Date: May 31, 2005
Calculator: Elisabeth Harrahy, Ph.D.

SECONDARY VALUES FOR METHYL TERT-BUTYL ETHER (CAS No. 1634-04-4)

A search was conducted for information on the chemical properties and toxicity of methyl tert-butyl ether (MTBE) 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). Recent journal articles were also obtained. This search yielded useful information on the properties and toxicity of MTBE.

FISH AND AQUATIC LIFE SECONDARY VALUES

ACUTE

To derive an acute toxicity criterion for fish and 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 MTBE to fish and other aquatic life, it was determined that data are available to meet all requirements for calculation of criteria. However, until such criteria can be promulgated, the criteria will be termed secondary values.

Cold Water

Genus mean acute values (GMAV; geometric mean of SMAVs), ordered from high to low and ranked (1 for the lowest, and 9 for the highest) are found below. The cumulative probability (P) was calculated for each GMAV as P=R/(N+1).

Rank (R)	Species	GMAV (μg/L)	P
9	Midge	1,742,000	0.9000
8	Bluegill	1,054,000	0.8000
7	Rainbow trout	887,000	0.7000
6	Fathead minnow	810,688	0.6000
5	Burrowing mayfly	581,000	0.5000
4	Pond snail	559,000	0.4000
3	Water flea (*D. magna*)	558,508	0.3000
2	Amphipod	473,000	0.2000
1	Water flea (*C. dubia*)	340,000	0.1000

Using the four GMAVs with Ps closest to 0.05 (*C. dubia* water flea, amphipod, *D. magna* water flea, and the pond snail), the acute toxicity criterion is calculated as follows:

Let EV = sum of the four ln GMAVs
= ln 340,000 + ln 473,000 + ln 558,508 + ln 559,000

= 12.7367 + 13.0669 + 13.2330 + 13.2339
= 52.2705

Let EW = sum of the four squares of the ln GMAVs
= $(12.7367)^2 + (13.0669)^2 + (13.2330)^2 + (13.2339)^2$
= 162.2235 + 170.7439 + 175.1123 + 175.1361
= 683.2158

Let EP = sum of the four Ps
= 0.1000 + 0.2000 + 0.3000 + 0.4000
= 1.0000

Let EPR = sum of the four square roots of P
= 0.3162 + 0.4472 + 0.5477 + 0.6325
= 1.9436

Let JR = square root of 0.05
= 0.2236

$S = ((EW - (EV)^2/4)/(EP-(EPR)^2/4))^{0.5}$
$= ((683.2158 - (52.2705)^2/4)/(1.0000 - (1.9436)^2/4))^{0.5}$
$= ((683.2158 - 683.0513)/(1.0000 - 0.9444))^{0.5}$
$= (0.1645/0.0556)^{0.5}$
$= (2.9586)^{0.5}$
= 1.7201

L = (EV - S(EPR))/4
= (52.2705 - 1.7201(1.9436))/4
= (52.2705 - 3.3432)/4
= 12.2318

A = (JR)(S) + L
= (0.2236)(1.7201) + 12.2318
= 12.6164

Final Acute Value (FAV) = e^A
$=e^{12.6164}$
=301,462.2259 (will round to **301,000**, based on the data)

Acute Toxicity Criterion = ATC = FAV/2
=301,462.2259
=150,731.1129

ATC for cold water = 150,731 µg/L

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

Because the four most sensitive species in the cold water database are all invertebrates and because none of these will drop out of the databases for any of the other water body use designations, the ATC for cold water will also apply for all other water body use designations.

CHRONIC

To derive a chronic toxicity criterion for aquatic life, chronic toxicity test results are required for at least one freshwater species in each of eight different families. Specific requirements and the data available to meet these requirements are found in Table 2. Complete data requirements for establishment of a chronic toxicity criterion for MTBE have not been met. However, it is also possible to calculate a chronic criterion using acute to chronic ratios. Acute and chronic tests were conducted by the same lab for each of the two species for which there are chronic data.

