3745-1-41 **Methodology for deriving bioaccumulation factors.**

[Comment: For dates of non-regulatory government publications, publications of recognized organizations and associations, federal rules and federal statutory provisions referenced in this rule, see rule 3745-1-03 of the Administrative Code.]

(A) The purpose of this rule is to describe procedures for deriving bioaccumulation factors (BAFs) to be used in the calculation of human health tier I criteria and tier II values and wildlife tier I criteria. A subset of the human health BAFs are also used to identify the chemicals that are considered bioaccumulative chemicals of concern (BCCs).

(B) Review and selection of data.

(1) Field-measured BAFs. The following procedural and quality assurance requirements shall be met for field-measured BAFs.

(a) The field studies used shall be limited to those conducted in the Great Lakes system with fish in trophic levels three or four.

(b) The trophic level of the fish species shall be determined.

(c) The site of the field study shall not be so unique such that the BAF cannot be extrapolated to other locations where the criteria and values will apply.

(d) For organic chemicals, the per cent lipid shall be either measured or reliably estimated for the tissue used in the determination of the BAF.

(e) The concentration of the chemical in the water shall be measured in a way that can be related to particulate organic carbon (POC) or dissolved organic carbon (DOC) and shall be relatively constant during the steady-state time period.

(f) For organic chemicals with log K_{ow} greater than four, the concentrations of POC and DOC in the ambient water shall be either measured or reliably estimated.

(g) For inorganic and organic chemicals, BAFs shall be used only if they are expressed on a wet weight basis; BAFs reported on a dry weight basis cannot be converted to wet weight unless a conversion factor is measured or reliably estimated for the tissue used in the determination of the BAF.

(2) Field-measured biota-sediment accumulation factors (BSAFs). The following procedural and quality assurance requirements shall be met for field-measured BSAFs.

(a) The field studies used shall be limited to those conducted in the Great Lakes system with fish in trophic levels three or four.

(b) Samples of surface sediments shall be from locations where there is net deposition of fine sediment (zero to one centimeter is ideal) and that are representative of average surface sediments in the vicinity of the organism.

(c) The K_{ow}s used shall be of acceptable quality as described in paragraph (B)(5) of this rule.

(d) The site of the field study shall not be so unique such that the resulting BAF cannot be extrapolated to other locations where the criteria and values will apply.

(e) The trophic level of the fish species shall be determined.

(f) The per cent lipid shall be either measured or reliably estimated for the tissue used in the determination of the BAF.

(3) Laboratory-measured BCFs. The following procedural and quality assurance requirements shall be met for laboratory-measured BCFs.

(a) The test organism shall not be diseased, unhealthy, or adversely affected by the concentration of the chemical.

(b) The total concentration of the chemical in the water shall be measured and shall be relatively constant during the steady-state time period.

(c) The organisms shall be exposed to the chemical using a flow-through or renewal procedure.

(d) For organic chemicals, the per cent lipid shall be either measured or reliably estimated for the tissue used in the determination of the BCF.

(e) For organic chemicals with log K_{ow} greater than four, the concentrations of POC and DOC in the test solution shall be either measured or reliably estimated.

(f) Laboratory-measured BCFs should be determined using fish species, but BCFs determined with molluscs and other invertebrates may be used if appropriate.

(g) In a bioconcentration test, if laboratory-measured BCFs increase or decrease as the concentration of the chemical increase in the test solutions, the BCF measured at the lowest test concentration that is

above concentrations existing in the control water shall be used (i.e., a BCF shall not be calculated from a control treatment). The concentrations of an inorganic chemical in a bioconcentration test shall be greater than normal background levels and greater than levels required for normal nutrition of the test species if the chemical is a micronutrient, but below levels that adversely affect the species.

(h) For inorganic and organic chemicals, BCFs shall be used only if they are expressed on a wet weight basis. BCFs reported on a dry weight basis cannot be converted to wet weight unless a conversion factor is measured or reliably estimated for the tissue used in the determination of the BAF.

