Site: Cities Oil
Location: West Bend
Receiving Water: Milwaukee River
Date: September 2002
Calculator: Elisabeth Harrahy, Ph.D.

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), CHEMFATE (environmental fate), BIOLOG (microbial degradation/toxicity), DATALOG (environmental fate bibliography), HSDB (Hazardous Substances Data Bank), CCRIS (Chemical Carcinogenesis Research Info System), GENE-TOX (mutagenicity database), TOXLINE (toxicology bibliography), TERA (Toxicology Excellence for Risk Assessment), and Ingenta (journal article search engine; since 1988). This search yielded some information on naphthalene's properties (vapor pressure, log octanol/water partition coefficient, Henry's Law, and water solubility), and 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. (Data are available for other species; however, these data either do not meet the quality requirements necessary for use in water quality criteria/secondary value calculations, or they are for saltwater species.)

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.					
Oncorhynchus kisutch	**coho salmon**	**96-h/LC50**	**3,220**	**13**	**AQUIRE**
Oncorhynchus kisutch	**coho salmon**	**96-h/LC50**	**2,100**	**14**	**AQUIRE**
Oncorhynchus kisutch	**coho salmon**	**96-h/LC50**	**5,600**	**10**	**AQUIRE**
SMAV = 3,358.05					
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**1,800**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**6,100**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**2,600**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**4,400**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**5,500**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**4,500**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**1,600**	**5**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**2,250**	**2**	**AQUIRE**
SMAV = 3,207.11					
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.					
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**6,080**	**9**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**1,990**	**12**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**6,140**	**8**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**7,900**	**5**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**4,900**	**2**	**AQUIRE**
SMAV = 4,917.56					

GMAV = 4,917.56

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

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

SMAV = 3,562.08

Daphnia pulex	**water flea**	**48-h/EC50**	**4,663**	**17**	**AQUIRE**

SMAV = 4,663

GMAV = 4,075.53

Diaptomus forbesi	**calanoid copepod**	**96-h/LC50**	**67,800**	**16**	**AQUIRE**

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).

Chironomus tentans	**midge**	**48-h/LC50**	**2,810**	**12**	**AQUIRE**

SMAV = 2,810

GMAV = 2,810

Tanytarsus dissimilis	**midge**	**48-h/LC50**	**20,700**	**4**	**AQUIRE**
Tanytarsus dissimilis	**midge**	**48-h/LC50**	**12,600**	**4**	**AQUIRE**
Tanytarsus dissimilis	**midge**	**48-h/LC50**	**13,700**	**3**	**AQUIRE**
Tanytarsus dissimilis	**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	**western mosquitofish**	**96-h/LC50**	**150,000**	**18**	**AQUIRE**

SMAV = 150,000

GMAV = 150,000

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

SMAV = 2,100

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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The Milwaukee River is designated as a warm water sport fish community, non-public water supply. However, it is necessary to calculate secondary values for both cold water and warm water first, for comparative purposes. If the secondary values are lower for warm water than for cold water, then the secondary values for cold water (complete database) will apply for the warm water. If the secondary values for warm water are higher than for cold water, then the secondary values for warm water will apply (and will offer some relief to warm water dischargers).

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*)

SAV = GMAV/SAF
= 2,100 µg/L /6.1
= 344.26 µg/L

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

SCV = SAV/SACR
= 344.26/18
= 19.12 µg/L

So, for naphthalene, the **secondary acute value is 344 µg/L** (rounded from 344.26) and the **secondary chronic value is 19 µg/L** (rounded from 19.12).

Warm Water

The salmonid category of fish drops out of the database when calculating secondary values for warm water.

SAF for four out of eight requirements met = 7.0

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

SAV = GMAV/SAF
= 2,100 µg/L /7.0

= 300 μg/L

A secondary chronic value may be calculated only by using default acute-chronic ratios.

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

SCV = SAV/SACR
= 300/18
= **16.67 μg/L**

Because secondary values for warm water cannot be lower than for cold water, the secondary values for all classes, in the case of naphthalene, will be set to the cold water values-- 344 and 19 μg/L. In other words, there is no relief for discharges to warm waters (in comparison to discharges to cold waters).

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 in Group C, a 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. In addition, there are aquatic organism bioaccumulation data (ECOTOX) available. Thus, there is sufficient data available at this time 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:

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

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

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

= 1/1.000479

= **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

If there is available a measured BAF from a field study, or a predicted BAF based on field measured BSAFs, then the final human threshold value will be a criterion. If the baseline BAF is greater than 1000, and is determined by using a laboratory BCF and a FCM, or by using a K_{ow} and a FCM, then the final human threshold value will be deemed a secondary value.

A baseline BAF was calculated for naphthalene using a K_{ow} and a food chain multiplier (FCM). (Melancon and Lech (1978) calculated a BCF for naphthalene in rainbow trout (listed in ECOTOX), but I have as yet, been unable to get a copy of this paper to see if it contains information on whether the tissue concentration was based on whole tissue residue or not, and whether a lipid value is presented.)

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. Given naphthalene's log Kow of 3.30, the FCM for trophic level 3 from the table is 1.053.

The anti-log of 3.30 = 1995

Warm Water Baseline BAF = $(FCM)(K_{ow})$

= (1.053)(1995)

= **2,100.7350**

3) Calculation of the human health BAF

For naphthalene (an organic substance) discharges to **warm water**, the equation to use is:

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

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

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

$= \{[(2{,}100.7350)(0.013)] + 1\}\ (0.9995)$

= 28.2954

4) Calculation of the human threshold secondary value

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

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 ~~DNR~~ (= 0.02 Kg/d)

BAF = human health BAF calculated in 3).

Warm water, non-public water supply

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

$= [(0.02\ mg/Kg/d)(70\ Kg)(0.8)]/[0.01\ L/d + (0.02\ Kg/d)(28.2954\ L/Kg)]$

$= 1.1200/0.5759$

$= 1.94478$ mg/L

= 1,944.78 µg/L

In water designated as warm water sportfish, non-public water supply, the human threshold secondary value for naphthalene is 1,945 µg/L.

ADDITIONAL REFERENCES

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