BIOTIC LIGAND MODEL WINDOWS® INTERFACE, RESEARCH VERSION 3.16.2.41: USER'S GUIDE AND REFERENCE MANUAL

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Table of Contents

Tables

Figures

Acronyms

Acronym	Definition
Ag	silver
BLM	Biotic Ligand Model
Ca	calcium
Ca^{2+}	calcium ion
$CaCO_3$	calcium carbonate
CCC	Criterion continuous concentration
CHESS	Chemical Equilibria in Soils and Solutions
Cl	chloride
CMC	Criterion maximum concentration
CO_3	carbonate
Cu	copper
DIC	dissolved inorganic carbon
DOC	dissolved organic carbon
EPA	US Environmental Protection Agency
FAV	final acute value
FMB	fixed monitoring benchmarks
H_2CO_3	carbonic acid
HC5	Concentration corresponding to the 5th percentile of the species sensitivity distribution (SSD)
HCO_3	bicarbonate
IWQC	instantaneous water quality criteria
K	potassium
LA50	accumulation of metal on the biotic ligand that is lethal to 50% of an exposed population
LC50	concentration that is lethal to 50% of an exposed population
Mg	magnesium
Na	sodium
NOM	natural organic matter
Pb	lead
QA/QC	quality assurance/quality control
SO_4	sulfate

SSD	Species sensitivity distribution showing the range in organism sensitivity to a toxicant ordered from most sensitive to least sensitive
TU	toxic unit
WER	water effect ratio
USGS	US Geological Survey
WHAM	Windermere Humic Aqueous Model
WQC	water quality criteria

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ADDITIONAL INFORMATION

Additional information can be found In the User's Guide, or online at:

http://www.windwardenv.com/biotic-ligand-model

Contact Information

For questions or problems, including bug reports, relating to the use and the application of the Biotic Ligand Model or the BLM Windows® Interface, please contact either:

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Additional information can be found online at:

http://www.windwardenv.com/biotic-ligand-model

1   Introduction to the BLM

1.1   INTRODUCTION

Metal bioavailability and toxicity have long been recognized to be a function of water chemistry (Sunda and Guillard 1976; Sunda and Hansen 1979). For example, the formation of inorganic and organic metal complexes and sorption on particle surfaces can reduce metal toxicity. As a result, metal toxicity can be highly variable and dependent on ambient water chemistry when expressed as total or dissolved metal concentrations. In contrast, the effects of water chemistry on metal toxicity can often be reduced or eliminated when metal toxicity is related to free metal ion concentrations (Sunda and Guillard 1976). Allen and Hansen (1996) have shown the relationship between metal speciation and toxicity and have used this relationship to predict the range of effects that site-specific water quality characteristics can have on copper (Cu) toxicity.

1.2   BLM FRAMEWORK AND CONCEPTUAL MODEL

The Biotic Ligand Model (BLM) was developed to incorporate metal speciation and the protective effects of competing cations into predictions of metal bioavailability and toxicity (Di Toro et al. 2001; Paquin et al. 1999; Santore et al. 2001; Santore et al. 2002). The BLM is based on a conceptual model similar to the gill site interaction model proposed by Pagenkopf (1983) and is conceptually similar to the Free Ion Activity Model (Morel and Hering 1993). The BLM incorporates a version of Chemical Equilibria in Soils and Solutions (CHESS) (Santore and Driscoll 1995) that has recently been modified to include the chemical and electrostatic interactions described in the Windermere Humic Aqueous Model (WHAM) (Tipping 1994). Metal toxicity is simulated as the accumulation of metal at a biologically sensitive receptor, the "biotic ligand," which represents the site of action of acute metal toxicity. Inorganic and organic ligands can also bind metal, however, thereby reducing accumulation at the biotic ligand. By incorporating the biotic ligand into a chemical equilibrium framework that includes aqueous metal complexation, the relation between free metal ion concentrations and toxicity is an inherent feature of the model.

The BLM framework also incorporates the competitive effects of other cations that interact with the biotic ligand to mitigate toxicity. For example, at a fixed free metal concentration, as hardness increases, the increased calcium ion (Ca^{2+}) competes with the free metal for binding sites at the biotic ligand. A higher free metal concentration is therefore required to achieve the same toxic effect in the presence of the elevated Ca^{2+} concentration. The BLM uses this competitive mechanism to simulate the reduction in metal toxicity due to elevated hardness concentrations. Thus, the BLM can effectively account for reduction in metal toxicity due to elevated levels of hardness cations (Meyer et al. 1999).

The BLM has been developed using published information on metal toxicity and biotic ligand accumulation as a function of water chemistry. The most comprehensive data compiled to date for use with the BLM is for Cu toxicity to fathead minnows (*Pimephales promelas*). The "biotic ligand" or site of acute Cu toxicity for fathead minnow has been identified as sodium (Na) ion uptake channels in the gill membrane (Playle et al. 1993a). Cu accumulation on the gill has been associated with respiratory distress and decreased blood plasma Na concentrations due to interference with these sites (Playle et al. 1992). The adsorption of Cu on gill surfaces in the BLM has been calibrated to measurements of Cu accumulation on the gill over a wide range of water quality conditions (Playle et al. 1992; Playle et al. 1993b). Additionally, MacRae (1999) established a dose response relationship necessary to determine the biotic ligand LC50 (concentration that is lethal to 50% of an exposed population) in rainbow trout. In the BLM, metal toxicity is defined as the amount of metal necessary to result in accumulation at the biotic ligand equal to the biotic ligand LC50. While others have developed models capable of predicting metal bioaccumulation on the gill in short term exposures (Playle et al. 1993a, b), the BLM is the first that includes a scheme for predicting toxicity. The BLM for other metals and organisms is based on a similar approach.

