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Calculator: Elisabeth Harrahy, Ph.D.

SECONDARY VALUES FOR METOLACHLOR (CAS No. 51218-45-2)

A search was conducted for information on the chemical properties and toxicity of metolachlor 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), BIODEG (degradation), HSDB (Hazardous Substances Data Bank), CCRIS (Chemical Carcinogenesis Research Info System), ATSDR ToxFAQs (Agency for Toxic Substances and Disease Registry chemical fact sheets), and EXTOXNET (Extension Toxicology Network's pesticide information project). This search yielded some useful information on metolachlor's properties and toxicity.

Fish and Aquatic Life Secondary Values

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

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 five out of eight requirements met = 6.1
Lowest GMAV = 3,900 µg/L (*Oncorhynchus mykiss*)

SAV = GMAV/SAF
= 3,900 µg/L / 6.1
= 639.34 µg/L

Chronic data is available for *Ceriodaphnia dubia*. Therefore, a secondary chronic value (SCV) may be calculated using a combination of this data and default ratios.

SACR (secondary acute-chronic ratio) = Geometric mean of three species mean acute-chronic ratios (SMACRs).

SMACR 1 = 15,930/8,840 = 1.80
SMACR 2 = 18 (default)
SMACR 3 = 18 (default)

SACR = geometric mean of 1.80, 18, and 18 = 8.35

SCV = SAV/SACR
= 639.34 µg/L / 8.35
= 76.57 µg/L

So for cold water-designated waters, the secondary acute value is 639 µg/L and the secondary chronic value is 77 µg/L for metolachlor.

Warm Water Sportfish

Cold water fish drop out of the database when calculating secondary values for warm water sportfish designated waters.

SAF for five out of eight requirements met = 6.1
Lowest GMAV = 4089.01 µg/L (*Chironomus plumosus*)

SAV = GMAV/SAF
= 4089.01 µg/L / 6.1
= 670.33 µg/L

SCV = SAV/SACR
= 670.33 µg/L / 8.35
= 80.28 µg/L

So for warm water sportfish-designated waters, the secondary acute value is 670 µg/L and the secondary chronic value is 80 µg/L for metolachlor.

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

Because the lowest GMAV in the warm water sportfish database was for an invertebrate (*Chironomus plumosus*), which will not drop out of the databases for any of the remaining water body use designations, the secondary acute and chronic values for warm water sportfish-designated waters will also apply for warm water forage fish, limited forage fish and limited aquatic life-designated waters.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for metolachlor, 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**	**3,900**	**1**	**AQUIRE**
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**	**10,000**	**1**	**AQUIRE**
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**4,900**	**1**	**AQUIRE**
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Ceriodaphnia dubia	**water flea**	**48-h/LC50**	**15,930**	**3**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**25,100**	**1**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**15,400**	**1**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**23,500**	**2**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**26,000**	**2**	**AQUIRE**
Species Mean Acute Value (SMAV) = 22,044.94					
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).					
Chironomus plumosus	**midge**	**48-h/EC50**	**3,800**	**2**	**AQUIRE**
Chironomus plumosus	**midge**	**48-h/EC50**	**4,400**	**2**	**AQUIRE**
SMAV = 4,089.01					
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**	**8,000**	**2**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**8,400**	**2**	**AQUIRE**
SMAV = 8,197.56					
Poecilia reticulata	**guppy**	**96-h/LC50**	**8,600**	**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]Office of Pesticide Programs. 2000. Environmental Effects Database (EEDB). Environmental Fate and Effects Division, U.S. EPA, Washington, D.C.

[2]Mayer, 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 No. 160. U.S. Department of Interior, U.S. Fish and Wildlife Service, Washington, D.C. 505 pp.

[3]Ort, M.P., J.F. Fairchild, and S.E. Finger. 1994. Acute and chronic effects of four commercial herbicide formulations on *Ceriodaphnia dubia*. Arch. Environ. Contam. Toxicol. 27(1):103-106.

Table 2. Requirements for calculation of a chronic toxicity criterion for protection of aquatic life for metolachlor, 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).					
Ceriodaphnia dubia	**water flea**	**7-d/MATC**	**8,840**	**1**	**AQUIRE**
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.					
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]Ort, M.P., J.F. Fairchild, and S.E. Finger. 1994. Acute and chronic effects of four commercial herbicide formulations on *Ceriodaphnia dubia*. Arch. Environ. Contam. Toxicol. 27(1):103-106.

