

Fact Sheet Date: March 12, 1998

**NEW YORK STATE
- HUMAN HEALTH FACT SHEET -**

**Ambient Water Quality Value
Based on Human Consumption of Fish**

SUBSTANCE: Chlorobenzene

CAS REGISTRY NUMBER: 108-90-7

AMBIENT WATER QUALITY VALUE: 400 ug/L

BASIS: Bioaccumulation

INTRODUCTION

This value applies to the water column and is designed to protect humans from the effects of waterborne contaminants that may bioaccumulate in fish; it is referred to as a Health (Fish Consumption) or H(FC) value. The H(FC) value is based on three components, the toxicity of the substance to humans, the extent to which it bioaccumulates in fish, and the rate of fish consumption.

SUMMARY OF INFORMATION

A. Toxicity

The toxicity of chlorobenzene relevant to human health is described in a separate fact sheet (NYS, 1997). That fact sheet, which supports an ambient water quality value for protection of sources of potable water, derives an acceptable daily intake (ADI) of 19 ug chlorobenzene/(kg · day) for non-oncogenic effects.

B. Bioaccumulation

A measurement of bioaccumulation is necessary to derive a value to protect human consumers of fish. Bioaccumulation is the process by which a substance becomes concentrated in an organism through the organism's exposure to the contaminant in food and water. Bioaccumulation is represented numerically by a bioaccumulation factor, or BAF, which is the ratio of the concentration of a substance in the organism to that in the water column.

The term bioconcentration also describes the concentration of a substance in an organism relative to the concentration in the water column. A bioconcentration factor (BCF), however, is measured with exposure to the contaminant by water only. A BCF may be equal to the BAF for many substances, but can substantially underestimate it for others.

U.S. EPA (1995a) has promulgated, as final Federal regulations, procedures for deriving bioaccumulation factors. The procedures are believed appropriate for deriving statewide values and are being used in this fact sheet.

A key aspect of this procedure is that bioaccumulation is believed to be related to the concentration of freely dissolved substance. Hydrophobic organic substances are considered to exist in water in three phases: freely dissolved, sorbed to dissolved organic matter and sorbed to suspended solids (U.S. EPA, 1995b). Because BAF determinations are often based on measurements of total or dissolved substance, a measured BAF must be adjusted based on the estimated fraction of freely dissolved material. In addition, because measured BAFs are determined based on the percent lipid in the species studied, they are adjusted, or normalized, to 100% lipid to allow comparison of BAFs derived from species with different tissue lipid fractions. A BAF adjusted for both fraction freely dissolved and normalized to 100% lipid is referred to as a "baseline BAF."

Although bioaccumulation is related to the freely dissolved substance, water quality criteria are based on total substance. A baseline BAF, therefore, is readjusted to a final BAF by the expected fraction freely dissolved and fish lipid content for the waters for which criteria are established. The relationship of field-measured or final BAF to the baseline BAF is shown in equation 1:

$$(Eq. 1) \quad \text{Baseline BAF} = \left[\frac{\text{Field or Final BAF}}{f_{fd}} \right] \left[\frac{1}{f_l} \right]$$

where f_l = fraction of tissue that is lipid and f_{fd} = fraction of substance that is freely dissolved.

U.S. EPA (1995b) presented the following equation for estimating f_{fd} :

$$(Eq. 2) \quad f_{fd} = \frac{1}{1 + \frac{(\text{DOC})(K_{ow})}{10} + (\text{POC})(K_{ow})}$$

where K_{ow} is the n-octanol-water partition coefficient of the substance in question, and DOC and POC are concentrations of dissolved and particulate organic carbon, respectively, in kg/L. The basis for this equation is described by U.S. EPA (1995b).

When deriving a baseline BAF from a field-measured BAF, DOC and POC levels

under which the field BAF was determined are used to calculate a f_{fd} . When the baseline BAF is readjusted to yield a final BAF, the DOC and POC levels appropriate for the applicability of the criterion are used.