1.3 BLM APPLICATIONS

In summary, the BLM can be used to calculate the chemical speciation of a dissolved metal, including complexation with inorganic and organic ligands, and the biotic ligand. The biotic ligand represents a discrete receptor or site of action on an organism where accumulation of metal leads to acute toxicity. The BLM can therefore be used to predict the amount of metal accumulation at this site for a variety of chemical conditions and metal concentrations (i.e., the inorganic, organic, and biotic speciation of metals in aquatic settings).

According to the conceptual framework of the BLM, the accumulation of metal at the biotic ligand at or above a critical threshold concentration leads to acute toxicity. This critical accumulation on the biotic ligand is also termed the LA50 (the accumulation of metal on the biotic ligand that is lethal to 50% of an exposed population) or, for example, the EA20 for chronic toxicity (the accumulation of metal on the biotic ligand that causes a defined effect in an exposed population). The LA50 is expressed in units of nmol/g wet weight of the biotic ligand. Since the BLM includes inorganic and organic metal speciation and competitive complexation with the biotic ligand, the amount of dissolved metal required to reach this threshold will vary, depending on the water chemistry. Therefore, in addition to calculating chemical speciation, the BLM can also be used to predict the concentration of metal that would result in toxicity within a given aquatic system.

2   Overview and Help File Layout

2.1   WHAT'S NEW IN THIS DISTRIBUTION?

Starting with Version 3.16.2.41, there is the capability to switch between freshwater and marine simulations. Two new file types have consequently been introduced for full-chemistry marine inputs and simple salinity-based chemistry inputs. A new salinity-based chemistry tab will become available in marine mode. Additionally, the metal and organism selection screen has been modified to accommodate chronic endpoints, where the user can choose between different endpoints and lifestages for organisms, where available. Finally, a feature has been added which allows the user to view the console windows that show the progress of the BLM calculation engine. This is particularly useful for determining when the engine is having trouble converging and getting "stuck".

2.2   HELP FILE LAYOUT

The remainder of this document describes the hardware and software requirements for installing and running the BLM Windows® Interface, details the data requirements of the BLM, and provides a step-by-step guide to using the various functionalities of the BLM Windows® Interface and a walk-through of the application using an example BLM data file.

3   Setup and Installation

3.1   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.

3.2   INSTALLING THE BLM WINDOWS® INTERFACE

Installing from a setup file – To install the BLM Windows® Interface from the setup file "BLM_3.16.2.41_setup.exe" simple double click on the file and follow the prompts. 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 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.

Installing from the compressed (.zip) file – To install the BLM Windows® Interface from the compressed file, simply unzip the entire package to a folder in the documents directory on your hard disk. If your zip utility asks if you would like to preserve paths, say "yes". Do not try to run it from the desktop or a server folder since that sometimes causes program errors. Once the zip file is unpacked, you can start the program by clicking on the file "BLM_UI.exe", which will have a BLM icon.
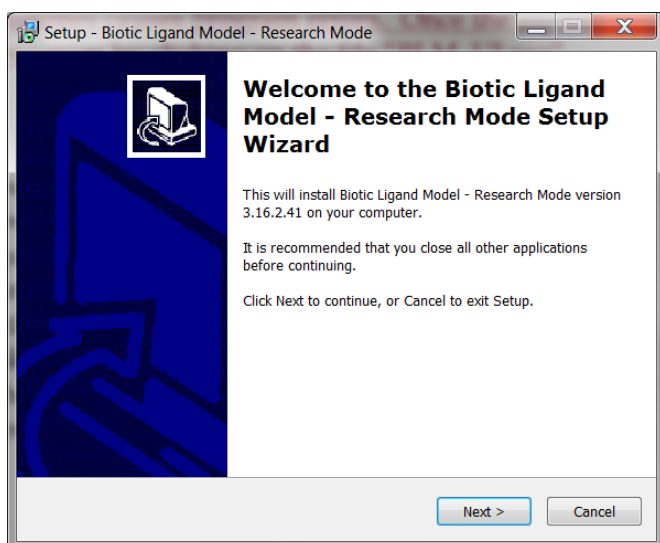

Figure 2-1.   Opening screen for the BLM setup program

4   Data Requirements

The BLM predicts metal 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, with certain parameters that may be measured in the field or laboratory depending on the purpose of the BLM simulation (e.g., pH and temperature as discussed below). This section describes the general physical and chemical data requirements for an application of the BLM to predict metal speciation, toxicity, or WQC in aquatic systems.

4.1   SITE CHEMISTRY

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

- ◆ Temperature
- ◆ pH
- ◆ Metal concentration
- ◆ Dissolved organic carbon (DOC)
- ◆ Major cations (calcium [Ca], magnesium [Mg], sodium [Na] and potassium [K])
- ◆ Major anions (sulfate [SO_4] and chloride [Cl])
- ◆ Alkalinity
- ◆ Sulfide
- ◆ Other components (possible with marine parameter files or user-created parameter files)

For a given metal, some of these chemical inputs have an important effect on metal 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. However, if some of the parameters are known to be absent in the water sample, a nominal, negligible concentration should be input (a value on the order of 1E-10 mg/L is typically sufficient) rather than a zero concentration.

