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

SECONDARY VALUES FOR XYLENES (CAS # 1330-20-7)

A search was conducted for information on the chemical properties and toxicity of xylenes (to human health and to fish and aquatic life) using the following databases: ECOTOX (toxicity to fish and aquatic life), IRIS (Integrated Risk Information System; toxicity to human health), CHEMFATE (environmental fate) and ChemFinder (chemical properties and links). This search yielded some information on properties of xylenes (vapor pressure, log octanol water partition coefficients, Henry's Law, and water solubility), and some information on their toxicity. In addition, two fact sheets on xylenes were printed from a U.S. EPA web site.

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 six of the eight requirements. Because there are no acceptable data available for at least one of the three genera in the family Daphnidae (*Ceriodaphnia* sp., *Daphnia* sp., or *Simocephalus* sp.), it is not possible to calculate secondary acute and chronic values for xylenes at this time. All available Daphnid test results are from tests with a 24-hour exposure duration, rather than the required 48-hour exposure duration. It may be possible to have the State Laboratory of Hygeine run a 48-hour Daphnid test with xylene in the near future to allow calculation of acute and chronic secondary values.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for xylenes, 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 mykiss	**rainbow trout**	**96-h/LC50**	**13,500**	**13**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**17,300**	**13**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**8,200**	**6**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**8,200**	**9**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**3,300**	**9**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**13,500**	**9**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**17,300**	**9**	**AQUIRE**
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warm water species.					
Cyprinus carpio	**common carp**	**96-h/LC50**	**780,000**	**11**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**24,500**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**15,700**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**20,870**	**10**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**19,000**	**3**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**13,500**	**6**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**13,500**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**8,600**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**12,000**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**13,300**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**12,000**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**12,000**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**16,100**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**17,400**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**15,000**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**14,400**	**9**	**AQUIRE**

Lepomis macrochirus	**bluegill**	**96-h/LC50**	**13,500**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**15,000**	**9**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**13,400**	**5**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**26,700**	**10**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**28,770**	**10**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**42,000**	**8**	**AQUIRE**

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

Diaptomus forbesi	**calanoid copepod**	**96-h/LC50**	**99,500**	**12**	**AQUIRE**

4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).

Asellus aquaticus	**aquatic sowbug**	**96-h/LC50**	**200,000**	**4**	**AQUIRE**
Gammarus fossarum	**scud**	**96-h/LC50**	**63,000**	**4**	**AQUIRE**

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.

Carassius auratus	**goldfish**	**96-h/LC50**	**16,940**	**2**	**AQUIRE**
Carassius auratus	**goldfish**	**96-h/LC50**	**36,810**	**10**	**AQUIRE**
Poecilia reticulata	**guppy**	**96-h/LC50**	**34,730**	**10**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**135,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**76,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**54,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**78,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**92,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**68,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**56,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**87,000**	**7**	**AQUIRE**
Xenopus laevis	**clawed toad**	**96-h/LC50**	**80,000**	**7**	**AQUIRE**

7. At least one organism from a family in a phylum other than Arthropoda or Chordata (e.g., Rotifera, Annelida, Mollusca).

Lymnaea stagnalis	**great pond snail**	**96-h/LC50**	**500,000**	**4**	**AQUIRE**

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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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). Xylenes are currently classified as Group D, not classifiable as to human carcinogenicity, in the U.S. EPA's IRIS database. No cancer slope factor is available, but the IRIS database does list an oral reference dose (RfD). There are no aquatic organism bioaccumulation data (ECOTOX) currently available; however, it is possible to calculate a BAF using the K_{ow} and a food chain multiplier. Thus, there is sufficient data available at this time to calculate a human threshold secondary value for xylene for the protection of human health. Commercial xylene usually contains a mixture of 40-65% *m*-xylene, and up to 20% each of *o*-xylene and *p*-xylene and ethylbenzene. (NR 105 contains a human threshold criterion for ethylbenzene.) Because the majority of the mixture is made up of *m*-xylene (CAS # 108-38-3), the human threshold secondary value for xylene is based on the K_{ow} for this isomer.

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 *m*-xylene, the K_{ow} = 1,585 and log K_{ow} = 3.20 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(1585)]\}$$

$$= 1/1.000380$$

$$\mathbf{= 0.9996}$$

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 *m*-xylene using a K_{ow} and a food chain multiplier (FCM).

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 *m*-xylene's log Kow of 3.20, the FCM for trophic level 3 from the table is 1.042.

The anti-log of 3.30 = 1585

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

= (1.042)(1585)

= 1651.5700

3) Calculation of the human health BAF

For xylene (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

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

$= \{[(1651.5700)(0.013)] + 1\} (0.9996)$

= 22.4614

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; = 2 mg/Kg/day for xylenes (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 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)]

= [(2 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(22.4614 L/Kg)]

= 112/0.4592

= 243.902439 mg/L

= 243,902.44 μg/L

In waters designated as warm water sportfish, non-public water supply, the human threshold secondary value for m-xylene is 243,900 μg/L.