

Date: March 2007

Calculator: Elisabeth Harrahy

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.

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. (This is still the case as of March 2007)

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.					
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	13,500	13	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	17,300	13	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	8,200	6	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	8,200	9	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	3,300	9	AQUIRE
<i>Oncorhynchus mykiss</i>	rainbow trout	96-h/LC50	13,500	9	AQUIRE
<i>Oncorhynchus mykiss</i>	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.					
<i>Cyprinus carpio</i>	common carp	96-h/LC50	780,000	11	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	24,500	1	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	15,700	1	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	20,870	10	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	19,000	3	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	13,500	6	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	13,500	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	8,600	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	12,000	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	13,300	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	12,000	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	12,000	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	16,100	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	17,400	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	15,000	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	14,400	9	AQUIRE

<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	13,500	9	AQUIRE
<i>Lepomis macrochirus</i>	bluegill	96-h/LC50	15,000	9	AQUIRE
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	13,400	5	AQUIRE
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	26,700	10	AQUIRE
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	28,770	10	AQUIRE
<i>Pimephales promelas</i>	fathead minnow	96-h/LC50	42,000	8	AQUIRE
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
<i>Diaptomus forbesi</i>	calanoid copepod	96-h/LC50	99,500	12	AQUIRE
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					
<i>Asellus aquaticus</i>	aquatic sowbug	96-h/LC50	200,000	4	AQUIRE
<i>Gammarus fossarum</i>	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.					
<i>Carassius auratus</i>	goldfish	96-h/LC50	16,940	2	AQUIRE
<i>Carassius auratus</i>	goldfish	96-h/LC50	36,810	10	AQUIRE
<i>Poecilia reticulata</i>	guppy	96-h/LC50	34,730	10	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	135,000	7	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	76,000	7	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	54,000	7	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	78,000	7	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	92,000	7	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	68,000	7	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	56,000	7	AQUIRE
<i>Xenopus laevis</i>	clawed toad	96-h/LC50	87,000	7	AQUIRE
<i>Xenopus laevis</i>	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).					
<i>Lymnaea stagnalis</i>	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.

-
- ¹Bailey, H.C., D.H.W. Liu and H.A. Javitz. 1985. Time/toxicity relationships in short-term, dynamic, and plug-flow bioassays. In: R.C. Bahner and D.J. Hansen (Eds.), Aquatic Toxicology and Hazard Assessment, 8th Symposium, ASTM STP 891, Philadelphia, PA:193-212.
- ²Brenniman, G. R. Hartung and W.J. Weber, Jr. 1976. A continuous flow bioassay method to evaluate the effects of outboard motor exhausts and selected aromatic toxicants on fish. *Water Res.* 10(2):165-169.
- ³Cope, O.B. 1965. Sport fishery investigations. In: Effects of Pesticides on Fish and Wildlife, U.S.D.I. Fish and Wildlife Circular 226:51-63.
- ⁴Erben, R. and Z. Pisl. 1993. Acute toxicity for some evaporating aromatic hydrocarbons for freshwater snails and crustaceans. *Int. Rev. Gesamten Hydrobiol.* 78(1):161-167.
- ⁵Geiger, D.L., L.T. Brooke and D.J. Call. 1990. Acute Toxicities of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vol. 5. Center for Lake Superior Environmental Studies, University of Wisconsin, Superior, WI. 332 pp.
- ⁶Johnson, W.W. and M.T. Finley. 1980. Handbook of Acute Toxicity of Chemicals to Fish and Aquatic Invertebrates. Resource Publication 137, Fish and Wildlife Service, U.S.D.I. Washington, D.C. 98 pp.
- ⁷Kononen, D.W. and R.A. Gorski. 1997. A method for evaluating the toxicity of industrial solvent mixtures. *Environmental Toxicology and Chemistry* 16(5):968-976.
- ⁸Mattson, V.R., J.W. Arthur and C.T. Walbridge. 1976. Acute toxicity of selected organic compounds to fathead minnows. *Ecol. Res. Ser.* EPA-600/3-76-097, Environ. Res. Lab., U.S. EPA, Duluth, MN. 12 pp.
- ⁹Mayer, F.L.J. and M.R. Ellersieck. 1986. Manual of Acute Toxicity: Interpretation and Data Base for 410 Chemicals and 66 Species of Freshwater Animals. Resource Publication Number 160, U.S.D.I., Fish and Wildlife Service, Washington, D.C. 505 pp.
- ¹⁰Pickering, Q.H. and C. Henderson. 1966. Acute toxicity of some important petrochemicals to fish. *J. Water Pollut. Control Fed.* 38(9):1419-1429.
- ¹¹Rao, T.S., M.S. Rao, and S.B.S. Prasad. 1975. Median tolerance limits of some chemicals to the fresh water fish *Cyprinus carpio*. *Indian J. Environ. Health* 17(2):140-146.
- ¹²Saha, M.K. and S.K. Konar. 1983. Acute toxicity of some petroleum pollutants to plankton and fish. *Environ. Ecol.* 1(1):117-119.
- ¹³Walsh, D.F., J.G. Armstrong, T.R. Bartley, H.A. Salman and P.A. Frank. 1977. Residues of emulsified xylene in aquatic weed control and their impact on rainbow trout, *Salmo gairdneri*. REC-ERC-76-11, Applied Sciences Branch, Eng. Res. Center, Denver, CO. 15 pp.