The BLM also allows estimation of major ions from hardness and ion ratios (see section 4.2) or salinity and base marine chemistry (see section 4.3), thereby allowing the model to run with only Temperature, pH, DOC, and hardness or salinity.

4.1.1 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. Note that laboratory temperature conditions would be relevant when the BLM is being used to explain or predict toxicity tests conducted in the laboratory. Field temperatures, on the other hand, would be more appropriate when using the model to extrapolate to field conditions.

4.1.2 pH

Accurate pH values are important to BLM results for most metals. The chemical speciation of many metals, such as Cu, is directly affected by pH. Sample pH is also important in determining the metal complexation capacity of dissolved organic matter. It is also important in determining the speciation of inorganic carbon, which relates to the formation of metal 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 metal toxicity, then it is preferable that the pH be measured within the test chamber during the exposure. As with temperature, it may be more appropriate to use laboratory pH when the BLM is being used to explain or predict toxicity tests conducted in the laboratory, and field pH to extrapolate to field conditions.

4.1.3 Dissolved organic carbon

Dissolved organic matter can play a critical role in determining metal 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. For water with low DOC, it is important to make sure that analytical detection limits are sufficiently low. 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 (NOM) 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 more complex organic molecules. Total organic matter can be broken down into particulate organic matter and dissolved organic matter. Although the exact cutoff is somewhat arbitrary, the standard is

dissolved organic matter can pass through a 0.45 micron filter and particulate organic matter gets caught in the filter. 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 purposes 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 the TOC.

It should not be expected that DOC from artificial sources (e.g. acetate, sugar, MOPS, etc…) behave as natural organic matter. The organic matter binding model that the BLM uses is based on natural sources of organic matter, and inputs should therefore not include known quantities of artificial organic matter. If there is a significant amount of artificial organic carbon in the solution, then a speciation model that includes that chemical component may be necessary to accurately model it.

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.

4.1.4 Metal concentrations

It is not necessary to input metal concentrations for the model to calculate toxicity or instantaneous WQC; however, metal concentrations are needed to run the model in speciation mode.

Future versions of the BLM will include the ability to predict Fixed Monitoring Benchmarks (FMBs; see HydroQual(2008). Users should be aware that metal concentrations will be required to calculate the FMB in subsequent versions.

4.1.5 Major cations

The cations Ca, Mg, Na, and K are all necessary inputs to the BLM. For Cu and silver (Ag), Ca and Na can directly compete with the metal at biotic ligand sites; these cations will, therefore, have a direct effect on predictions of metal 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 metal toxicity in the BLM and can be estimated if measurements do not exist. Although K does not have direct effects on metal 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 effect the metal toxicity – typically, but not always, to a small extent.

4.1.6 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 4.1.7). 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 are not available, however, the concentrations can be estimated. For Cu and most other metals simulations, Cl is only important as a contribution to ionic strength, but for Ag simulations, Cl can have additional importance due to the formation of silver-chloride complexes. Therefore, it is preferable that only measured Cl concentrations be used for BLM applications involving Ag, while estimates can be used for applications involving other metals.

4.1.7 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. The one exception is Ag, which does not form carbonate complexes, and so DIC is not a critical input to BLM applications for Ag. Unfortunately, measurements of DIC are not often made in natural water samples, but it can be estimated from alkalinity and pH measurements, as in Equation 4-1.

$$DIC = Alk \cdot \frac{\dfrac{[H]}{K_1} + 1 + \dfrac{K_2}{[H]}}{1 + \dfrac{2 \cdot K_2}{[H]}}$$

Equation 4-1

where:

Alk   =   alkalinity in equivalents/L

   = 2×10^{-5} x alkalinity (as mg calcium carbonate [$CaCO_3$]/L)

$$[H] = 10^{-pH}$$

$$K_1 = 10^{-6.352}$$

$$K_2 = 10^{-10.329}$$

The BLM Windows® Interface uses this expression to calculate the DIC internally, and so only the alkalinity and the pH need to be specified. Alkalinity should be measured on filtered samples to eliminate potential contribution from suspended $CaCO_3$ and specified in units of mg/L of $CaCO_3$. If there are chemical additions that affect alkalinity but would not affect DIC, those quantities should be excluded from the input alkalinity concentrations. However, depending on the inorganic carbon option selected, the user may also opt to specify DIC concentrations directly, or choose to have the BLM calculate the DIC that would result from atmospheric CO_2 being in equilibrium with the site chemistry. This last method assumes a pCO_2 of 3.5, and calculations are done within the BLM engine. It differs from the atmospheric alkalinity calculation done when converting between simple and full site chemistry (see Section 4.2.4) in that all of the chemical equilibria equations will be considered, not just carbonate equilibria equations.

4.1.8 Sulfide

Although it has traditionally been assumed that sulfide concentrations are negligible in aerated waters, recent evidence suggests that appreciable sulfide concentrations persist in both marine and fresh waters. Waters affected by wastewater treatment plant effluents in particular can have elevated sulfide concentrations. Sulfide has a strong affinity for many metals and is therefore an important consideration in determining metal speciation and bioavailability. Therefore, if it is present, measured sulfide should be considered a required input to the BLM, especially when sulfide concentrations are similar to the predicted effect levels for a given metal and organism.

