Fact Sheet Date: March 12, 1998

NEW YORK STATE
- HUMAN HEALTH FACT SHEET -

Ambient Water Quality Value
Based on Human Consumption of Fish

SUBSTANCE: 2,4-Dimethylphenol **CAS REGISTRY NUMBER:** 105-67-9

AMBIENT WATER QUALITY VALUE: 1000 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

U.S. EPA (1995a) conducted a comprehensive evaluation of the oncogenic and non-oncogenic effects of 2,4-dimethylphenol as part of its criteria development for the Great Lakes Water Quality Initiative (GLI). The GLI was a joint undertaking by U.S. EPA and the Great Lakes States and included representatives of interest groups. Its final regulations and the criteria document for this substance received extensive public review in a formal rule making process. U.S. EPA's documentation for their criteria for 2,4-dimethylphenol has been reviewed. U.S. EPA does not consider 2,4-dimethylphenol to be carcinogenic, and the Department concludes that 2,4-dimethylphenol is not an oncogen under New York's definition in 6 NYCRR 700.1.

The Department reviewed the toxicological basis for U.S. EPA's non-oncogenic criteria and concludes it is appropriate for the derivation of a statewide value. Exhibit I, excerpted from U.S. EPA (1995a), provides the scientific basis for their non-oncogenic criteria. These data will be used to derive an acceptable daily intake for 2,4-dimethylphenol using New York State procedures as described below.

U.S. EPA (1995a) selected the results of the study by U.S. EPA (1989) as the most appropriate for deriving a water quality value based on non-oncogenic effects. From these, they calculated an acceptable daily exposure (ADE) of 16.7 ug 2,4-dimethylphenol/(kg · day), equivalent to an acceptable daily intake (ADI) developed under NYS procedures (702.5).

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 (1995b) 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, 1995c). 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) $$\text{Baseline BAF} = \left[\frac{\text{Field or Final BAF}}{f_{fd}} {}_{-1} \right] \left[\frac{1}{f_l} \right]$$

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

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

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

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 (1995c).

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 (1995c), 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, 1995b,c) provide a hierarchy of methods to calculate a baseline BAF. The only baseline BAF presented by U.S. EPA (1995c) for 2,4-dimethylphenol 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:

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

The predicted baseline BAFs for trophic levels 3 and 4 for 2,4-dimethylphenol from U.S. EPA (1995c) are shown in Table 1.

Table 1 Baseline BAFs for 2,4-Dimethylphenol (U.S. EPA, 1995c)	
Trophic Level	Baseline BAF (L/kg)
3	202
4	200

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).

Log K_{ow} is 2.30 (U.S. EPA, 1995c); K_{ow} = 200

The FCMs, from U.S. EPA (1995b) are 1.008 and 1.001 for trophic levels 3 and 4, respectively.

Predicted Baseline BAF_{TL3} = (FCM_{TL3}) (K_{ow})

= (1.008) (200) = 202 L/kg

Predicted Baseline BAF_{TL4} = (FCM_{TL4}) (K_{ow})

= (1.001) (200) = 200 L/kg

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 16.7 ug 2,4-dimethylphenol/(kg · day) as described above. The acceptable daily intake from fish consumption is:

0.2 x 16.7 ug 2,4-dimethylphenol/(kg · day) =

3.34 ug 2,4-dimethylphenol/(kg · 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:

Final BAF = [(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 (1995b) 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 (1995b) 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:

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

With a K_{ow} of 200, the fraction freely dissolved is calculated to be 1.000

As described above, the baseline BAFs for 2,4-dimethylphenol for trophic levels 3 and 4 are 202 and 200 L/kg respectively.

The final BAF for trophic level 3 is calculated as:

Final BAF_{TL3} = [(baseline BAF_{TL3})($f_{l\,TL3}$) + 1](f_{fd}) =

Final BAF_{TL3} = [(202 L/kg)(0.0182) + 1](1.000) = 4.68 L/kg

The final BAF for trophic level 4 is calculated as:

Final BAF_{TL4} = [(baseline BAF_{TL4})($f_{l\,TL4}$) + 1](f_{fd}) =

Final BAF_{TL4} = [(200 L/kg)(0.0310) + 1](1.000) = 7.20 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.

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

$$WQV = \frac{3.34 \text{ ug 2,4-dimethylphenol/(kg} \cdot \text{day)} \times 70 \text{ kg}}{[(4.68 \text{ L/kg})(0.24) + (7.20 \text{ L/kg})(0.76)] \times 0.033 \text{ kg/day}}$$

= 1070 ug/L, rounded to 1000 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.