(i) BCFs for organic chemicals may be based on measurement of radioactivity only when the BCF is intended to include metabolites or when there is confidence that there is no interference due to metabolites.

(j) The calculation of the BCF shall address growth dilution.

(k) Other aspects of the methodology used shall be similar to those described in "Standard Guide for Conducting Bioconcentration Tests with Fishes and Saltwater Bivalve Molluscs. Standard E1022."

(4) Predicted BCFs. The following procedural and quality assurance requirements shall be met for predicted BCFs.

(a) The K_{ow} used shall be of acceptable quality as described in paragraph (B)(5) of this rule.

(b) The predicted baseline BCF shall be calculated using the equation

Predicted baseline BCF = K_{ow}

Where:

K_{ow} = octanol-water partition coefficient.

(5) Octanol-water partition coefficient (K_{ow}).

(a) The value of K_{ow} used for an organic chemical shall be determined by giving priority to the experimental and computational techniques used as shown in table 41-1 of this rule.

(b) A value of K_{ow} that seems to be different from the others may be considered an outlier and not used. The value of K_{ow} used for an organic chemical shall be either the geometric mean of the available

s with highest priority or the arithmetic mean of the available log K_{ow}s with the highest priority. Because it is an intermediate value in the derivation of a BAF, the values used for the K_{ow} and log K_{ow} of a chemical shall not be rounded to fewer than three significant digits after the decimal point.

(C) 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 an FCM.

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

For comparative purposes, baseline BAFs shall be derived for each chemical by as many of the four methods as available data allow.

(D) Calculation of baseline BAFs for organic chemicals.

(1) Lipid normalization.

(a) It is assumed that BAFs and BCFs for organic chemicals can be extrapolated on the basis of per cent lipid from one tissue to another and from one aquatic species to another in most cases.

(b) Because BAFs and BCFs for organic chemicals are related to the per cent lipid, it does not make any difference whether the tissue sample is whole body or edible portion, but both the BAF (or BCF) and the per cent lipid must be determined for the same type of tissue. The per cent lipid of the tissue should be measured during the BAF or BCF study, but in some cases it may be reliably estimated from measurements on tissue from other organisms. If per cent lipid is not reported for the test organisms in the original study, it may be obtained from the author. 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.

(c) The lipid-normalized concentration (C_l) of a chemical in tissue is defined using the following equation:

$$C_l = \frac{C_B}{f_l}$$

Where:

C_B = concentration of the organic chemical in the tissue of aquatic biota (either whole organism or specified tissue) expressed in micrograms per gram.

f_l = fraction of the tissue that is lipid.

(2) Bioavailability. By definition, baseline BAFs and BCFs for organic chemicals, whether measured or predicted, are 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 rule, the relationship between the total concentration of the chemical in the ambient 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.

The fraction of the total chemical in the ambient water that is freely dissolved (f_{fd}), shall be calculated using the following equation:

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

Where:

DOC = concentration of dissolved organic carbon, expressed as kilograms of dissolved organic carbon per liter of water.

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

POC = concentration of particulate organic carbon, expressed as kilograms of particulate organic carbon per liter of water.

(3) Food-chain multiplier (FCM). In the absence of a field-measured BAF or a predicted BAF derived from a BSAF, an FCM shall be used to calculate the baseline BAF for trophic levels three and four from a laboratory-measured or predicted BCF. For an organic chemical, the FCM used shall be derived from table 41-2 of this rule using the chemical's log K_{ow} and linear interpolation. An 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.

(4) Calculation of a baseline BAF from a field-measured BAF. A baseline BAF shall be calculated from a field-measured BAF using the following equation:

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

Where:

BAF^t= BAF based on total concentration in tissue and water.

f_l = 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 measured 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 measured baseline BAFs shall be calculated. If a baseline BAF based on a measured BAF is available for either trophic level three or four, but not both, a measured baseline BAF for the other trophic level shall be calculated using the ratio of the FCMs that are obtained by linear interpolation from table 41-2 of this rule for the chemical.