At the present time, researchers at several universities are still looking into the nature of sulfide-metal complexes in aqueous systems. The persistence of sulfide in aerated waters may be linked to the formation of stable metal-sulfide clusters, and these clusters may not be detected by traditional sulfide measurements. Alternatively, strong metal complexes that are believed to be due to sulfide compounds may be due to other forms of reduced sulfur that are also missed by traditional sulfide measurements. Suitable analytical methods that measure the target form of sulfide and do not measure other non-reduced forms of sulfur are under development. Also, sulfide levels in some locations may be known to be low and well below the effect levels of interest for a given metal. Therefore, sulfide measurements may not be critical in all instances. Since these research questions are still being addressed, metal-sulfide reactions have not yet been incorporated into the BLM. The sulfide column in the input file is a reminder that these interactions are likely to be added to a subsequent

version of the model. Sulfide concentrations added in that column will not affect the BLM calculation. For typical users we recommend that a near-zero concentration is entered as a default value (i.e., 1.0E-10 mg/L). When sulfide reactions are omitted from model simulations, the BLM will always predict a lower (i.e., more protective) estimate of a concentration associated with toxicity.

4.1.9 Other Components

The current marine chemistry file also includes phosphate (PO_4) as a component. Phosphate does have reactions associated with it, and measured concentrations should be entered if available. Parameter files for silver include a nitrate (NO_3) component as well. It is also possible through the use of a user-generated parameter file to have other non-standard components (only advanced users should attempt this). Typically when a non-standard component is included in a parameter file, it is because it will have a significant effect, and the measured concentrations should be entered whenever possible.

4.2 SIMPLIFIED SITE CHEMISTRY (HARDNESS-BASED)

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
- Metal concentration *[speciation mode only]*
- DOC
- Hardness
- Ion ratios (default values may be used if unknown)
- pCO_2 (defaults to atmospheric)

The requirements for Temperature, pH, metal concentration, and DOC are the same as in the "Site Chemistry" tab (see previous section).

4.2.1 Hardness

The hardness measurement, in addition to pH and ion ratios is used to estimate the major cations and anions. Hardness is typically the total Ca and Mg ion concentrations, although 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 $CaCO_3$.

4.2.2 Ion Ratios

The Ion Ratios are inserted 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 region being considered, use the default values in the boxes. Additionally, the we have calculated median ion ratios for across the U.S. and Canada, including at the country and state/provincial spatial scale. The user may find and use the most appropriate value from these tables provided in Section 9.

4.2.3 pCO₂

The pCO₂ (negative logarithm of ambient CO_2 concentration in atmospheres) is inserted in a box to the right of the grid, below the ion ratios. Alkalinity is estimated from pH assuming an open system in equilibrium with CO_2 in the atmosphere. The relatively small differences between indoor and outdoor CO_2 concentrations may significantly affect the calculated alkalinity. For this reason, the user is allowed to adjust the pCO₂ value. In most natural settings, it is a reasonable assumption that the CO_2 concentration will be $10^{-3.5}$ atmospheres (pCO₂ of 3.5), but for indoor settings such as where many toxicity tests are performed this might not be the case. The CO_2 concentrations are typically higher indoors, resulting in a lower pCO₂ value. Most indoor air quality standards suggest CO_2 to be at concentrations of less than 10^{-3} atmospheres, so the pCO₂ value should generally be greater than 3 and less than 3.5. The indoor CO_2 concentration depends on the amount of ventilation and respiration occurring in the building. There would not be any physical effects from CO_2 until it reached much higher concentrations than 10^{-3} atmospheres, so it is possible to have pCO₂ values less than 3 but not likely.

4.2.4 Simple to Full Chemistry Conversion Process

When the user switches from the Simplified Site Chemistry tab to the full Site Chemistry tab, the software copies the labels, temperature, pH, DOC, and copper concentrations to the full chemistry input grid. Then the pH and pCO₂ 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 atmospheric CO_2, following Henry's Law. The following equations perform this operation:

$$[H_2CO_3^*] = K_H * 10^{-pCO_2}$$

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

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

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

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 $10^{-1.5}$ mol/L/atm), so that with the default pCO_2 value of 3.5, the concentration of $[H_2CO_3^*]= 10^{-5}$ mol/L The alkalinity is then pH dependent, with the alkalinity being 2.23 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 arbitrary low alkalinity of 1 mg/L $CaCO_3$ to avoid errors.

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:

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

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 an arbitrary low number (10^{-7} mol/L) before calculating [Cl$^-$] in order to avoid errors.

4.3 SIMPLIFIED SITE CHEMISTRY (SALINITY-BASED)

The "Simplified Site Chemistry (Salinity)" view is another alternate place where the user can save chemical characterization of the water chemistry in marine environments. It differs from the "Site Chemistry" tab in that there are fewer inputs required for each site, making data collection easier, and differs from the "Simplified Site Chemistry" tab in that it uses salinity in place of ions rather than hardness. The ambient water quality information required to run the BLM with this tab are:

- ◆ Temperature
- ◆ pH
- ◆ Metal concentration *[speciation mode only]*
- ◆ DOC
- ◆ Salinity
- ◆ Base marine chemistry

The requirements for Temperature, pH, metal concentration, and DOC are the same as in the "Site Chemistry" tab (see section 4.1).

