Environment and Climate Change Canada | Environnement et Changement climatique Canada

Federal Water Quality Guideline for Copper

Biotic Ligand Model (BLM) Tool and User Manual

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Environment and Climate Change Canada
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Acronyms

Acronym	Definition
BLM	Biotic Ligand Model
Ca	calcium
Ca^{2+}	calcium ion
$CaCO_3$	calcium carbonate
CEC	Commission for Environmental Cooperation
Cl	chlorine
CO_3	carbonate
Cu	copper
DIC	dissolved inorganic carbon
DOC	dissolved organic carbon
ECCC	Environment and Climate Change Canada
FWQG	Federal Water Quality Guideline
GEV	Generalized extreme value (distribution)
H_2CO_3	carbonic acid
HC_5	5^{th} percentile of the species sensitivity distribution
HCO_3	bicarbonate
K	potassium
Mg	magnesium
Na	sodium
NOM	natural organic matter
pCO_2	partial pressure of carbon dioxide in the atmosphere
QA/QC	quality assurance/quality control
SO_4	sulfate
SSD	species sensitivity distribution
TOC	total organic carbon
WHAM	Windermere Humic Aqueous Model

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1 Introduction

The Biotic Ligand Model (BLM) software of the Environment and Climate Change Canada (ECCC) calculates the federal water quality guideline (FWQG) for copper, while considering the chronic toxicity database for fish, invertebrates and plants. The BLM is used to normalize the toxicity database to site-specific chemical conditions, considering the effects of water quality parameters on bioavailability. The normalized chronic toxicity database becomes the basis for developing a species sensitivity distribution (SSD) that characterizes the range in sensitivity of aquatic organisms. The 5th percentile of the SSD (HC_{5}/FWQG) is estimated using a range of distribution models and the user friendly outputs are provided. A detailed technical description of FWQG for copper is presented in ECCC (2021).

2 Setup and installation

2.1 System requirements

The BLM Windows® Interface is designed for use on the PC family of computers running Microsoft Windows®. The memory requirements of the BLM Windows® Interface are modest and should not interfere with other resident programs.

2.2 Installing the BLM Windows® Interface

To install the BLM Windows® Interface from the setup file "BLM_EnvCanCu_Users_1.20_setup.exe" simply double click on the file and follow the prompts. The first prompt will be to select which language to use during installation and for the starting language of the BLM Windows® Interface. The user can change the BLM interface's language later if needed (see section 4.4.6). The setup program (Figure 2-1) will guide the user through a fairly straightforward installation process, querying the user for information on where to install the necessary files. During the installation, a shortcut to the BLM Windows® Interface application will be added to the 'Programs' sub-menu within the 'Start' menu on the Microsoft Windows® desktop. In addition, the BLM Windows® Interface application will also be registered in the system registry so that the BLM data files created by the user can be accessed directly by just double-clicking on the file name.

Figure 2-1. Opening screen for the BLM tool setup program

3 Starting the application

To start using the BLM Windows® Interface, the user should select the application using 'Start -----> Programs -----> Biotic Ligand Model -----> Environment and Climate Change Canada Chronic Cu BLM, Version 1.20 on the Microsoft Windows® desktop. After starting the program, the user can switch between English or French version of the interface by clicking on the "Language" tab shown in Figure 3-1.

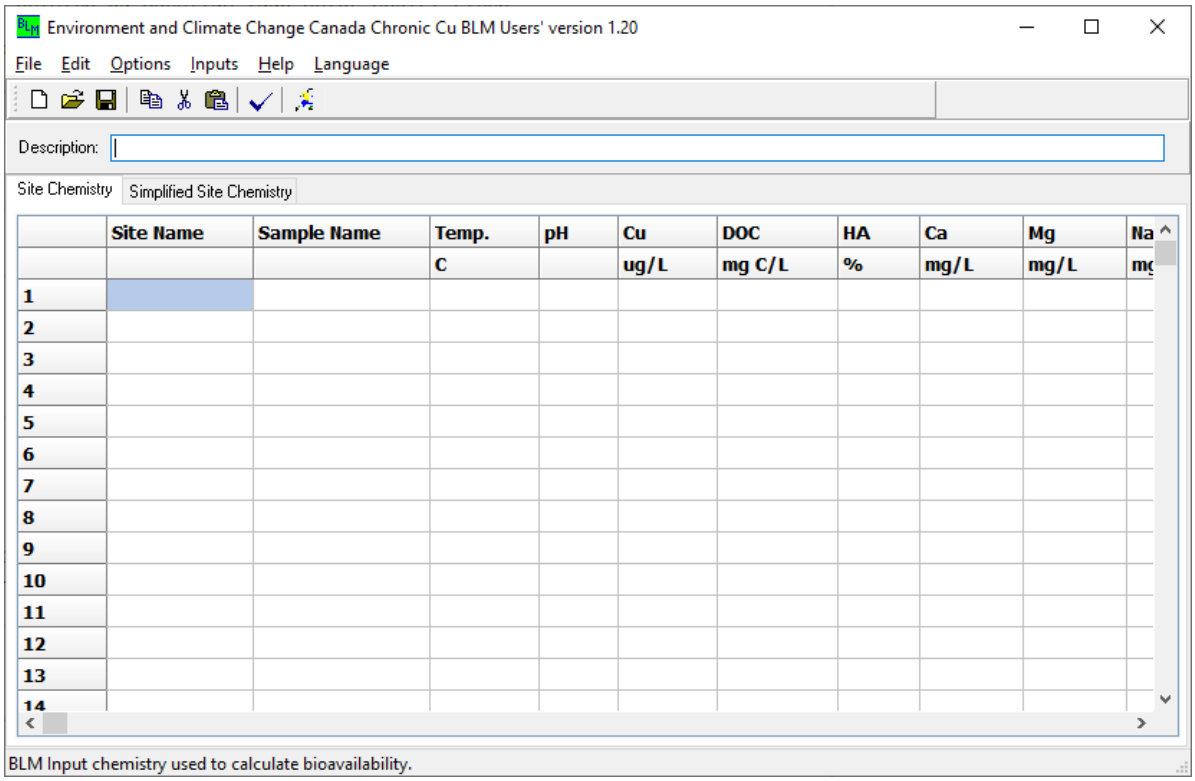

Figure 3-1. Opening screen for the BLM Windows® interface application

In case the user already has a BLM data file created using the BLM Windows® Interface, the file can be opened directly by just double-clicking on the file name through a file system manager, such as Microsoft Windows® Explorer.

4 Running the application

The following subsections describe the various functions and features available in the BLM Windows® Interface and the use of the BLM with its various predictive capabilities.

4.1 Description of interface

Figure 4-1 shows a snapshot of the BLM Windows® Interface application. The main purpose of this section of the interface application is to provide an easy-to-use editor to develop input files containing water chemistry information for the BLM, facilitate checks and validate user inputs for the various parameters, perform checks on whether the values entered for any given parameter are within the range for which the BLM has been calibrated, and run the BLM for calculating the site-specific/water sample specific FWQG for copper.

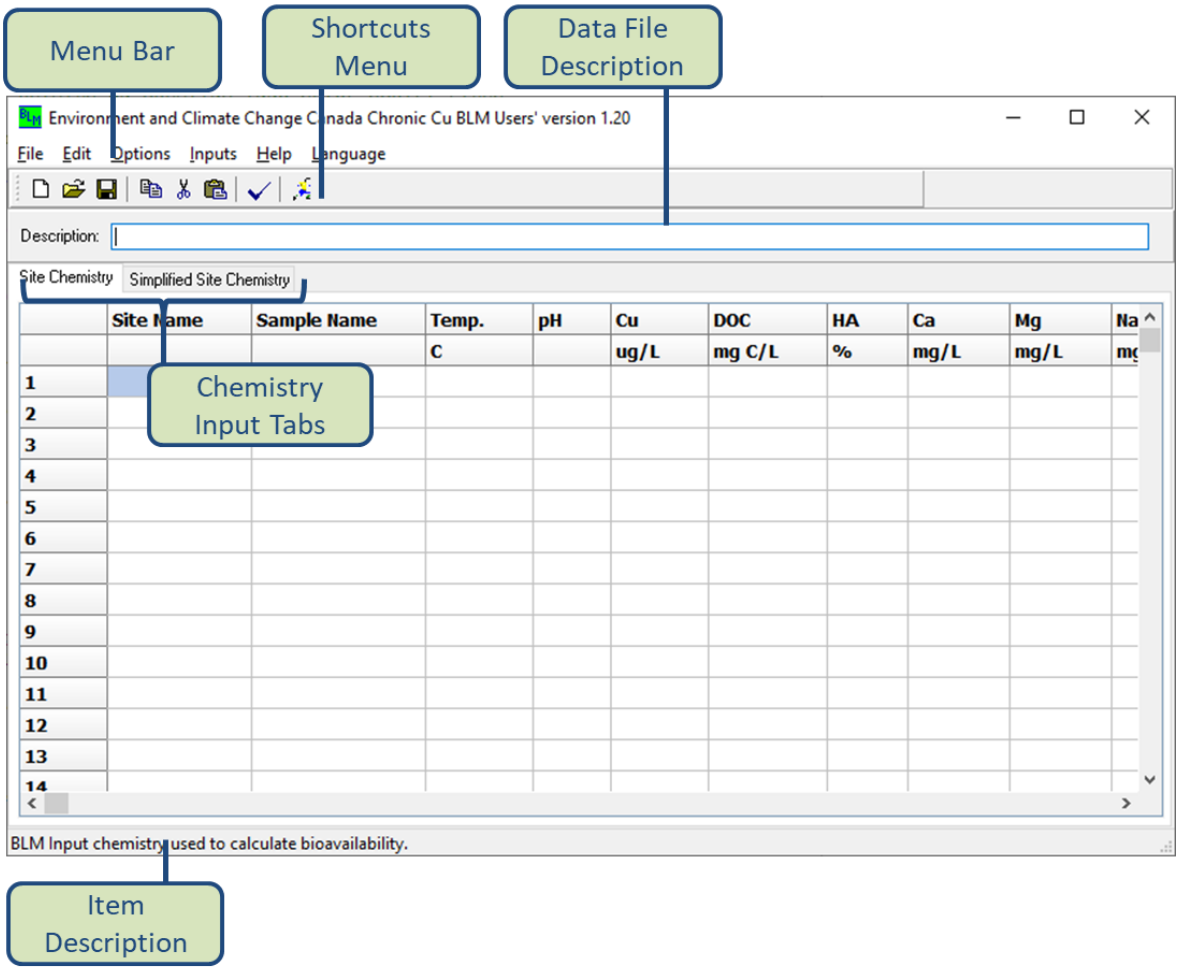

Figure 4-1. Snapshot of the BLM Windows® interface

As shown in Figure 4-1, the interface window is divided into five areas broadly based on their functionality. Each of these is described in the subsections that follow.

4.2 Site chemistry inputs tab

This region of the interface window contains a spreadsheet-based editor, which organizes the various BLM input parameters in a columnar format such that the chemistry for each discrete water sample can be specified on a separate row. Apart from the water chemistry information, two additional columns are also provided for labeling the sites and the samples described in a given BLM data file. Figure 4-2 shows the various columns typically available for user input.

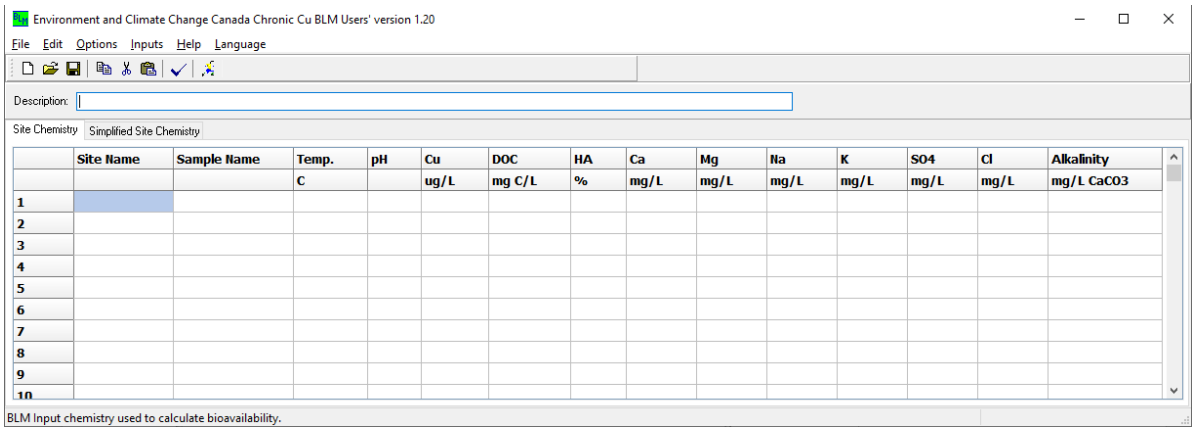

Figure 4-2. Columns for data input in the BLM Windows® interface

The BLM predicts copper toxicity and speciation for a particular site based on the ambient water quality. Therefore, the user will be expected to provide data describing the physical and chemical properties of the site water. The data requirements of the BLM are conventional physical and chemical parameters that are easily measurable in the laboratory. This section describes the general physical and chemical data requirements for an application of the BLM to predict copper speciation and toxicity in aquatic systems.

The ambient water quality information required to run the BLM is listed below:

- Temperature
- pH
- Dissolved organic carbon (DOC)
- Major cations (calcium [Ca], magnesium [Mg], sodium [Na] and potassium [K])
- Major anions (sulfate [SO_4] and chloride [Cl])
- Alkalinity

Some of these chemical inputs have an important effect on copper speciation, while other chemical inputs have only minor effects on BLM predictions. The user should be aware of the relative importance of each of the chemical inputs to decide whether adequate information is available for a meaningful application of the BLM. The guidelines described in the subsequent subsections may be helpful in that assessment.

