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SECONDARY VALUES FOR NAPHTHALENE (CAS # 91-20-3)

A search was conducted for information on the chemical properties and toxicity of naphthalene (to human health and to fish and aquatic life) using the following databases and search engines: ECOTOX (toxicity to fish and aquatic life), IRIS (Integrated Risk Information System; toxicity to human health), and CHEMFATE (environmental fate). This search yielded some information on naphthalene's properties, its biodegradation, and a significant amount of information on its toxicity.

FISH AND AQUATIC LIFE

To calculate an acute toxicity criterion for aquatic life, acute toxicity test results are required for at least one species in each of eight different families. Specific requirements and the data available to meet these requirements are found in Table 1. Following an extensive search, it was determined that data are available to meet only five out of the eight requirements. Because there are data available for *Daphnia magna*, it is possible to calculate secondary acute and chronic values for naphthalene.

Cold Water

To calculate a secondary acute value (SAV), the lowest genus mean acute value (GMAV) in the database is divided by the secondary acute factor (SAF; an adjustment factor corresponding to the number of satisfied requirements).

SAF for five out of eight requirements met = 6.1

Lowest GMAV = 2,100 µg/L (*Xenopus laevis*)

$$\begin{aligned}\text{SAV} &= \text{GMAV}/\text{SAF} \\ &= 2,100 \text{ µg/L} / 6.1 \\ &= \mathbf{344.26 \text{ µg/L}}\end{aligned}$$

There are currently no chronic data for naphthalene which meet suitability requirements. (MATC data are available for Coho salmon; however, the exposure duration was too short and the exposure was static rather than flow-through, as required.) Therefore, a secondary chronic value may be calculated only by using default acute-chronic ratios.

SACR = Geometric mean of 18, 18, and 18 = 18

$$\begin{aligned}\text{SCV} &= \text{SAV}/\text{SACR} \\ &= 344.26/18 \\ &= \mathbf{19.12 \text{ µg/L}}\end{aligned}$$

Warm Water Sport Fish, Warm Water Forage Fish, Limited Forage Fish, and Limited Aquatic Life

Because the lowest GMAV in the cold water database is for an amphibian, secondary values calculated for cold water will also apply to all other water body use designations.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for naphthalene, and corresponding acute toxicity data.

Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference #	Source
1. At least one salmonid fish in the family Salmonidae, in the class Osteichthyes.					
<i>Oncorhynchus kisutch</i>	coho salmon	96-h/LC50	3,220	13	AQUIRE
<i>Oncorhynchus kisutch</i>	coho salmon	96-h/LC50	2,100	14	AQUIRE
<i>Oncorhynchus kisutch</i> SMAV = 3,358.05	coho salmon	96-h/LC50	5,600	10	AQUIRE
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warm water species.					
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	1,800	7	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	6,100	7	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	2,600	7	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	4,400	7	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	5,500	7	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	4,500	7	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	1,600	5	AQUIRE
<i>Oncorhynchus mykiss</i> SMAV = 3,207.11	rainbow trout	96-h/LC50	2,250	2	AQUIRE
GMAV = 3,281.71					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warm water species.					
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	6,080	9	AQUIRE
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	1,990	12	AQUIRE
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	6,140	8	AQUIRE
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	7,900	5	AQUIRE
<i>Pimephales promelas</i> SMAV = 4,917.56	fathead minnow	96-h/LC50	4,900	2	AQUIRE

GMAV = 4,917.56

3. At least one planktonic crustacean (e.g., cladoceran, copepod).

<i>Daphnia magna</i>	water flea	48-h/EC50	3,845	1	AQUIRE
<i>Daphnia magna</i>	water flea	48-h/EC50	16,662	1	AQUIRE
<i>Daphnia magna</i>	water flea	48-h/EC50	2,194	15	AQUIRE
<i>Daphnia magna</i>	water flea	48-h/EC50	1,600	11	AQUIRE
<i>Daphnia magna</i>	water flea	48-h/EC50	2,550	11	AQUIRE

SMAV = 3,562.08

<i>Daphnia pulex</i>	water flea	48-h/EC50	4,663	17	AQUIRE
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SMAV = 4,663

GMAV = 4,075.53

<i>Diaptomus forbesi</i>	calanoid copepod	96-h/LC50	67,800	16	AQUIRE
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SMAV = 67,800

GMAV = 67,800

4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).

