Minnesota’s aquatic life screening values
Their purpose and derivation.
Principal Authors
Mark Jankowski and Summer Streets

Author(s)
Steven Hennes

Contributors/acknowledgements
MPCA Steering Committee - Mark Ferrey, Paul Hoff, Elizabeth Kaufenberg, Katrina Kessler, Sharon Kroening, Shannon Lotthammer, Bruce Monson, Phil Monson, Catherine O’Dell, Angela Preimesberger, Laura Solem, and Mark Tomasek

Minnesota Department of Health
U.S. Environmental Protection Agency
Mid-Continent Ecology Division

Editing and graphic design
Scott Andre
Sherry Mottonen
Jennifer Holstad

The MPCA is reducing printing and mailing costs by using the Internet to distribute reports and information to a wider audience. Visit our website for more information.

MPCA reports are printed on 100% post-consumer recycled content paper manufactured without chlorine or chlorine derivatives.
## Contents

**Executive summary** .......................................................... 1

I. **Introduction** ................................................................. 2
   - What are aquatic life screening values? .......................... 2
   - What are contaminants of emerging concern? .................. 2
   - What is aquatic life? ...................................................... 3
   - How will aquatic life screening values be used? ............... 3
   - How will aquatic life screening values be derived? ........... 3

II. **Prioritize chemicals for ALSV derivation** ....................... 4
   - Occurrence data ......................................................... 4
   - Toxicity screening ...................................................... 4
   - Priority categories .................................................... 4

III. **Gather and evaluate data** ............................................ 6
   - Relevant toxicological effects ....................................... 6
   - Exposure duration ..................................................... 6
   - Exposure pathways .................................................... 7
   - Toxicity value selection .............................................. 7
   - Aquatic life screening value derivation worksheet .......... 8
   - Evaluate data ........................................................... 9
   - What if there are no toxicity data? ............................... 9

IV. **Derive the aquatic life screening value** ............................ 9
   - Which type of aquatic life screening value should be derived? 10
   - When should an acute aquatic life screening value be derived? 10
   - Convert toxicity values ............................................. 10
   - Data guidelines ........................................................ 11
   - Assessment factors .................................................. 12
   - Derive an ALSV\textsubscript{WATER} .................................. 13
   - Derive an ALSV\textsubscript{SEDIMENT} ......................... 13
   - Derive an ALSV\textsubscript{BIOTA} ................................. 13
   - Mixtures .................................................................... 17

V. **Application** ............................................................... 18
   - Action triggers ......................................................... 18
   - Recommendations .................................................. 18
   - Gaps and opportunities ............................................. 18

VI. **Literature cited** .......................................................... 20
Executive summary

The Minnesota Pollution Control Agency (MPCA) has been collecting occurrence data for a large number of contaminants of emerging concern (CECs) for several years. While it is apparent that many of these chemicals are detected in many of Minnesota's aquatic environments, it is difficult to describe the ecological risks associated with these contaminants because there are very few risk-based screening values that can be used to provide context to the occurrence data. For this reason, the MPCA requested and received funds to develop methods to derive risk-based screening values. This document describes the methodology developed by the MPCA to derive aquatic life screening values (ALSVs), the rationale for the methods, and the expected and appropriate uses of ALSVs.

ALSVs are risk-based chemical concentrations specific to water, sediment, or biota. If a chemical's environmental concentration is found to exceed the ALSV, there is a potential for harm to aquatic life. Follow-up action will then be recommended. This action may include additional monitoring, effects assessments, source identification, or identifying opportunities for pollution control and prevention.

CECs are a highly diverse set of chemicals that have been found in the environment, sometimes at concentrations that are significantly different than expected. ALSVs will initially be derived for CECs that have been previously monitored by the MPCA. Additional contaminants will be added to the list over time depending on legislative interest, societal concern, scientific literature, and best scientific judgment.

Chemicals on the initial list will be prioritized for ALSV derivation based on their occurrence in the aquatic environment as well as information about potential impacts to aquatic life. Depending on the nature of the chemical and its potential hazard, an ALSV may be derived for water, sediment, and/or biota.

To derive an ALSV, the lowest toxicity value (LTV) for a chemical is selected and an assessment factor (AF) is applied according to how many taxa are represented in the available toxicity data. A range of AFs are used to account for uncertainty associated with having only a small amount of toxicity data. Once the ALSV is derived, it will be used by the MPCA as a formalized, risk-based framework to prioritize the agency's monitoring and other follow-up actions.
I. Introduction

The MPCA has been collecting occurrence data for selected CECs for several years. It is apparent that many of these chemicals are present in the aquatic environment at detectable concentrations across all of Minnesota. However, it is difficult to describe the ecological risks associated with these contaminants as there are very few toxicity-based screening values, no promulgated methods to rapidly develop screening values for these types of chemicals, and little toxicity data to provide context to much of Minnesota’s CEC occurrence data.

Despite a lack of national guidance, the MPCA needs to be able to characterize the risk to aquatic life due to chemical exposure in order to make more informed decisions about its monitoring program and to determine appropriate follow-up action. As such, we have constructed a methodology for deriving ALSVs which will be used to evaluate ecological risk. Our approach is an amalgamation of numerous existing methods selected from both promulgated and un-promulgated guidance documents (Appendix D) that we tailored to address the special considerations associated with CECs in Minnesota.

What are aquatic life screening values?

ALSVs are risk-based chemical concentrations specific to water, sediment, or biota that account for a chemical’s environmental fate and toxicity. Environmental concentrations above the ALSV may indicate harm to aquatic life. Chemicals found to exceed the ALSV are prioritized for follow-up action, which may include additional monitoring for chemical occurrence or effects, source identification, or identifying opportunities for pollution reduction or prevention.

What are contaminants of emerging concern?

ALSVs will initially be derived for CECs, a loosely defined, highly diverse set of chemicals that can include pharmaceuticals and personal care products, flame retardants and many other chemicals detected at very low concentrations in the ambient environment. These chemicals may act to disrupt the endocrine or other physiological systems of organisms under chronic, low-level concentrations. Knowledge of the occurrence and possible adverse effects of exposure to many of these chemicals is rather limited.

Although a small proportion of CECs may be acutely toxic to aquatic life and released at a concentration sufficient to induce rapid harm - such as during a spill - the available toxicity data coupled with the low concentrations typically found in the environment suggest that most of these chemicals may induce sub-lethal effects to aquatic life following chronic, low-level exposure.

Furthermore, many of the identified sub-lethal effects associated with exposure to CECs are not considered “traditional” effects of concern (i.e., growth, reproduction, or survival). Therefore, quantitative ways to consider these data are not available when setting water quality standards or other regulatory benchmarks. For example, many chemicals have been shown to elicit toxic effects through their interaction with the endocrine system of biota. This phenomenon is commonly known as endocrine disruption. However, endocrine disruption is not typically considered by regulatory agencies in the evaluation of risk posed by a given chemical in the environment because it is not clear how or if the observed effects are manifested at the population scale, which is the scale of concern most often used by regulators. Adverse outcome pathways [1] are being developed to address this issue, but much scientific work remains before these methods can be used for environmental regulation and water quality standard setting. Thus, to be conservative and to reflect the potential for endocrine disruption...
and other sub-lethal effects, we developed methods to derive screening values that will enhance our understanding of the potential ecological risks of environmental contaminants based on both "traditional" and "non-traditional" effects reported in the literature.

Currently, the methods are primarily focused on organic chemicals because most new chemicals of concern are organic. Also, the risks posed by many inorganic contaminants are often dependent on a chemical’s ionic state, which usually depends on site-specific conditions such as water hardness, pH, or other biogeochemical factors, making the derivation of ALSVs for this class of contaminants much more complex. Additionally, inorganic chemicals of concern are generally already addressed through Minnesota’s water quality standards [2]. It is possible that an ALSV will be derived for an inorganic compound, if the need arises. In that case, potential guidance documents for derivation of an ALSV for an inorganic compound include those identified in Appendix D [2-5].