Each water sample has to be fully described in terms of the above water quality inputs before the BLM can be used. If users are missing some of the input values, there is a simplified version (see Section 4.3) which requires only 4 inputs to estimate the remaining parameters. Users can use this tab alone or to supplement the full chemistry tab if only some chemistry is missing. Copper concentration is not a required input, since the BLM will predict the amount of copper that results in toxicity to the specified organism(s). For all other water quality inputs, any row with a missing input will be flagged as incomplete, and no BLM predictions will be made for that row.

4.2.1 Site name and sample name

The very first column, 'Site Name,' is meant to contain information about the site under consideration. For example, it could be the name of the river or site ID if the same file contains water chemistry data for more than one location along a particular river. The 'Sample Name' field can be used to distinguish the various water chemistry samples available for a particular site. For instance, at a given site, this field could represent the date and time at which the site water samples were collected. For both the site and the sample descriptor fields, the maximum number of characters allowed in each field is 20.

4.2.2 Temperature

Temperature measurements are typically the most common and basic of all water quality measurements and therefore available in most laboratory characterizations of site water chemistry. Because the BLM is based on a thermodynamic chemical equilibrium-modeling framework, temperature measurements are important in determining the relevant thermodynamic reaction rates.

4.2.3 pH

Accurate pH values are important to BLM results for most metals, preferably reported to at least the nearest 0.1 pH units. The chemical speciation of Cu is directly affected by pH. However, pH is also important in determining the complexation capacity of copper with dissolved organic matter. It is also important in determining the speciation of inorganic carbon, which relates to the formation of copper carbonate complexes. For these reasons, pH is considered a required chemical input to the BLM. If BLM results are to be compared with laboratory measurements of copper toxicity, then it is preferable that the pH be measured within the test chamber during the exposure.

4.2.4 Dissolved organic carbon

Dissolved organic matter can play a critical role in determining copper speciation and bioavailability. In the BLM, the presence of dissolved organic matter is specified as a DOC concentration in mg/L and is considered a required input for the BLM, preferably reported to at least the nearest 0.1 mg/L. For water with low DOC, it is important to make sure that analytical detection limits are sufficiently low, preferably less than 0.5 mg/L. In toxicity studies, the test organisms themselves may be a significant source of organic matter, depending on the number of organisms and the volume of the test chamber.

Natural organic matter is any organic components of the water, for example leaf litter and detritus is a common source of organic matter. NOM is a complex mixture of organic acids, proteins and many complex organic molecules. Total organic matter can be splitted into particulate organic matter and dissolved organic matter. The commonly-used operational definition is that dissolved organic matter can pass through a 0.45-micron filter while particulate organic matter is retained by the filter, although the exact size cutoff is somewhat arbitrary Dissolved organic carbon is a way of quantifying dissolved organic matter, and is simply the mass of carbon present in the mixture of organic compounds. Sometimes total organic carbon (TOC) is reported instead of DOC. For the purpose of use in the BLM, DOC

is preferred but TOC can be used in lieu of DOC with the understanding that the actual amount of DOC will be less than or equal to the TOC.

4.2.5 Humic acid fraction of DOC

The BLM uses a description of organic matter chemistry developed for WHAM, Version 1.0 (Tipping 1994), which characterizes metal complexation with both humic and fulvic organic matter sources. (Note that this version of WHAM is sometimes called WHAM Model V, due to a change in the version numbering around that time). To be able to make use of this capability, it is necessary to specify the distribution of humic and fulvic acids in the organic matter present in a given water. Unfortunately, natural organic matter composition is not routinely characterized and information on humic and fulvic acid content is not likely to be available. In the absence of chemical characterization, a value of 10% humic acid content is recommended for most natural waters. The variability of the dissolved organic matter content in diverse water sources has not been found to be an especially critical parameter, and little benefit is achieved by characterizing natural organic matter (NOM) beyond DOC concentrations.

4.2.6 Copper concentrations

It is not necessary to input copper concentrations for the model to calculate an HC_5, however this field is retained to allow compatibility, and to allow for easy comparison with the results. Copper concentrations entered here will not affect the FWQG calculations.

4.2.7 Major cations

The cations Ca, Mg, Na and K are all necessary inputs to the BLM. Ca and Na can directly compete with the metal at biotic ligand sites and these cations, therefore, have a direct effect on predictions of copper toxicity. For some organisms, Mg may play a critical role as well. These cations, therefore, should be considered required inputs to the BLM. On the other hand, K currently has no direct effect on copper toxicity in the BLM and can be estimated if measurements do not exist. Although K does not have a direct effect of the copper toxicity, it is still often present in large enough quantities that it can affect the charge balance and ionic strength of the water. This would indirectly affect the copper toxicity – typically, but not always, to a small extent.

Although major cations, anions, and alkalinity are required inputs, they can be estimated from hardness, pH and geochemical ion ratios as discussed in Section 4.3.

4.2.8 Major anions

The anions SO_4 and Cl are necessary inputs to the BLM (although bicarbonate is also an important anion, as discussed in Section 4.2.9). In fresh waters, SO_4 may be the dominant anion and is, therefore, important for determining charge balance and ionic strength. The chemistry of metals and natural organic matter is dependent to varying degrees on ionic strength, and so SO_4 has some importance as a BLM input. If measurements of SO_4 and chloride are not available, the concentrations can be estimated, including by using geochemical ion ratios as discussed in Section 4.3

4.2.9 Alkalinity

Inorganic carbon species in the BLM include carbonate (CO_3^{2-}), bicarbonate (HCO_3^-) and carbonic acid (H_2CO_3). The sum of these species is referred to as dissolved inorganic carbon (DIC). Bicarbonate is usually the most important DIC species in natural waters because it is the dominant species between pH 6.35 and 10.33. Inorganic carbon is a critical input to the BLM because many metals form carbonate complexes. Unfortunately, measurements of DIC are not often made in natural water samples. It can be estimated, however, from alkalinity and pH measurements, as in Equation 4-1.

$$DIC = Alk \cdot \frac{\frac{[H]}{K_1} + 1 + \frac{K_2}{[H]}}{1 + \frac{2 \cdot K_2}{[H]}} \qquad \text{Equation 4-1}$$

where:

Alk	=	alkalinity in equivalents/L
	=	2×10^{-5} x alkalinity (as mg calcium carbonate [$CaCO_3$]/L)
[H]	=	10^{-pH}
K_1	=	$10^{-6.352}$
K_2	=	$10^{-10.329}$

4.3 Simple chemistry input tab

By clicking on the 'Simplified Site Chemistry' tab, a grid similar to the full site chemistry data input will be displayed, as shown in Figure 4-3. The "Simplified Site Chemistry" view is an alternate place where the user can save chemical characterization of the water chemistry. It differs from the "Site Chemistry" tab in that there are fewer inputs required for each site, making data collection easier. The ambient water quality information required to run the BLM with this tab are:

- Temperature
- pH
- DOC
- Hardness
- Ion ratios (default values may be used if unknown)
- pCO_2 (defaults to 3.2 or 3.0 (plants/algae); cannot be changed by user)

The requirements for temperature, pH and DOC are the same as in the "Site Chemistry" tab (see previous section). The ion ratios inputs can be viewed and edited in a side bar with editable boxes. The default values are median Canadian values. These values can be changed to match the particular conditions of the site or test, and can be returned to the starting values at any time by clicking the 'Restore Default Values' button.

While in this tab, clicking the 'Open' option will filter for files with the extension '.blme' rather than '.blm'. This type of file optionally lists the ion ratios and pCO_2. An example file is included.

After the simplified site chemistry data has been entered into this grid, simply run the BLM as normal. Alternatively, select the 'Site Chemistry' tab again to have the full site chemistry estimated for you. This is helpful if only some of the chemistry needs to be estimated, since the user can use any measured values to replace the estimated values in the 'Site Chemistry' tab, which ultimately should result in a better prediction of toxicity.

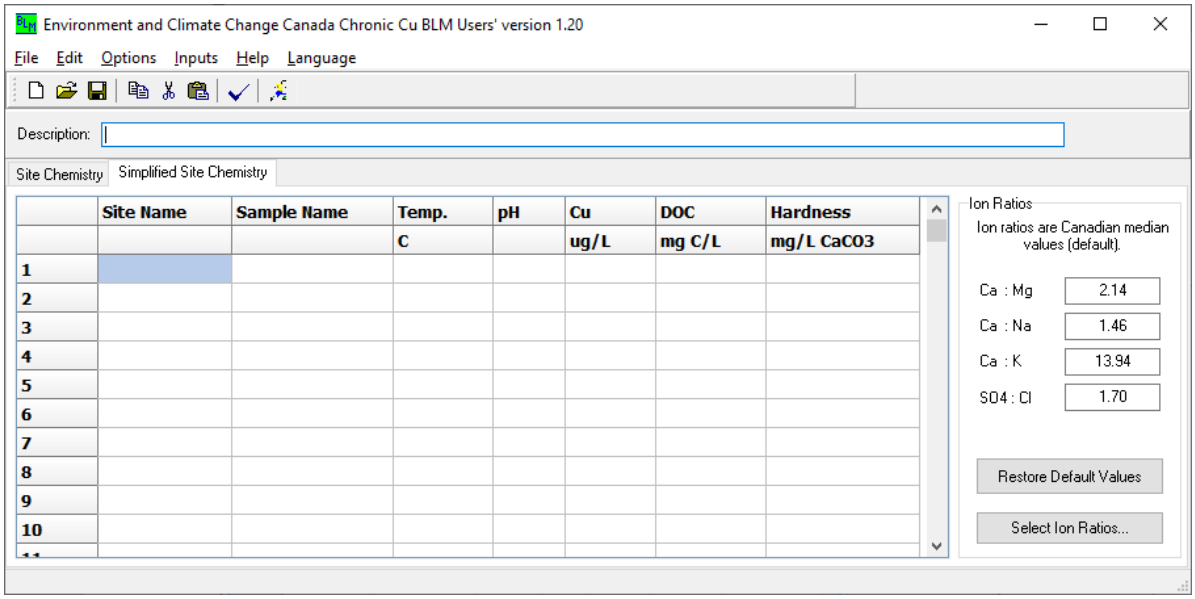

Figure 4-3. Snapshot of simplified site chemistry inputs and ion ratios

4.3.1 Hardness

The hardness measurements, in addition to pH and ion ratios, are used to estimate the major cations and anions. Hardness is typically the total Ca and Mg ion concentrations, although if hardness is measured directly then sometimes other ions can also affect it. For this calculation, hardness is assumed to be equivalent to Ca + Mg, specified in units of mg/L as $CaCO_3$.

4.3.2 Ion ratios

The ion ratios are entered in the group of boxes to the right of the grid. They determine the proportion of each ion that makes up hardness and the charge balance of the water, so "Ca: Mg" is the ratio of calcium ions to magnesium ions (in mol/L). These will vary between water

samples depending on watershed geology and various inputs. If unknown for the water source being considered, use the Canadian default values in the boxes or select the ecozone the water source is in from the "Select Ion Ratios..." dialog. The default values are median values based on water quality monitoring data from across Canada (Figure 4-4). The data used to calculate these values are discussed further in the Appendix. The median North American ion ratios are based on Canadian (Appendix 1) and the United States Geological Survey's National Water Quality Assessment dataset. These values can easily be returned to the boxes by pressing the "Restore Default Values" button below the group of boxes. An option for the median North American ion ratios is also available for using this tool outside Canada. The second button, "Select Ion Ratios..", will open a dialog when pressed so that the user may select values specific to a Canadian ecozone (ESWG 1995). These values are also shown in

Table 4-1, and came from the same data set as the Canadian median values, but have instead been grouped by ecozone before calculating a median. Insufficient data were available for Ca, Mg, Na and K in the Taiga Cordillera ecozone to determine median ion ratios for the cations. The Commission for Environmental Cooperation (CEC 1997) has a similar system of delineating ecologically- and geologically-similar regions, which they do at three spatial scales – Level I being the broadest scale and Level III being the finest scale. Canadian ecozones generally have the same or close to the same borders as the CEC Level I ecological regions, with a few ecozones corresponding to Level II ecological regions instead. The Taiga Cordillera ecozone corresponds to the CEC Level II ecological region of the same name, which is part of the Taiga CEC Level I ecological region, so the missing ion ratios for the Taiga Cordillera ecozone were filled in with the ion ratios from the Taiga CEC Level I ecological region.