4.3.1 Salinity

Salinity should be input with units of parts per thousand (ppt). The full chemistry is calculated from Salinity and the base marine chemistry. It should be noted that the BLM interface estimates full ion chemistry from salinity under the assumption that estuarine water is essentially diluted sea water with negligible ionic inputs from the freshwater source. This assumption is not valid in some cases, namely when the estuarine water's salinity approaches that of freshwater and when the estuary's freshwater source has a high hardness. For example, when the freshwater input to an estuary has a hardness of 100 mg/L as CaCO3 and the estuarine water has a salinity of 10 ppt, the estimated ion concentrations will differ from actual by about 14% for Ca, 2% for Mg, 0.3% for Na, 1% for K, 6% for SO4, and 1% for Cl. However, a similar magnitude of departure from actual concentrations is seen at only about 25 ppt when the freshwater input has a hardness of 500 mg/L CaCO3.

4.3.2 Base Marine Chemistry

The base marine chemistry is the chemistry that would be expected from full-strength sea water. This defaults to sea water with a salinity of 35 ppt, Ca of 10.02 mmol/L, Mg of 51.48 mmol/L, Na of 457.12 mmol/L, K of 9.950 mmol/L, SO$_4$ of 27.52 mmol/L, Cl of 532 mmol/L, DIC of 1.998 mmol/L, and PO$_4$ of 2.33 mmol/L.

4.3.3 Simple to Full Chemistry Conversion Process (Salinity)

The Ca, Mg, Na, K, SO4, Cl, and PO4 ions and dissolved inorganic carbon (DIC) are all calculated from salinity and the base marine chemistry. The calculation assumes that the contribution from freshwater is negligible, and therefore the concentrations of ions and DIC are proportional to the base chemistry as per the following equation:

$$[X] = \frac{(Salinity) * [X]_{base}}{(Salinity)_{base}}$$

where [X] is the concentration of one of the ions or DIC and "base" denotes the values from the base marine chemistry. As noted previously, this relationship breaks down when the freshwater source has high hardness, or when the site is near the freshwater source (i.e. it has a low salinity). In those cases, it would be best to measure the full chemistry of each sample, or to manually estimate the full chemistry while taking the freshwater source's ions into account.

4.4   MINIMUM DATA REQUIREMENTS

The BLM can be run with any number of observations from 1 to 1,000. In toxicity mode a corresponding number of instantaneous WQC values will be calculated. Any observations with missing chemistry will be skipped in the calculation process. Missing metal concentrations will not prevent an observation from being run in toxicity mode, since the metal concentration is the component being calculated.

4.5   DATA TEMPLATE

To assist users in collecting and organizing the information required to run the BLM, we now have a BLM Data Template available on our website (www.windwardenv.com/biotic-ligand-model/). The template is in Microsoft Excel® .xlsx format, and contains two data template sheets in the workbook, one for toxicological data ("Toxicity Data Template") and one for site chemistry ("Site Chars Data Template"). The word "METAL" in some of the column headers should be replaced with the metal of concern when entering data. Although it is expected that the data in the Site Chars Data Template sheet will mostly be used in toxicity mode, metal concentration columns are still included in this sheet to make it easier to compare to the predicted HC5/WQC, and also so that the template will be usable to set up inputs for FMB calculations when the feature becomes available.

The user should fill in this template to the furthest extent possible when preparing data for use in the BLM. If water quality parameters need to be estimated, it is suggested that the green columns are copied to the right of the table and filled in with the estimated values there so it is clear which ones are the estimated values, and which are the measured/reported.

5   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.

5.1   STARTING THE APPLICATION

To start using the BLM Windows® Interface, the user should select the application using 'Start -----> Programs -----> Biotic Ligand Model -----> Biotic Ligand Model, Version 3.16.2.41' on the Microsoft Windows® desktop. The user will be presented with the screen shown in Figure 5-1, which contains the user input areas and the various functions implemented in this version of the BLM Windows® Interface.
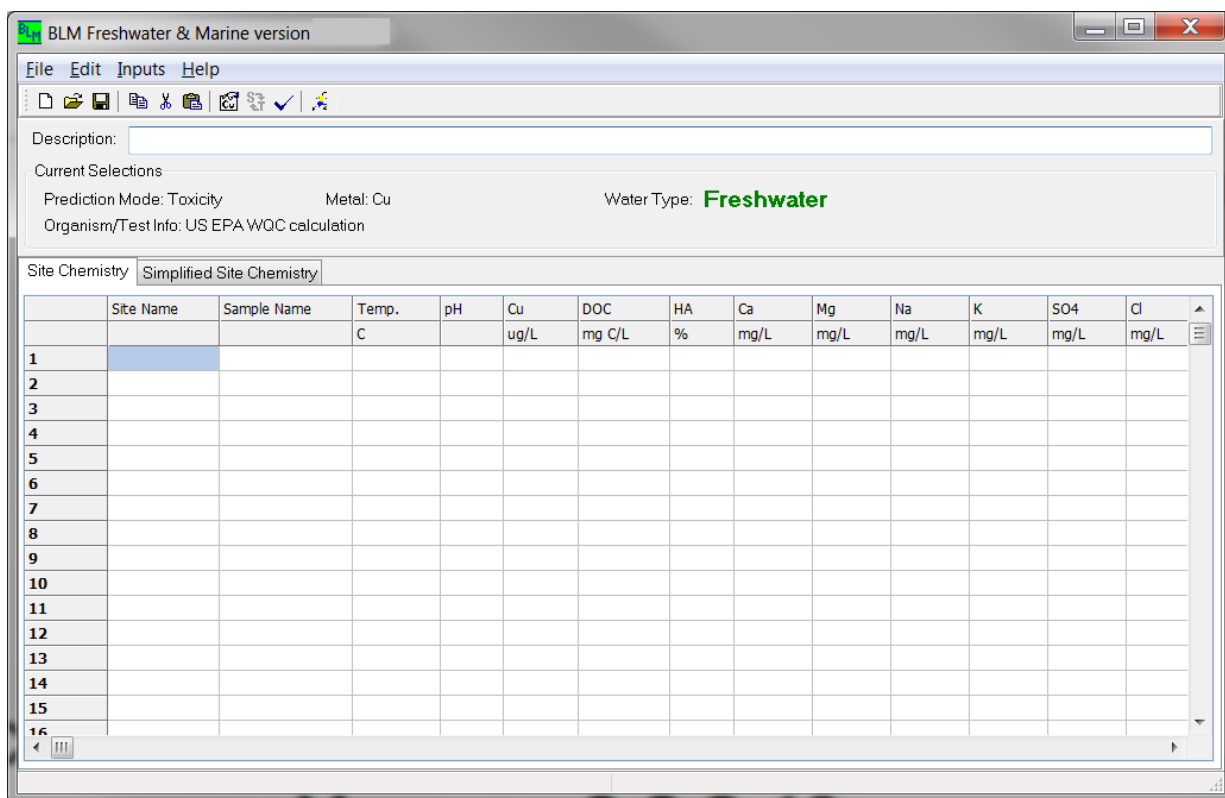