Derivation of Baseline BAFs

U.S. EPA (1995b), as part of the documentation for the Great Lakes Water Quality Initiative, presents baseline BAFs for a number of substances. The procedures (U.S. EPA, 1995a,b) provide a hierarchy of methods to calculate a baseline BAF. The only baseline BAF presented by U.S. EPA (1995b) for chlorobenzene is a predicted baseline BAF that is based on a predicted BCF and food chain multiplier (FCM). For this, a 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:

$$\text{Predicted Baseline BAF} = (\text{FCM}) (K_{ow})$$

The predicted baseline BAFs for trophic levels 3 and 4 for chlorobenzene from U.S. EPA (1995b) are shown in Table 1.

Table 1	
Baseline BAFs for Chlorobenzene (U.S. EPA, 1995b)	
Trophic Level	Baseline BAF (L/kg)
3	747
4	740

These values have been reviewed and are believed appropriate for both the Great Lakes and the rest of the State. The data U.S. EPA used and calculations needed to derive these values are shown below. (Note: The readjustment of these baseline BAFs to final BAFs is described under Derivation of Water Quality Values).

$$\text{Predicted Baseline BAF} = (\text{FCM}) (K_{ow})$$

$\log K_{ow}$ is 2.865 (U.S. EPA, 1995b); $K_{ow} = 733$

The FCMs, from U.S. EPA (1995a) are 1.023 and 1.006 for trophic levels 3 and 4, respectively.

$$\text{Predicted Baseline BAF}_{TL3} = (\text{FCM}_{TL3}) (K_{ow})$$

$$= (1.023) (733) = 750 \text{ L/kg}$$

$$\text{Predicted Baseline BAF}_{\text{TL4}} = (\text{FCM}_{\text{TL4}}) (K_{\text{ow}})$$

$$= (1.006) (733) = 737 \text{ L/kg}$$

These values are slightly different than the Table 1 values; the differences are insignificant and believed due to rounding. Because the values are sufficiently close, and to be consistent with U.S. EPA, this fact sheet will use the Table 1 values of 747 and 740 as the baseline BAFs for chlorobenzene for trophic levels 3 and 4, respectively.

DERIVATION OF WATER QUALITY VALUE

As required by 6 NYCRR 702.8(a) the water quality value must equal the acceptable daily intake from fish consumption divided by a bioaccumulation factor and by a fish consumption rate of 0.033 kg/day.

A. Acceptable Daily Intake From Fish Consumption

As required by 6 NYCRR 702.8(b), the most stringent acceptable daily intake from fish consumption is 20% of the ADI for non-oncogenic effects, as determined from 6 NYCRR 702.5. This value is 19 ug chlorobenzene/(kg · day) from NYS (1997) as described above. The reader will note that the health (water source) value derived in NYS (1997) is not based on 702.5 but rather is based on a principal organic contaminant class (702.3). The regulations for deriving H(FC) values require that the acceptable daily intake from fish consumption be based on either an oncogenic or non-oncogenic effect.

The acceptable daily intake from fish consumption is:

$$0.2 \times 19 \text{ ug chlorobenzene}/(\text{kg} \cdot \text{day}) = 3.8 \text{ ug chlorobenzene}/(\text{kg} \cdot \text{day})$$

B. Final BAF

As described above, a baseline BAF is adjusted by the fish lipid fraction and the fraction freely dissolved to yield a final BAF for the substance. Equation 1 (above) is rearranged to solve for final BAF:

$$\text{Final BAF} = [(\text{baseline BAF})(f_l) + 1](f_{fd})$$

where values for f_l and f_{fd} are appropriate to criteria for New York State. Because, as described below, humans are exposed to fish from two trophic levels, this calculation is performed to generate final BAFs for trophic levels 3

and 4.

A fish lipid content of 3% had previously been used when calculating BAFs for deriving criteria for New York State. U.S. EPA (1995a) apportions daily fish consumption between fish of trophic levels 3 and 4. Specifically, 24% is assigned to trophic level 3 fish, with a standardized lipid fraction of 0.0182 (1.82%), and 76% to trophic level 4 fish, with a standardized lipid fraction of 0.0310 (3.1%). The weighted average lipid fraction of trophic level 3 and 4 fish is thus 0.028 (2.8%), which is very close to the value of 3% that had been used in New York State. U.S. EPA's apportionment approach is believed to be protective of human consumers of fish statewide, and will be used in the derivation of the water quality value in this fact sheet to achieve consistency with requirements for the Great Lakes System.