5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).

<i>Chironomus tentans</i>	midge	48-h/LC50	2,810	12	AQUIRE
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SMAV = 2,810

GMAV = 2,810

<i>Tanytarsus dissimilis</i>	midge	48-h/LC50	20,700	4	AQUIRE
<i>Tanytarsus dissimilis</i>	midge	48-h/LC50	12,600	4	AQUIRE
<i>Tanytarsus dissimilis</i>	midge	48-h/LC50	13,700	3	AQUIRE
<i>Tanytarsus dissimilis</i>	midge	48-h/LC50	12,200	3	AQUIRE

SMAV = 14,449.58

GMAV = 14,449.58

6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.

Gambusia affinis
SMA V = 150,000
western mosquitofish **96-h/LC50** **150,000** **18** **AQUIRE**

GMAV = 150,000

Xenopus laevis
Xenopus laevis
SMA V = 2,100
clawed toad **96-h/LC50** **2,100** **6** **AQUIRE**
clawed toad **96-h/LC50** **2,100** **6** **AQUIRE**

GMAV = 2,100

7. At least one organism from a family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).

8. At least one organism from a family in any order of insect or any other phylum not already represented in subdivisions 1 through 7.

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HUMAN HEALTH

To calculate a criteria or secondary value for the protection of human health, it is first necessary to determine if the substance has been shown to be carcinogenic (which will result in the calculation of a human cancer criteria or secondary value) or not (which will result in the calculation of a human threshold criteria or secondary value). Naphthalene is currently classified as a class C carcinogen (possible human carcinogen) in EPA's IRIS database. No cancer slope factor is available because of a lack of chronic oral studies. However, an oral reference dose (RfD) is listed in the IRIS database. Therefore, it is possible to calculate a human threshold secondary value for naphthalene for the protection of human health.

There are several steps to calculating a human threshold secondary value: 1) calculation of the fraction of freely dissolved chemical; 2) calculation of the "baseline BAF"; 3) calculation of the "human health BAF"; and 4) calculation of the human threshold secondary value.

1) Calculation of the freely-dissolved fraction = f_{fd}

Given a standard dissolved organic carbon (DOC) concentration of 0.000002 Kg/L and a particulate organic carbon (POC) concentration of 0.00000004 Kg/L in water, the equation

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

can be reduced to:

$$= 1 / \{ 1 + [(0.00000024 \text{ Kg/L})(K_{ow})] \}$$

For naphthalene, the $K_{ow} = 1995$, and $\log K_{ow} = 3.30$ (CHEMFATE database).

$$f_{fd} = 1 / \{ 1 + [(0.00000024 \text{ Kg/L})(1995)] \}$$

$$= 1 / 1.000479$$

$$= \mathbf{0.9995}$$

2) Calculation of the baseline BAF

The baseline BAF is calculated according to the equations contained in 40 CFR part 132 (Final Water Quality Guidance for the Great Lakes System), Appendix B, using BAF data that was collected in one of four ways (listed in order of most preferred to least preferred):

- a measured BAF from a field study
- a predicted BAF based on field-measured BSAFs
- a predicted BAF using a laboratory-measured bioconcentration factor (BCF) and a food chain multiplier (FCM)
- a predicted BAF using a K_{ow} and a FCM

A baseline BAF was calculated for naphthalene using a K_{ow} and a food chain multiplier (FCM).

FCM = food chain multiplier, from Table B-1, in 40 CFR Part 132

For discharges into water classified as warm water, the FCM will be for trophic level 3. For discharges into water classified as cold water, the FCM will be for trophic level 4. Given naphthalene's log K_{ow} of 3.30, the FCM for trophic level 3 from the table is 1.053, and for trophic level 4, 1.012.