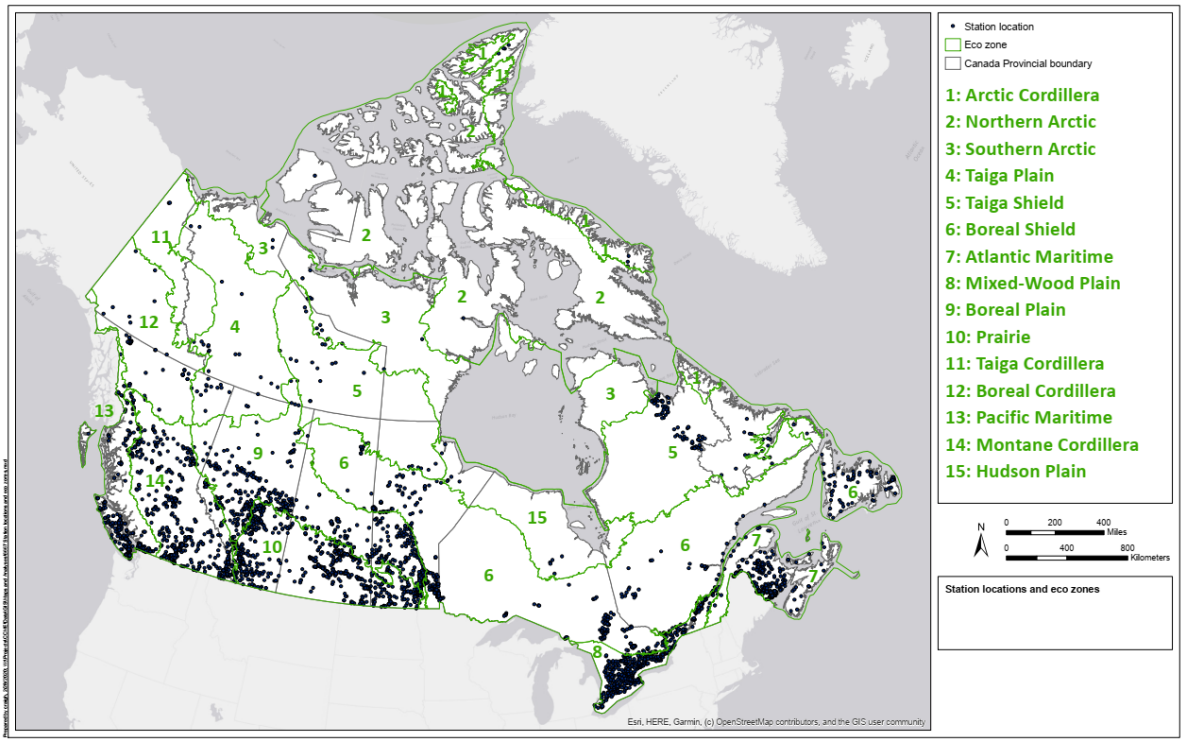

Figure 4-4. Map of Canada showing ecozones used as spatial units for calculating ion ratios for Table 4-1. Black circles show where samples were collected for surface water quality monitoring data

Table 4-1. Median ion ratios for Canada, North America and Canadian ecozones

Geographic Unit	Ca : Mg	Ca : Na	Ca : K	SO4 : Cl
Canada	2.14	1.46	13.94	1.70
North America	1.98	1.57	11.47	1.95
Canadian Ecozones				
1 Arctic Cordillera	3.71	3.08	5.03	7.75
2 Northern Arctic	4.57	10.25	30.14	10.61
3 Southern Arctic	1.19	1.61	3.25	1.05
4 Taiga Plain	2.14	3.26	33.31	6.99
5 Taiga Shield	1.87	2.12	6.42	0.96
6 Boreal Shield	2.10	0.99	6.71	0.67
7 Atlantic Maritime	3.87	1.11	13.77	0.33
8 Mixed-Wood Plain	2.53	2.03	25.98	4.14
9 Boreal Plain	1.82	1.66	16.26	2.88
10 Prairie	1.20	0.84	8.48	3.31
11 Taiga Cordillera	1.98	2.19	7.14	10.06
12 Boreal Cordillera	2.51	8.19	31.09	23.30
13 Pacific Maritime	4.07	1.46	28.05	0.81
14 Montane Cordillera	2.43	5.13	29.63	4.76
15 Hudson Plain	2.46	4.02	20.17	0.52

4.3.3 pCO_2

The pCO_2 (ambient CO_2 concentration in atmospheres) is pre-set in this version of the software and cannot be edited by the user. The value that is entered is the negative logarithm of the actual CO_2 concentration. Alkalinity is estimated from pH assuming an open system in equilibrium with CO_2 in the atmosphere. The differences between indoor and outdoor CO_2 concentrations may significantly affect the calculated alkalinity.

The partial pressure of atmospheric CO_2 gas has been steadily rising in recent decades. In the 1950s average atmospheric CO_2 concentrations were around 300 ppm[1] (partial pressure of 3.5) but as of January 2020 concentrations are now around 413 ppm[2] (partial pressure of 3.4). Indoor air quality, however, often has atmospheric CO_2 concentrations that are much higher

[1] https://climate.nasa.gov/climate_resources/24/graphic-the-relentless-rise-of-carbon-dioxide/
[2] https://www.co2levels.org/

than outdoor air quality and may range as high as 2,500 ppm (Seppänen et al. 1999). Since toxicity tests are almost always conducted indoors, the enriched CO_2 concentrations that are typical of indoor air quality may be more relevant for predicting CO_2 solubility in aquatic toxicity tests. The variability in indoor air quality makes it difficult to assign a value that would be appropriate for all conditions.

Natural waters are also frequently supersaturated with CO_2 relative to the atmosphere which is another factor to consider when assigning a pCO_2 value. We have found that a pCO_2 of 3.2 tends to best represent the relationship between pH and alkalinity in natural waters. An exception, however, is that for plants and algae we use a somewhat higher CO_2 concentration, corresponding to a pCO_2 of 3.0. The reason for this difference, is that plants and algae are more sensitive to the impact of pCO_2 on the toxicity of copper and a value of 3.0 is more protective. For this reason, the software uses separate pCO_2 values for estimating inorganic carbon when alkalinity measurements are not available.

4.3.4 Simple to full chemistry conversion process

When the user switches from the Simplified Site Chemistry tab to the Full Site Chemistry tab, the tool copies the labels, temperature, pH, DOC and copper concentrations to the full chemistry input grid. Then the pH and pCO_2 are used to estimate alkalinity, and the hardness and ion ratios are used to estimate the major ion concentrations.

Alkalinity is estimated with the assumption that carbonate species are in equilibrium with the selected pCO_2, following Henry's Law. The following equations perform this operation:

$$[H_2CO_3^*] = K_H * P_{CO_2}$$

$$[HCO_3^-] = 10^{-6.352} * \frac{[H_2CO_3^*]}{[H^+]}$$

$$[CO_3^{2-}] = 10^{-10.329} * \frac{[HCO_3^-]}{[H^+]}$$

$$\left[Alk\left(\frac{mg}{L}\ as\ CaCO_3\right)\right] = ([HCO_3^-] + 2 * [CO_3^{2-}] + [OH^-] - [H^+]) * \left(\frac{100086}{2}\right)$$

where $[H_2CO_3^*]$ is the sum of dissolved CO_2 gas and the H_2CO_3 species, K_H is Henry's Law constant (equal to $10^{-1.5}$ $M/_{atm}$), so that with the default pCO_2 value of $10^{-3.2}$, the concentration of $[H_2CO_3^*] = 10^{-4.8}\ M$. The alkalinity is then pH dependent, with the alkalinity being 4.44 mg/L as $CaCO_3$ when the pH is 7, as an example. At low pH, this calculation will often yield a negative alkalinity, which we replace with an alkalinity of 1 mg/L $CaCO_3$ to avoid computational inconsistencies.

The hardness is converted to ion concentrations using the ion ratios and a charge balance. Calcium concentrations are calculated first, as:

$$[Ca^{2+}] = \left(\frac{Hardness\ as \frac{mg}{L} CaCO_3}{100086 \frac{mg}{mol}} \right) * \left(\frac{Ca{:}\,Mg}{Ca{:}\,Mg + 1} \right)$$

The remaining cations are calculated as:

$$[X] = \frac{[Ca^{2+}]}{Ca{:}\,X}$$

where X is Mg, Na or K. The anions, SO_4 an Cl, are calculated by first calculating the anion deficit:

$$\begin{aligned} &Deficit\ \left(\frac{eq}{L}\right) = 2 * [SO_4^{2-}] + [Cl^-] \\ &= \Sigma(charge * Cations) - \Sigma(\text{charge} * \text{Anions}) \\ &= \ (2 * [Ca^{2+}] + 2 * [Mg^{2+}] + [Na^+] + [K^+] + [H^+]) \\ &\qquad - ([OH^-] + [HCO_3^-] + 2 * [CO_3^{2-}]) \end{aligned}$$

Then, the concentration of SO_4 and Cl are then calculated as follows:

$$[SO_4^{2-}] = \frac{Deficit}{2 + \frac{1}{SO_4{:}\,Cl}}$$

$$[Cl^-] = \frac{[SO_4^{2-}]}{SO_4{:}\,Cl}$$

If there is a negative deficit, the concentration of SO_4 would be calculated as a negative number – an impossible condition. In these cases, $[SO_4^{2-}]$ is set to an arbitrary low number (10^{-7} M) before calculating $[Cl^-]$ in order to avoid computational inconsistencies.

4.4 Menu bar

Located at the very top of the interface window, the menu bar provides the user with a range of functions and features including:

- Mechanism for managing the BLM data files
- Text editing functions
- Functions to select between various units for data inputs
- A help function

These features are described below.

4.4.1 File

Figure 4-5 shows the functions available under this menu item. Basic file management utilities to create a new BLM data file, open an existing BLM data file and save a BLM data file are provided. The user can also open a dialog to run batches from this menu (see section 4.9), or open a file that was previously used (only the last five files are saved this way).

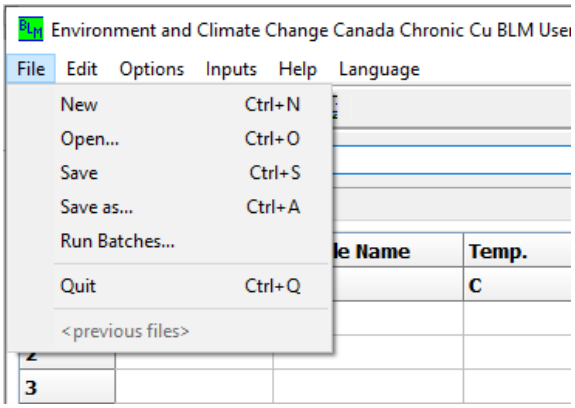

Figure 4-5. Snapshot of file menu item

Shortcut keys (shown to the right of each item) are also available for some of the different functions in this menu item.

For ease of access, BLM data files can also be opened directly by double-clicking on the BLM data file in a file system manager, such as Microsoft Windows® Explorer. This avoids having to first start the application and then navigate through the file menu to locate the BLM data file of interest.

Note that the BLM data files created by the interface application are given a '.blm' extension by default. Even though the BLM data file created by the interface application basically is an ASCII text file, it is recommended that the user not modify this file using a program other than the BLM Windows® Interface application. Doing so may result in the BLM data file becoming corrupted. If this happens, the next time the user tries to edit that BLM data file using the BLM Windows® Interface, the file may not be read correctly by the BLM interface application.

4.4.2 Edit

Figure 4-6 shows the editing functions available in the BLM Windows® Interface. Basic editing functions such as 'Cut,' 'Copy,' 'Paste' and 'Delete,' are available in the interface application. The editing functions can be performed on a single cell or multiple cells by highlighting and dragging the cell(s) or by using the Shift and Arrow functions on the keyboard. These editing functions can also be accessed by using the shortcut keys shown to the right of each. Note that it is also possible to copy and paste data from external programs, such as a spreadsheet application into the BLM Windows® Interface.

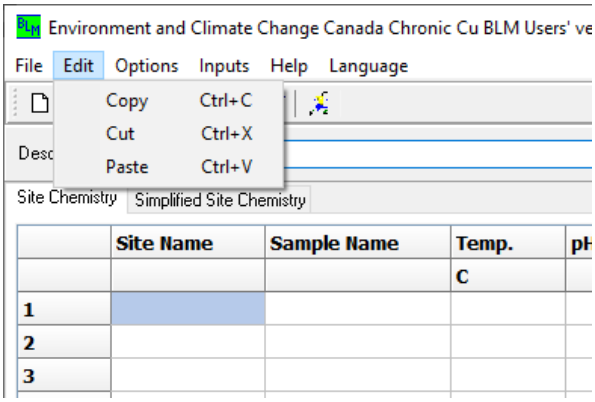

Figure 4-6. Snapshot of edit menu item

4.4.3 Options

Figure 4-8 shows the 'Options' menu, which currently only contains the option 'Show Engine Runs'. The 'Show Engine Runs' option can be selected so that the command line windows that are normally hidden when the BLM engine runs will be visible on the screen, which can be useful for finding where an issue is if the BLM calculations seem to be getting "stuck".

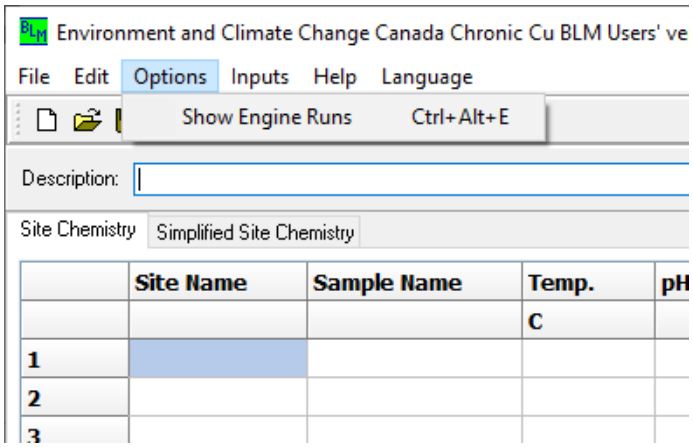

Figure 4-7. Snapshot of options menu item

4.4.4 Inputs

Figure 4-8 shows the options available under the Inputs menu item. The units for all parameters can be changed by selecting the "Set Units" menu item. The "Set Inorganic Carbon" menu item can be selected to change how the user inputs inorganic carbon in the full Site Chemistry tab. There are two options for closed systems, inputting inorganic carbon as either DIC or alkalinity. The third option is for an open system, in which the inorganic carbon is in equilibrium with the atmosphere (hence, an open system is "open to the atmosphere" which means gaseous CO_2 can dissolve and affect the aqueous composition).

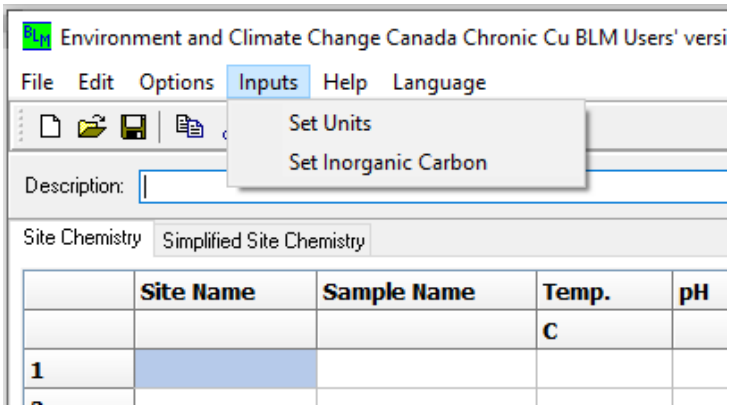

Figure 4-8. Snapshot of inputs menu item

4.4.5 Help

Figure 4-9 shows the various features available under the Help menu item.

