**Site:** Cities Oil
**Location:** West Bend
**Receiving Water:** Milwaukee River
**Date:** September 2002
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## SECONDARY VALUES FOR BENZO[A]PYRENE (CAS # 50-32-8)

A search was conducted for information on the chemical properties and toxicity of benzo[a]pyrene (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 benzo[a]pyrene's properties (vapor pressure, log octanol/water partition coefficient, Henry's Law, and water solubility), its biodegradation, and some 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 two out of the eight requirements. Because there are data available for *Daphnia pulex*, it is possible to calculate secondary acute and chronic values for benzo[a]pyrene. (Data are available for many 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 benzo[a]pyrene, 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. | | | | | |
| 3. At least one planktonic crustacean (e.g., cladoceran, copepod). | | | | | |
| ***Daphnia pulex*** | **water flea** | **96-h/LC50** | **5** | **1** | **AQUIRE** |
| 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. | | | | | |
| ***Xenopus laevis*** | **clawed toad** | **96-h/EC50** | **8,700** | **2** | **AQUIRE** |
| ***Xenopus laevis*** | **clawed toad** | **96-h/EC50** | **9,600** | **2** | **AQUIRE** |
| SMAV = 9,138.93 | | | | | |
| GMAV = 9,138.93 | | | | | |
| 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. | | | | | |

[1]Trucco, R.G., F.R. Engelhardt and B. Stacey. 1983. Toxicity, accumulation and clearance of aromatic hydrocarbons in *Daphnia pulex*. Environ. Pollut. Ser. A Ecol. Biol. 31(3):191-202.

[2]Propst, T.L., D.J. Fort and E.L. Stover. 1997. Evaluation of the developmental toxicity of benzo[a]pyrene and 2-acetylaminofluorine using *Xenopus*: Modes of biotransformation. Drug Chem. Toxicol. 20(1/2):45-61.

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 = 5 µg/L (*Daphnia pulex*)

**SAV** = GMAV/SAF
= 5 µg/L /13.0
= **0.3846 µg/L**

There are currently no chronic toxicity data for benzo[a]pyrene which meet suitability requirements. 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
= 0.3846/18
= **0.0214 µg/L**

So, for benzo[a]pyrene, the **secondary acute value is 0.38 µg/L** (rounded from 0.3846) and the **secondary chronic value is 0.02 µg/L** (rounded from 0.0214).

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 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). Benzo[a]pyrene is currently classified in Group B2, a probable human carcinogen, in EPA's IRIS database. A cancer oral slope factor is available; therefore, it is possible to calculate a human cancer secondary value for the protection of human health.

There are several steps to calculating a human cancer secondary value: 1) calculation of the risk associated dose (RAD); 2) calculation of the fraction of freely dissolved chemical; 3) calculation of the "baseline BAF"; 4) calculation of the "human health BAF"; and 5) calculation of the human cancer secondary value.

**1) Calculation of the risk associated dose (RAD):**

$RAD = (1/q_1^*)(0.00001)$

where

RAD = risk associated dose in milligrams toxicant per kilograms body weight per day (mg/Kg/d)

$q_1^*$ = upper 95% confidence limit (one-sided) of the carcinogenic potency factor in milligrams toxicant per kilograms body weight per day (mg/Kg/d) = Cancer slope factor

RAD = (1/7.3 mg/Kg/d)(0.00001)

= **0.000001 mg/Kg/d**

**2) 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 benzo[a]pyrene, the $K_{ow}$ = 933,254 and log $K_{ow}$ = 5.97 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(933,254)]\}$$

= 1/1.22398

= **0.8170**

**3) 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 benzo[a]pyrene using a $K_{ow}$ and a food chain multiplier (FCM). (Lu et al. (1977) calculated a BCF for benzo[a]pyrene in Western mosquitofish (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 benzo[a]pyrene's log Kow of 5.97, the FCM for trophic level 3 from the table is interpolated to be 10.304.

The anti-log of 5.97 = 933,254

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

= (10.304)(933,254)

= **9,616,249.**

**4) Calculation of the human health BAF**

For benzo[a]pyrene (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

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

$= \{[(9{,}616{,}249)(0.013)] + 1\}\ (0.8170)$

$=$ **102,135**

**5) Calculation of the human cancer secondary value**

Human Cancer Secondary Value = $[(RAD)(70\ Kg)]/[W_H + (F_H)(BAF)]$

where

RAD = risk associated dose in milligrams toxicant per kilogram body weight per day (mg/Kg/d) that is associated with a lifetime incremental cancer risk equal to one in 100,000 as derived in 1) (above).

70 Kg = average weight of an adult male

$W_H$ = 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 4) (above).

**Warm water, non-public water supply**

Human Cancer Secondary Value = $[(RAD)(70\ Kg)]/[W_H + (F_H)(BAF)]$

$= [(0.000001\ mg/Kg/d)(70\ Kg)]/[0.01\ L/d + (0.02\ Kg/d)(102{,}135\ L/Kg)]$

$= 0.000070/2{,}042.7100$

$= 3.43E\text{-}8\ mg/L$

**$= 3.43E\text{-}5\ \mu g/L$ (or $0.0000343\ \mu g/L$)**

$= 0.0343\ ng/L$

**$= 3.43\ pg/L$**

**In water designated as warm water sportfish, non-public water supply, the human threshold secondary value for benzo[a]pyrene is 3.42 pg/L. (NOTE: UNITS ARE NOT IN µg/L)**

ADDITIONAL REFERENCES

Lu, P.Y., R.L. Metcalf, N. Plummer, and D. Mandel. 1977. The environmental fate of three carcinogens: benzo-(alpha)-pyrene, benzidine, and vinyl chloride evaluated in laboratory model ecosystems. Archives of Environmental Contamination and Toxicology 6(2-3):129-142.