**What is aquatic life?**

The term 'aquatic life' includes all organisms that reside in water for all or most of their life such as fish, aquatic invertebrates, and plants. It also includes aquatic-dependent wildlife, such as amphibians, aquatic birds, and mammals that rely on aquatic systems in some way - either as a source of food or for the completion of some portion of their life cycle. This holistic definition of aquatic life provides a basis to consider the potential range of species affected by contaminants in Minnesota’s water.

**How will aquatic life screening values be used?**

The MPCA intends to use ALSVs for rapid screening purposes only. ALSVs are not regulatory standards, site-specific cleanup levels, or remediation goals. As such, the methods used to derive ALSVs differ in some respects from methods used to derive water quality standards or other risk-based water quality values. For example, we are able to derive ALSVs from very limited datasets, including modeled data, and can consider non-traditional effects such as endocrine disruption and behavioral changes. We will also consider effects of mixtures that have a common mode of action.

**How will aquatic life screening values be derived?**

The initial list of contaminants to be considered for ALSV derivation is comprised of chemicals that are currently (i.e., Minnesota fiscal year 2015) analyzed for the MPCA by the following laboratories: Axys Analytical Services, Ltd., U.S. Geological Survey, and the Minnesota Department of Health (MDH). Other contaminants will be added to the initial list over time based on legislative interest, societal concern, scientific literature, and best scientific judgment.

Chemicals on this initial list will be rapidly evaluated based on their occurrence and toxicity and given a rank of high, intermediate, or low priority for ALSV derivation. Chemicals determined to be highest priority will be the first to be fully evaluated for an ALSV, followed by chemicals deemed to be of intermediate then low priority. A standardized literature search and vetting process will be used to identify physicochemical and ecotoxicity data that will be used for ALSV derivation.

Depending on the nature of the chemical and its potential hazard, an ALSV may be set for water, sediment, or biota. Given that ALSVs are rapidly derived and intended to grossly identify chemicals of highest concern, we will make recommendations that may include additional monitoring, source identification, communication, education, outreach, and opportunities for pollution prevention and reduction. Figure 1 provides a brief overview of the ALSV process and application.
II. Prioritize chemicals for ALSV derivation

Two key factors are used to prioritize chemicals for ALSV derivation:

1. observed or expected occurrence in the environment
2. risk of adverse effects to aquatic life

The prioritization methods are generally based on methods described by the U.S. Geological Survey (USGS) [6].

Occurrence data

Existing data for the occurrence of chemicals in the environment will be used to prioritize chemicals for ALSV derivation. In general, chemicals will be placed higher on the priority list when they have been found to occur more often and at higher concentrations.

Toxicity screening

A rapid search of U.S. Environmental Protection Agency’s (EPA’s) ECOTOX database will be conducted for each chemical on the initial prioritization list. The LTV will be used, without regard for its reliability or relevance. The point is to simply get an idea of how toxic a chemical might be and place it into the appropriate priority category (PC), as described below, without yet doing a full toxicity evaluation. If no data are available for a given chemical in ECOTOX [7], then a value modeled in ECOSAR [8] can be used.

Priority categories

Each chemical is evaluated and placed in a PC, based on its occurrence, toxicity, and physicochemical properties. For cases in which several chemicals fall under the same PC, the more criteria a chemical meets, the higher priority it will receive for ALSV derivation. If needed, to further prioritize chemicals for ALSV derivation within a PC, we will develop a rapid hazard quotient (RHQ). The RHQ will be calculated by selecting the maximum detected concentration for a chemical in any media and dividing this value by
its toxicity rank (1 for high, 2 for intermediate, and 3 for low) as in Tables 1 and 2. The higher the RHQ, the higher it will be placed on the priority list.

**PC 1** - Highest priority for ALSV derivation is based on the potential for a chemical to occur in water, sediment, or biota and/or its potential to adversely affect aquatic life.

Chemicals that are included in PC 1 meet one or more of the following criteria (the more criteria a chemical meets, the higher it will be placed on the priority list within PC 1):

- large detection frequency in the environment, defined as ≥10%
- high production volume chemicals (>1 million pounds per year produced or imported to the U.S.) [9]
- indication, either observed or predicted, that a chemical is persistent (half-life >60 days in water or sediment)
- indication, either observed or predicted, that a chemical is bioaccumulative (e.g., log BAF ≥4, log K\text{OW} ≥4)
- observed or predicted toxicity that meets the high toxicity threshold shown in aquatic or dietary toxicity tables (Tables 1 or 2, respectively)

**PC 2** - Intermediate priority for ALSV derivation because there is evidence of lower likelihood of occurrence and/or lower likelihood to adversely affect aquatic life.

Chemicals that are included in PC 2 meet one or more of the following criteria (the more criteria a chemical meets, the higher it will be placed on the priority list within PC 2):

- detected in the environment, but not frequently, according to ALSV prioritization criteria (i.e., <10% detection)
- observed or predicted toxicity that meets the intermediate toxicity threshold described in aquatic or dietary toxicity tables (Tables 1 or 2, respectively)

**PC 3** - Low or not a priority for ALSV derivation because of evidence of non-occurrence and/or lack of adverse effects on aquatic life.

Chemicals that are included in PC 3 meet one or more of the following criteria:

- not detected in the environment
- no evidence of detection in peer-reviewed literature
- observed or predicted toxicity that meets the low toxicity threshold shown in aquatic or dietary toxicity tables (Tables 1 or 2, respectively)

**Table 1. Aquatic toxicity ranks for chemical concentration in water**.

<table>
<thead>
<tr>
<th>Toxicity rank(^b)</th>
<th>Acute thresholds(^c) (μg/L)</th>
<th>Chronic thresholds(^d) (μg/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>High (1)</td>
<td>&lt;100</td>
<td>&lt;10</td>
</tr>
<tr>
<td>Intermediate (2)</td>
<td>100 – 100,000</td>
<td>10-10,000</td>
</tr>
<tr>
<td>Low (3)</td>
<td>&gt;100,000</td>
<td>&gt;10,000</td>
</tr>
</tbody>
</table>

\(^a\) Ranking categories are from EPA (2001) Labeling Requirements for Pesticides and Devices [10]
\(^b\) Toxicity rank is given a numeric rank value for the purposes of estimating a rapid hazard quotient as described in document.
\(^c\) Acute thresholds are based on LC50 or EC50.
\(^d\) Chronic thresholds are based on the no-observable-effect concentration, NOEC.
Table 2. Dietary toxicity ranks for chemical concentrations in food.

<table>
<thead>
<tr>
<th>Toxicity rank&lt;sup&gt;b&lt;/sup&gt;</th>
<th>Acute thresholds&lt;sup&gt;c&lt;/sup&gt; (mg/kg)</th>
<th>Chronic thresholds&lt;sup&gt;c&lt;/sup&gt; (mg/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>High (1)</td>
<td>≤50</td>
<td>≤5</td>
</tr>
<tr>
<td>Intermediate (2)</td>
<td>51 – 4999</td>
<td>5.1 – 499.9</td>
</tr>
<tr>
<td>Low (3)</td>
<td>≥5000</td>
<td>≥500</td>
</tr>
</tbody>
</table>

<sup>a</sup> Ranking categories are from EPA (2001) Labeling Requirements for Pesticides and Devices [10]

<sup>b</sup> Toxicity rank is given a numeric rank value for the purposes of estimating a rapid hazard quotient as described in document.

<sup>c</sup> Thresholds are based on LD50 or LC50.

## III. Gather and evaluate data

### Relevant toxicological effects

In accordance with the Clean Water Act and other regulatory authorizations, many government agencies develop water quality standards based on impacts of chemicals to the growth, reproduction, or survival of exposed organisms, sometimes called “traditional” effects. The primary reason for focusing on these effects for regulatory purposes is that they can potentially be linked to population level effects, which is the level of concern for species not managed under special protections such as those listed in the Migratory Bird Treaty Act or the Endangered Species Act. ALSV derivation procedures will therefore consider these effects.