HUMAN HEALTH

Note: new oral reference dose as of 2003. Therefore, these secondary values are different than those previously calculated.

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:

$$= 1 / \{ 1 + [(0.00000024 \text{ Kg/L})(K_{ow})] \}$$

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

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

$$= 1 / 1.000380$$

$$= \mathbf{0.9996}$$

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

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. For discharges into water classified as cold, the FCM will be for trophic level 4. Given *m*-xylene's log K_{ow} of 3.20, the FCM for trophic level 3 is 1.042 and for trophic level 4 is 1.009.

The anti-log of 3.20 = 1585

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

$$= (1.042)(1585)$$

$$= \mathbf{1651.5700}$$

Cold Water Baseline BAF = (FCM) (K_{ow})

$$= (1.009) (1585)$$

$$= \mathbf{1599.2650}$$

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

$$\begin{aligned}
 \text{BAF}_{\text{TL3}}^{\text{HH}} &= \{[(\text{baseline BAF})(0.013)] + 1\} (f_{\text{fd}}) \\
 &= \{[(1651.5700)(0.013)] + 1\} (0.9996) \\
 &= \mathbf{22.4614}
 \end{aligned}$$

For xylene (an organic substance) discharges to **cold water**, the equation to use is:

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

where

baseline BAF = the baseline BAF calculated in 2)

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

f_{fd} = fraction freely dissolved

$$\begin{aligned}
 \text{BAF}_{\text{TL4}}^{\text{HH}} &= \{[(\text{baseline BAF})(0.044)] + 1\} (f_{\text{fd}}) \\
 &= \{[(1599.2650)(0.044)] + 1\} (0.9996) \\
 &= \mathbf{71.3391}
 \end{aligned}$$

4) Calculation of the human threshold secondary value

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

where

ADE = acceptable daily exposure (= oral reference dose, or RfD; = 0.2 mg/Kg/day for xylenes (IRIS 2003))

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

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.2 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(22.4614 \text{ L/Kg})] \\ &= 11.2/2.4492 \\ &= 4.5729 \text{ mg/L} \\ &= \mathbf{4,573 \mu\text{g/L}}\end{aligned}$$

Cold water, Public Water Supply

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.2 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[2 \text{ L/d} + (0.02 \text{ Kg/d})(71.3391 \text{ L/Kg})] \\ &= 11.2/3.4268 \\ &= 3.2684 \text{ mg/L} \\ &= \mathbf{3,268 \mu\text{g/L}}\end{aligned}$$

Warm Waters, Non-Public Water Supply

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.2 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(22.4614 \text{ L/Kg})] \\ &= 11.2/0.4592 \\ &= 24.3902 \text{ mg/L} \\ &= \mathbf{24,390 \mu\text{g/L}}\end{aligned}$$

Cold Water, Non-Public Water Supply

$$\begin{aligned}\text{Human Threshold Secondary Value} &= [(ADE)(70 \text{ Kg})(RSC)]/[W_H + (F_H)(BAF)] \\ &= [(0.2 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d} + (0.02 \text{ Kg/d})(71.3391 \text{ L/Kg})] \\ &= 11.2/1.4368\end{aligned}$$

$$= 7.7951 \text{ mg/L}$$

$$= \mathbf{7,795 \text{ }\mu\text{g/L}}$$

Limited Aquatic Life, Non-Public Water Supply

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

$$= [(0.2 \text{ mg/Kg/d})(70 \text{ Kg})(0.8)]/[0.01 \text{ L/d}]$$

$$= 11.2/0.01$$

$$= 1,120 \text{ mg/L}$$

$$= \mathbf{1,120,000 \text{ }\mu\text{g/L}}$$