Date: January 21, 2007
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SECONDARY VALUES FOR PYRENE (CAS # 129-00-0)

A search was conducted in 2002 for information on the chemical properties and toxicity of 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), 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 was repeated in 2006 to look for updates.

FISH AND AQUATIC LIFE

To derive 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 for information on the toxicity of pyrene to fish and other aquatic life (volumes 19 and 20 (to date) of *Environmental Toxicology and Chemistry*, Chemfate, and AQUIRE and HSDB databases), it was determined that data are available to meet only two out of the eight requirements; but because there are data for *Daphnia* sp., it is possible to calculate a secondary acute value for pyrene.

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 = 1820.34 (*Daphnia magna*)

SAV = GMAV/SAF
= 1820 / 13
= 140.0

There are currently no chronic data for pyrene. 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
= 140.0 / 18

= **7.778**

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

Because the lowest GMAV in the cold water database is for *Daphnia magna*, an invertebrate, and because this species will not drop out for any of the other use classifications, secondary values for warm water sport fish, warm water forage fish, limited forage fish and limited aquatic life waters will be the same as for cold waters.

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

	Species Name	Common Name	Duration/ Endpoint	Value µg/L	Reference #[a]	Source
1.	At least one salmonid fish in the family Salmonidae, in the class Osteichthyes.					
	Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>2000**	**2**	**AQUIRE**
2.	At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
3.	At least one planktonic crustacean (e.g., cladoceran, copepod).					
	Daphnia magna	**water flea**	**48-h/EC50**	**9 mmol/m^3 = 1820.34 µg/L**	**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.					
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]Bobra, A.M., W.Y. Shiu, and D. MacKay. 1983. A predictive correlation for the acute toxicity of hydrocarbons and chlorinated hydrocarbons to the water flea (*Daphnia magna*). Chemosphere 12(9-10):1121-1129.

[2]Kennedy, C.J. 1990. Toxicokinetic studies of chlorinated phenols and polycyclic aromatic hydrocarbons in rainbow trout (*Oncorhynchus mykiss*). Ph.D. Dissertation. Simon Fraser University, Canada. 188 pp. Diss. Abstr. Int. B Sci. Eng. 53(1):18 (1992).

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). Pyrene is currently classified as "D", not classifiable, by the U.S. EPA (IRIS) based on inadequate data from animal bioassays and no human data. Both an oral reference dose (RfD; IRIS) and a BAF are available; therefore, a human threshold secondary value can be calculated for this substance.

There are several steps to calculating a human threshold criterion or 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 criterion or 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 pyrene, the K_{ow} = 151,356 and log K_{ow} = 5.18 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(151356)]\}$$

$$= 1/1.0363$$

$$= \mathbf{0.9650}$$

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 BCF and a FCM
-a predicted BAF using a K_{ow} and a FCM

Using a field-measured BAF:

Baseline BAF = [Measured BAF^{t}_{T}/f_{fd} - 1] [$1/f_{l}$]

where

BAF^{t}_{T} = BAF based on total concentration in tissue and water

f_{l} = fraction of tissue that is lipid

f_{fd} = fraction of total chemical in water that is freely dissolved

Burkhard and Lukasewycz (2000) calculated BAFs and BSAFs for five different PAHs, including pyrene, based on field studies conducted by Baker and Eisenreich (1989), Baker and Eisenreich (1990) and Zabik et al. (1996). They report a log BAF value of 4.02 for pyrene in lake trout. The antilog of 4.02 is 10,471.2855. They also report a lipid value of 20.5%, or 0.205.

Baseline BAF = [10,471.2885/0.9650 - 1] [1/0.205]

= (10,850.0762)(4.8780)

= 52,926.6717

3) Calculation of the human health BAF

a) Human health BAF for warm water:

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

where

BAF^{HH}_{TL3} = human health BAF for trophic level 3 (warm water)

baseline BAF = the baseline BAF calculated in 3)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL3} = {[(52,927.67)(0.013)] + 1} (0.9650)

= 664.9426

b) Human health BAF for cold water:

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

where

BAF^{HH}_{TL4} = human health BAF for trophic level 4 (cold water)

baseline BAF = the baseline BAF calculated in 3)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL4} = {[(52,927.67)(0.044)] + 1} (0.9650)

= 2,248.2739

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; =0.03 mg/Kg/day for pyrene (IRIS))

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

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

= [0.03 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(664.9426)]

= 0.1098 mg/L

= 109.8 µg/L

Cold Water, Public Water Supply

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

= [0.03 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(2248.2739)]

= 0.0358 mg/L

= 35.8 μg/L

Warm waters, Non-Public Water Supply

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

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(664.9426 L/Kg)]

= 0.1262 mg/L

= 126.2 μg/L

Cold Water, Non-Public Water Supply

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

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(2248.2739 L/Kg)]

= 0.0374 mg/L

= 37.4 μg/L

Limited Aquatic Life, Non-Public Water Supply

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

= [(0.03 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(0 L/Kg)]

= 168 mg/L

= 168,000 μg/L