For deriving f_{fd} values for the Great Lakes, U.S. EPA (1995a) procedures use DOC and POC values of 2 and 0.04 mg/L respectively. The POC level of 0.04 mg/L is on the low end for the Great Lakes but U.S. EPA selected it to ensure protection throughout the System.

Data on levels of DOC and POC were examined for fresh and marine waters in New York State. Levels of DOC vary somewhat through the State but are fairly close to 2 mg/L. The f_{fd} is not very sensitive to changes in concentration of DOC. Levels of POC in New York State range from zero to several mg/L, but a sufficient number of near-zero values were found such that the level that EPA uses for the Great Lakes System seems appropriate for statewide standards and at the same time provides consistency with the Federal requirements for the Great Lakes System.

Using these values for DOC and POC, equation 2 (above) becomes:

$$f_{fd} = \frac{1}{1 + (0.0000024 \text{ kg/L})(K_{ow})}$$

With a K_{ow} of 733, the fraction freely dissolved is calculated to be 1.000.

As described above, the baseline BAFs for chlorobenzene for trophic levels 3 and 4 are 747 and 740 L/kg respectively.

The final BAF for trophic level 3 is calculated as:

$$\text{Final BAF}_{TL3} = [(\text{baseline BAF}_{TL3})(f_{TL3}) + 1](f_{fd}) =$$

$$\text{Final BAF}_{TL3} = [(747)(0.0182) + 1](1.000) = 14.6 \text{ L/kg}$$

The final BAF for trophic level 4 is calculated as:

$$\text{Final BAF}_{\text{TL4}} = [(\text{baseline BAF}_{\text{TL4}})(f_{\text{TL4}}) + 1](f_{\text{fd}}) =$$

$$\text{Final BAF}_{\text{TL4}} = [(740)(0.0310) + 1](1.000) = 23.9 \text{ L/kg}$$

C. Human Exposure (Fish Consumption)

6 NYCRR 702.8 requires that H(FC) values be based on a fish consumption rate of 0.033 kg/day.

D. Calculation of Water Quality Value

The water quality value (WQV) is derived using a human body weight of 70 kg and a daily fish consumption rate of 0.033 kg as shown below. The fish consumption is apportioned as 24% trophic level 3 and 76% trophic level 4.

$$\text{WQV} = \frac{\text{Acceptable Daily Intake from Fish Consumption} \times 70 \text{ kg}}{[(\text{BAF}_{\text{TL3}})(0.24) + (\text{BAF}_{\text{TL4}})(0.76)] \times 0.033 \text{ kg/day}}$$

$$\text{WQV} = \frac{3.8 \text{ ug chlorobenzene/kg} \cdot \text{day} \times 70 \text{ kg}}{[(14.6 \text{ L/kg})(0.24) + (23.9 \text{ L/kg})(0.76)] \times 0.033 \text{ kg/day}}$$

$$= 372 \text{ ug/L, rounded to } 400 \text{ ug/L}$$

REFERENCES

6 NYCRR (New York State Codes, Rules and Regulations). Water Quality Regulations, Surface Water and Groundwater Classifications and Standards: Title 6 NYCRR, Chapter X, Parts 700-705. Albany, NY: Department of Environmental Conservation.

NYS (New York State). 1997. Human Health Fact Sheet. Ambient Water Quality Value for Protection of Sources of Potable Water. Chlorobenzene. Albany, NY: Department of Health.

U.S. EPA (Environmental Protection Agency). 1995a. Final Water Quality Guidance for the Great Lakes System. 60 Federal Register: 15366-15425. March 23, 1995.

U.S. EPA (Environmental Protection Agency). 1995b. Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors. Office of Water. EPA-820-B95-005.

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