Cold Water

Species	Acute Value	Chronic Value	Acute to Chronic Ratio
Daphnia magna	472,000	41,600	11.3462
Pimephales promelas	980,000	289,400	3.3863

Final Acute to Chronic Ratio (FACR) = Geometric Mean of ACRs = 6.1985

Final Chronic Value (FCV) = Final Acute Value (FAV)/FACR
= 301,462.2259 / 6.1985
= 48,634.7061 µg/L

FCV for cold water = 48,635 µg/L (will round to **49,000**, based on the data)

Warm Water Sportfish, Warm Water Forage Fish, Limited Forage Fish

Because both the fathead minnow and the water flea would remain in the database for warm water sportfish, warm water forage fish and limited forage fish designated waters, the final chronic value would remain the same for these use designations as for cold water.

Limited Aquatic Life

The fathead minnow would drop out of the database.

Species	Acute Value	Chronic Value	Acute to Chronic Ratio
Daphnia magna	472,000	41,600	11.3462

Final Acute to Chronic Ratio (FACR) = 11.3462

Final Chronic Value (FCV) = Final Acute Value (FAV)/FACR
= 301,462.2259 / 11.3462
= 26,569.4440 µg/L

FCV for limited aquatic life = 26,569 µg/L. However, because this is lower than for cold water, the FCV for cold water would also apply for limited aquatic life-designated waters.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for MTBE, 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**	**887,000**	**1**	**journal**
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**	**1,054,000**	**1**	**journal**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Ceriodaphnia dubia	**water flea**	**48-h/LC50**	**340,000**	**1**	**journal**
Daphnia magna	**water flea**	**48-h/EC50**	**472,000**	**1**	**journal**
Daphnia magna	**water flea**	**48-h/EC50**	**542,000**	**1**	**journal**
Daphnia magna	**water flea**	**48-h/EC50**	**681,000**	**1**	**journal**
Species Mean Acute Value (SMAV) = 558,508					
4. At least one benthic crustacean (e.g., ostracod, isopod, amphipod, crayfish).					
Hyalella azteca	**amphipod**	**96-h/LC50**	**473,000**	**1**	**journal**
5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).					
Hexagenia limbata	**burrowing mayfly**	**96-h/LC50**	**581,000**	**1**	**journal**
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**	**672,000**	**1**	**journal**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**706,000**	**1**	**journal**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**929,000**	**1**	**journal**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**980,000**	**1**	**journal**

SMAV = 810,688

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

Physa gyrina	**snail**	**96-h/LC50**	**559,000**	**1**	**journal**

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.

Chironomus tentans	**midge**	**48-h/LC50**	**1,742,000**	**1**	**journal**

---

[1]Mancini, E.R., A. Steen, G.A. Rausina, D.C.L. Wong, W.R. Arnold, F.E. Gostomski, T. Davies, J.R. Hockett, W.A. Stubblefield, K.R. Drottar, T.A. Springer, and P. Errico. 2002. MTBE ambient water quality criteria development: A public/private partnership. Environmental Science and Technology 36(2):125-129.

Table 2. Requirements for calculation of a chronic toxicity criterion for protection of aquatic life for MTBE, and corresponding chronic 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.					
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**	**21-d/IC20**	**41,600**	**1**	**journal**
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.					
Pimephales promelas	**fathead minnow**	**31-d/IC20**	**289,400**	**1**	**journal**
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]Mancini, E.R., A. Steen, G.A. Rausina, D.C.L. Wong, W.R. Arnold, F.E. Gostomski, T. Davies, J.R. Hockett, W.A. Stubblefield, K.R. Drottar, T.A. Springer, and P. Errico. 2002. MTBE ambient water quality criteria development: A public/private partnership. Environmental Science and Technology 36(2):125-129.

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). MTBE has not yet been classified as to its carcinogenicity so no cancer slope factor is available. In addition, no oral reference dose is available with which to calculate a human threshold value for the protection of human health (U.S. EPA's IRIS database).

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
MTBE	1634-04-4	Fish and Aquatic	Acute	Cold, WWSF, WWFF, LFF, LAL	FAV= 301,000 ATC = 151,000
MTBE	1634-04-4	Fish and Aquatic	Chronic	Cold, WWSF, WWFF, LFF, LAL	FCV = 49,000
MTBE	1634-04-4	Human Health	Human Threshold	-	Insufficient Data

Cold = cold water designated water bodies
WWSF = warm water sportfish designated water bodies
WWFF = warm water forage fish designated water bodies
LFF = limited forage fish designated water bodies
LAL = limited aquatic life designated water bodies (includes wetlands)