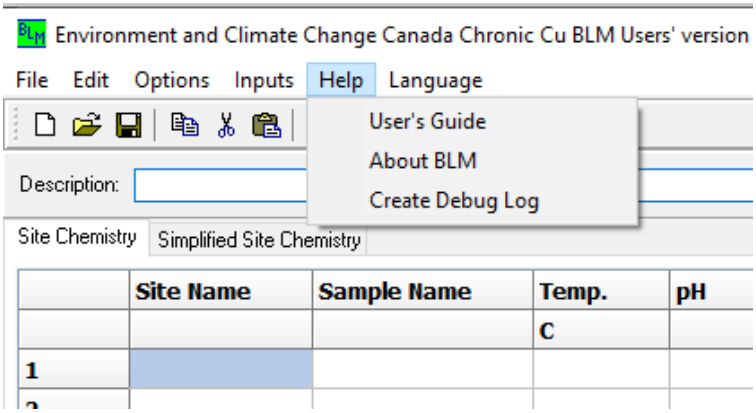

Figure 4-9. Snapshot of help menu item

The User's Guide for the BLM Windows® Interface can be accessed via this menu item. In addition, under the 'About BLM' sub-item, there is also information on contacts for technical support. The "Create Debug Log" option will make it so the program makes a detailed log of everything that happens in it, which is useful for sending to the developers if a problem is occurring.

4.4.6 Language

Figure 4-10 shows the options available under the Language menu.

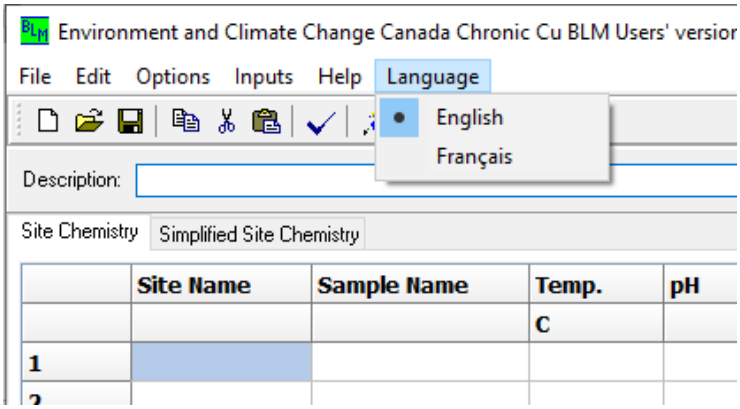

Figure 4-10. Snapshot of language menu item

The user can use this menu to select English or French language option for the BLM interface and output. The BLM interface will remain in the chosen language (even if restarted) until the user switches it again. Note that switching the language will reset the program and clear the input grid, so save any work before doing so.

4.5 Shortcuts menu

Icons located on the toolbar provide shortcuts to some of the menu bar items, as well as additional functions that are not available on the menu bar.

Figure 4-8 shows the various icons and their functions; brief descriptions are provided in the subsections that follow.

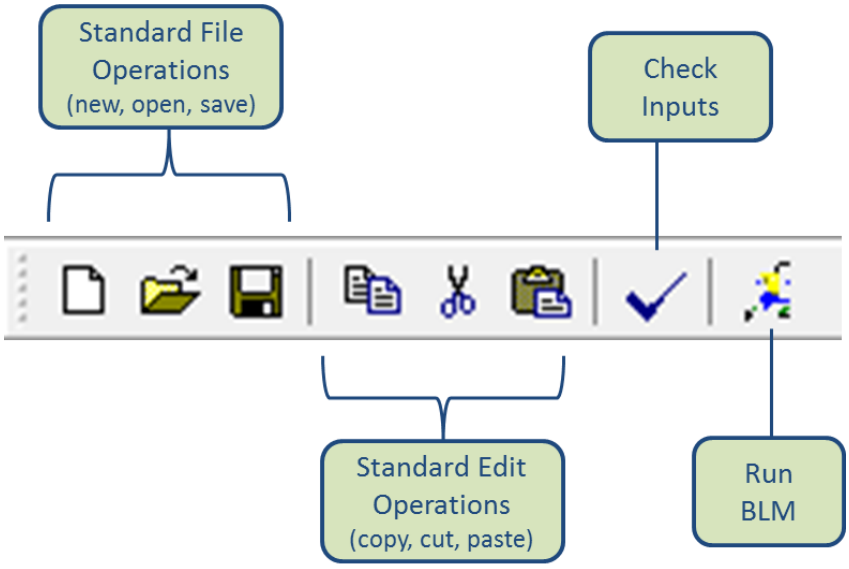

Figure 4-8. Shortcut menu icons

4.5.1 Open file

This is a shortcut to the menu bar item under 'File -----> Open' and is serves as a quick mode of access to the BLM data files. If the BLM data file being edited has changed since the last time it was saved and the user tries to open another file, the user will be queried as to whether the current data file should be saved prior to opening another data file.

4.5.2 Save file

This is a shortcut to the menu bar item under 'File -----> Save' and serves as a quick mode of saving the BLM data file. The data file will be saved with the same, existing name. If the user wishes to save the file under a different file name, the menu bar item 'File -----> Save As' should be chosen.

4.5.3 Check inputs

After creating a BLM data file, the user may wish to check the water chemistry inputs to verify whether the parameter values are within the overall range for which the BLM has been calibrated and check to see whether all the parameters necessary for a BLM prediction have been specified. Clicking on this icon generates an input check report that contains information on which parameters are out of range (i.e., too high or too low when compared with the range for which the BLM has been calibrated) and which parameters are missing for any given input row. The ranges prescribed for each of the BLM input parameters are shown in Table 4-2. Figure 4-9 shows an example of an input check report. If the user input water chemistry is outside the ranges prescribed in Table 4-2, the BLM will substitute the lower or upper bound before normalizing the data.

Table 4-2. Prescribed ranges for BLM input parameters

Parameter	Lower Bound	Upper Bound	Importance
Temperature (°C)	8.5	27	Low
pH	5.5	8.75	High
DOC (mg/L)	0.2	33.4	High
Humic acid content (%)	0.01	24.1	Low
Calcium (mg/L)	2.2	160.3	High
Magnesium (mg/L)	0.49	36.3	High
Sodium (mg/L)	1.2	505.8	High
Potassium (mg/L)	0.2	10.4	Low
Sulfate (mg/L)	0.5	330	Low
Chloride (mg/L)	0.2	989.1	Low
Alkalinity (mg/L)	0.007	325.91	High
DIC (mmol/L)	0.0162	6.37	High
Hardness (mg/L)	7.9	525	High

DIC – dissolved inorganic carbon
DOC – dissolved organic carbon

The ranges represent the minimum and maximum of the parameter values observed in chronic toxicity studies of acceptable quality according to CCME (2007). DIC is included because it is an alternate input rather than alkalinity. Since the conversion to DIC from alkalinity is pH-dependent, a separate range was determined for alkalinity. While these ranges are based on the actual values used in toxicity tests for model evaluation, it would be unusual to experience conditions where all model inputs were at their highest or lowest values.

The range of temperature values reflects the conditions used in toxicity tests, and do not represent field conditions. Temperature effects on copper toxicity are relatively minor, and the use of temperature values outside this range are common in field conditions and should not be a concern.

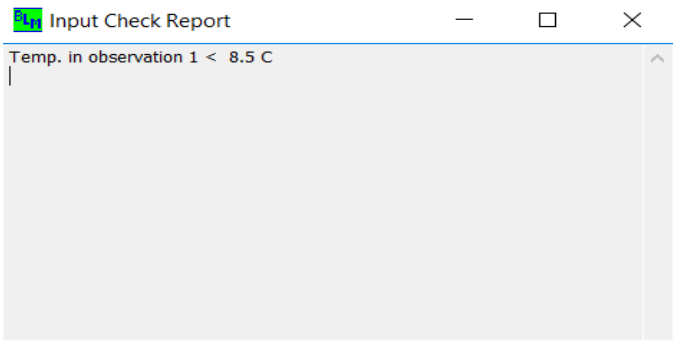

Figure 4-9. Example of an input check report generated by the check inputs function

4.5.4 Run BLM

This icon is used to launch the BLM program to calculate FWQG for the user-specified selections for the site water chemistry described in the BLM data file currently open in the BLM Windows® Interface. If the BLM data file has changed since the last time it was saved and the user tries to run the BLM, the user will be queried as to whether the current file should be saved prior to the BLM run.

4.6 Data file description

This area is provided for the user to insert comments describing the BLM data file, which will then be saved along with the water chemistry parameters input by the user. Although this function is not of critical importance to the use of the BLM, for record-keeping and possibly quality assurance/quality control (QA/QC) purposes, it is useful.

4.7 Item description

Located at the very bottom of the interface window, this area is designed to display a brief description of the icon/image/area over which the cursor is currently positioned. For the example shown in Figure 4-1, the cursor is positioned over the Site Chemistry area. Similar messages are displayed when the cursor is moved over other areas of the interface window.

4.8 Description of output files

Various outputs will be written in the same location where input files are saved, and with the same name as the input file with '.output' appended. For example, using the input file 'Example.blm' would create a Microsoft Excel® output file 'Example.output.xls'. The output file will have the full chemistry inputs repeated in the first several columns, followed by the best probabilistic distribution, the HC_5 (FWQG) and the lower confidence limit (LCL) and upper confidence limit (UCL) of the HC_5 value. The distribution model is automatically chosen as the best-fit of four log space models (lognormal, log-logistic, log-Gumbel and log-generalized extreme value (GEV). The best-fit species sensitivity distribution (SSD) model is selected based on which of the four models results in the lowest sum of squared residuals on the probability axis and this model is saved as one or multiple bitmap files (Figure 4-13). For example, if 'Example.blm' from before had two lines of input, it would produce two bitmap files that might be named 'Example.blm_site 1_day 1_1.bmp' and 'Example.blm_site 2_ day

1_2.bmp'. Notice that the row number is also appended so that each file will have a unique name in case they have the same site and sample labels. The SSD plot shows relative sensitivity of individual fish, invertebrate and plant species, selected distribution model, HC_5 (FWQG) value and the lower and upper confidence limits. In addition, an output file with normalized toxicity data that is plotted in the SSD will be created (Figure 4-14) and saved as a text file in the Data folder. This output file has information about the site chemistry, each SSD, and the individual toxicity observations that have been selected for use in the FWQG, as described in the following subsections. In the Excel and text output files and the Output tab, the lower HC_5 is capped at "0.2*"µg/L (i.e., where the HC_5 is calculated below 0.2 µg/L, the software provides a FWQG value of 0.2 µg/L). Setting this lower limit was necessary because calculated FWQGs were extremely low for waters of very high Cu bioavailability (e.g., low DOC).). It is to be noted that for these waters, the BLM calculated HC_5 value will be still presented in SSD graphs and users can consider them on case-by-case basis.

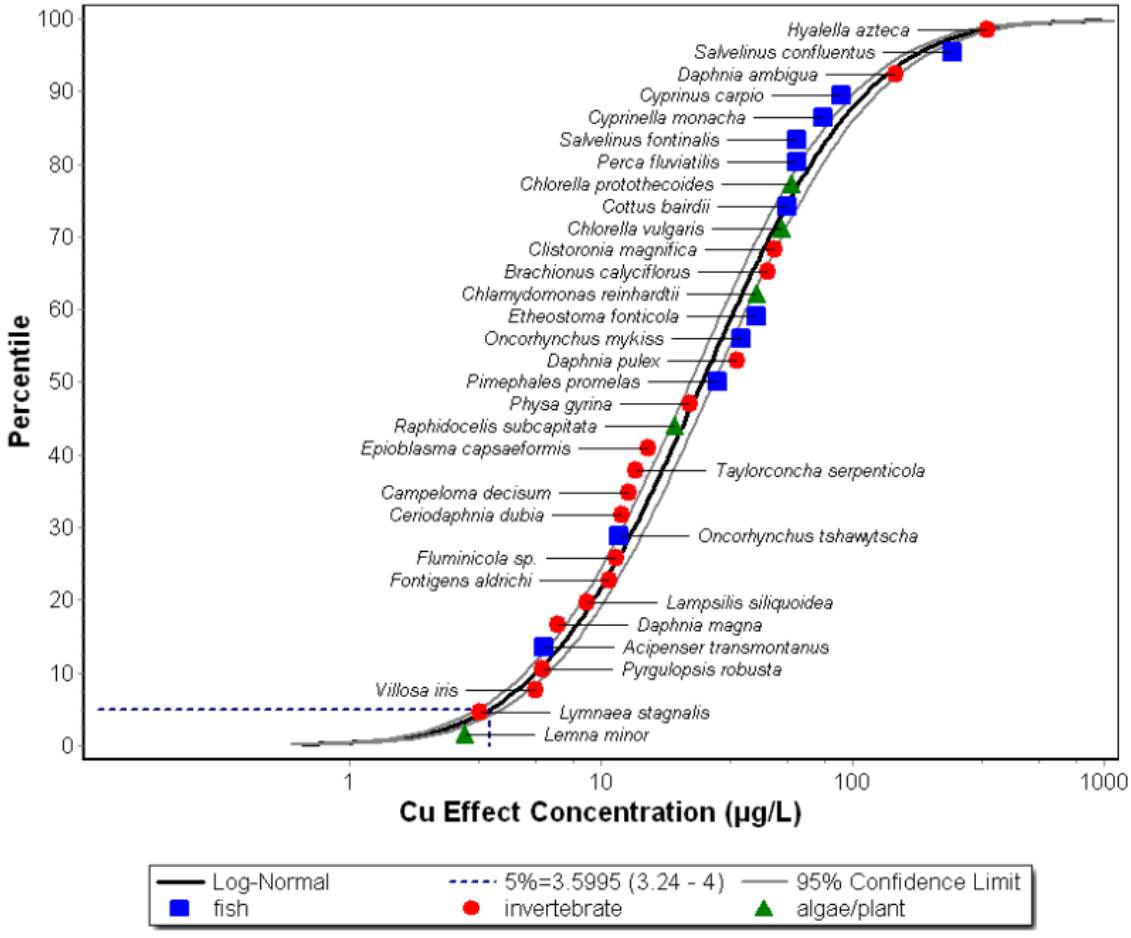

Figure 4-13. Site-specific species sensitivity distribution (SSD) for copper, based on best model fitting the long-term toxicity endpoints of 33 aquatic species

Example_Chronic.results.txt - Notepad

File Edit Format View Help

Chronic Copper Biotic Ligand Model (BLM)

Federal Water Quality Guideline (FWQG) for Copper Version 1.20

For the following calculation, the BLM is used in conjunction with acceptable chronic toxicity data for copper.