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). Metolachlor has been classified as a Class C carcinogen (possible human carcinogen); however, no cancer slope factor is available with which to calculate a human secondary cancer value for the protection of human health (U.S. EPA's IRIS database). Because an oral reference dose and a log octanol water partition coefficient are available, a human threshold secondary value can be calculated for metolachlor.

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:

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

A log K_{ow} of 3.13 (K_{ow} of 1,348.9629) has been established for metolachlor (National Institutes of Health, Hazardous Substance Database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(1{,}348.9629)]\}$$

$$= 1/1.000324$$

$$\mathbf{= 0.9997}$$

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) a measured BAF from a field study
b) a predicted BAF based on field-measured BSAFs
c) a predicted BAF using a laboratory-measured bioconcentration factor (BCF) and a food chain multiplier (FCM)
d) a predicted BAF using a K_{ow} and a FCM

Currently, there are no BAFs, BSAFs, or BCFs available for metolachlor; therefore, the baseline BAF was calculated using the K_{ow} and a food chain multiplier (method d above).

Given metolachlor's log K_{ow} of 3.13 (K_{ow} of 1,348.9629), the FCMs (taken from table B-1 in GLI) are 1.034 for trophic level 3 (warm waters) and 1.007 for trophic level 4 (cold waters).

a) Cold Water

Baseline BAF = (FCM)(Kow)

= (1.007)(1,348.9629)

= 1,358.4056

b) Warm Waters

Baseline BAF = (FCM)(Kow)

= (1.034)(1,348.9629)

= 1,393.8276

3) Calculation of the human health BAF

a) Cold Water

BAF^{HH}_{TL4} = {[(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 (for cold waters) calculated in 2)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL4} = {[(1,358.4056)(0.044)] + 1} (0.9997)

= **60.7516**

b) Warm Waters

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

where

BAF^{HH}_{TL3} = Human health BAF for trophic level 3 (warm waters)

baseline BAF = the baseline BAF (for warm waters) calculated in 2)

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

f_{fd} = fraction freely dissolved

BAF^{HH}_{TL3} = {[(1,393.8276)(0.013)] + 1} (0.9997)

= **19.1140**

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; = 0.15 mg/Kg/day for metolachlor (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).

a) Public Water Supply/Cold Water

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

= [(0.15 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(60.7516 L/Kg)]

= 2.6127 mg/L

= 2,612.7 µg/L

b) Public Water Supply/Warm Water Sportfish

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

= [(0.15 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(19.1140 L/Kg)]

= 3.5264 mg/L

= 3,526.4 µg/L

c) Non-Public Water Supply/Cold Water

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

= [(0.15 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(60.7516 L/Kg)]

= 6.8571 mg/L

= 6,857.1 µg/L

d) Non-Public Water Supply/Warm Waters (Warm Water Sportfish, Warm Water Forage Fish, and Limited Forage Fish designated waters)

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

= [(0.15 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(19.1140 L/Kg)]

= 21.4122 mg/L

= 21,412.2 µg/L

e) Non-Public Water Supply/Limited Aquatic Life

Note: The Limited Aquatic Life classification applies to water bodies with no (or very few) fish present. Therefore, calculation of a human health threshold value for water bodies with this classification does not include a human health BAF since it is assumed that humans will not be exposed to metolachlor through consumption of fish in these areas.

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

$= [(0.15\ mg/Kg/d)(70\ Kg)(0.8)]/[\mathbf{0.01}\ L/d + (0)]$

= 840 mg/L

= 840,000 µg/L

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Metolachlor	51218-45-2	Fish and Aquatic	Acute	Cold	639
Metolachlor	51218-45-2	Fish and Aquatic	Chronic	Cold	77
Metolachlor	51218-45-2	Fish and Aquatic	Acute	WWSF, WWFF, LFF, LAL	670
Metolachlor	51218-45-2	Fish and Aquatic	Chronic	WWSF, WWFF, LFF, LAL	80
Metolachlor	51218-45-2	Human Health	Human Threshold	Public Water Supply/Cold	2,613
Metolachlor	51218-45-2	Human Health	Human Threshold	Public Water Supply/WWSF	3,526
Metolachlor	51218-45-2	Human Health	Human Threshold	Non-Public Water Supply/Cold	6,857
Metolachlor	51218-45-2	Human Health	Human Threshold	Non-Public Water Supply/WWSF, WWFF, LFF	21,412
Metolachlor	51218-45-2	Human Health	Human Threshold	Non-Public Water Supply/LAL	840,000

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)