Figure 5-1.   Opening screen for the BLM Windows® Interface application

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.

5.2   DESCRIPTION OF INTERFACE

Figure 5-2 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 predictions of aquatic speciation or toxicity for a variety of metals and organisms.
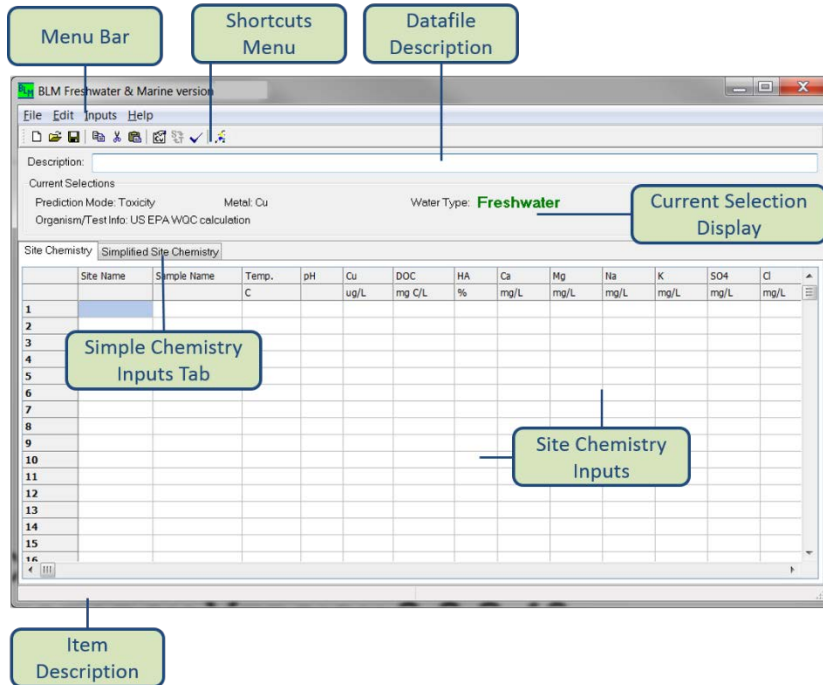

Figure 5-2.   Snapshot of the BLM Windows® Interface

As shown in Figure 5-2, the interface window is divided into seven areas broadly based on their functionality. Each of these is described in the subsections that follow.

5.3   SITE CHEMISTRY INPUTS

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 5-3 shows the various columns typically available for user input.
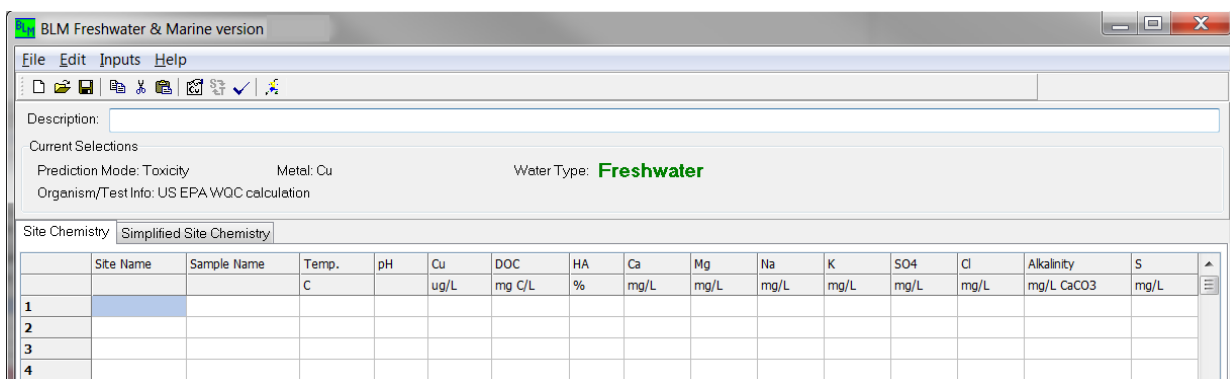
Figure 5-3.   Columns for data input in the BLM Windows® Interface

5.3.1   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 it could be the mile point along a river 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 dates and times 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.