The anti-log of 3.30 = 1995

$$\begin{aligned}\text{Warm Water Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (1.053)(1995) \\ &= \mathbf{2,100.7350}\end{aligned}$$

$$\begin{aligned}\text{Cold Water Baseline BAF} &= (\text{FCM})(K_{ow}) \\ &= (1.012)(1995) \\ &= \mathbf{2,018.9400}\end{aligned}$$

3) Calculation of the human health BAF

For Warm Water:

$$\text{BAF}_{\text{TL3}}^{\text{HH}} = \{[(\text{baseline BAF})(0.013)] + 1\} (f_{\text{fd}})$$

where

baseline BAF = the baseline BAF calculated in 2)

0.013 = fraction lipid value for warm water fish and aquatic life communities

f_{fd} = fraction freely dissolved

$$\begin{aligned}\text{BAF}_{\text{TL3}}^{\text{HH}} &= \{[(\text{baseline BAF})(0.013)] + 1\} (f_{\text{fd}}) \\ &= \{[(2,100.7350)(0.013)] + 1\} (0.9995) \\ &= \mathbf{28.2954}\end{aligned}$$

For Cold Water:

$$\text{BAF}_{\text{TL4}}^{\text{HH}} = \{[(\text{baseline BAF})(0.044)] + 1\} (f_{\text{fd}})$$

where

baseline BAF = the baseline BAF calculated in 2)

0.044 = fraction lipid value for cold water fish and aquatic life communities

f_{fd} = fraction freely dissolved

$$\begin{aligned}\text{BAF}_{\text{TL4}}^{\text{HH}} &= \{[(\text{baseline BAF})(0.044)] + 1\} (f_{\text{fd}}) \\ &= \{[(2,018.9400)(0.044)] + 1\} (0.9995) \\ &= \mathbf{89.7884}\end{aligned}$$

4) Calculation of the human threshold secondary value

$$\text{Human Threshold Secondary Value} = [(ADE)(70 \text{ Kg})(RSC)]/[W_{\text{H}} + (F_{\text{H}})(\text{BAF})]$$

where

ADE = acceptable daily exposure (= oral reference dose, or RfD; = 0.02 mg/Kg/day for naphthalene (IRIS 1998))

70 Kg = average weight of an adult

RSC = relative source contribution to account for other routes of exposure (= 0.8 in the absence of other data)

W_{H} = average per capita daily water consumption (= 2 L/d for public water supplies, and 0.01 L/d for non-public water supplies)

F_{H} = average consumption of sport-caught fish in Wisconsin (= 0.02 Kg/d)

BAF = human health BAF calculated in 3).

Warm Waters, Public Water Supply

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)/[W_H + (F_H)(BAF)]] \\ &= [0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(28.2954)] \\ &= 1.1200/2.5659 \\ &= 0.4365 \text{ mg/L} \\ &= 436.5 \text{ }\mu\text{g/L}\end{aligned}$$

Cold Water, Public Water Supply

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)/[W_H + (F_H)(BAF)]] \\ &= [0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(89.7884)] \\ &= 1.1200/3.7958 \\ &= 0.2951 \text{ mg/L} \\ &= 295.1 \text{ }\mu\text{g/L}\end{aligned}$$

Warm waters, Non-Public Water Supply

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(28.2954 \text{ L/Kg})] \\ &= 1.1200/0.5759 \\ &= 1.94478 \text{ mg/L} \\ &= 1,944.78 \text{ }\mu\text{g/L}\end{aligned}$$

Cold Water, Non-Public Water Supply

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(89.7884 \text{ L/Kg})] \\ &= 1.1200/1.8058\end{aligned}$$

$$= 0.6202 \text{ mg/L}$$

$$= 620.2 \text{ } \mu\text{g/L}$$

Limited Aquatic Life, Non-Public Water Supply

$$\text{Human Threshold Secondary Value} = [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)]$$

$$= [(0.02 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(0 \text{ L/Kg})]$$

$$= 1.1200/0.01$$

$$= 112.00 \text{ mg/L}$$

$$= \mathbf{112,000} \text{ } \mu\text{g/L}$$