The BLM calculations here are resulting from three steps. In the first step, the BLM predicts bioavailability effects to adjust observed chronic toxicity values (EC10, MATC, NOEC, etc.) to values appropriate for the water chemistry of new water body. In the second step, most preferred endpoints along with the geometric means (where possible) for individual species are selected following the CCME protocol (2007). Finally, a HC5 is derived from these selected endpoints (one endpoint per species) as the 5-percentile value, using Log-Normal, Log-Logistic, Log-Gumbel and Log-Extreme Value (GEV) distribution models.

BLM Cu toxicity values normalized to chemistry found in the file:
C:\Users\DixitS\Desktop\Ver.1.20_EnvCanCu_Users\Data\Example.blm

Site Characteristics:

Site Name	Sample Name	Temp. C	pH	DOC mg C/L	HA %	Alkalinity mg/L CaCO3
Bow at Chuny	1	7.6*	8.05	2.2	10	141

Site Name	Sample Name	Ca mg/L	Mg mg/L	Na mg/L	K mg/L	SO4 mg/L	Cl mg/L
Bow at Chuny	1	49.4	15.8	15	1.83	54.8	14.9

*The lower limit of this parameter was used in the model because input value was too low.
**The upper limit of this parameter was used in the model because input value was too high.

Results for observation 1, Bow at Chuny, 1

Species	Taxonomic Group	Duration	Quant.	Effect	Log Effect Conc.	Effect Conc.	N
Lemna minor	algae/plant	7 d	EC10	root length	0.457	2.864	4
Lymnaea stagnalis	invertebrate	30 d	EC10	growth	0.5188	3.302	1
Villosa iris	invertebrate	28 d	EC10	dry weight	0.7406	5.503	3
Pyrgulopsis robusta	invertebrate	28 d	EC10	growth	0.7705	5.896	1
Acipenser transmontanus	fish	24 d	EC10	growth	0.7753	5.96	1
Daphnia magna	invertebrate	21 d	EC10	reproduction	0.829	6.745	4
Lampsilis siliquoidea	invertebrate	28 d	IC10	survival	0.9437	8.785	1
Fontigens aldrichi	invertebrate	28 d	EC10	survival	1.031	10.73	1
Fluminicola sp.	invertebrate	28 d	EC20	mortality	1.063	11.56	1
Oncorhynchus tshawytscha	fish	14 weeks	EC10	growth	1.072	11.81	1
Ceriodaphnia dubia	invertebrate	7 d	EC10	reproduction	1.081	12.06	4
Campeloma decisum	invertebrate	42 d	EC10	survival	1.113	12.97	2
Taylorconcha serpenticola	invertebrate	28 d	LC20	survival	1.139	13.79	1
Epioblasma capsaeformis	invertebrate	28 d	IC10	survival	1.187	15.37	1
Raphidocelis subcapitata	algae/plant	72 hr	MATC	growth	1.293	19.63	4
Physa gyrina	invertebrate	28 d	EC10	growth	1.353	22.56	1
Pimephales promelas	fish	30 d	IC10	growth	1.465	29.16	2
Daphnia pulex	invertebrate	42 d	NOEC	survival	1.54	34.71	9
Oncorhynchus mykiss	fish	200 hr	LC10	survival	1.556	35.97	1
Etheostoma fonticola	fish	30 d	IC10	survival	1.617	41.44	1
Chlamydomonas reinhardtii	algae/plant	3 d	EC10	growth	1.618	41.53	3
Brachionus calyciflorus	invertebrate	48 hr	EC10	intrinsic rate of...	1.663	46.05	1
Clistoronia magnifica	invertebrate	8 mo.	EC10	life cycle	1.693	49.29	1
Chlorella vulgaris	algae/plant	3 d	EC10	growth	1.716	51.99	17
Cottus bairdii	fish	28 d	EC10	biomass	1.742	55.18	1
Chlorella protothecoides	algae/plant	72 hr	MATC	growth	1.756	57	4
Perca fluviatilis	fish	30 d	MATC	growth	1.778	59.96	1
Salvelinus fontinalis	fish	30 d	EC10	reproduction	1.781	60.46	1
Cyprinella monacha	fish	30 d	IC10	biomass	1.882	76.15	1
Cyprinus carpio	fish	168 h	MATC	survival	1.959	90.89	1
Daphnia ambigua	invertebrate	10 d	EC10	reproduction	2.171	148.2	1
Salvelinus confluentus	fish	60 d	MATC	survival	2.397	249.3	1
Hyalella azteca	invertebrate	10 d	NOEC	survival	2.537	344.3	5

Estimated HC5 (5-percentile) based on:
Log-Normal Distribution Model (best) ..... 3.5995 (3.2360 - 4.0038)

Figure 4-10. Example output text file of site water chemistry normalized data plotted in SSD

4.8.1 Site characteristics

The text output file begins with a summary of the chemistry used for normalization, labeled as ‘Site Characteristics’. This includes the water chemistry inputs on every observation (line) in the site chemistry input file. If the model was run from the ‘Simplified Site Chemistry’ tab,

there will first be a list of the ion ratios used, the simplified data, and finally the estimated chemistry that was ultimately used in the BLM normalization.

4.8.2 Results

The results are presented as a series of sections showing a summary of the normalized SSD for each observation in the chemistry input file. It shows the species name, taxonomic group, test duration, endpoint quantifier, effect, log effect and effect concentrations, and number of database entries (labeled as 'N') for each species. The effect concentration selected for each species is the most preferred endpoint following CCME (2007), and is the value plotted in the SSD graphs. After each SSD, the estimated HC_5 values are given.

4.8.3 Appendix I

This section details the BLM-normalized critical values for each entry in the database, for each chemistry observation.

4.9 Batch mode

The BLM's batch mode dialog can be accessed from the File menu by clicking the "Run Batches..." menu item. The BLM can only accept 250 site chemistry observations at a time (because of memory issues), but monitoring datasets often contain many times that in observations. Because of this, a way to import large amounts of data and save and/or run it in (up to) 250-observation batches is useful. A screenshot of this dialog is shown in Figure 4-11 and the components seen there are explained below.

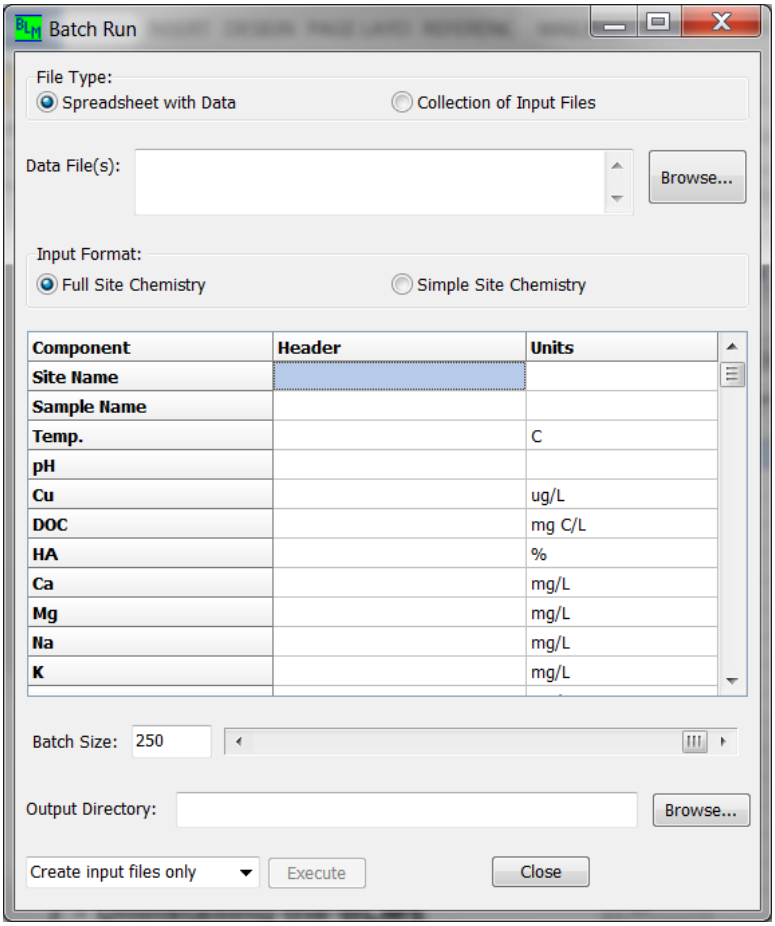

Figure 4-11. The batch run utility dialog

4.9.1 File type

In this section of the dialog, you can choose between the two file type options: "Spreadsheet with Data" or "Collection of Input Files". With the "Spreadsheet with Data" option, you can import data from a *.csv or *.xls file and have the program create BLM input files for you, and then optionally run the BLM with those files. The "Collection of Input Files" option will allow you to choose one or more BLM input files that have already been created and run each of them in sequence. The "Input Format", Component-Mapping Grid, and "Batch Size" sections will disappear when the "Collection of Input Files" option is selected, since they are only relevant when importing data to create input files.

4.9.2 Data file(s)

The "Data File(s)" section has a box where the name of the single data file or the list of BLM input files that is/are selected will appear. Click the "Browse..." button next to this box to select which file(s) to use. Note that only one data file can be selected, but multiple BLM input files can be selected. A data file should have all relevant site chemistry data in columns (i.e., a column for temperature, a column for pH, etc.) in one of the accepted units used for that component (go to the Inputs menu and click "Set Units" to see these options). The

columns should correspond to either full site chemistry components (temperature, pH, Cu, DOC, HA, Ca, Mg, Na, K, SO4, Cl and alkalinity) or simple chemistry components (temperature, pH, Cu, DOC and hardness) and should have unique names indicated in the first row. Accepted file types for data files are *.csv (comma-separated values) and *.xls (1997-2003 Microsoft® Excel). Conversely, the "Collection of Input Files" option will allow you to select any number and combination of *.blm (full BLM chemistry) and *.blme (simple BLM chemistry) files that it will then open and run in sequence.

4.9.3 Input format

This section only appears when the "Spreadsheet with Data" file type is selected. Here you can select which set of chemical components you would like to use, i.e. full or simple chemistry. If you select to use simple chemistry, then all of the input files that are created will use the ion ratios that are currently selected in the simple chemistry tab. You do not need to close the Batch Run dialog to change the ion ratio selection.

4.9.4 Component-mapping grid

This section only appears when the "Spreadsheet with Data" file type is selected. When you have selected a data file, the program will read the first row of the file for the column headers. These headers will now appear as drop-down box options in the column labeled "Header" of the component-mapping grid. The program makes guesses wherever possible to fill in these options (e.g., if you have a column called "DOC (mg/L)", it's going to fill that header in as the one to use for the DOC component). Check these assignments (the computer is only *slightly* smart) and fill in any that are missing by selecting an appropriate column header from the drop-down box that appears when you go to edit a cell. Also make sure to check that the units are correct – they should match the units of the data in your data file. All of the components need to have a header assignment in order to run batch mode. The same header can be used twice (e.g., if you only have one "ID" column, you can use that as both "Site Name" and "Sample Name").

4.9.5 Batch size

This section only appears when the "Spreadsheet with Data" file type is selected. The "Batch Size" section of the dialog has a small text box and a slider for selecting the size of the batches you would like the program to parse the data out into. It defaults to the maximum number of observations possible in one input file (250), but can be adjusted just in case a smaller number of observations per file is desired. Move the slider or type a number in the box to change the batch size. If the number of observations is not a multiple of the batch size, then the last batch will be smaller than the batch size number.

4.9.6 Output directory

The "Output Directory" section is for choosing and/or displaying where the files are going to be saved. With the "Spreadsheet with Data" option selected, you can choose a different directory for the newly created BLM input files and their associated output files to be saved in, or keep the default directory (the same directory the data file is in). Clicking the "Browse..." button will open a separate dialog, which the user can use to navigate to an

existing directory. A new directory can be created by modifying the "Directory Name" field of the selection dialog. With the "Collection of Input Files" option selected, the output directory will not be something that can be changed, but is just displayed for clarity – it will be the same directory that the input files come from.

4.9.7 Execute

The "Execute" button tells the program to perform the action displayed in the drop-down box next to the "Execute" button. The "Create input files only" option is available only when the "Spreadsheet with Data" file type option is selected. With this option selected, the program will not normalize any of the data, but will just make the input files and stop. If a "Run..." option is selected instead, then the program will do the equivalent of reading in an input file and clicking the Run button in the main interface. When all batches are finished running, a message will pop up that tells the user when it finished and how long it took. It takes about an hour to run one 250-observation batch, but the exact amount of time depends on computing power and how difficult the chemistry is for the BLM engine to converge on. Be patient and remember that the BLM engine is doing around 80 chemical equilibria calculations consisting of more than 100 chemical reactions, more than 25 mass balances, and solving a non-linear optimization algorithm, for each *one* site chemistry observation.