However, “non-traditional” effects of concern will also be considered for ALSV derivation because of the unique way in which many of these chemicals impact organisms. Sub-lethal effects that will be considered may include significant changes in gene expression, behavioral changes, or increased susceptibility to infectious disease. Also, because ALSVs will be based on effects that are detectable in individual organisms rather than on populations of organisms, our approach will provide early indications of potential threats to populations.

### Exposure duration

Many chemicals for which ALSVs will be derived may exert biological effects upon low-level chronic exposure rather than high-level, short-term exposures [11]. Thus, chronic data are preferred over acute data for the derivation of a chronic ALSV. However, CECs, like any other chemical, may occur in the ambient environment at concentrations that present an acute risk to organisms, spurring the need to derive an acute ALSV. In this case, acute data will be required.

Careful classification of studies as acute or chronic in duration is important. We consider an exposure to be chronic if it encompassed ≥10% of the exposed species typical life span [12]. Also, an organism’s life stage can greatly affect its sensitivity to chemical exposure. Therefore, data that result from exposures for the full life cycle (FLC) of an organism are preferred. In addition, data collected from exposures during the organism’s most sensitive life stage (if known) can be considered chronic studies. Any study that was not conducted for ≥10% of a species’ typical life-span, was not conducted during the organism’s most sensitive life stage, or was not a FLC test, is considered to be of acute duration.
Exposure pathways

We prefer toxicity data from studies conducted under environmentally-relevant (realistic) exposure scenarios. Environmental relevance is based, in part, on the physicochemical properties of a particular chemical. However, data from all media and exposure pathways will be considered for ALSV derivation because these data can provide toxicity information that may otherwise be unavailable. Although organisms vary in their sensitivity to chemicals, toxicity data can often be applied across taxa to, at a minimum, inform on modes of action and target organs.

Toxicity value selection

Toxicity values are the statistical summaries of experimental results. Note that EPA ECOTOX database uses the term endpoint where we use the term toxicity value. The reason we have chosen to use the term toxicity value is to reduce confusion, as endpoint can also be used when referring to an effect.

Common acute toxicity values

- LC50 or EC50
- IC50 for immobility (invertebrates)

Where:
L/E/IC50 = lethal/effective/immobilizing concentration impacting 50% of the exposed individuals

Common chronic toxicity values

- ECx
- LOEC
- NOEC
- MATC

Where:
ECx = Effective concentration impacting x % of the individuals tested
NOEC = No observed effect concentration
LOEC = Lowest observed effect concentration
MATC = Maximum acceptable toxicant concentration (geometric mean of NOEC and LOEC values)

Traditional effects

Toxicity values calculated from studies reporting effects to growth, reproduction, and survival will be converted to NOEC, as described in Section IV.

Non-traditional effects

At this time, the available technical information is not adequate to enable the systematic conversion of toxicity values for non-traditional effects to NOECs, as will be done for traditional effects using the Dutch methods shown in Section IV. Therefore, we will use the following logic, guided by the "Minnesota Department of Health Simplification of Exhibit A.3, Compendium of Critical Effects Table" (Appendix C) for toxicity value conversion for non-traditional effects:

1. If the literature reports on a direct link between a non-traditional effect and a traditional effect, we will convert all toxicity values to NOECs as in Section IV.
2. If the literature does not report a direct link as above, but
   a. the observed non-traditional effect has a severity score ≥4 (i.e., only irreversible effects; scale is 1-9, with 1 being no effect and 9 being death), toxicity values will be converted to a NOEC as in Section IV; or,
   b. the observed non-traditional effect has a severity score <4 (i.e., only reversible effects), toxicity values will not be converted and will not be used directly in ALSV derivation.

In a case in which toxicity data are identified that fall under 2b above, the toxicity value will not be used to derive the ALSV, but an additional AF of 5 will be assigned in order to reflect the potential for effects not directly considered in ALSV derivation.

Aquatic life screening value derivation worksheet

A worksheet will be used to house all relevant information used in deriving individual ALSVs. The worksheet describes a contaminant’s physicochemical properties, the ecotoxicity data gathered in the initial search, the data that were used to derive the final ALSV, and notes to provide important supporting information. The worksheet can be found in Appendix A.

Physicochemical properties

For each chemical, physical and chemical property information will be gathered and inserted into the ALSV derivation worksheet. These data will be used specifically to guide ALSV development as described in the derivation methods. Estimations Program Interface Suite (EPI Suite, EPA), will be used to collect all necessary physicochemical properties.

Toxicity data sources

There are several sources that may provide data useful to ALSV derivation. See Table 3 for the data sources to search. Those sources given a priority ranking of 1 must always be searched. Sources marked with a 2 can be accessed in cases where societal interest in understanding the potential hazard associated with a chemical is high, but no data can be located using higher ranking sources, and modeled toxicity data are deemed inadequate.
Table 3. Initial sources of ecotoxicity data for ALSV derivation.

<table>
<thead>
<tr>
<th>Search ranking</th>
<th>Source</th>
<th>Details/notes</th>
<th>Currency</th>
<th>Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ECOTOX</td>
<td>EPA database containing coded aquatic and terrestrial toxicity data</td>
<td>Up to one year lag time from publication to entry</td>
<td><a href="http://cfpub.epa.gov/ecotox/">http://cfpub.epa.gov/ecotox/</a></td>
</tr>
<tr>
<td>1</td>
<td>ECHA</td>
<td>EU chemical registration data</td>
<td>Varies by chemical</td>
<td><a href="http://echa.europa.eu/information-on-chemicals;jsessionid=1240D5DFC763E407051FE017AFDA3B07.live1">http://echa.europa.eu/information-on-chemicals;jsessionid=1240D5DFC763E407051FE017AFDA3B07.live1</a></td>
</tr>
<tr>
<td>1</td>
<td>TOXLINE</td>
<td>NIH Library of Medicine</td>
<td>Up to one week lag time from publication to entry</td>
<td><a href="http://toxnet.nlm.nih.gov/newtoxnet/toxline.htm">http://toxnet.nlm.nih.gov/newtoxnet/toxline.htm</a></td>
</tr>
<tr>
<td>1</td>
<td>Scholar</td>
<td>Google database</td>
<td>Minimal delay</td>
<td><a href="http://scholar.google.com">http://scholar.google.com</a></td>
</tr>
<tr>
<td>2</td>
<td>Manufacturer provided data</td>
<td>EPA Office of Pesticide Programs. May be proprietary, require Freedom of Information Act request and thus not be feasible</td>
<td>Varies by chemical</td>
<td><a href="http://www.ipmcenters.org/ecotox/">www.ipmcenters.org/ecotox/</a></td>
</tr>
<tr>
<td>2</td>
<td>Other jurisdictions</td>
<td>The evaluator may contact other states or countries for data, as warranted</td>
<td>Varies by chemical</td>
<td>Case-by-case basis</td>
</tr>
</tbody>
</table>

*Other, as-yet undetermined reputable data sources may be accessed if it is discovered that these listed sources are not sufficiently comprehensive.

Evaluate data

After all relevant studies are obtained and iteratively evaluated (Appendix B), the ALSV derivation worksheet will be populated (Appendix A). Studies must be evaluated for reliability first [13] using ToxRTool [14] (Appendix B) and if reliable, relevance will be assessed [13]. Only reliable and relevant studies will be used for ALSV derivation. Studies performed according to good laboratory practices [15-17] can be accepted without further evaluation. The study with the LTV that is found to be both relevant and reliable will be used to derive the final ALSV. Note that if all data guidelines are satisfied, adoption of a water quality standard may be warranted.

What if there are no toxicity data?

The Ecological Structure Activity Relationship (ECOSAR, EPA) Class Program and EPI Suite will be used to generate modeled data if an ALSV must be developed but no measured toxicity data are available.

