Date: July 26, 2005
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SECONDARY VALUES FOR METHYL ETHYL KETONE (CAS No. 78-93-3)

A search was conducted for information on the chemical properties and toxicity of methyl ethyl ketone 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), and CHEMFATE (environmental fate). This search yielded some information on methyl ethyl ketone's properties and toxicity.

Fish and Aquatic Life Secondary Values

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 methyl ethyl ketone to fish and other aquatic life, it was determined that data are available to meet two out of the eight requirements. Because data are available for a Daphnid species, it is possible to calculate a secondary acute value for methyl ethyl ketone.

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 = 1,627,059 µg/L (*Daphnia magna*)

SAV = GMAV/SAF
= 1,627,059 µg/L /13
= 125,158 µg **/L**

SACR = 18 (default)

SCV = SAV/SACR
= 125,158 µg/L /18
= 6,953 µg/L

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

Because the lowest GMAV in the cold water database is for an invertebrate (*Daphnia magna*), and because invertebrates do not drop out of the database for any other use designation, the acute and chronic secondary values will be the same for all other use designations as for cold water.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for methyl ethyl ketone, 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 warmwater species.					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**5,091,000**	**a**	**ECOTOX**
Daphnia magna	**water flea**	**48-h/LC50**	**>520,000**	**b**	**ECOTOX**
SMAV = 1,627,059					
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.					
Gambusia affinis	**western mosquitofish**	**96-h/LC50**	**5,600,000**	**c**	**ECOTOX**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**3,220,000**	**d**	**ECOTOX**
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.					

[a]Randall, T.L. and P.V. Knop. 1980. Detoxification of specific organic substances by wet oxidation. J. Water Pollut. Control Fed. 52(8):2117-2130.

[b]LeBlanc, G.A. 1980. Acute toxicity of priority pollutants to water flea (*Daphnia magna*). Bull. Environ. Contam. Toxicol. 24(5):684

-691.
[c]Wallen, I.E., W.C. Greer, and R. Lasater. 1957. Toxicity to *Gambusia affinis* of certain pure chemicals in turbid waters. Sewage Ind. Wastes 29(6):695-711.
[d]Brooke, L.T., D.J. Call, D.L. Geiger and C.E. Northcott. 1984. Acute toxicities of organic chemicals to fathead minnows (*Pimephales promelas*), Vol. 1. Center for Lake Superior Environmental Studies, University of Wisconsin-Superior, Superior, WI:414.

Human Health Secondary Values

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). Methyl ethyl ketone is currently classified as "D", not classifiable, by the U.S. EPA (IRIS, 2004) based on inconclusive data in humans and no animal data. An oral reference dose (RfD; IRIS, 2004) 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:

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

For methyl ethyl ketone, the K_{ow} = 1.9498, and the log K_{ow} = 0.29 (CHEMFATE database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(1.9498)]\}$$

$$= 1/1.0000$$

$$= \mathbf{1.0000}$$

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

No field-measured BAFs or BSAFs, and no laboratory-measured BCFs are available for methyl ethyl ketone. Therefore, a baseline BAF was calculated for using a K_{ow} and a FCM.

The FCM will be for trophic level 3 for a discharge to a water body classified as warm water, and the FCM will be for trophic level 4 for a discharge to a water body classified as cold water. Given methyl ethyl ketone's log Kow of 0.29, the FCM from the table is 1.000 both trophic levels 3 and 4.

For warm water:

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

= (1.000)(1.9498)

= 1.9498

For cold water:

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

= (1.000)(1.9498)

= 1.9498

3) Calculation of the human health BAF

Because methyl ethyl ketone is an organic substance, the equations to use are as follows (depending on whether the discharge is to a water body classified as warm water or cold water):

For warm water:

BAF^{HH}_{TL3} = {[(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} = {[(1.9498)(0.013)] + 1} (1.0000)

= **1.0253**

For cold water:

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

BAF^{HH}_{TL4} = {[(1.9498)(0.044)] + 1} (1.0000)

= 1.0858

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)
= 0.6 mg/Kg/day for methyl ethyl ketone (IRIS 2005)

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 Waters, Public Water Supply

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

= [(0.6 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(1.0253 L/Kg)]

= 33.6/2.0205

= 16.6295 mg/L

= 16,630 μg/L

Cold water, Public Water Supply

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

= [(0.6 mg/Kg/d)(70 Kg)(0.8)]/[2 L/d + (0.02 Kg/d)(1.0858 L/Kg)]

= 33.6/2.0217

= 16.6197 mg/L

= 16,620 μg/L

Warm Waters, Non-Public Water Supply

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

= [(0.6 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(1.0253 L/Kg)]

= 33.6/0.0305

= 1101.6393 mg/L

= 1,101,600 μg/L

Cold Water, Non-Public Water Supply

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

= [(0.6 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d + (0.02 Kg/d)(1.0858 L/Kg)]

= 33.6/0.0317

= 1059.9369 mg/L

= 1,059,900 μg/L

Limited Aquatic Life, Non-Public Water Supply

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

= [(0.6 mg/Kg/d)(70 Kg)(0.8)]/[0.01 L/d]

= 33.6/0.01

= 3360 mg/L

= 3,360,000 μg/L