5 Example Application

The BLM Windows® Interface installation also features an example application for demonstration purposes. This file, named 'Example.blm,' is installed along with the BLM interface application and is located in the BLM data directory asked for during installation (by default within the 'My Documents' folder). The file can be opened directly, by double-clicking on the file name through a file-system manager such as Microsoft Windows® Explorer or by first starting the BLM Windows® Interface application and selecting the file through the 'File -----> Open' action. This example data file contains the water quality observation from an example site.

This data file 'Example.blm' can be used to normalize the SSD for Cu. Once the user has defined the scope of the BLM predictions, the BLM can be run using the shortcut Menu button 'Run BLM.' Depending on the number of lines of inputs in the BLM data file and the database, the runtime for the BLM predictions can vary from a few seconds to a couple hours. Upon completion of the BLM run, the user is informed of the names and the locations of the output files, and given the option to open the directory, as shown in Figure 5-1.

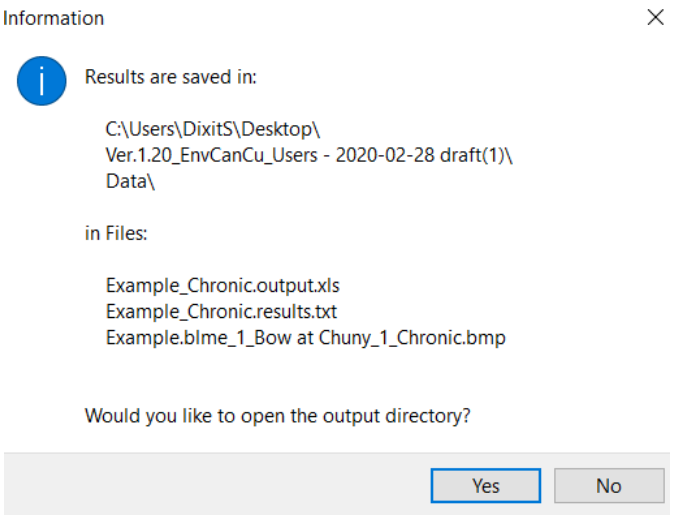

Figure 5-1. Example of notification window shown at completion of BLM run

The contents of the output files have been described in Section 4.8 – Description of output file.

6 Uninstalling the BLM

To uninstall the BLM Windows® Interface, select the uninstall utility using 'Start -----> Programs -----> Environment Canada Chronic Cu BLM-----> Uninstall.' All program files installed by the BLM during setup will be uninstalled. However, none of the files created by the user and saved in the BLM installation directory will be deleted during the uninstallation process. These will have to be deleted manually by the user, if so desired.

7 References

CCME. 2007. Canadian water quality guidelines for the protection of aquatic life: A protocol for the derivation of water quality guidelines for the protection of aquatic life 2007. Canadian Council of Ministers of the Environment, Winnipeg, MB.

[CEC] Commission for Environmental Cooperation. 1997. Ecological regions of North America. Toward a common perspective. Commission for Environmental Cooperation, Montreal, Quebec, Canada.

[ECCC] Environment and Climate Change Canada. 2021. Federal Environmental Quality Guidelines for Copper. Environment and Climate Change Canada, National Guidelines and Standards Office, Gatineau, Quebec.

[ESWG] Ecological Stratification Working Group. 1995. A national ecological framework for Canada. Agriculture and Agri-Food Canada, Research Branch, Centre for Land and

Biological Resources Research and Environment Canada, State of the Environment Directorate, Ecozone Analysis Branch, Ottawa, Canada.

Seppänen, O.A., W.J. Fisk and M.J. Mendell. 1999. Association of ventilation rates and CO_2 concentrations with health and other responses in commercial and institutional buildings. Indoor Air 9: 226-252.

Tipping, E. 1994. WHAM - a chemical equilibrium model and computer code for waters, sediments, and soils incorporating a discrete site/electrostatic model of ion-binding by humic substances. Comput. Geosci. 20: 973-1023.

Appendix: Parameter Ranges in Canada

Canadian water quality monitoring data summarized here, including copper concentrations (Table A- 1, ECCC 2021), were compiled by the Environment and Climate Change Canada. Data sources included ECCC monitoring programs and datasets provided by the provinces and territories. Every province and ecozone has data with temperatures below the model minimum of 8.5°C, a result that is not unexpected (Table A- 2). A few of the provinces have temperatures above the model maximum of 27°C, but they occur less than 10% of the time in the data. Nova Scotia, Ontario, and the Boreal Shield ecozone show more than 10% of observations with a pH value below the model minimum of 5.5, and Saskatchewan and the Northern Arctic ecozone show observations with more than 10% above the model maximum of 8.75 (Table A- 3). The DOC values in the monitoring data rarely fall outside the model range of 0.2 to 33.4 mg C/L, with less than 10% of data in each province and ecozone being outside the range (Table A- 4). The hardness values in the monitoring data are below the model minimum >50% of the time in Nova Scotia and >75% of the time in the Arctic Cordillera ecozone (Table A- 5). Other areas that tended to have soft waters were Newfoundland and Labrador (>25%), Nunavut (>25%), Northwest Territories (>10%), Ontario (>10%), and the Boreal Shield (>25%), Southern Arctic (>25%) and Taiga Shield (>25%) ecozones. Saskatchewan and the Prairie ecozone were alone in showing particularly hard waters, with >25% of monitoring data above the model maximum in Saskatchewan, and >10% in the Prairie ecozone. The individual cations tended to follow this same trend (Table A- 6 through Table A- 9), although sodium concentrations tended to be relatively lower across the board, in particular in the Arctic ecozones, and potassium concentrations tended to conform to the model bounds more closely. Sulfate concentrations (Table A- 10) were rarely lower than the model minimum, with <10% below the model minimum in all provinces and ecozones. Sulfate concentrations were high in Saskatchewan (>25% above the model maximum), British Columbia (>10%), and the Prairie (>10%) ecozone. Chloride concentrations are almost always within the model bounds in the monitoring data, with <10% outside the bounds in all ecozones and provinces (Table A- 11). The alkalinity values in the monitoring data were very rarely below the model minimum, and were only above the model maximum significantly often in Saskatchewan (>25% above model maximum), Manitoba (>25%), and the Boreal Plain (>25%) and Prairie (>10%) ecozones (Table A- 12). However, DIC from the monitoring data was higher than the model maximum by a significant amount in the majority of provinces and ecozones (Table A- 13).

Table A- 1. Ranges and quantiles of copper concentrations from Canadian monitoring data (units are µg/L).

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	347/5909	0.02	0.21	0.47	0.77	1.14	1.94	19
British Columbia	751/19018	0.02	0.25	0.44	0.7	1.38	3.33	4600
Manitoba	170/5045	0.2	0.8	1.11	1.82	3.36	6.47	2270
New Brunswick	320/4138	0.2	0.5	0.5	0.5	0.7	1	23
Newfoundland and Labrador	99/4680	0.02	0.19	0.26	0.44	1.35	2.22	30
Northwest Territories	53/2930	0.06	0.3	0.5	1	2	3.70	218
Nova Scotia	13/591	0.03	0.17	0.25	0.4	0.82	1.44	158
Nunavut	10/147	0.03	0.32	0.66	1.27	2.58	3.81	50
Ontario	539/29752	0.002	0.37	0.7	1	2.14	4.07	2320
Prince Edward Island	3/76	0.09	0.2	0.22	0.31	0.5	1.13	3
Quebec	164/1673	0.025	0.36	0.73	1.1	1.5	2.8	25
Saskatchewan	317/4293	0.02	0.17	0.9	1.5	2.71	8.29	5273
Yukon	11/1266	0.16	0.36	0.49	0.91	1.84	4.2	46
Summary by Ecozone								
Arctic Cordillera	2/21	0.37	0.44	0.99	2.1	2.62	3.09	10
Atlantic Maritime	346/4910	0.03	0.48	0.5	0.5	0.78	1.05	158
Boreal Cordillera	65/1291	0.05	0.32	0.46	0.83	1.53	3.8	46
Boreal Plain	297/5209	0.02	0.31	0.6	1	1.82	4	253
Boreal Shield	375/19489	0.002	0.23	0.4	0.7	1.23	2.62	2270
Hudson Plain	9/75	0.39	0.56	0.84	1.03	1.95	2.41	14
Mixedwood Plain	444/17144	0.021	1	1	1.52	2.72	4.39	2320
Montane Cordillera	462/14428	0.02	0.2	0.38	0.63	1.23	3	4600
Northern Arctic	7/70	0.03	0.20	0.61	1.29	3.15	6.53	50
Pacific Maritime	262/5447	0.05	0.37	0.52	0.81	1.5	3.72	400
Prairie	397/7827	0.05	0.54	0.91	1.66	2.74	6.09	5273
Southern Arctic	14/428	0.1	0.3	0.47	0.7	1.55	2	7
Taiga Cordillera	2/97	0.2	0.28	0.6	1.7	2.64	4.94	16
Taiga Plain	31/894	0.06	0.3	0.6	1.4	2.4	5	39
Taiga Shield	89/2176	0.05	0.25	0.4	0.7	1.1	2	40

Table A- 2. Ranges and quantiles of temperature from Canadian monitoring data (units are degrees Celsius). Acceptable ranges of model inputs for temperature are 8.5 to 27 degrees Celsius.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	685/14392	0	0	1.64	9.85	16	19.61	28
British Columbia	374/18780	0	0.2	2.5	6	11	15.5	28
Manitoba	207/14908	0	3.3	13.1	18.9	21.5	23.1	33
New Brunswick	64/2357	0	5.5	11.2	15.1	19.8	22.8	30
Newfoundland and Labrador	94/4136	0	0.3	2.61	8.76	14.76	18.52	26
Northwest Territories	13/221	0.08	2.13	6.87	12.17	16.27	19.09	23
Nova Scotia	12/760	0	0.18	2.73	10.96	17.18	20.49	26
Nunavut	-	-	-	-	-	-	-	-
Ontario	552/54265	0	2.9	4.8	10.2	17.9	21.8	38
Prince Edward Island	3/211	0	0.5	3.1	9.7	12.8	14.56	19
Quebec	151/955	0	7.48	11.23	15.76	19.05	22.5	27
Saskatchewan	244/3433	0	0.3	4.4	13	18.8	21.6	31
Yukon	10/1228	0	0	0	2.1	10	13	22
Summary by Ecozone								
Arctic Cordillera								
Atlantic Maritime	88/3382	0	2.3	9	14	18.8	22.1	30
Boreal Cordillera	11/1140	0	0	0	2	9.15	13	18
Boreal Plain	410/12603	0	0.04	7.56	15.5	20.1	22.3	30
Boreal Shield	323/36727	0	0.92	4.4	8	17	21.2	37
Hudson Plain	9/94	0	0	9.56	14.88	18.28	19.86	22
Mixedwood Plain	490/25510	0	4.5	8.3	14.8	19.8	22.7	38
Montane Cordillera	336/15394	0	0	1.9	5.2	9.9	15	28
Northern Arctic	-	-	-	-	-	-	-	-
Pacific Maritime	96/4129	0	3	5.1	9	13.5	17	25
Prairie	569/14345	0	0	3.03	11.9	18.2	21.7	31
Southern Arctic	4/29	5.9	8.95	10.62	11.48	14.74	16.25	17
Taiga Cordillera	2/92	0	0	0	4	12	16	22
Taiga Plain	2/16	0	2.35	5.13	10.45	12.25	13.6	22
Taiga Shield	75/728	0	1.185	6	12.35	16.29	18.6	23

Table A- 3. Ranges and quantiles of pH from Canadian monitoring data. Acceptable ranges of model inputs for pH are 5.5 to 8.75.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	699/15931	3.65	7.6	7.91	8.2	8.4	8.61	11
British Columbia	708/19008	4.3	7.3	7.6	7.9	8.1	8.3	10
Manitoba	205/8336	3.2	7.77	8.01	8.24	8.41	8.56	11
New Brunswick	320/4153	4.48	6.81	7.11	7.44	7.8	8.04	8.9
Newfoundland and Labrador	90/3856	3.63	5.57	6.1	6.59	7.03	7.45	9.8
Northwest Territories	53/2977	4.15	6.76	7.11	7.53	8	8.26	10
Nova Scotia	12/756	3.22	4.7	6.03	6.6	6.99	7.27	8.7
Nunavut	10/122	4.3	6.12	6.85	7.48	8.18	8.59	10
Ontario	585/36539	3.06	5.21	6.27	7.81	8.19	8.44	12
Prince Edward Island	3/204	6.8	7.2	7.5	7.8	8	8.2	10
Quebec	151/943	3	6.62	7.25	7.8	8.1	8.2	9.4
Saskatchewan	417/7437	4.45	7.72	8.04	8.32	8.58	8.8	11
Yukon	11/903	6.7	7.77	7.94	8.08	8.16	8.2	13
Summary by Ecozone								
Arctic Cordillera	2/17	5.77	5.86	6.4	6.9	7.47	7.88	8.3
Atlantic Maritime	343/5168	3.22	6.5	7	7.35	7.76	8.02	10
Boreal Cordillera	25/857	6.7	7.77	7.94	8.09	8.15	8.2	8.5
Boreal Plain	453/10739	3.65	7.57	7.9	8.2	8.43	8.67	11
Boreal Shield	373/20361	3.2	4.78	5.53	6.3	7.15	8	13
Hudson Plain	9/75	7.4	7.88	8.08	8.19	8.27	8.32	8.4
Mixedwood Plain	485/22736	3.06	7.54	7.83	8.09	8.31	8.53	13
Montane Cordillera	529/15932	4.9	7.5	7.8	8	8.2	8.3	10
Northern Arctic	7/63	4.3	6.06	6.95	7.98	8.41	8.94	10
Pacific Maritime	215/4474	4.3	6.9	7.3	7.57	7.8	8	9.6
Prairie	698/17459	5.34	7.77	8.04	8.28	8.48	8.67	10
Southern Arctic	14/414	5.64	6.54	6.66	6.84	7.47	8.2	13
Taiga Cordillera	2/46	7.43	7.76	7.95	8.05	8.16	8.24	8.3
Taiga Plain	30/924	6.44	7.51	7.84	8.11	8.30	8.55	9.6
Taiga Shield	86/1899	3	6.63	6.93	7.32	7.58	7.91	9.7