IV. Derive the aquatic life screening value

After all relevant toxicity data have been collected and evaluated an ALSV will be derived according to the following steps:

1. determine relevant media for ALSV derivation
2. determine if an acute ALSV should be derived (for water and sediment only)
3. convert all relevant and reliable toxicity values to a NOEC
4. select the LTV
5. apply an appropriate AF according to the number of data guidelines that are met

**Which type of aquatic life screening value should be derived?**

The most relevant media for which an ALSV will be derived depends on the nature of the chemical. Sometimes, a chemical will not be detectable in water due to its low water solubility, but it will be present in sediment or biota at detectable concentrations of potential concern. Therefore, derivation triggers will be used to determine the media for which an ALSV will be derived (Fig. 2).

![Figure 2. Overview of decision process for derivation of ALSVs by media. Derivation triggers based on a contaminant’s physicochemical properties will be used to determine the relevant environmental compartments for ALSV derivation.](image)

**When should an acute aquatic life screening value be derived?**

An acute ALSV (water or sediment only) may be developed for some chemicals. As concentrations of a chemical in biota reflect a time- and space-integrated exposure, an acute ALSV<sub>BIOTA</sub> is not appropriate. Chemicals with an EC50 or LC50 <0.1 mg/L, and/or chemicals that may be released via high concentration pulses are subject to the derivation of an acute ALSV in addition to a chronic ALSV. Although some chemicals will not generally be released in large pulses most of the year, some releases may be seasonal or otherwise predictable, in which case an acute ALSV may be advised, especially if acute toxicity exceeds 0.1 mg/L.

**Convert toxicity values (water and sediment)**

Toxicity values based on traditional and non-traditional effects from some studies may have to be recalculated or converted in order to be comparable to toxicity values from other studies (i.e., reflect similar levels of toxicity). Conversions given on the following page are relevant to water and sediment data only, as dietary data (biota) are generally reported using the same toxicity values. See the ALSV<sub>BIOTA</sub> section for more information. Our selected conversion procedures are based on an approach used in the Netherlands [18], as regulators in that country have developed the most rigorous, data-based approach that could be found.
In order of preference, we will:

- Calculate a given toxicity value such as an ECx from full datasets if provided in a report (for all effect types).
- Convert to NOEC when full datasets are not available.

**NOEC conversion procedures [18]:**

- Highest tested concentration with effects not statistically different from controls is the NOEC.
- Highest concentration showing 10% effect or less is considered the NOEC if statistical evaluation is not possible.
- Reported LOECs are converted to NOEC as follows (can be adjusted if justified by data):
  - NOEC = LOEC/2 for cases where 10% effect < LOEC < 20% effect
  - NOEC = EC10 for cases where: LOEC ≥ 20% effect and dose-response relationship is available
  - NOEC = LOEC/3 for cases where: 20% < LOEC < 50% effect
  - NOEC = LOEC/10 for cases where: 50% ≤ LOEC ≤ 80% effect
  - NOEC is not estimated when percent effect is unknown for a LOEC
  - NOEC = EC10
- NOEC is the lowest value in a range of MATC values.
- NOEC = MATC/2 when MATC expressed as a single value.

To derive an ALSV\textsubscript{WATER} or ALSV\textsubscript{SEDIMENT}, the LTV for a chemical after being converted to a NOEC, is selected and an AF is applied according to completeness of the available toxicity data.

**Data guidelines**

Data guidelines (DGs) are similar to minimum data requirements (MDRs) used in water quality standard guidance in that they provide guidance in the collection of taxonomically representative toxicity data. DGs differ in that they are more flexible than MDRs and are primarily used to gauge the breadth of available data and to select the appropriate AFs from Tables 4 or 5. DGs are based on EPA [5] and European Union (EU) [4] guidance documents while recognizing the need to be more flexible than requirements described in these two documents.

It is recognized that receptors of potential concern [11] in Minnesota will vary depending on a chemical’s release pattern, environmental fate, and mode of action. Thus, in addition to data from aquatic species exposures, data relevant to aquatic-dependent terrestrial species, such as fish- or invertebrate-eating birds, are often useful and will therefore be used for ALSV derivation. Professional judgment will be used when deciding how data from a terrestrial species will be used to establish an ALSV. For example, dietary exposures in one vertebrate (e.g., mice) can provide information for the toxicity of a compound in another vertebrate (e.g., fish) if the compound primarily impacts biota through dietary rather than aqueous exposures. Lastly, data from studies including species that are not native to Minnesota or North America will be used to fulfill a DG.
Recommended data guidelines

- fish (cold or warm water)
- second organism in a family in the phylum Chordata (for example, fish, amphibian, mammal, bird)
- benthic crustacean
- planktonic crustacean
- insect
- aquatic family in a phylum other than Arthropoda or Chordata (for example, rotifer, mollusc, annelid)
- aquatic plant (e.g., algae, duck weed, macrophyte)
- Open and not already represented above. Selection should be based on a chemical’s fate and mode of action, if known (e.g., plant if an herbicide or insect if an insecticide). Terrestrial or aquatic species may be used.

Assessment factors

Depending on how many data guidelines are fulfilled and the relevant exposure duration (acute and/or chronic), an AF will be selected from Tables 4 and 5, and applied to the LTV. For example, if the chemical being evaluated is not acutely toxic and two chronic NOEC values are found in the literature for the same DG, the ALSV would be calculated by dividing the LTV from those two studies by 50, as indicated in Table 6. We developed the AFs listed below based on an integration of EU [4] and EPA Great Lakes Initiative [19] approaches. The EU has established an AF of 1000 when three DGs for acute data are fulfilled while the EPA approach provides guidance for situations in which data are only available for one or two DGs. The numerical ratio from one AF to the next is guided by ratios established by the EPA.

Table 4. Assessment factors for calculation of an acute ALSV_{WATER} or acute ALSV_{SEDIMENT} [4, 19].

<table>
<thead>
<tr>
<th>Available data</th>
<th>Assessment factors</th>
</tr>
</thead>
<tbody>
<tr>
<td># of DGs fulfilled</td>
<td>1</td>
</tr>
<tr>
<td>Assessment factor</td>
<td>300</td>
</tr>
</tbody>
</table>

Table 5. Assessment factors for calculation of a chronic ALSV_{WATER} or chronic ALSV_{SEDIMENT} [4, 19].

<table>
<thead>
<tr>
<th>Available data</th>
<th>Assessment factors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Only acute data</td>
<td># of DGs fulfilled</td>
</tr>
<tr>
<td>Assessment factor</td>
<td>3000</td>
</tr>
<tr>
<td>One DG chronic NOEC</td>
<td>100</td>
</tr>
<tr>
<td>Two DGs chronic NOEC</td>
<td>50</td>
</tr>
<tr>
<td>≥ Three DGs, chronic NOEC</td>
<td>10</td>
</tr>
<tr>
<td>Field data or model ecosystems</td>
<td>Reviewed on a case by case basis</td>
</tr>
</tbody>
</table>
Derive an ALSV\textsubscript{WATER}

An ALSV\textsubscript{WATER} will be derived when toxicity to an organism is likely to occur through direct exposure to a chemical in the water column. Any of the following derivation triggers would indicate likely presence of a chemical in the water column. Derivation triggers were based on EU guidance [4].

- $\log_{10}$ octanol-water partition coefficient ($K_{OW}$) < 4
- $\log_{10}$ organic carbon-water partition coefficient ($K_{OC}$) < 4

An ALSV\textsubscript{WATER} can be derived according to the following equation:

\textbf{Equation 1.}

$$\text{ALSV}_{\text{WATER}} = \frac{LTV}{AF}$$

Where:

$LTV$ is the lowest toxicity value selected according to the hierarchy described previously; $AF$ is the assessment factor selected based on the number of data guidelines that were met (Tables 4 and 5).

Derive an ALSV\textsubscript{SEDIMENT}

Sediment can act as both a sink and a source for contaminants. Benthic invertebrates and fish that feed on particulates can be adversely affected by contaminants in sediment. Evidence in the literature of high toxicity to aquatic- or sediment-dwelling organisms or evidence of accumulation in sediment from monitoring data would also trigger derivation of an ALSV\textsubscript{SEDIMENT}. In general, any of the following derivation triggers would be considered adequate evidence of potential to accumulate in sediments. Derivation triggers were selected from the EU [4].

