdot 0.030 + 1] \cdot 0.8223 = 45,862.41 \text{ L/kg-tissue}$$

The corresponding values for TLs 2 and 3 were computed as 4,611.98 and 35,570.31 L/kg-tissue, respectively. Rounding the values to two significant figures yields national BAF values of 4,600, 36,000, and 46,000 L/kg-tissue for TLs 2, 3, and 4, respectively.

## 7.2 BAF and BCF Methods: Fluorene

The Log  $K_{ow}$  for fluorene from ATSDR is 4.18 ( $K_{ow} = 10^{4.18}$ ) (see BAF Calculation Table.xlsx, Chemical-Level Reference tab). Based on the FCMs presented in Table 1, the FCMs for TLs 3 and 4 were interpolated to be 1.346 and 1.122, respectively. The FCM for TL 2 is 1.0.

The calculation of  $f_{fd}$  for fluorene is shown below:

$$f_{fd} = \frac{1}{1 + \text{POC} \cdot K_{ow} + \text{DOC} \cdot 0.08 \cdot K_{ow}}$$

$$f_{fd} = \frac{1}{1 + 0.5 \times 10^{-6} \cdot 10^{4.18} + 2.9 \times 10^{-6} \cdot 0.08 \cdot 10^{4.18}} = 0.9890$$

The  $f_{fd}$  term is part of the equations for the BAF method, BCF method, and the national BAF equation. Calculations of fluorene's baseline and national BAFs using the BAF and BCF methods for TL 2 are explained in the sections that follow.

### 7.2.1 BAF Method

One field sample was available for fluorene with a BAF of 79,432.8 L/kg for an amphipod (*Pontoporeia hoyi*) (TL 2). No BAF samples were available for TLs 3 and 4. A baseline BAF is calculated for each field sample available. The fraction lipid ( $f_l$ ) in this equation is determined as described in section 6.4, Lipid Content. In this example,  $f_l$  was not provided with the source data and was estimated as 0.03 based on data from the TSD's Tables 4-5 and 6-3 (USEPA 2003a). The calculation of baseline BAF using the BAF method for fluorene is shown below:

$$(\text{Baseline BAF})_i = \left[ \frac{\text{BAF}_T^t}{f_{fd}} - 1 \right] \cdot \frac{1}{f_l}$$

$$(\text{Baseline BAF})_i = \left[ \frac{79432.8}{0.9890} - 1 \right] \cdot \frac{1}{0.03} = 2,677,062.70 \text{ L/kg-lipid}$$

If multiple baseline BAFs were derived, they were averaged prior to computing the national BAF by calculating a geometric mean first by species, then by TL. In this example for fluorene, however, only one field sample was available.

Thus, the calculated baseline BAF above, the  $f_{fd}$  value, and the national default trophic-specific value for fraction lipid ( $f_l$ ) are substituted into the national BAF equation. Continuing with the fluorene example and TL 2 ( $f_{l(TL 2)}=0.019$ ), the national BAF is calculated using the following equation:

$$\text{National BAF}_{(TL 2)} = [(\text{Final Baseline BAF})_{TL 2} \cdot (f_l)_{TL 2} + 1] \cdot (f_{fd})$$

$$\text{National BAF}_{(TL 2)} = [2,677,062.7 \cdot 0.019 + 1] \cdot 0.9890 = 50,307.82 \text{ L/kg-tissue}$$

Rounding this value to two significant figures yields a national BAF value using the BAF method of 50,000 L/kg-tissue for TL 2.

### 7.2.2 BCF Method

Twelve laboratory-derived BCF values were available for fluorene for six species at all three TLs. Focusing on TL 2 for this example, six BCF values were available for two species: an oligochaete (*Lumbriculus variegatus*) and a water flea (*Daphnia magna*). The oligochaete laboratory-derived BCF values are 330, 380, 490, 405, and 500 L/kg. The water flea BCF value is 506 L/kg. In the BCF method, a baseline BAF is calculated for each laboratory-measured BCF value. Calculation of the baseline BAF using the BCF method for fluorene using the BCF value of 330 L/kg is shown below:

$$(\text{Baseline BAF})_i = (\text{FCM})_{TL n} \cdot \left[ \frac{\text{BCF}_T^t}{f_{fd}} - 1 \right] \cdot \frac{1}{f_l}$$

$$(\text{Baseline BAF})_i = 1 \cdot \left[ \frac{330}{0.9890} - 1 \right] \cdot \frac{1}{0.03} = 11,088.54 \text{ L/kg-lipid}$$

The other oligochaete baseline BAF values calculated using the BCF method are 12,773.67, 16,480.96, 13,616.24, and 16,817.99 L/kg-lipid. The water flea baseline BAF value calculated using the BCF method is 10,212.12 L/kg-lipid. Multiple  $(\text{Baseline BAF})_i$  are averaged to a  $(\text{Baseline BAF})_{TL n}$  by taking a geometric mean first by species, then by TL. For fluorene at TL 2, a geometric mean of 13,983.01 L/kg-lipid was calculated for the oligochaete and only one water flea baseline BCF value of 10,212.12 L/kg-lipid was available. The geometric mean of those two values is 11,949.74 L/kg-lipid, which is the derived baseline BAF for fluorene TL 2 using the BCF method. The corresponding values for TLs 3 and 4 were computed as 17,652.38 and 23,784.77 L/kg-lipid, respectively.

The calculated baseline BAF values above, the  $f_{fd}$  value, and the national default trophic-specific value for fraction lipid ( $f_l$ ) are substituted into the national BAF equation. Continuing with the

fluorene example and TL 2 ( $f_{i(TL\ 2)}=0.019$ ), the national BAF is calculated using the following equation:

$$\text{National BAF}_{(TL\ 2)} = [(\text{Final Baseline BAF})_{TL\ 2} \cdot (f_{\rho})_{TL\ 2} + 1] \cdot (f_{fd})$$

$$\text{National BAF}_{(TL\ 2)} = [11,949.74 \cdot 0.019 + 1] \cdot 0.9890 = 225.55 \text{ L/kg-tissue}$$

The corresponding values for TLs 3 and 4 were computed as 454.92 and 706.71 L/kg-tissue, respectively. Rounding the values to two significant figures yields national BAF values using the BCF method of 230, 450, and 710 L/kg-tissue for TLs 2, 3, and 4, respectively.



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