Table A- 4. Ranges and quantiles of dissolved organic carbon (DOC) from Canadian monitoring data (units are mg C/L). Acceptable ranges of model inputs for DOC are 0.2 to 33.4 mg C/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	519/10780	0.01	0.8	1.8	3.8	10	17.7	5950
British Columbia	632/16378	0.2	0.5	1	1.9	3.7	6.7	500
Manitoba	141/7438	1	7	8.8	10.9	13.7	17	99
New Brunswick	317/4156	1	2.5	3.6	5.9	8.1	10.9	34
Newfoundland and Labrador	99/4685	1	2.7	3.6	5.1	6.8	9.2	43
Northwest Territories	49/2009	0.5	1.8	2.6	4.3	6.4	7.9	56
Nova Scotia	13/1127	1	3.8	5.3	7.8	11.1	14.7	30
Nunavut	10/145	0.5	0.5	0.8	1.8	3.7	4.8	9.3
Ontario	319/21447	0.1	2.7	3.7	5.5	8.6	16.9	84
Prince Edward Island	3/111	0.5	1	1.3	2.2	4.3	8.7	13
Quebec	153/933	0.2	2.4	3	4.6	7.2	11.8	32
Saskatchewan	400/6019	1	5.3	10.2	14.6	20.2	28	2666
Yukon	10/1066	0.3	0.5	0.8	1.7	2.9	5.8	29
Summary by Ecozone								
Arctic Cordillera	2/21	0.5	0.5	0.5	0.6	0.9	1.4	1.8
Atlantic Maritime	341/5447	0.5	2.5	3.8	6.2	8.6	12.2	34
Boreal Cordillera	38/1007	0.3	0.5	0.7	1.5	2.5	4.1	29
Boreal Plain	363/7929	0.2	2.2	5.4	10	14.7	21	374
Boreal Shield	330/19565	0.5	2.8	4	6.3	10.2	18	84
Hudson Plain	9/75	5.6	6.9	7.8	8.7	9.5	12.5	20
Mixedwood Plain	231/8366	0.1	2.6	3.4	4.7	6.2	8.1	29
Montane Cordillera	423/13095	0.01	0.5	0.8	1.6	3.6	7	5950
Northern Arctic	7/67	0.5	0.5	0.7	1.2	1.9	3.4	8.4
Pacific Maritime	221/4351	0.5	0.8	1.3	2.2	3.3	5.1	500
Prairie	575/13427	0.3	2	4.2	10.9	15.8	21.1	2666
Southern Arctic	14/431	0.5	1.9	2.3	2.8	3.5	4.5	16
Taiga Cordillera	2/94	0.5	0.8	1.6	7.5	10.3	13.3	27
Taiga Plain	29/671	0.5	1.1	1.9	3.9	7.2	20	61
Taiga Shield	87/1747	0.9	2.6	3.6	5.2	6.5	7.3	35

Table A- 5. Ranges and quantiles of hardness from Canadian monitoring data (units are mg/L CaCO3). Acceptable ranges of model inputs for hardness are 7.9 to 525 mg/L CaCO3.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	550/10646	23.4	100	130	170	220	280	2270
British Columbia	682/18160	0.4	21.98	39.38	64	110	170	3400
Manitoba	173/5419	1.4	52.28	129	269	379	474	2990
New Brunswick	320/4135	1.2	8.78	12	22.9	46.6	68.2	361
Newfoundland and Labrador	99/4732	0.5	4.16	6.03	9.54	30	53.3	4055
Northwest Territories	53/2998	0.007	7	15	34.8	114.6	206.6	2280
Nova Scotia	13/1126	1.18	3.24	3.97	5.57	20.27	51.48	131
Nunavut	10/147	2.12	5.37	7.86	16.21	41.97	58.25	115
Ontario	543/30703	0.06	5.07	8.5	103	245	297	1510
Prince Edward Island	3/235	23.38	63.53	82.07	104	131.3	136.9	146
Quebec	154/954	4.02	10.23	23.23	67.24	105	117.8	235
Saskatchewan	407/6054	6	176	214	395	629	1643	60300
Yukon	10/1082	29.2	50.41	75.93	99.9	154.8	228	773
Summary by Ecozone								
Arctic Cordillera	2/21	2.16	4.06	5.48	6.41	7.59	8.26	16
Atlantic Maritime	344/5549	1.18	4.59	9.95	20.9	47.7	79.7	361
Boreal Cordillera	65/1111	0.5	48.9	62.4	97.2	155	268	773
Boreal Plain	387/7199	1.5	99.48	123	170	253	464.5	34890
Boreal Shield	379/20306	0.06	4.51	6.36	9.17	26.6	71	4055
Hudson Plain	9/75	43	68.96	83.3	92.5	120	134.4	151
Mixedwood Plain	440/16758	3.034	97.8	171	236.1	280	322	1510
Montane Cordillera	431/13818	0.4	36	56	79.5	132	200	2270
Northern Arctic	7/69	2.12	3.72	9.56	39.99	63.1	82.23	108
Pacific Maritime	247/5276	0.5	10.5	21	36	60	120	3400
Prairie	587/12535	7	160	190	264.9	427	651.7	60300
Southern Arctic	14/432	0.01	4.62	6.28	9.39	26.25	114.2	350
Taiga Cordillera	2/95	30.6	70.26	99.95	123	198	207.5	250
Taiga Plain	19/889	0.22	96.9	108	140.2	201.5	233.7	362
Taiga Shield	89/2245	0.5	4.5	7.34	16.24	29.4	65.12	158

Table A- 6. Ranges and quantiles of calcium from Canadian monitoring data (units are mg/L). Acceptable ranges of model inputs for calcium are 2.2 to 160.3 mg/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	503/9998	2.49	24.5	32.7	44	54	66	373
British Columbia	673/15094	0.05	6.8	11.2	18	30.1	49	420
Manitoba	173/5611	2.35	14.1	30.2	54	77	94.5	1160
New Brunswick	320/4134	0.26	2.71	3.81	7.47	15.48	22.8	67.6
Newfoundland and Labrador	99/4729	0.26	0.99	1.51	2.62	9.37	17.2	265
Northwest Territories	53/2993	0.07	1.49	4.03	9.3	31.8	53.6	824
Nova Scotia	13/1126	0.19	0.66	0.81	1.19	6.15	16.77	44
Nunavut	10/147	0.57	1.64	2.19	4.27	11.05	19.34	36
Ontario	480/24766	0.02	1.26	1.96	7.72	65.5	84.7	326
Prince Edward Island	3/235	5.7	14.4	18.88	25.5	44	46.9	51
Quebec	154/954	0.85	2.8	6.8	19	30	34	65
Saskatchewan	407/6055	1	36	47	65	92	124	566
Yukon	3/104	15.3	25.89	30.87	44.35	67.1	90.62	194
Summary by Ecozone								
Arctic Cordillera	2/21	0.7	1.33	1.75	1.99	2.32	2.63	5.2
Atlantic Maritime	344/5548	0.19	1.04	3.06	6.65	15.6	24.5	68
Boreal Cordillera	60/228	0.05	9.77	15	34	73.03	180	220
Boreal Plain	351/6641	2	25.7	31	42	55.4	82.1	824
Boreal Shield	376/19847	0.02	1.14	1.56	2.48	7.15	20	1160
Hudson Plain	9/75	13.2	20	24.65	27.5	30.45	31.62	37.5
Mixedwood Plain	381/11346	0.74	27.65	47.2	67.8	81.8	95	326
Montane Cordillera	426/11653	0.05	11	16	22	38	56	420
Northern Arctic	7/69	0.57	0.94	2.89	14.3	20.4	24.16	36
Pacific Maritime	245/4515	0.05	2.71	6.35	10.2	17	26	270
Prairie	574/12429	1	37	46	58.4	78	101	566
Southern Arctic	14/432	0.4	0.9	1.2	2.1	6.57	29.72	110
Taiga Cordillera	-	-	-	-	-	-	-	-
Taiga Plain	19/886	0.07	26.7	30.6	39	52.45	61.15	92
Taiga Shield	89/2243	0.5	1.10	1.81	4.35	7.61	17	177

Table A- 7. Ranges and quantiles of magnesium from Canadian monitoring data (units are mg/L). Acceptable ranges of model inputs for magnesium are 0.49 to 36.3 mg/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	433/9254	1.3	8.03	11	15	19.5	29.9	330
British Columbia	740/15276	0.01	0.8	1.95	4.1	7.6	15.4	650
Manitoba	173/5419	0.84	4.18	11.9	28.5	45.5	60.6	330
New Brunswick	320/4135	0.13	0.45	0.62	1.07	1.91	2.87	67
Newfoundland and Labrador	99/4729	0.14	0.36	0.46	0.77	1.66	2.66	824
Northwest Territories	53/2997	0.01	0.8	1.2	2.8	9.04	16.74	93
Nova Scotia	13/1126	0.17	0.38	0.46	0.59	1.13	2.37	4.9
Nunavut	10/147	0.1	0.31	0.52	1.1	2.34	4.25	8.1
Ontario	533/26837	0.002	0.36	0.58	3.12	15.6	22.6	168
Prince Edward Island	3/235	1.51	4.25	4.55	7.52	10.05	11.7	14
Quebec	154/954	0.29	0.75	1.5	4.3	7.3	8.37	24
Saskatchewan	407/6054	0.5	17	23	52	98	335	14600
Yukon	3/104	3.1	4.4	5.2	6.9	13.2	19.32	42
Summary by Ecozone								
Arctic Cordillera	2/21	0.1	0.18	0.29	0.33	0.41	0.54	0.8
Atlantic Maritime	344/5549	0.13	0.43	0.58	0.99	1.99	3.45	67
Boreal Cordillera	60/228	0.05	3.47	4.9	9.6	18.27	32	42
Boreal Plain	291/6040	1	6.9	10	15.5	29	59.2	8342
Boreal Shield	376/19890	0.002	0.33	0.46	0.7	1.58	4.6	824
Hudson Plain	9/75	2.46	4.64	5.01	6.11	11.65	13.68	14
Mixedwood Plain	432/13304	0.24	4.07	9.38	15.3	21	25.8	168
Montane Cordillera	468/11533	0.01	2	3.57	5.45	10.7	17	270
Northern Arctic	7/69	0.17	0.3	0.47	1.33	2.53	4.90	11
Pacific Maritime	255/4581	0.01	0.36	0.72	1.4	3.33	5.51	650
Prairie	568/12390	1	13.8	17.5	29.1	56	97.6	14600
Southern Arctic	14/432	0.2	0.6	0.7	1.1	2.34	8.71	24
Taiga Cordillera	-	-	-	-	-	-	-	-
Taiga Plain	31/901	0.01	6.77	7.72	10.2	16.4	21.2	38
Taiga Shield	89/2241	0.1	0.4	0.61	1.3	2.42	5.1	14

Table A- 8. Ranges and quantiles of sodium from Canadian monitoring data (units are mg/L). Acceptable ranges of model inputs for sodium are 1.2 to 505.8 mg/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	302/7235	0.33	2.4	5.7	13	31	78	2200
British Columbia	452/9081	0.05	0.94	1.59	2.6	5	10.6	5300
Manitoba	170/5163	0.03	2.52	6.01	23	61.7	106	773
New Brunswick	320/4134	0.53	1.42	1.86	2.59	3.9	6.02	558
Newfoundland and Labrador	97/1595	0.2	0.61	1.39	3.05	23.4	82.62	786
Northwest Territories	53/2376	0.03	0.5	0.8	1.72	2.7	8.16	3460
Nova Scotia	13/1126	2.02	3.21	3.62	4.28	8.89	21.81	310
Nunavut	10/147	0.09	0.32	0.45	0.58	0.69	1.03	3.03
Ontario	573/24597	0.005	0.61	0.86	2.4	12.6	41.6	5480
Prince Edward Island	3/76	3.19	5.68	7.27	8.17	9.42	9.99	11
Quebec	154/954	0.25	0.92	2.2	7.5	12	14	84
Saskatchewan	407/5754	0.3	13	26.1	77	183	491	25990
Yukon	3/81	0.4	1.24	2.7	3.3	4.1	5.9	11
Summary by Ecozone								
Arctic Cordillera	2/21	0.15	0.25	0.33	0.39	0.46	0.55	0.75
Atlantic Maritime	344/5389	0.53	1.51	2.09	3.08	4.55	9.48	558
Boreal Cordillera	50/157	0.52	0.932	2	3.5	9	14	540
Boreal Plain	215/5124	0.41	2.6	6.3	15	40.02	150.7	11980
Boreal Shield	375/16316	0.005	0.58	0.72	1.35	2.64	6.77	786
Hudson Plain	7/73	1.29	1.60	1.87	3.21	16.3	21.5	43.2
Mixedwood Plain	471/11711	0.04	1.7	5.88	12.6	32.2	75.8	5480
Montane Cordillera	307/6508	0.05	0.93	1.5	2.4	4.14	8.39	1700
Northern Arctic	7/69	0.09	0.29	0.39	0.58	1.06	1.69	3
Pacific Maritime	119/2761	0.05	0.86	1.66	3.36	7.8	15	5300
Prairie	544/11570	0.3	7.36	16	42.8	97.15	202	25990
Southern Arctic	14/409	0.03	0.4	0.5	0.6	0.8	1.1	3
Taiga Cordillera	-	-	-	-	-	-	-	-
Taiga Plain	19/384	0.35	1.5	2.92	5.33	8.61	13	32
Taiga Shield	88/1814	0.1	0.5	0.67	1.47	2.1	2.5	35