- $\log_{10} K_{OW} \geq 3$
- $\log_{10} K_{OC} \geq 3$

Sediment toxicity data are often very limited. If reliable toxicity data are available, then Equation 1 is used to calculate an ALSV\textsubscript{SEDIMENT}; however, if no reliable sediment toxicity data are available, an equilibrium partitioning approach can be used to derive an ALSV\textsubscript{SEDIMENT} [4]. An ALSV\textsubscript{WATER} must be calculated first in order to calculate an ALSV\textsubscript{SEDIMENT}.

\textbf{Equation 2.}

$$\text{ALSV}_{\text{SEDIMENT}} = (\text{ALSV}_{\text{WATER}} \times K_{OC}) \times 0.01$$

Where:

- $\text{ALSV}_{\text{SEDIMENT}}$ is the dry weight sediment concentration (μg/kg);
- $\text{ALSV}_{\text{WATER}}$ is the water screening value calculated above (μg/L);
- $K_{OC}$ is the log organic carbon-water partition coefficient (L/kg\textsubscript{OC});
- 0.01 is the factor to normalize the concentration per unit mass of organic carbon to the default value of 1% organic carbon (0.01 kg\textsubscript{OC}/kg)

Derive an ALSV\textsubscript{BIOTA}

The ALSV\textsubscript{BIOTA} is a concentration of a chemical in the aquatic food chain that can be used to estimate the risk to upper trophic level organisms from secondary poisoning due to food-chain transfer of bioaccumulative chemicals. Dietary data are often available only for terrestrial species such as birds and mammals but not fish. However, by incorporating AFs, the ALSV derivation process assumes that all
aquatic and terrestrial vertebrate consumers are considered when an ALSV\textsubscript{BIOTA} is calculated from feeding studies in vertebrate taxa. If available, data from fish or other aquatic organism feeding studies will be considered on a case-by-case basis.

An ALSV\textsubscript{BIOTA} will be derived when a chemical has low water solubility and is known or predicted to bioaccumulate in the food chain. In addition, evidence of bioaccumulation from monitoring data or evidence of high chronic dietary toxicity (Table 2) would also trigger derivation of an ALSV\textsubscript{BIOTA}. If available information suggests that aqueous toxicity to a chemical is high, a water column value will be derived in addition to a biota value.

In general, any of the following derivation triggers would be considered adequate evidence of bioaccumulation potential. Derivation triggers are based on guidance from the EU [4] and EPA [20].

- log bioaccumulation factor (BAF) \( \geq 4 \)
- biomagnification factor (BMF) >1
- bioconcentration factor (BCF) \( \geq 100 \)
- log \( K_{OW} \) \( \geq 4 \)

The process for deriving an ALSV\textsubscript{BIOTA} is different and more complex than the process for deriving an ALSV\textsubscript{WATER} or ALSV\textsubscript{SEDIMENT}. The general steps for deriving and ALSV\textsubscript{BIOTA} are as follows:

1. Convert the lowest no observable adverse effect level (NOAEL) to a NOEC\textsubscript{ORAL} (Equation 3).
2. Select the appropriate TOX\textsubscript{ORAL} and the associated AF\textsubscript{ORAL} from Table 7.
3. Calculate ALSV\textsubscript{BIOTA} as in equation 4.

The following list includes organisms for which data are required to derive an ALSV\textsubscript{BIOTA}. If not available, an AF is applied as in Table 7:

- birds (class aves)
- mammals (class mammalia)
- vertebrate class not yet represented (e.g., class amphibia or reptilia)

Dietary exposures are often quantified as the mass of the chemical normalized to the mass of the organism per day (e.g., mg\textbullet \( k_{gbw} \textbullet d^{-1} \)). A common resulting summary statistic is the NOAEL, but we will consider other toxicity values that are similarly conservative. A NOAEL may be used to estimate toxicity values (e.g., NOEC) reflecting chemical concentrations in dietary items (mg/k\textsubscript{FOOD}) or water (µg/L). We will use the conservative assumption that 100% of the chemical is bioavailable through dietary exposures.

A NOAEL can be converted to an exposure concentration (NOEC\textsubscript{H\textsubscript{\textsc{IV}}, ORAL} expressed in mg/k\textsubscript{FOOD}) using the following equation:

**Equation 3.**

\[ \text{NOEC}_{HIV, \text{ORAL}} = \text{NOAEL}_{i, \text{ORAL}} \times \text{CONV}_i \]

Where:
- \( i \) is the class of vertebrate (bird, mammal, or third vertebrate) for which a NOEC\textsubscript{ORAL} is being estimated;
- NOAEL\textsubscript{i, ORAL} is the dietary toxicity value (in mg\textbullet \( k_{gbw} \textbullet \textbullet d^{-1} \)) for vertebrate \( i \);
- CONV\textsubscript{i} is a conversion factor with units of \( g_{gbw} \textbullet g_{food}^{-1} \textbullet d^{-1} \).

Table 6 displays conversion factors for mammals, birds, amphibians, and reptiles [4, 21]. NOECs derived from NOAELs using this approach are assumed to be equivalent to directly measured NOECs.
Table 6. Factors for converting NOAELs (dose) into NOECs (concentration) from toxicity studies performed on birds, mammals, amphibians and reptiles.

<table>
<thead>
<tr>
<th>Species</th>
<th>Age/study</th>
<th>Conversion factor (body weight/daily food intake)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rat (Rattus norvegicus)</td>
<td>&gt;6 weeks</td>
<td>20&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Rat</td>
<td>&lt;6 weeks</td>
<td>10&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Rat</td>
<td>28 and 90 days</td>
<td>10&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Rat</td>
<td>Two generation study first mating&lt;sup&gt;a&lt;/sup&gt;</td>
<td>12.5&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Rat</td>
<td>Two generation study overall</td>
<td>8.3&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Mouse (Mus musculus)</td>
<td>28 and 90 days</td>
<td>8.3&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Vole (Microtus spp)</td>
<td>-</td>
<td>8.3&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Rabbit (Oryctolagus cuniculus)</td>
<td>-</td>
<td>33.3&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Dog (Canis domesticus)</td>
<td>Adult/all</td>
<td>40&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Monkey (Macaca spp)</td>
<td>-</td>
<td>20&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Chicken (Gallus domesticus)</td>
<td>-</td>
<td>8&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>Bufflehead (Bucephala albeola)</td>
<td>-</td>
<td>2.4&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Common goldeneye (Bucephala clangula)</td>
<td>-</td>
<td>3.2&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Mallard (Anas platyrhynchos)</td>
<td>-</td>
<td>4.3&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Long-tailed duck (Clangula hyemalis)</td>
<td>-</td>
<td>3.2&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Wood duck (Aix sponsa)</td>
<td>-</td>
<td>2.9&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>American wigeon (Anas americana)</td>
<td>-</td>
<td>3.1&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Lesser scaup (Aythya affinis)</td>
<td>-</td>
<td>3.1&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Common merganser (Mergus merganser)</td>
<td>-</td>
<td>3.7&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Red-breasted merganser (Mergus serrator)</td>
<td>-</td>
<td>4.8&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Bald eagle (Haliaeetus leucocephalus)</td>
<td>-</td>
<td>9.1&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Osprey (Pandion haliaetus)</td>
<td>-</td>
<td>5.0&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Belted kingfisher (Megaceryle alcyon)</td>
<td>-</td>
<td>2.0&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Common loon (Gavia immer)</td>
<td>-</td>
<td>5.6&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Common tern (Sterna hirundo)</td>
<td>-</td>
<td>1.6&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Herring gull (Larus argentatus)</td>
<td>-</td>
<td>3.4&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Ring-billed gull (Larus delawarensis)</td>
<td>-</td>
<td>5.9&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Great blue heron (Ardea herodias)</td>
<td>-</td>
<td>4.5&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>American mink (Neovison vison)</td>
<td>-</td>
<td>4.2&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>River otter (Lontra canadensis)</td>
<td>-</td>
<td>10.0&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>Snapping turtle (Chelydra serpentina)</td>
<td>-</td>
<td>76.9&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>American bullfrog (Rana catesbeiana)</td>
<td>-</td>
<td>62.5&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
</tbody>
</table>


<sup>b</sup> From the Protocol for derivation of Canadian tissue residue guidelines for protection of wildlife that consume aquatic biota [21]
The ALSV\textsubscript{BIOTA} is the threshold concentration of a chemical in the food of a consumer. To derive an ALSV\textsubscript{BIOTA}, an appropriate AF (Table 7) must be applied to the calculated NOEC\textsubscript{ORAL}. The LTV will be used to calculate the ALSV\textsubscript{BIOTA}. Data from chronic exposures are preferred for ALSV\textsubscript{BIOTA} derivation. Studies are considered to be of chronic duration if they occurred for the full life cycle of the organism, covered ≥10% of the organism’s life span, or occurred during the most sensitive life stage of the organism (if known).

