Date: January 21, 2007
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SECONDARY VALUES FOR FLUORENE (CAS # 86-73-7)

A search was conducted in 2004 for information on the chemical properties and toxicity of fluorene (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 fluorene's properties (vapor pressure, log octanol/water partition coefficient, Henry's Law, and water solubility), its biodegradation, and a significant amount of information on its toxicity. A search was again conducted in July 2006 to look for any 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 a search for information on the toxicity of fluorene to fish and other aquatic life, it was determined that data are available to meet six out of the eight requirements. Because there are data for *Daphnia* sp., it is possible to calculate a secondary acute value for fluorene.

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 six out of eight requirements met = 5.2

Lowest GMAV = 302 µg/L (*Daphnia* sp.)

SAV = GMAV/SAF
= 301 µg/L /5.2
= 58.1 µg/L

There are currently no chronic data for fluorene 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
= 58.1 µg/L /18
= **3.23 µg/L**

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* sp., which are invertebrates, and because these 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 fluorene, 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**	**820**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**>2000**	**2**	**AQUIRE**
Species mean acute value (SMAV): 1280.6248					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**910**	**1**	**AQUIRE**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**430**	**1**	**AQUIRE**
Daphnia pulex	**water flea**	**48-h/EC50**	**212**	**3**	**AQUIRE**
Genus mean acute value (GMAV): 301.9271					
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					
Gammarus pseudolimnaeus	**scud**	**96-h/LC50**	**600**	**1**	**AQUIRE**
5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).					
Chironomus thummi	**midge**	**48-h/EC50**	**2350**	**1**	**AQUIRE**
6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.					
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**>100000**	**1**	**AQUIRE**
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] Finger, S.E., E.F. Little, M.G. Henry, J.F. Fairchild and T.P. Boyle. 1985. Comparison of laboratory and field assessment of fluorene- Part 1: Effects of fluorene on survival, growth, reproduction and behavior. In: Validation and Predictability of Laboratory Methods for Assessing the Fate and Effects of Contaminants in Aquatic Ecosystems, 1st Symposium. T.P. Boyle, editor. ASTM STP 865, Philadelphia, PA. Pp. 120-133.

[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).

[3] 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 aquatic biota. Journal of Great Lakes Research 14(4):394-404.

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). Fluorene is currently classified as "D", not classifiable, by the U.S. EPA (IRIS) based on inadequate data from animal bioassays and no human data. An oral reference dose (RfD; IRIS, last revised in 1990) is available, and it is possible to calculate a predicted baseline bioaccumulation factor (BAF); therefore, a human threshold secondary value may be calculated for this substance.

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 fluorene, the K_{ow} = 15136, and log K_{ow} = 4.18 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024 \text{ Kg/L})(15136)]\}$$

$$= 1/1.003633$$

$$\mathbf{= 0.9964}$$

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 BCF is available with which to calculate a BAF. A 28-day laboratory study conducted with fathead minnows by Carlson et al. (1979) produced a log BCF of 3.17. The antilog of 3.17 is 1479. The authors report a lipid range of 4.4 to 4.8%. The mean of these figures is 4.6%, or 0.046.

Using the BCF from the laboratory study and a FCM:

Baseline BAF = (FCM) [(measured BCF^t_T/f_{fd}) - 1] [$1/f_l$]

where

BCF^t_T = BCF 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

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

Fluorene log Kow = 4.18
Kow = 15,136
FCM for trophic level 3 = 1.380
FCM for trophic level 4 = 1.130

a) Baseline BAF for warm water

Baseline BAF = (1.380) [(1479/0.9964) - 1] [1/0.046]

= (1.380) (1484.3436) (21.7391)

= 44,530

b) Baseline BAF for cold water

Baseline BAF = (1.130) [(1479/0.9964) - 1] [1/0.046]

= (1.130) (1484.3436) (21.7391)

= 36,463

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) for warm water (using the octanol-water partition coefficient method)

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

f_{fd} = fraction freely dissolved

$BAF^{HH}_{TL3} = \{[(44{,}530)(0.013)] + 1\}\ (0.9964)$

= 577.80

b) Human health BAF for cold water:

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

where

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

baseline BAF = the baseline BAF calculated in 3) for cold water (using the octanol-water partition coefficient method)

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

f_{fd} = fraction freely dissolved

$BAF^{HH}_{TL4} = \{[(36{,}463)(0.044)] + 1\}\ (0.9964)$

= 1,599.59

4) Calculation of the human threshold secondary value

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

where

ADE = acceptable daily exposure (= oral reference dose, or RfD; =0.04 mg/Kg/day for fluorene (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)]

= [0.04 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(577.80)]

= 2.24 / 13.55

= 0.1653 mg/L

= 165.3 µg/L

Cold Water, Public Water Supply

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

= [0.04 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(1599.59)]

= 2.24 / 33.99

= 0.0659 mg/L

= 65.9 µg/L

Warm waters, Non-Public Water Supply

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

= [(0.04 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(577.80 L/Kg)]

= 2.24 / 11.57

= 0.1936 mg/L

= 193.6 μg/L

Cold Water, Non-Public Water Supply

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

= [(0.04 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(1599.59 L/Kg)]

= 2.24 / 32.00

= 0.0700 mg/L

= 70 μg/L

Limited Aquatic Life, Non-Public Water Supply

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

= [(0.04 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(0 L/Kg)]

= 2.24 / 0.01

= 224.00 mg/L

= 224,000 μg/L

REFERENCES

Carlson, R.M., A.R. Oyler, E.H. Gerhart, R. Caple, K.J. Welch, H.L. Kopperman, D. Bodenner, and D. Swanson. 1979. Implications to the aquatic environment of polynuclear aromatic hydrocarbons liberated from northern Great Plains coal. EPA-600/3-79-093. U.S. Environmental Protection Agency, Duluth, MN.

National Institute of Health. Chemical Carcinogenesis Research Information System (CCRIS). http://toxnet.nlm.nih.gov

National Institute of Health. Hazardous Substances Data Bank (HSDB). http://toxnet.nlm.nih.gov

Oak Ridge National Laboratory. Risk Assessment Information System (RAIS). http://risk.lsd.ornl.gov

Syracuse Research Corporation. CHEMFATE database. http://esc.syrres.com/efdb.htm

U.S. EPA. Aquatic Toxicity Information Retrieval (AQUIRE) database. http://www.epa.gov/med/databases.html

U.S. EPA. Integrated Risk Information System (IRIS) database.
http://www.epa.gov/ngispgm3/iris/index.html)

U.S. EPA. 1999. National recommended water quality criteria- correction. EPA 822-Z-99-001. U.S. Environmental Protection Agency, Washington, D.C.

U.S. EPA Region 6 website. Chemical-specific input data tables.
http://www.epa.gov/earth1r6/6pd/rcra_c/protocol/volume_2/