(5) Calculation of a baseline BAF from a field-measured BSAF.

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

$$(\text{Baseline BAF})_i = (\text{Baseline BAF})_r \cdot \frac{(\text{BSAF})_i \cdot (K_{ow})_i}{(\text{BSAF})_r \cdot (K_{ow})_r}$$

Where:

$(BSAF)_i$ = BSAF for chemical "i".

$(BSAF)_r$ = 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".

(b) A BSAF shall be calculated using the following equation:

$$\text{BSAF} = \frac{C_\ell}{C_{SOC}}$$

Where:

C_l = the lipid-normalized concentration of the chemical in tissue.

C_{soc} = the organic carbon-normalized concentration of the chemical in sediment.

(c) The organic carbon-normalized concentration of a chemical in sediment (C_{soc}), shall be calculated using the following equation:

$$C_{soc} = \frac{C_s}{f_{oc}}$$

Where:

C_S = concentration of chemical in sediment (expressed as micrograms per gram sediment).

f_{OC} = fraction of the sediment that is organic carbon.

(d) Predicting BAFs from BSAFs requires data from a steady-state (or near steady-state) condition between sediment and ambient water for both a reference chemical "r" with a field-measured BAF^{fd}_{1} and other chemicals "N=i" for which BSAFs are to be determined.

(e) 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 derived using BSAFs shall be calculated.

(f) If a baseline BAF based on a measured BSAF is available for either trophic level three or four, but not both, a baseline BAF for the other trophic level shall be calculated using the ratio of the FCMs that are obtained by linear interpolation from table 41-2 of this rule for the chemical.

(6) Calculation of a baseline BAF from a laboratory-measured BCF. A baseline BAF for trophic level three and a baseline BAF for trophic level four shall be calculated from a laboratory-measured BCF of acceptable quality and an FCM using the following equation:

$$\text{Baseline BAF} = (\text{FCM})\left[\frac{\text{Measured BCF}_T^{\,t}}{f_{fd}} - 1\right]\left(\frac{1}{f_l}\right)$$

Where:

BCF^t = BCF based on total concentration in tissue and water.

f_l = fraction of the tissue that is lipid.

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

FCM = the food-chain multiplier obtained from table 41-2 of this rule by linear interpolation for trophic level three or four, 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 based on laboratory-measured BCFs shall be calculated.

(7) Calculation of a baseline BAF from an octanol-water partition coefficient. A baseline BAF for trophic level three and a baseline BAF for trophic level four shall be calculated from a K_{ow} of acceptable quality and an FCM using the following equation:

Baseline BAF = (FCM) (predicted baseline BCF)

= (FCM) (K_{ow})

Where:

FCM = the food-chain multiplier obtained from table 41-2 of this rule by linear interpolation for trophic level three or four, as necessary.

K_{ow} = octanol-water partition coefficient.

(E) Human health and wildlife BAFs for organic chemicals.

(1) 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 to yield the fraction freely dissolved (f_{fd}) using the following equations:

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

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

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

(2) The human health BAFs for an organic chemical shall be calculated using the equations.

(a) For trophic level three

Human health BAF^{HH}_{TL3} = [(baseline BAF) (0.0182)+1] (f_{fd})

and

(b) For trophic level four

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 three and four, respectively, that are used to derive human health criteria and values pursuant to rule 3745-1-42 of the Administrative Code.

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

(a) For trophic level three:

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

(b) For trophic level four:

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

Where:

0.0646 and 0.1031 are the standardized fraction lipid values for trophic levels three and four, respectively, that are used to derive wildlife criteria pursuant to rule 3745-1-43 of the Administrative Code.

(F) Human health and wildlife BAFs for inorganic chemicals.