**Equation 4.**

\[
\text{ALSV}\textsubscript{BIOTA} = \frac{\text{TOX}_{\text{ORAL}}}{\text{AF}_{\text{ORAL}}}
\]

Where:

TOX\textsubscript{ORAL} is the NOEC\textsubscript{ORAL} for a bird or mammal (or other species if advised and available).

**Table 7. Assessment factors for the calculation of the ALSV\textsubscript{BIOTA}\textsuperscript{a} [4, 19].**

<table>
<thead>
<tr>
<th>Available data</th>
<th>Assessment factors</th>
</tr>
</thead>
<tbody>
<tr>
<td>Only acute data</td>
<td># of DGs fulfilled</td>
</tr>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>Assessment factor</td>
</tr>
<tr>
<td></td>
<td>3000</td>
</tr>
<tr>
<td></td>
<td>1500</td>
</tr>
<tr>
<td></td>
<td>1000</td>
</tr>
<tr>
<td>One DG, chronic NOEC\textsubscript{ORAL}</td>
<td>100</td>
</tr>
<tr>
<td>Two DGs, chronic NOEC\textsubscript{ORAL}</td>
<td>50</td>
</tr>
<tr>
<td>≥ Three DGs, chronic NOEC\textsubscript{ORAL}</td>
<td>10</td>
</tr>
</tbody>
</table>

\textsuperscript{a} AFs are based on the same considerations and references [4, 19] as presented for in Tables 4 and 5 above for water and sediment while incorporating fewer three rather than eight DGs.

It may be warranted to convert the ALSV\textsubscript{BIOTA} (mg/kg) to an ALSV\textsubscript{WATER} (µg/L). This step is necessary when direct toxicity through water exposure is likely but there are no toxicity studies using the water exposure pathway.

The following equations can be used to convert the ALSV\textsubscript{BIOTA} to an ALSV\textsubscript{WATER}:

**Equation 5.**

\[
\text{ALSV}\textsubscript{WATER} = \frac{\text{ALSV}\textsubscript{BIOTA}}{\text{BAF}}
\]

If a measured field BAF is not available then:

**Equation 6.**

\[
\text{BAF} = \text{BCF} \ast \text{BMF}
\]

If a measured field BMF is not available, then a BMF value modeled in EPI Suite can be used.
**Mixtures**

Chemicals that occur in mixtures can be assessed as recommended by many guidance documents including the EU WFD 27 [4] and the University of California Methodology [22].

Two circumstances may trigger a mixture assessment using the toxic unit (TU) or toxic equivalent (TEQ) approaches outlined below, provided an ALSV can be derived for each individual chemical:

1. when chemicals with a common mode of action are released together or monitoring data indicate that they regularly occur together
2. when an environmental degradate or metabolite is formed and for which a toxicity value is available

**Equation 7.**

\[ TU_i = \frac{C_i}{ALSV_i} \]

**Equation 8.**

\[ TU_{MIXTURE} = \sum TU_i \]

Where:
- TU is the toxic unit;
- \( C_i \) is the concentration of chemical \( i \) in the relevant medium.
- ALSV\(_i\) is the ALSV for chemical \( i \) in the relevant medium

If \( TU_{MIXTURE} > 1 \), further mixture assessment is indicated.

Provided sufficient information exists, the TEQ concentration approach may be used to modify the above TU calculation. This applies to groups of chemicals that act through the same mode of action.

**Equation 9.**

\[ TEF_i = \frac{ALSV_i}{ALSV_{LOWEST}} \]

**Equation 10.**

\[ TEQ_{MIXTURE} = \sum (TEF_i * C_i) \]

Where:
- TEF\(_i\) is the toxic equivalency factor for chemical \( i \);
- ALSV\(_i\) is the ALSV for chemical \( i \);
- ALSV\(_{LOWEST}\) is the ALSV for the chemical in the group with the lowest ALSV;
- TEQ\(_{MIXTURE}\) is the toxic equivalent concentration for the mixture.

If the \( TEQ_{MIXTURE} > 1 \), further mixture assessment is indicated.
V. Application

Aquatic life screening values are intended for use primarily by the MPCA. Using the ALSVs to give context to our CEC monitoring data will inform our decision making and help us prioritize contaminants that require follow-up action.

Action triggers

A simple risk quotient approach will be used to determine if concentrations of a chemical detected in the environment pose a potential risk to aquatic life:

Equation 11.

\[ \text{ATQ} = \frac{C_m}{\text{ALSV}_j} \]

Where:
- ATQ is the action trigger quotient. If the ATQ >1, appropriate follow-up action will be recommended;
- \( j \) is the environmental compartment of interest;
- \( C_m \) is the geometric mean concentration of a chemical measured in compartment \( j \);
- \( \text{ALSV}_j \) is the aquatic life screening value for compartment \( j \).

If the ATQ is >1, we conservatively assume that harm to aquatic life is possible.

Recommendations

ALSVs will be used as a formalized, risk-based framework to prioritize the agency’s CEC efforts. When the exceedance of an ALSV triggers follow-up action, recommendations will be developed to further MPCA’s understanding of how the chemical may impact aquatic life. Recommended activities may include specific monitoring, source identification, identifying opportunities for pollution prevention and reduction, identifying opportunities to partner with Universities and researchers to gain a better understanding of toxic effects induced by chemicals of concern, and communication efforts including education and outreach activities with internal and external partners and other stakeholders.

ALSVs will also be used to refine and prioritize all future CEC monitoring within the MPCA with a focus on understanding the potential for risk to aquatic life. This approach will help allocate limited funds toward gaining a better understanding of the most problematic chemicals. The guidance documents that we have referenced specifically recommend a process for the validation of environmental quality guidelines like ALSVs. Validation activities such as more focused monitoring in the most relevant environmental media, effects assessments, or toxicity tests may therefore be included in recommendations for a given chemical.

Gaps and opportunities

We recognize that these methods are somewhat limited in scope and should be updated as new scientific information and methods become available. In particular, the negative impacts to protected species (i.e., special status species) and selection of biota for chemical monitoring are issues that may warrant further examination as new resources and information become available.

Depending on the nature and occurrence of a chemical, special status species may be of particular concern due to adverse impacts related to chemical exposure. Protection of special status species is mandated by laws such as the Minnesota Endangered Species Statute, Federal Endangered Species Act,
or Migratory Bird Treaty Act. These laws mandate protection of listed species at the level of the individual organism. The data used to derive ALSVs will likely include effects detected at the level of the organism or lower, suggesting a satisfactory assessment of risk to organisms and thus populations. However, it may be found that a special status species is more sensitive to a chemical than the species upon which an ALSV is based. In such a case, a more species-specific assessment would be recommended.

