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SECONDARY VALUES FOR ANTHRACENE (CAS # 120-12-7)

A search was conducted for information on the chemical properties and toxicity of anthracene (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), and ChemFinder (chemical properties). This search yielded some information on anthracene's properties (vapor pressure, log octanol/water partition coefficient, Henry's Law, and water solubility), and 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 two out of the eight requirements. Because there are data available for *Daphnia magna* and *Daphnia pulex*, it is possible to calculate secondary acute and chronic values for anthracene. (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 anthracene, 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.					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warm water species.					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**2.78**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**4.5**	**2**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**7.47**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**1.27**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**7.97**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**6.78**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**3.74**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**8.27**	**3**	**AQUIRE**
SMAV = 4.59					
GMAV = 4.59					
Result excluded because LC50 was more than 10X the others:					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**46**	**2**	**AQUIRE**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**35.65**	**4**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**95**	**5**	**AQUIRE**
SMAV = 58.20					

Daphnia pulex	**water flea**	**48-h/EC50**	**754**	**6**	**AQUIRE**

SMAV = 754
GMAV = 209.48

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).

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

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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[1]Oris, J.T., Jr. 1985. The photoenhanced toxicity of anthracene to juvenile sunfish (*Lepomis* spp.). Aquatic Toxicology 6(2):133-146.

[2]Oris, J.T., Jr. 1986. Photoinduced toxicity of anthracene to juvenile bluegill sunfish (*Lepomis macrochirus* Rafinesque): Photoperiod effects and predictive hazard. Environmental Toxicology and Chemistry 5(8):761-768.

[3]McCloskey, J.T. and J.T. Oris. 1991. Effect of water temperature and dissolved oxygen concentration on the photoinduced toxicity of anthracene to juvenile bluegill sunfish (*Lepomis macrochirus*). Aquatic Toxicology 21:145-156.

[4]Abernethy, S., A.M. Bobra, W.Y. Shiu, P.G. Wells, and D. MacKay. 1986. Acute lethal toxicity of hydrocarbons and chlorinated hydrocarbons to two planktonic crustaceans: The key role of organism-water partitioning. Aquatic Toxicology 8(3):163-174.

[5]Munoz, M.J. and J.V. Tarazona. 1993. Synergistic effect of two- and four-component combinations of the polycyclic aromatic hydrocarbons: Phenanthrene, anthracene, naphthalene, and… Bulletin of Environmental Contamination and Toxicology 50(3):363-368.

[6]Smith, S.B., J.F. Savino, and M.A. Blouin. 1988. Acute toxicity to *Daphnia pulex* of six classes of chemical compounds potentially hazardous to Great Lakes biota. Journal of Great Lakes Research 14(4):394-404.

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 two out of eight requirements met = 13.0

Lowest GMAV = 4.59 (*Lepomis macrochirus*)

SAV = GMAV/SAF
= 4.59 µg/L /13.0
= 0.353 µg/L

There are currently no chronic data for anthracene. 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
= 0.353/18
= **0.0196 µg/L**

So, for anthracene, the **secondary acute value is 0.35 µg/L** (rounded from 0.353) and the **secondary chronic value is 0.02 µg/L** (rounded from 0.0196).

Warm Water

Because no species will drop out of the cold water database for warm water, the acute and chronic secondary values will be the same for both cold water and warm water.

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). Anthracene is currently listed as Group D, not classifiable as to human carcinogenicity, in EPA's IRIS database. No cancer slope factor is available because of a lack of 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 anthracene 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 anthracene, the K_{ow} = 28,183.8293, and log K_{ow} = 4.45 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(28{,}183.8293)]\}$$

$$= 1/1.006764$$

$$\mathbf{= 0.9932}$$

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 for anthracene may be calculated in the future using laboratory BCFs and a food chain multiplier (FCM). Hall and Oris (1991) calculated two BCFs for fathead minnows (*Pimephales promelas*). (A baseline BAF would be calculated for each of these BCFs, and then the geometric mean of the baseline BAF was used to calculated the human health BAF (step 3)). However, until we get a copy of this paper (ordered from the library 9/19/02) to confirm that anthracene was measured in only the edible portions of the fish tissue, and that lipid content was measured, we'll have to calculate a baseline BAF using the K_{ow} and a food chain multiplier.

The seep from Cities Oil is discharging into the Milwaukee River, which is classified as warm water sportfish, non-public water supply, so the FCM will be for trophic level 3. Given anthracene's log K_{ow} of 4.45 (K_{ow} of 28,184), the FCM from the table (for trophic level 3) is interpolated to be 1.674.

Baseline BAF = (FCM)(Kow)

Baseline BAF = (1.674)(28,184)

= 47,180.0160

3) Calculation of the human health BAF

For anthracene (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

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

$= \{[(47{,}180.0160)(0.013)] + 1\}\ (0.9932)$

= 610.1627

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; = 0.3 mg/Kg/day for anthracene (IRIS 2002))

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 water, non-public water supply

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

= [(0.3 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(610.1627 L/Kg)]

= 16.8000/12.2132

= 1.37561 mg/L

= 1,375.61 μg/L

In water designated as warm water sportfish, non-public water supply, the human threshold secondary value for anthracene is 1,376 μg/L.

<u>REFERENCES</u>

Hall, J.T. and J.T. Oris. 1991. Anthracene reduces reproductive potential and is maternally transferred during long-term exposure in fathead minnows. Aquatic Toxicology 19(3): 249-264.