(1) For inorganic chemicals, the baseline BAFs for trophic levels three and four are both assumed to equal the BCF determined for the chemical with fish, i.e., the FCM is assumed to be 1.0 for both trophic levels three and four. However, an FCM greater than 1.0 might be applicable to some metals, such as mercury, if, for example, an organometallic form of the metal biomagnifies.

(2) BAFs for human health criteria and values.

(a) Measured BAFs and BCFs used to determine human health BAFs for inorganic chemicals shall be based on edible tissue of freshwater fish unless it is demonstrated that whole-body BAFs or BCFs are similar to edible-tissue BAFs or BCFs. BCFs and BAFs based on measurements of aquatic plants and invertebrates should not be used in the derivation of human health criteria and values.

(b) If one or more field-measured baseline BAFs for an inorganic chemical are available from studies conducted in the Great Lakes system with the edible tissue of fish, then for each trophic level:

(i) A species mean measured baseline BAF shall be calculated as the geometric mean if more than one measured BAF is available for a given species.

(ii) The geometric mean of the species mean measured baseline BAFs shall be used as the human health BAF for that chemical.

(c) If an acceptable measured baseline BAF is not available for an inorganic chemical and one or more acceptable edible-portion laboratory-measured BCFs are available for the chemical, a predicted baseline BAF shall be calculated by multiplying the geometric mean of the BCFs times an FCM. The FCM shall be 1.0 unless chemical-specific biomagnification data support using a multiplier other than 1.0. The predicted baseline BAF shall be used as the human health BAF for that chemical.

(3) BAFs for wildlife criteria.

(a) Measured BAFs and BCFs used to determine wildlife BAFs for inorganic chemicals shall be based on whole-body freshwater fish and invertebrate data unless it is demonstrated that edible-tissue BAFs or BCFs are similar to whole-body BAFs or BCFs.

(b) If one or more field-measured baseline BAFs for an inorganic chemical are available from studies conducted in the Great Lakes system with whole body fish or invertebrates, then:

(i) For each trophic level, a species mean measured baseline BAF shall be calculated as the geometric mean if more than one measured BAF is available for a given species.

(ii) For each trophic level, the geometric mean of the species mean measured baseline BAFs shall be used as the wildlife BAF for that chemical.

(iii) If an acceptable measured baseline BAF is not available for an inorganic chemical and one or more acceptable whole-body laboratory-measured BCFs are available for the chemical, a predicted baseline BAF shall be calculated by multiplying the geometric mean of the BCFs times an FCM. The FCM shall be 1.0 unless chemical-specific biomagnification data support using a multiplier other than 1.0. The predicted baseline BAF shall be used as the wildlife BAF for that chemical.

(G) Final review. For both organic and inorganic chemicals, human health and wildlife BAFs for both trophic levels shall be reviewed for consistency with all available data concerning the bioaccumulation, bioconcentration, and metabolism of the chemical. BAFs derived in accordance with this methodology shall be modified if changes are justified by available data.

Table 41-1. Priorities for K_{ow} experimental and computational techniques for organic chemicals.

Priority		Technique
Log $K_{ow} \leq 4.0$	Log $K_{ow} > 4.0$	
1	1	Slow-stir
1	1	Generator-column
1	4	Shake-flask
2	2	Reverse-phase liquid chromatography on C18 chromatography packing with extrapolation to zero per cent solvent
3	3	Reverse-phase liquid chromatography on C18 chromatography packing without extrapolation to zero per cent solvent
4	5	Calculated by the CLOGP program (a computer program available from Pomona college)

Table 41-2. Food-chain multipliers for trophic levels 2, 3 and 4.

Log K_{ow}	Trophic level 2	Trophic[1] 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
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

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

Replaces: 3745-1-37

Effective:

Five Year Review (FYR) Dates:

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Certification

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Date

Promulgated Under:	119.03
Statutory Authority:	6111.041
Rule Amplifies:	6111.041
Prior Effective Dates:	10/31/1997, 8/10/2016