At this time, the MPCA uses fish for most of its biota monitoring. However, fish may not always be the most appropriate biota for chemical monitoring. For example, wetlands do not contain fish, so invertebrate or plant samples would be more suited to detecting the presence of bioaccumulative chemicals that may impact higher trophic level species such as birds and mammals that are dependent on wetland ecosystems. Or, it may be more appropriate to measure bioaccumulative chemicals that are of particular concern to predatory birds directly, via serum or eggs. For pharmaceuticals in particular, the blood plasma concentration of the active pharmaceutical ingredient may best reflect biological risk, based on what is known about therapeutic doses in humans. Careful consideration should be given to selecting the most appropriate species and tissue to use in chemical monitoring.
VI. Literature cited


This page left blank intentionally.
Appendix A: Aquatic life screening value derivation worksheet
Aquatic life screening value derivation worksheet

**Chemical information**

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>IUPAC name</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CAS number</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SMILES</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Chemical formula</td>
<td></td>
<td></td>
</tr>
<tr>
<td>High production volume chemical? (yes or no)</td>
<td></td>
<td><a href="http://www.epa.gov/hpv/hpvis/index.html">http://www.epa.gov/hpv/hpvis/index.html</a></td>
</tr>
<tr>
<td>Molecular weight (g/mol)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Melting point (°C)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Boiling point (°C)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Density (g/mL)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Vapor pressure (Pa)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Henry's Law Constant (Pa*m³/mol)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water solubility (mg/L)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>pKa</td>
<td></td>
<td></td>
</tr>
<tr>
<td>log K_{OW} (octanol/water partition coefficient)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>log K_{OC} (organic carbon/water partition coefficient)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>log K_{P} (sediment/water partition coefficient)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>log K_{SP} (suspended particulate/water partition coefficient)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Released as a part of a mixture?</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Known formation of toxic degradates or metabolites?</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mode of action (if known)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Data table – water

<table>
<thead>
<tr>
<th>Genus species</th>
<th>Data guideline category</th>
<th>Acute or chronic?</th>
<th>Toxicity value type &amp; concentration (μg/L)</th>
<th>Toxicity value conversion?</th>
<th>Notes</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Data table – sediment

<table>
<thead>
<tr>
<th>Genus species</th>
<th>Data guideline category</th>
<th>Acute or chronic?</th>
<th>Toxicity value type &amp; concentration (μg/L)</th>
<th>Toxicity value conversion?</th>
<th>Notes</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Data table – biota

<table>
<thead>
<tr>
<th>Genus species</th>
<th>Data guideline category</th>
<th>Acute or chronic?</th>
<th>Toxicity value type &amp; concentration (μg/L)</th>
<th>Toxicity value conversion?</th>
<th>Notes</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Final aquatic life screening value derivation

<table>
<thead>
<tr>
<th>Toxicity value</th>
<th>AF</th>
<th>Final ALSV (units)</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATQ</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix B: Literature evaluation
How to evaluate toxicity studies

Reliability

Evaluation of the reliability of toxicity studies for use in the derivation of ALSVs is an iterative process. Using the ToxRTool worksheet included in this appendix, each study identified in the data gathering phase is evaluated for its reliability and then assigned to a reliability category (Table 1C) as follows:

1. Search EPA’s ECOTOX database to rapidly identify available toxicity data for the chemical.
2. Evaluate one study at a time for each data guideline (DG), starting with the study with the LTV and assign a reliability category (1-4).
3. If the study is deemed unreliable (category 3 and 4), evaluate the study with the next LTV for the same DG. It is possible that DGs will be lost during this process.
4. Repeat Step 3 above until one qualified study is found per DG or no more studies are available.
5. Select relevant LTV as described below.

Relevance

Relevance is evaluated against the following four conditions:

1. Is the testing strategy (e.g. organism, exposure, or scenario) aligned with the occurrence and the persistence of the test substance in the environment?
2. Is it possible to derive useful information from data obtained from experiments with non-standard organisms?
3. Are physicochemical properties of the test substance sufficiently considered in light of the selected test design?
4. Have all pertinent factors been considered, based on the evaluator’s professional judgment?

An ALSV can be derived once a reliable and relevant study has been identified. A fully vetted study with the LTV will be used as the basis for ALSV derivation.

Table 1B. The data evaluation process is performed according to Klimisch et al. [13] and leads to the assignment of all studies to one of the four Reliability Categories. ToxRTool [14] was built to facilitate this evaluation.

<table>
<thead>
<tr>
<th>Reliability category</th>
<th>Interpretation</th>
<th>Description</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Reliable without restriction</td>
<td>Studies conducted according to or in accordance with accepted testing guidelines</td>
<td>Use data with high confidence</td>
</tr>
<tr>
<td>2</td>
<td>Reliable with restrictions</td>
<td>Not conducted according to testing guidelines but are well documented and scientifically acceptable</td>
<td>Narrower scope for use then Cat 1. Use data if suited for intended purpose</td>
</tr>
<tr>
<td>3</td>
<td>Not reliable</td>
<td>Studies designed and conducted in a way that makes their conclusions invalid or contain insufficient documentation to assess validity</td>
<td>Do not use</td>
</tr>
<tr>
<td>4</td>
<td>Not assignable</td>
<td>Insufficient details such that the study can’t be rated</td>
<td>Do not use</td>
</tr>
</tbody>
</table>
Appendix C: Severity scores for sub-lethal non-traditional effects
<table>
<thead>
<tr>
<th>Severity score</th>
<th>Score definition</th>
<th>Compendium of critical effects</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>No adverse effect</td>
<td>No observed effect(s) or adverse effect(s) related to treatment. Absence of biologically significant adverse effect(s) or gross light microscopic histopathological change(s).</td>
</tr>
<tr>
<td>2</td>
<td>Cosmetic effect (Interpretation: Consider those effects that alter the appearance of the body without affecting structure or functions)</td>
<td>Dental fluorosis; abnormal appearance; facial flushing; dermal sensitization; changes in skin (argyria, pigmentation, hyperpigmentation, keratosis); and alopecia (hair loss)</td>
</tr>
</tbody>
</table>
| 3              | Reversible effects; differences in organ weights or size, body weights or changes in biochemical parameters with minimal clinical significance. (Interpretation: Transient, adaptive effects) | * Changes in body weight and or body-weight gain; changes in absolute or relative organ weights; decreased growth.  
* Gastrointestinal disturbances (e.g., diarrhea, nausea, vomiting)  
* Irritation/irritability  
* Biochemical changes (e.g., alterations in clinical chemistry; changes in glucose, triglyceride or enzyme levels)  
* Hematological effects (e.g., abnormal pigments in blood, changes in blood cell counts/volumes, meth- or carboxyhemoglobin, hemosiderosis, iron deposits and elevated Heinz bodies in liver).  
* Cholinesterase effects (plasma/RBC cholinesterase decreases/inhibition without cholinergic symptoms or signs)  
* Hormone changes  
* Cellular vacuolization  
* Other (e.g., changes in teeth and supporting structures, sensory organ effects, inhibition of the concentration of beneficial bacteria in the gastrointestinal microflora) |
| 4              | Cellular/physiological changes that could lead to disorders (risk factors or precursor effects). (Interpretation: Considers cellular/physiological changes in the body that are used as indicators of disease susceptibility) | * Hematological effects (e.g., jaundice, anemia, hemolytic anemia, hemolysis)  
* Immunological effects (e.g., a delayed hypersensitivity, cellular or humoral immune response)  
* Liver effects (e.g., fatty cyst - liver and elevated liver enzymes, cell enlargement or alteration)  
* Renal effects (e.g, proteinuria, renal cytomegaly)  
* Cholinergic effects (cholinesterase inhibition with cholinergic symptoms or signs)  
* Other effects (e.g., hypothermia, mild CNS effects) |
| 5              | Significant functional changes that are reversible or permanent changes of minimal toxicological significance. (Interpretation: Consider those disorders in which the removal of chemical exposure will restore health back to prior condition) | * Increased cholinergic effects (e.g., sweating, diarrhea, hypotention, and/or fishy inhibition with or without signs or symptoms)  
* Hematological effects (e.g., GI bleeding, coagulation defects, extramedulary hematopoesis)  
* Single or multiple organ effects (e.g., cytomegaly; renal/liver/thyroid functional impairment; inflammation, fatty changes)  
* Ocular effects  
* Neurological effects (e.g., mild neurological signs, alteration of classic conditioning, brain ChE inhibition, myelin degeneration, CNS depression, tremors, dyspnea, changes in motor activity, ataxia)  
* Other effects (e.g., chronic pneumonitis, nonneoplastic lesions - splenic capsule) |
<table>
<thead>
<tr>
<th>Severity score</th>
<th>Score definition</th>
<th>Compendium of critical effects</th>
</tr>
</thead>
</table>
| 6             | Significant, irreversible, nonlethal conditions or disorders. *(Interpretation: Consider those disorders that persist for over a long period of time but do not lead to death)* | * Single or multiple organ effects (e.g., histopathological effects, dysfunction)  
* Sensory and neurological effects (a brain/brain to body weight ratio, degenerative changes for brain/other coverings, neuropathy, nerve damage, sensory neuropathy, minimal lens opacity and cataracts, nasal olfactory lesions)  
* Cardiac effects (e.g., cardiomyopathy, including infarction, vascular complications, atrial dilation, mild histological lesions)  
* Other effects (e.g., GI necrotic changes, chronic irritation with histopathology findings, bladder toxicity, bone marrow toxicity) |
| 7             | Developmental or reproductive effects leading to major dysfunction. *(Interpretation: Considers those chemicals that cause permanent developmental effects or that impact the ability of a population to reproduce)* | * Reproductive organ effects (e.g., testicular and uterine effects (weight changes, histopathological, functional)  
* Maternal toxicity  
* Fertility effects (e.g., spermatogenic effects, reduced numbers of corpora allata, a fertility/litter size)  
* Growth inhibition (e.g., reduced offspring weight gain, total litter weight, or litter size, decreased lactation indices, decreased crown-rump length)  
* Decreased offspring viability  
* Developmental effects (e.g., fetal toxicity/malformations, skeletal or visceral abnormalities, delayed ossification, neurodevelopmental effects, mixed sexual differentiation or imbalance in sex ratio. |
| 8             | Tumors or disorders likely leading to death *(Interpretation: Considers chemical exposures that result in a fatal disorder and all types of tumors).* | Suspected carcinogenicity (including short latency periods and rare tumors).  
Cancer (any type) |