5.3.2   Water chemistry inputs

The subsequent columns are the data input areas for the water quality parameters described in Section 4, Data Requirements. For predictions of metal toxicity, metal concentration is not a required input, since the BLM will predict the amount of metal that results in acute toxicity to the specified organism(s). For predictions of metal speciation, the metal concentration is a required input; if no metal concentration is specified, the row will be considered incomplete and no BLM predictions will be made for that row. 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.

5.4   SIMPLE CHEMISTRY INPUTS TAB

By clicking on the 'Simplified Site Chemistry' tab, a grid similar to the full site chemistry data inputs will be displayed, as shown in Figure 5-4a. Additionally, there is a side bar with boxes where the ion ratios and pCO_2 can be set. The default values are median North American values and atmospheric, respectively. 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 this tab, clicking the 'Open' option will filter for files with the extension '.blme' rather than '.blm'. This type of file saves the ion ratios and pCO2 selections,

and is in other ways similar to the regular '.blm' file type, i.e. an ASCII text file that is space and/or comma delimited. An example file is included with the software download.

After the simplified site chemistry data has been inserted into this grid, the user can save the file as a '.blme' file and run the model (see section 5.6.6 for information on running the model). The chemistry will be converted to full chemistry and saved in an additional file called "<filename>.blme.blm" in the same directory before the program runs the model. Alternatively, the user can select the 'Site Chemistry' tab again to convert the simple inputs into full site chemistry before running the BLM as normal. This step may be desirable so that the user can check that the full chemistry estimates are reasonable before running the model, and perhaps make changes where better information is available (e.g. including measured alkalinity instead of using the calculated values). Because of this possibility, switching from the simplified tab to the full chemistry tab is a one-way conversion – *the user cannot go back to the simple chemistry inputs after converting*.

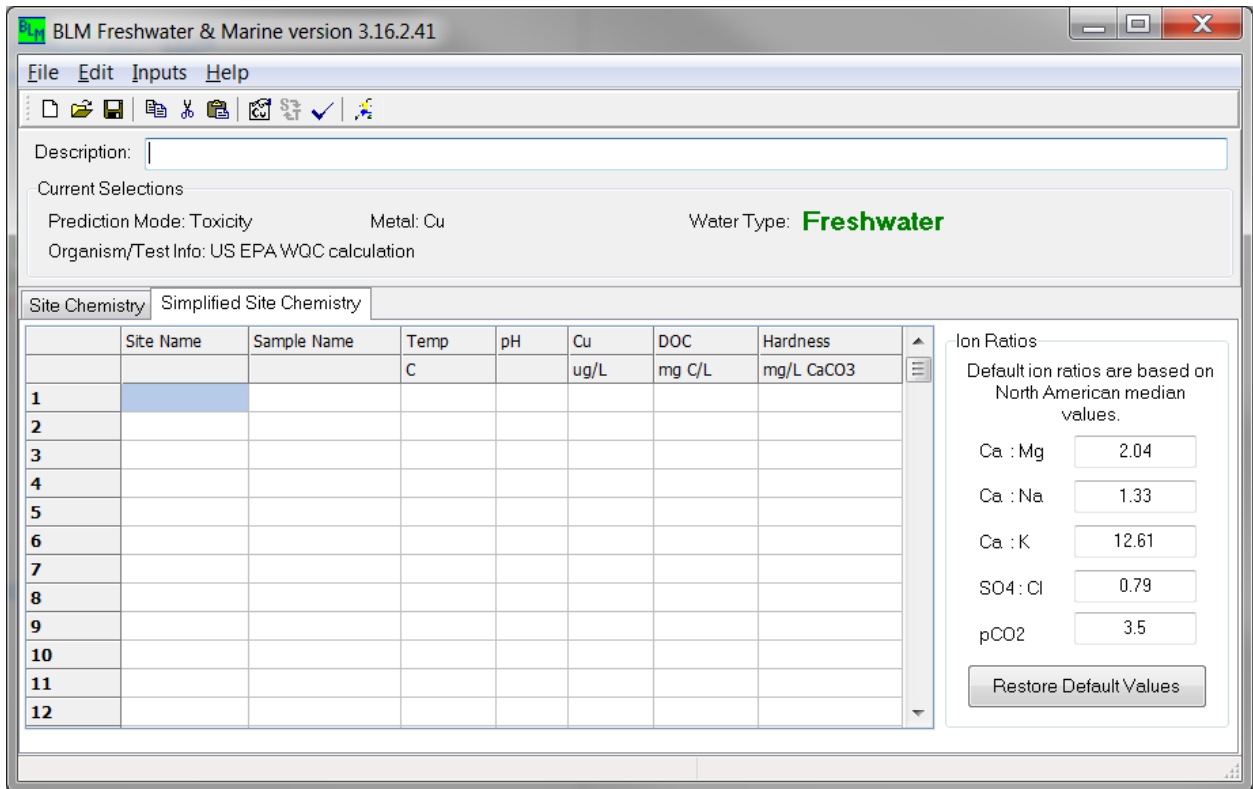**Figure 5-4a. Snapshot of Simplified Site Chemistry inputs and ion ratios**

By clicking the 'Simplified Site Chemistry (Salinity)' tab in marine mode, a grid will appear that is similar in function to the hardness-based simple site chemistry tab for freshwater, as shown in Figure 5-3b. The file extensions while in marine mode will be '.swblm' for full chemistry and '.swblme' for simple chemistry.

