Date: March 25, 2009
Calculator: James Schmidt (updated to account for variability within species)

SECONDARY VALUES FOR ALACHLOR (CAS No. 15972-60-8)

A search was conducted for information on the chemical properties and toxicity of alachlor 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 useful information on alachlor'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 alachlor to fish and other aquatic life, it was determined that data are available to meet six out of the eight requirements. Because data are available for a Daphnid species, it was possible to calculate a secondary acute value for alachlor.

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 six out of eight requirements met = 5.2
Lowest GMAV = 2,035.32 µg/L (*Onchorhynchus mykiss*)

SAV = GMAV/SAF
= 3,587.48 µg/L / 5.2
= 391.41 µg/L

Chronic data are available for alachlor which meet acceptability requirements and which were collected along with corresponding acute data (Table 2). Therefore, a secondary chronic value (SCV) may be calculated using some actual chronic data, rather than through default ratios only.

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

SMACR 1 (*Ceriodaphnia dubia*) = 7,900 µg/L /3,852.27 µg/L = 2.0507

SMACR 2 (default) = 18
SMACR 3 (default) = 18

SACR = geometric mean of 2.0507, 18, and 18 = 8.73

SCV = SAV/SACR
= 391.41 µg/L / 8.73
= 44.83 µg/L

So for cold water designated waters, the secondary acute value is 391 µg/L and the secondary chronic value is 44.8 µg/L for alachlor.

Because the lowest acute value was for a coldwater fish, and because the next lowest acute value was for an amphibian, another value will be calculated and applied to the remaining use designations.

SAF for six out of eight requirements met = 5.2
Lowest GMAV = 3,587.48 µg/L (*Bufo americanus*)

SAV = GMAV/SAF
= 3,587.48 µg/L / 5.2
= 689.90 µg/L

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

SMACR 1 (*Ceriodaphnia dubia*) = 7,900 µg/L /3,852.27 µg/L = 2.0507
SMACR 2 (default) = 18
SMACR 3 (default) = 18

SACR = geometric mean of 2.0507, 18, and 18 = 8.73

SCV = SAV/SACR
= 689.90 µg/L / 8.73
= 79.03 µg/L

So for warmwater sport fish and forage fish, limited forage fish, and limited aquatic life waters, the secondary acute value is 690 µg/L and the secondary chronic value is 79 µg/L for alachlor.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for alachlor, 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**	**1,400**	**9**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**2,400**	**9**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**9,100**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**1,800**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**3,600**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**3,700**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**4,200**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**240**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**1,000**	**7**	**AQUIRE**
# ***Oncorhynchus mykiss***	**rainbow trout**	**96-h/LC50**	**>104,000**	**7**	**AQUIRE**
# ***Oncorhynchus mykiss***	**rainbow trout**	**96-h/LC50**	**>100,000**	**7**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**1,400**	**4**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**2,400**	**4**	**AQUIRE**
# - Deleted from the database because the LC50s varied by over a factor of 10 and the remaining values tended towards the lower end of the extremes.					
Species Mean Acute Value (SMAV) = 2,035.32					
2. At least one non-salmonid fish from another family in the class Osteichthyes, preferably a commercially or recreationally important warmwater species.					
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**16,700**	**1**	**AQUIRE**
Ictalurus punctatus	**channel catfish**	**96-h/LC50**	**6,500**	**7**	**AQUIRE**
SMAV = 10,418.73					

Lepomis macrochirus	**bluegill**	**96-h/LC50**	**3,200**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**4,300**	**9**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**2,800**	**7**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**6,200**	**7**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**6,400**	**7**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**7,600**	**7**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**12,400**	**7**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**5,600**	**7**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**3,200**	**4**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**4,300**	**4**	**AQUIRE**

SMAV = 5,064.53

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

Ceriodaphnia dubia	**water flea**	**48-h/LC50**	**7,900**	**2**	**AQUIRE**
Ceriodaphnia dubia	**water flea**	**48-h/LC50**	**14,360**	**3**	**AQUIRE**

SMAV= 10,651.01

Daphnia magna	**water flea**	**48-h/EC50**	**27,000**	**7**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**10,000**	**7**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**35,000**	**7**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**22,000**	**7**	**AQUIRE**
# *Daphnia magna*	**water flea**	**48-h/EC50**	**>104,000**	**7**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**21,000**	**4**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**7,700**	**4**	**AQUIRE**

- Deleted from the database because the EC50s varied by over a factor of 10 and the remaining values tended towards the lower end of the extremes.

SMAV = 17,965

Daphnia pulex	**water flea**	**48-h/EC50**	**10,400**	**8**	**AQUIRE**
Daphnia pulex	**water flea**	**48-h/EC50**	**9,000**	**8**	**AQUIRE**

SMAV = 9,674.71

Genus Mean Acute Value (GMAV; for *Daphnia* sp.) = 13,183.35

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

***Procambarus* sp.**	**crayfish**	**96-h/LC50**	**19,500**	**7**	**AQUIRE**

SMAV = 19,500

5. At least one insect (e.g., mayfly, dragonfly, damselfly, stonefly, caddisfly, mosquito, midge).

Chironomus plumosus	**midge**	**48-h/EC50**	**3,200**	**4**	**AQUIRE**
Chironomus plumosus	**midge**	**48-h/EC50**	**2,500**	**4**	**AQUIRE**

SMAV = 2,828.43

Chironomus thummi	**midge**	**48-h/EC50**	**10,000**	**5**	**AQUIRE**
Chironomus thummi	**midge**	**48-h/EC50**	**12,500**	**5**	**AQUIRE**

SMAV = 11,180.34

GMAV (for *Chironomus* sp.) = 5,623.42

6. At least one fish or amphibian from a family in the phylum Chordata not already represented in one of the other subdivisions.