U.S. EPA (Environmental Protection Agency). 1995a. Great Lakes Water Quality Initiative Criteria Documents for the Protection of Human Health. Office of Water. EPA-820-B-95-006

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

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

New York State Department of Environmental Conservation
Division of Water
SJS
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ATTACHMENT

GREAT LAKES WATER QUALITY INITIATIVE
TIER 1 HUMAN HEALTH CRITERIA FOR
2,4-DIMETHYLPHENOL
CAS NO. 105-67-9

Tier 1 Human Noncancer Criterion

A review of the available literature indicates that HNV derivation for 2,4-dimethylphenol (2,4-DMP) is most appropriately based on the subchronic oral mouse study conducted by EPA (1989). Groups consisting of 30 male and 30 female albino mice were administered 2,4-DMP by gavage at dose levels of 0, 5, 50 or 250 mg/kg/day for 90 days. At day 30, an interim sacrifice was performed on at least 8 males and 9 females from each group. Effects examined included mortality, clinical signs, body weights, food consumption, ophthalmology, hematology, clinical chemistry, organ weights, and gross histopathology. Toxicologically relevant clinical signs observed only after week 6 at 250 mg/kg/day in both sexes included squinting, lethargy, prostration, and ataxia, with onset shortly after dosing. Statistically significant lower mean corpuscular volume and mean corpuscular hemoglobin concentrations were observed in female mice at 250 mg/kg/day during the final but not during the interim sacrifice. At interim sacrifice, the blood urea nitrogen (BUN) levels for females at 50 and 250 mg/kg/day were significantly lower than the vehicle controls, while at the final sacrifice, the BUN levels for females at 50 mg/kg/day were significantly higher than the vehicle control group. For only the low-dose (5 mg/kg/day) males at the interim sacrifice, cholesterol levels were significantly higher than the vehicle control group. Increased adrenal weights were observed in low-dose (5 mg/kg/day) but not mid- to high-dose females when compared to vehicle control animals. Since the reported changes in BUN, serum cholesterol and adrenal weights were not dose- or time-dependent, they may be interpreted to be spurious findings. The NOAEL and LOAEL for this study were 50 and 250 mg/kg/day, respectively, based on clinical signs and hematological changes.

The database is judged to be sufficient for Tier 1 HNC derivation because the key study (EPA, 1989) provides a subchronic NOAEL. However, there is a paucity of supplemental and supportive data. No useful chronic, reproductive or developmental studies are available. The overall findings from the 90-day study (EPA, 1989) compare favorably with the results of a 14-day mice gavage study (EPA, 1987; as cited in EPA, 1989; EPA, 1990) conducted at the same laboratory. In the 14-day study, the only toxicological signs observed in males and females administered 250 mg/kg/day were lethargy, prostration, and ataxia. This is the same dose at which critical effects were found in the 90-day study (EPA, 1989).

The HNV is derived from the NOAEL dose of 50 mg/kg/day from the 90-day gavage mouse study by EPA (1989) with an uncertainty factor of 3000. This approach is consistent with the derivation of the oral RfD for 2,4-DMP by EPA (1990).

$$ADE = \frac{NOAEL}{UF} = \frac{50\ mg/kg/d}{3000} = 1.67 \times 10^{-2}\ mg/kg/d$$

Where: Uncertainty Factor = 3000, composed of:

10x for interspecies variability
10x for intraspecies differences
10x for subchronic exposure duration
3x for substantial gaps in the database

References:

U.S. Environmental Protection Agency (EPA). 1990. Integrated Risk Information System (IRIS database). Chemical file for 2,4-dimethylphenol (105-67-9). Verification Date 2/21/90. Last Reviewed 2/21/90.

U.S. Environmental Protection Agency (EPA). 1989. Ninety-Day Gavage Study in Albino Mice Using 2,4-Dimethylphenol. Study No. 410-2831, prepared by Dynamac Corporation, Rockville, MD, for the Office of Solid Waste and Emergency Response, Washington, DC.

U.S. Environmental Protection Agency (EPA). 1987. Fourteen-Day Gavage Study in Albino Mice Using 2,4-Dimethylphenol. Study No. 410-2830, prepared by Dynamac Corporation, Rockville, MD, for the Office of Solid Waste and Emergency Response, Washington, DC. As cited in EPA (1989, 1990).

U.S. Environmental Protection Agency (EPA). 1980. Ambient Water Quality Criteria for 2,4-Dimethylphenol. Office of Water Regulations and Standards, Criteria and Standards Division, Washington, DC. EPA 440/5-80-044. PB81-117558.