The above table is the MDH Simplification of Exhibit A.3. Compendium of Critical Effects Table (from Health Advisories & IRIS) For Scoring Severity, EPA 815-R-09-008 (August 2009), Final CCL 3 Chemicals Classification of the PCCL to CCL. It does not represent official MDH Policy.
This page left blank intentionally.
Appendix D: Critical guidance documents
Important links

The following are links (URLs) to guidance documents that were relied upon for ALSV method development:


X:\Agency_Files\Outcomes\Emerging Issues\2013-15 Projects\CEC ALSV Project\Existing Methods\Evaluate\TGD-EQS CIS-WFD 27 EC 2011.pdf

The University of California Davis Methodology for Deriving Aquatic Life Pesticide Water Quality Criteria

Monitoring Strategies for Chemicals of Emerging Concern in California’s Aquatic Ecosystems


Protocol for the derivation of Canadian tissue residue guidelines for the protection of wildlife that consume aquatic biota, 1999


EPA Science Advisory Board on Aquatic Life Water Quality Criteria for Contaminants of Emerging Concern, 2008
Appendix E: Species sensitivity distribution considerations
Species sensitivity distributions

Water quality criteria are generally derived by the AF or species sensitivity distribution (SSD) approach, depending on the availability of toxicity data. In general, the more data that are available, the more likely a SSD is used. The methods described above have been focused solely on the AF approach.

Many regulatory jurisdictions provide decision criteria for the derivation of water quality criteria (WQC) using SSDs, generally based on the quantity of qualified data. To derive a WQC using the SSD approach, all qualified data are plotted and then a statistical distribution is fit to the data. From the equation resulting from the fitted distribution, a chemical concentration corresponding to a percentile of species in the distribution can be estimated. The selected value is called the hazardous concentration (HCp) and is interpreted as the chemical concentration that is hazardous to \( p \) percentile of organisms. For example, if the decision is to set a WQC that is protective of 95% of the species in a community, an HC5 would be calculated from the SSD. In such a situation, 5% of the species in a community may be negatively affected by waters meeting WQC.

Although the SSD approach suggests a level of quantification not present in the AF method, the MPCA has decided to derive ALSVs using the AF approach for the following reasons:

- Species sensitivity distributions are statistical distributions that may obfuscate one’s impression of how species actually vary in their sensitivity to a given contaminant. There is no known biological basis for the sensitivity of species to fit any one statistical distribution.
- Often, when the HC5 value is greater than the LTV (as it should be given the strict definition of HC5), all jurisdictions reviewed provide a means of reducing the value such that it is lower than the LTV, based on the abundance and diversity of data and the level of certainty; this method is akin to the AF approach.
- Most CECs will not fulfill the data requirements for SSDs. Some of these requirements are:
  - Toxicity values for \( \geq 8 \) taxonomic groups (e.g., EPA 1985 Guidelines [5] and EU Water Framework Directive (WFD) [4])
  - Toxicity values for \( \geq 5 \) taxonomic groups [22] and Canadian Water Quality Guidelines for the Protection of Aquatic Life [3]
  - EPA Midcontinent Ecology Division statisticians have calculated that at least 30 data points from at least 8 taxa are needed for a biologically and statistically certain SSD (Etterson M, personal communication)
  - The EU WFD Technical Guidance Document #27 [4] requires at least 15 data points from 8 taxa
  - 5th percentile values cannot actually be calculated with fewer than 20 data points [23].
- If there are enough data to reliably produce an SSD, then there are enough data to generate a standard rather than an ALSV.
- The numerous chronic endpoints available in the literature for CECs are not easily converted to values that would be suitable for SSD construction.
- The intended use for the ALSVs does not require the amount of rigor associated with standard development.
- SSDs generate values that can be less conservative than values from the AF procedure (i.e., higher), a result that is not desired given the intended use of the ALSVs.
- Therefore, the time and effort required for SSD generation is high while the resulting value is often no different or is less conservative than what would be generated via the AF procedure.
Abbreviations

AF  Assessment factor
ALSV  Aquatic life screening value
ATQ  Action trigger quotient
BAF  Bioaccumulation factor
BCF  Bioconcentration factor
BMF  Biomagnification factor
CEC  Contaminants of emerging concern
DG  Data guidelines
ECx  Concentration that results in an effect on x% of individuals tested
ICx  Concentration that immobilized x% of individuals tested
KOW  Octanol-water partition coefficient
KOC  Organic carbon-water partition coefficient
LCx  Concentrations that is lethal to x% of individual tested
LOEC  Lowest observed effect concentration
LTV  Lowest toxicity value
MATC  Maximum acceptable toxicant concentration
MPCA  Minnesota Pollution Control Agency
NOAEL  No observable adverse effect level
NOEC  No observed effect concentration
NOEL  No observed effect level
SSD  Species sensitivity distribution
TEF  Toxic equivalency factor
TEQ  Toxic equivalent
TU  Toxic unit
EPA  United States Environmental Protection Agency

Definitions

Aquatic Life - all biological organisms that reside in water for all or most of their life. It also includes organisms that rely on aquatic systems in some way - either as a source of food or for the completion of some portion of their life cycle.

Aquatic Life Screening Values (ALSVs) - risk-based chemical concentrations specific to water, sediment, or biota. Environmental concentrations above the ALSV may indicate harm to aquatic life.

Contaminants of emerging concern (CECs) - a loosely defined, highly diverse set of chemicals that can include pharmaceuticals and personal care products, flame retardants and many other chemicals detected at very low concentrations in the ambient environment. These chemicals may act to disrupt the endocrine or other physiological systems of organisms under chronic, low-level concentrations. Knowledge of the occurrence and possible adverse effects of exposure to many of these chemicals is rather limited.