Table A- 9. Ranges and quantiles of potassium from Canadian monitoring data (units are mg/L). Acceptable ranges of model inputs for potassium are 0.2 to 10.4 mg/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	377/7849	0.2	0.5	0.8	1.5	3.2	8.6	123
British Columbia	484/9540	0.01	0.18	0.38	0.63	1.1	2	210
Manitoba	170/5162	0.02	1.01	2.33	7.01	11.6	14.9	57
New Brunswick	320/4134	0.05	0.25	0.31	0.38	0.52	0.78	22
Newfoundland and Labrador	97/1594	0.08	0.17	0.23	0.4	0.76	1.65	11
Northwest Territories	53/2377	0.1	0.4	0.53	0.86	1.1	1.44	12
Nova Scotia	13/1126	0.17	0.27	0.34	0.4	0.62	1.5	5
Nunavut	10/147	0.09	0.27	0.36	0.43	0.54	0.84	3.7
Ontario	537/24820	0.005	0.18	0.33	0.69	2	3.74	172
Prince Edward Island	3/76	0.56	0.85	0.99	1.16	1.25	1.32	2.5
Quebec	154/954	0.03	0.28	0.51	1.2	1.58	1.9	34
Saskatchewan	407/5754	0.2	3	6.74	14	23	61	3510
Yukon	3/81	0.27	0.57	1	1.3	1.5	1.9	3
Summary by Ecozone								
Arctic Cordillera	2/21	0.14	0.19	0.33	0.43	0.56	0.67	0.94
Atlantic Maritime	344/5389	0.05	0.26	0.31	0.4	0.54	0.94	22
Boreal Cordillera	53/160	0.19	0.4	0.78	1.3	2.28	8.3	110
Boreal Plain	255/5434	0.1	0.6	1	2.63	8.57	14.7	746
Boreal Shield	373/16458	0.005	0.14	0.24	0.38	0.59	1.24	35.5
Hudson Plain	4/70	0.44	0.53	0.60	0.96	2.83	3.18	3.4
Mixedwood Plain	440/11794	0.06	0.86	1.32	2.07	3.37	4.99	172
Montane Cordillera	341/6986	0.05	0.33	0.5	0.67	1.2	2	103
Northern Arctic	7/69	0.09	0.23	0.31	0.41	0.53	0.79	3.7
Pacific Maritime	137/2965	0.01	0.10	0.17	0.34	0.84	2	210
Prairie	556/11646	0.27	1.1	2.3	8	15	23	3510
Southern Arctic	14/409	0.1	0.34	0.4	0.5	0.6	0.7	2.3
Taiga Cordillera	-	-	-	-	-	-	-	-
Taiga Plain	19/384	0.13	0.48	0.77	1.01	1.41	2.17	7.5
Taiga Shield	88/1816	0.03	0.33	0.46	0.8	1.08	1.2	4.4

Table A- 10. Ranges and quantiles of sulfate from Canadian monitoring data (units are mg/L). Acceptable ranges of model inputs for sulfate are 0.5 to 330 mg/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	466/9810	0.5	10	21.42	41.45	64	120	7750
British Columbia	57/9894	0.5	2.5	6.2	11	41.18	580	740
Manitoba	171/5199	0.3	2.38	11.95	69.4	189	287	2800
New Brunswick	320/4179	0.12	1.69	2.32	3.52	5.91	10.1	139
Newfoundland and Labrador	99/4714	0.2	0.6	0.83	1.68	6.7	12.6	111
Northwest Territories	53/2966	0.3	2	3	5	27.2	60.55	1840
Nova Scotia	13/1550	0.7	1.33	1.68	2.23	6.47	17.7	52
Nunavut	10/146	0.3	0.69	1.14	2.44	6.2	10.85	47
Ontario	110/12659	0.05	0.6	2.4	3.7	5.1	6.81	213
Prince Edward Island	3/281	2.11	4.34	5	6.9	9.6	10.8	13
Quebec	16/102	0.6	1.2	1.6	2.15	3.43	7.2	13
Saskatchewan	405/5888	0.4	51.97	95.18	270	590	1919	98300
Yukon	11/1294	2.9	6.9	12.92	17.85	47	88.07	541
Summary by Ecozone								
Arctic Cordillera	2/21	0.72	2.14	2.66	2.99	3.82	5.14	12
Atlantic Maritime	336/6015	0.12	1.56	2.11	3.37	6.20	11.41	139
Boreal Cordillera	8/1164	2.9	6.9	12.3	16.9	40	90	541
Boreal Plain	345/6495	0.5	6	17	40	78.4	238.6	57730
Boreal Shield	288/17539	0.05	0.64	1.62	3.4	5.2	8.74	1570
Hudson Plain	4/70	0.3	0.5	0.52	5.85	26.38	36.12	38.5
Mixedwood Plain	20/676	0.05	2.95	3.49	4.75	19.18	34.5	213
Montane Cordillera	71/8603	0.5	4.09	8.29	14.5	57	580	740
Northern Arctic	7/68	0.55	1.1	4.46	7.82	10.72	18.68	47
Pacific Maritime	14/2272	0.5	1.1	2.82	7.2	11	18.5	54
Prairie	571/12195	0.3	31.3	53	120	290	635.1	98300
Southern Arctic	14/432	0.3	1	1.79	2	3	10	205
Taiga Cordillera	2/97	3.5	11.9	21.9	43	52	60.8	90
Taiga Plain	18/875	1	19	25.6	40.4	58.65	78.58	135
Taiga Shield	39/2147	0.2	0.61	1	2.9	4	7	48

Table A- 11. Ranges and quantiles of chloride from Canadian monitoring data (units are mg/L). Acceptable ranges of model inputs for chloride are 0.2 to 989.1 mg/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	345/8090	0.04	0.8	1.2	3.7	9.2	20	1500
British Columbia	462/12679	0.02	0.5	0.6	1.3	3.1	7.1	11000
Manitoba	171/5349	0.1	1.1	3.54	15.4	30.6	80.32	1410
New Brunswick	320/4179	0.07	0.9	1.51	2.87	4.39	8.64	898
Newfoundland and Labrador	99/4714	0.07	0.24	2.05	5.3	43.18	154	2770
Northwest Territories	53/2923	0.05	0.35	0.7	1.54	2.7	7.31	5750
Nova Scotia	13/1550	0.1	4.5	5.15	6.6	14.88	39.41	526
Nunavut	10/146	0.07	0.12	0.19	0.35	1.06	1.45	2.42
Ontario	594/37300	0.002	0.3	1.61	12.7	35.9	82	18200
Prince Edward Island	3/282	5.76	11.95	14.1	15.45	22.4	23.6	27
Quebec	89/525	0.06	0.37	1.2	3.6	9.6	24	170
Saskatchewan	391/4847	0.2	3.8	8.5	22.8	57.7	137.9	24460
Yukon	11/1296	0.05	0.12	0.2	0.3	0.5	0.8	6.8
Summary by Ecozone								
Arctic Cordillera	2/21	0.09	0.1	0.13	0.16	0.2	0.21	0.66
Atlantic Maritime	344/6064	0.07	1.11	2.14	3.94	7.13	17.9	898
Boreal Cordillera	46/1244	0.05	0.11	0.2	0.3	0.5	0.8	1000
Boreal Plain	250/5390	0.2	1	2	5.96	19.48	115.1	5750
Boreal Shield	378/20523	0.004	0.24	0.38	1.96	5.8	23.8	2770
Hudson Plain	4/70	0.1	0.76	0.98	1.64	17.32	21.37	25
Mixedwood Plain	478/22700	0.002	7.4	14	27.3	54.9	111	18200
Montane Cordillera	332/10223	0.02	0.42	0.5	1.1	2.4	4.6	200
Northern Arctic	7/68	0.07	0.1	0.15	0.23	0.53	2.38	4.1
Pacific Maritime	138/3499	0.1	0.5	0.8	2.1	6.2	14	11000
Prairie	514/10562	0.1	2.3	6	14	31.2	72.66	24460
Southern Arctic	14/409	0.1	0.26	0.4	0.7	0.8	1.35	25
Taiga Cordillera	2/96	0.1	0.29	0.6	1.35	4.93	5.85	6.8
Taiga Plain	18/875	0.05	0.18	0.36	1.84	5.07	8.43	49
Taiga Shield	39/2123	0.07	0.18	0.4	1	1.72	2.2	11

Table A- 12. Ranges and quantiles of alkalinity from Canadian monitoring data with missing data filled in by converting DIC and pH to alkalinity (units are mg/L CaCO3). Acceptable ranges of model inputs for alkalinity are 0.007 to 325.91 mg/L CaCO3.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	464/10103	0.1	90.42	120	150	206	300	2750
British Columbia	501/11730	0.001	12	26.92	51.9	90	140	2062
Manitoba	193/8031	5.7	57.9	130	254	1018	1958	7113
New Brunswick	320/4187	0.009	6.04	8.54	18.4	38.4	57	167
Newfoundland and Labrador	99/4764	0.01	2	3.63	7.6	18.4	25.77	200
Northwest Territories	53/2935	1.2	4.3	13	29.6	88.25	144	362
Nova Scotia	13/1474	0.02	1.7	20	20	20	26.94	68
Nunavut	10/146	1.2	3.5	5.95	16.9	37.85	48.1	66
Ontario	595/35497	0.002	2.2	5.45	113	209	241	6254
Prince Edward Island	3/130	22.25	51.75	66.61	83	92.14	119.3	1047
Quebec	15/75	8	9	11	17	27	34	54
Saskatchewan	404/5897	6.11	140	168	246	328	413	10300
Yukon	11/1302	22.7	44.7	65.1	85.6	103	140	806
Summary by Ecozone								
Arctic Cordillera	2/21	1.5	2.8	3	3.9	5	5.4	6.2
Atlantic Maritime	336/5795	0.009	5.6	9.6	20	35.1	56	1047
Boreal Cordillera	44/1248	7.2	44	63	84.8	102	145	806
Boreal Plain	353/7906	7.1	94.85	129.2	174	347	1300	5817
Boreal Shield	358/21372	0.002	1.3	2.8	5.75	20.2	75	4470
Hudson Plain	9/75	40	69.4	74.8	91.3	101	113.2	121
Mixedwood Plain	436/20485	0.5	96.6	153	201	230	254	6254
Montane Cordillera	363/8918	0.001	30	49	64.25	109	150	2062
Northern Arctic	7/68	1.2	3.54	6.05	32.35	50.45	63.84	86
Pacific Maritime	129/3755	0.5	6.5	11	21	40	96.41	1043
Prairie	576/13085	5.4	130	160	230	303	444	10300
Southern Arctic	14/431	1.2	3.3	3.8	5.5	24.85	98.4	232
Taiga Cordillera	2/96	22.7	50.9	64.6	93.35	158	166	394
Taiga Plain	20/865	14.7	68.2	80.9	101	146	170	244
Taiga Shield	39/2150	0.1	3.65	5.9	15.5	23.87	60.41	99

Table A- 13. Ranges and quantiles of dissolved inorganic carbon (DIC) from Canadian monitoring data with missing data filled in by converting alkalinity and pH to DIC (units are mmol/L). Acceptable ranges of model inputs for DIC are 0.0162 to 6.37 mmol/L.

Geographic Unit	Numbers (sites/samples)	Minimum	10%	25%	50%	75%	90%	Maximum
Summary by Province								
Alberta	462/10010	0.11	1.86	2.43	3.05	4.17	6.11	102
British Columbia	431/11735	0.01	0.33	0.80	1.90	11	22.2	77
Manitoba	193/8011	0.17	2.77	11.8	31	53.2	68.7	568
New Brunswick	320/4165	0.003	0.15	0.21	0.41	0.81	1.19	38
Newfoundland and Labrador	99/4718	0.05	0.7	1.1	1.7	3.1	6.1	48
Northwest Territories	53/2893	0.03	0.13	0.3	0.63	1.82	2.94	263
Nova Scotia	13/1312	0.42	0.5	0.69	1.59	5.7	9.1	543
Nunavut	10/119	0.03	0.08	0.17	0.46	0.83	1.17	106
Ontario	583/33840	0.002	0.11	0.24	3.4	7.3	49.5	4233
Prince Edward Island	3/98	0.78	6.81	12.19	18.2	20.95	22.96	29
Quebec	15/42	0.23	0.32	0.39	0.55	0.68	0.79	1.1
Saskatchewan	404/5857	0.14	2.82	3.37	4.91	6.62	8.38	724
Yukon	11/1192	0.75	2.55	10.5	17.9	22.5	33.8	52
Summary by Ecozone								
Arctic Cordillera	2/17	0.037	0.06	0.07	0.13	0.16	0.29	0.44
Atlantic Maritime	336/5577	0.003	0.17	0.26	0.6	1.08	4.4	543
Boreal Cordillera	24/1094	0.16	2.33	10.4	17.7	22.2	28.78	48
Boreal Plain	354/7909	0.14	1.96	2.66	3.98	21.8	41.52	724
Boreal Shield	354/20790	0.002	0.08	0.15	0.39	1.8	10	568
Hudson Plain	9/75	9.2	15.22	16.65	19.9	22.9	25.52	29
Mixedwood Plain	428/19354	0.002	2.23	3.73	4.87	44.2	53.9	4233
Montane Cordillera	329/9127	0.02	0.83	1.19	2.25	11.5	21.1	50
Northern Arctic	7/60	0.03	0.08	0.36	0.76	1.17	1.86	106
Pacific Maritime	110/3469	0.01	0.2	0.27	0.56	6.4	20.26	77
Prairie	576/13057	0.11	2.65	3.29	4.90	8.95	58.7	331
Southern Arctic	14/412	0.03	0.09	0.10	0.16	0.54	1.98	5
Taiga Cordillera	2/98	4.6	11.49	14.92	20.85	37.55	39.2	52
Taiga Plain	20/842	0.35	1.44	1.67	2.11	2.98	3.60	13
Taiga Shield	39/2110	0.04	0.14	0.32	0.51	1.3	2.3	63