Date: May 1, 2003
Calculator: Elisabeth Harrahy, Ph.D.

SECONDARY VALUES FOR ACETOCHLOR (CAS No. 34256-82-1)

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

Secondary acute values were calculated for cold water, warm water sportfish, warm water forage fish, limited forage fish and limited aquatic life designated water bodies. (Acetochlor is not a bioaccumulative chemical of concern (BCC); therefore, it will not be necessary to automatically apply cold water criteria.)

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 three out of eight requirements met = 8.0
Lowest GMAV = 576.42 µg/L (*Oncorhynchus mykiss*)

SAV = GMAV/SAF
= 576.42 µg/L / 8.0
= 72.05 µg/L

No chronic data are available for acetochlor which meet acceptability requirements. Therefore, a secondary chronic value (SCV) may be calculated using default ratios only.

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

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

SCV = SAV/SACR
= 72.05 µg/L /18
= 4.00 µg/L

So, for cold water designated waters, the secondary acute value is 72 µg/L and the secondary chronic value is 4 µg/L for acetochlor.

Warm Water Sportfish

The salmonid category of fish drops out of the database when calculating secondary values for warm water.

Lowest GMAV = 1,461.23 µg/L (*Lepomis macrochirus*)

SAV = GMAV/SAF
= 1,461.23 µg/L / 8.0
= 182.65 µg/L

SCV = SAV/SACR
= 182.65 µg/L /18
= 10.15 µg/L

So, for warm water sportfish designated waters, the secondary acute value is 183 µg/L and the secondary chronic value is 10 µg/L for acetochlor.

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

Cold water and warm water game fish species drop out of the database, leaving only toxicity data for *Daphnia magna*. Because this species will not drop out of the databases for Limited Forage Fish or Limited Aquatic Life designated waters, the secondary values will be the same for each of these types of water bodies.

Lowest GMAV = 9,384.80 µg/L (*Daphnia magna*)

SAV = GMAV/SAF
= 9,384.80 µg/L / 8.0
= 1,173.10 µg/L

SCV = SAV/SACR
= 1,173.10 µg/L /18
= 65.17 µg/L

So, for warm water forage fish, limited forage fish, and limited aquatic life designated waters, the secondary acute value is 183 μg/L and the secondary chronic value is 10 μg/L for acetochlor.

Table 1. Requirements for calculation of an acute toxicity criterion for protection of aquatic life for acetochlor, 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**	**1,200**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**380**	**1**	**AQUIRE**
Oncorhynchus mykiss	**rainbow trout**	**96-h/LC50**	**420**	**1**	**AQUIRE**
Genus Mean Acute Value (GMAV) = 576.42					
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**	**1,500**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**1,600**	**1**	**AQUIRE**
Lepomis macrochirus	**bluegill**	**96-h/LC50**	**1,300**	**1**	**AQUIRE**
GMAV = 1,461.23					
3. At least one planktonic crustacean (e.g., cladoceran, copepod).					
Daphnia magna	**water flea**	**48-h/EC50**	**8,200**	**1**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**7,200**	**1**	**AQUIRE**
Daphnia magna	**water flea**	**48-h/EC50**	**14,000**	**1**	**AQUIRE**
GMAV = 9,384.80					
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]Dow AgroSciences, LLC. July 1998. Clopyralid: A North American Technical Profile. Dow AgroSciences, LLC, 9330 Zionsville Road, Indianapolis, IN 46268.

[2]Vardia, H.K. and P.S. Rao. 1986. Pesticidal effects on chironomid larvae. Rev. Biol. (Lisb.) 13(1-4):113-115.

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). Acetochlor has been classified as a class B2 carcinogen (probable human carcinogen; 40 CFR Part 180, Vol. 59, No. 56. Rules and Regulations, March 23, 1994); however, there is currently 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 acetochlor.

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 acetochlor, the K_{ow} = 1,071.5193, and log K_{ow} = 3.03 (National Institutes of Health Hazardous Substance Database).

$$f_{fd} = 1/\{1 + [(0.00000024\ Kg/L)(1{,}071.5193)]\}$$

$$= 1/1.000257$$

$$\mathbf{= 0.9997}$$

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 acetochlor; therefore, the baseline BAF was calculated using the K_{ow} and a food chain multiplier (method d above).

Given acetochlor's log K_{ow} of 3.03 (K_{ow} of 1,071.5193), the FCMs (taken from table B-1 in GLI) are 1.028 for trophic level 3 (warm waters) and 1.007 trophic level 4 (cold waters).

a) Cold Water

Baseline BAF = (FCM)(Kow)

= (1.007)(1,071.5193)

= 1,079.0199

b) Warm Waters

Baseline BAF = (FCM)(Kow)

= (1.028)(1,071.5193)

= 1,101.5218

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} = {[(1,079.0199)(0.044)] + 1} (0.9997)

= **48.4623**

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} = {[(1,101.5218)(0.013)] + 1} (0.9997)

= **15.3152**

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; = 0.02 mg/Kg/day for acetochlor (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 = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.02 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(**48.4623** L/Kg)]

= 0.3772 mg/L

= 377.2 µg/L

b) Public Water Supply/Warm Water Sportfish

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

= [(0.02 mg/Kg/d)(70 Kg)(0.8)]/[**2** L/d + (0.02 Kg/d)(**15.3152** L/Kg)]

= 0.4856 mg/L

= 485.6 µg/L

c) Non-Public Water Supply/Cold Water

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

= [(0.02 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(**48.4623** L/Kg)]

= 1.1438 mg/L

= 1,143.8 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 = $[(ADE)(70\ Kg)(RSC)]/[W_H + (F_H)(BAF)]$

= [(0.02 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0.02 Kg/d)(**15.3152** L/Kg)]

= 3.5409 mg/L

= 3,540.9 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 acetochlor through consumption of fish in these areas.

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

= [(0.02 mg/Kg/d)(70 Kg)(0.8)]/[**0.01** L/d + (0)]

= 112.0000 mg/L

= **112,000 µg/L**

Chemical	CAS #	Category	Type of Secondary Value	Water Body Classification	Value (µg/L)
Acetochlor	34256-82-1	Fish and Aquatic	Acute	Cold	72
Acetochlor	34256-82-1	Fish and Aquatic	Acute	WWSF	183
Acetochlor	34256-82-1	Fish and Aquatic	Acute	WWFF, LFF, LAL	1,173
Acetochlor	34256-82-1	Fish and Aquatic	Chronic	Cold	4
Acetochlor	34256-82-1	Fish and Aquatic	Chronic	WWSF	10
Acetochlor	34256-82-1	Fish and Aquatic	Chronic	WWFF, LFF, LAL	65
Acetochlor	34256-82-1	Human Health	Human Threshold*	Public Water Supply/Cold	377
Acetochlor	34256-82-1	Human Health	Human Threshold*	Public Water Supply/WWSF	486
Acetochlor	34256-82-1	Human Health	Human Threshold*	Non-Public Water Supply/Cold	1,144
Acetochlor	34256-82-1	Human Health	Human Threshold*	Non-Public Water Supply/WWSF, WWFF, LFF	3,541
Acetochlor	34256-82-1	Human Health	Human Threshold*	Non-Public Water Supply/LAL	112,000

*Acetochlor has been classified as a class B2 carcinogen (probable human carcinogen) by the U.S. EPA. However, there is currently 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)