Bufo americanus	**American toad**	**96-h/LC50**	**3,900**	**1**	**AQUIRE**
Bufo americanus	**American toad**	**96-h/LC50**	**3,300**	**1**	**AQUIRE**

SMAV =3,587.48

Cyprinus carpio	**common carp**	**96-h/LC50**	**4,600**	**6**	**AQUIRE**

SMAV = 4,600

Pimephales promelas	**fathead minnow**	**96-h/LC50**	**5,000**	**10**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**5,000**	**11**	**AQUIRE**
Pimephales promelas	**fathead minnow**	**96-h/LC50**	**5,000**	**12**	**AQUIRE**

SMAV = 5,000

Rana pipiens	**leopard frog**	**96-h/LC50**	**11,500**	**1**	**AQUIRE**
Rana pipiens	**leopard frog**	**96-h/LC50**	**3,500**	**1**	**AQUIRE**

SMAV = 6,344.29

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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Table 2. Requirements for calculation of a chronic toxicity criterion for protection of aquatic life for alachlor, 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**	**2,800**	**1**	**AQUIRE**
Ceriodaphnia dubia	**water flea**	**7-d/MATC**	**5,300**	**1**	**AQUIRE**
Species Mean Chronic Value (SMCV) = 3,852.27					
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]Oris, J.T., R.W. Winner and M.V. Moore. 1991. A four-day survival and reproduction toxicity test for *Ceriodaphnia dubia*. Environmental Toxicology and Chemistry 10(2):217-224.

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). Alachlor has been classified as a class B2 carcinogen since 1984 (probable human carcinogen; National Institute of Health's Hazardous Substance Database); however, there is no cancer slope factor available with which to calculate a human cancer secondary value. Because an oral reference dose and a log octanol water partition coefficient are available, a human threshold secondary value can be calculated for alachlor.

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 alachlor, log K_{ow}s of 2.63 and 3.53 have been published (National Institutes of Health, Hazardous Substance Database). The arithmetic mean of these is 3.08, which gives a K_{ow} of 1,202.2644.

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(1{,}202.2644)]\}$$

$$= 1/1.000289$$

$$\mathbf{= 0.9997}$$

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 alachlor that meet data acceptability requirements; therefore, the baseline BAF was calculated using the K_{ow} and a food chain multiplier (method d above).

Given alachlor's average log K_{ow} of 3.08 (K_{ow} of 1,202.2644), the FCMs (taken from table B-1 in GLI) are 1.034 for trophic level 3 (warm waters) and 1.007 trophic level 4 (cold waters).

a) Cold Water

Baseline BAF = (FCM)(Kow)

= (1.007)(1,202.2644)

= 1,210.6802

b) Warm Waters

Baseline BAF = (FCM)(Kow)

= (1.034)(1,202.2644)

= 1,243.1414

3) Calculation of the human health BAF

a) Cold Water

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

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

$BAF^{HH}_{TL4} = \{[(1,210.6802)(0.044)] + 1\} (0.9997)$

= **54.2536**

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} = {[(1,243.1414)(0.013)] + 1} (0.9997)

= **17.1557**

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; = 0.01 mg/Kg/day for alachlor (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)]

= [(0.01 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(**54.2536** L/Kg)]

= 0.1815 mg/L

= 181.5 µg/L

b) Public Water Supply/Warm Water Sportfish

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

= [(0.01 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(**17.1557** L/Kg)]

= 0.2390 mg/L

= 239 µg/L

c) Non-Public Water Supply/Cold Water

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

= [(0.01 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(**54.2536** L/Kg)]

= 0.5411 mg/L

= 541.1 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)]

= [(0.01 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(**17.1557** L/Kg)]

= 1.5859 mg/L

= 1,585.9 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 alachlor through consumption of fish in these areas.

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

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

$= \mathbf{56}\ mg/L$

$= \mathbf{56{,}000\ \mu g/L}$

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Alachlor	15972-60-8	Fish and Aquatic	Acute	Cold, WWSF, WWFF, LFF, LAL	690
Alachlor	15972-60-8	Fish and Aquatic	Chronic	Cold, WWSF, WWFF, LFF, LAL	79
Alachlor	15972-60-8	Human Health	Human Threshold*	Public Water Supply/Cold	182
Alachlor	15972-60-8	Human Health	Human Threshold*	Public Water Supply/WWSF	239
Alachlor	15972-60-8	Human Health	Human Threshold*	Non-Public Water Supply/Cold	541
Alachlor	15972-60-8	Human Health	Human Threshold*	Non-Public Water Supply/WWSF, WWFF, LFF	1,586
Alachlor	15972-60-8	Human Health	Human Threshold*	Non-Public Water Supply/LAL	56,000

*Alachlor has been classified as a class B2 carcinogen (probable human carcinogen) by the U.S. EPA. However, there no cancer slope factor available with which to calculate a human cancer secondary value (would likely be more stringent than a human threshold secondary value).

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)