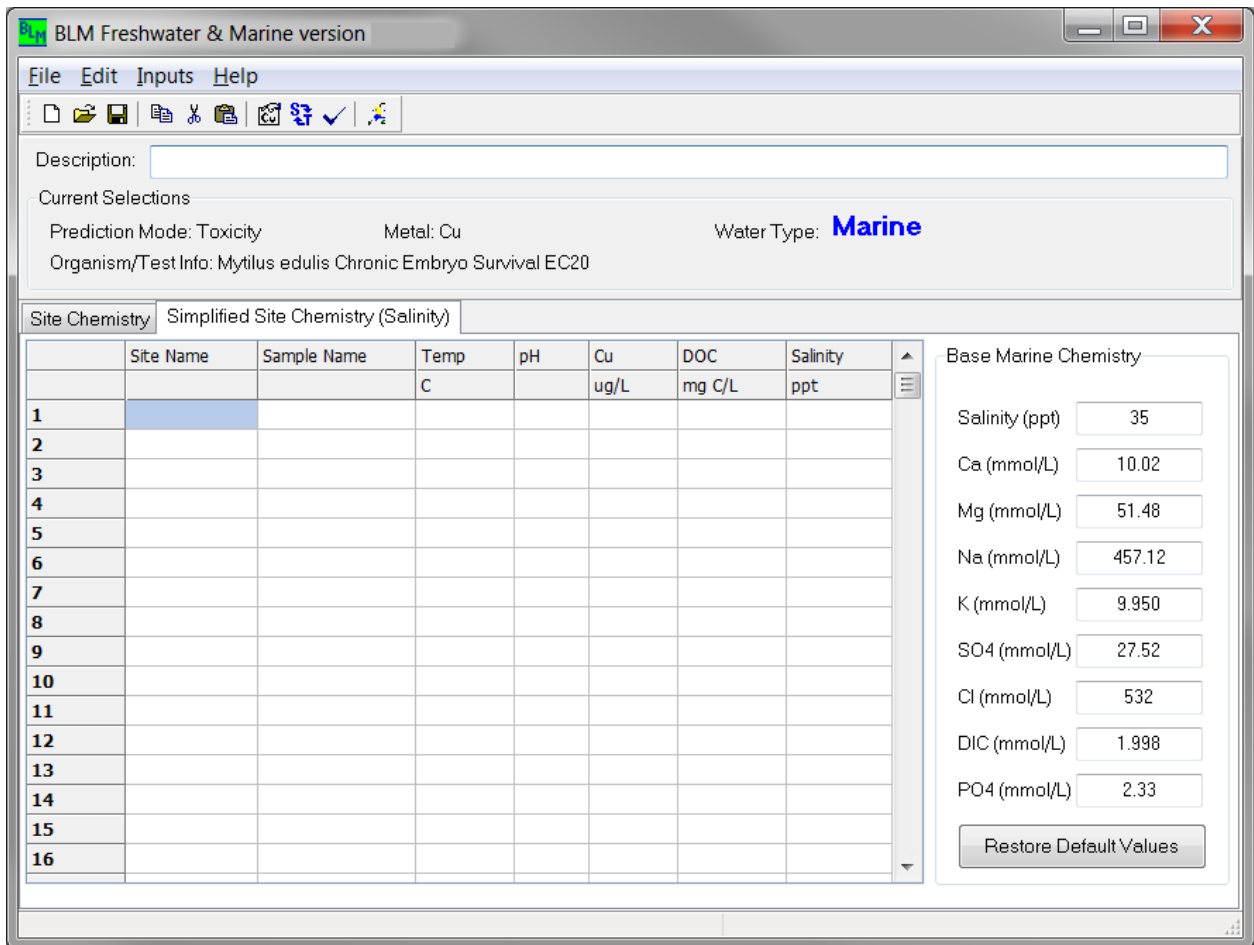**Figure 5-4b. Snapshot of Simplified Site Chemistry (Salinity) inputs and base marine chemistry**

5.5 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 and miscellaneous options

◆ Options relating to data inputs

◆ A help function

These features are described below.

5.5.1 File

Figure 5-5 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.
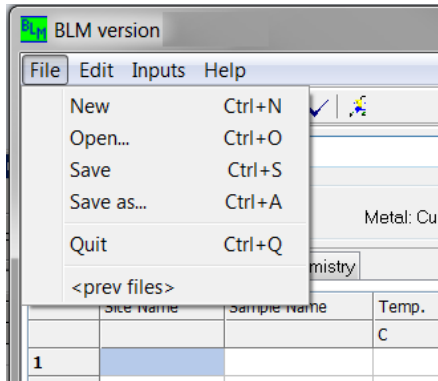

Figure 5-5.   Snapshot of file menu item

Shortcut keys (shown to the right of each item) are also available for all 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 of interest 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 in freshwater mode and '.swblm' extension in marine mode 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.

5.5.2 Edit

Figure 5-6 shows the editing functions available in the BLM Windows® Interface. Basic editing functions such as 'Cut,' 'Copy,' and 'Paste,' 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.

Additionally, there are the options to have output saved as Microsoft ® Excel (as opposed to an ASCII text file), and to show the BLM 'engine' windows while it's running. The latter option has been added so that the user can see when the BLM run "gets stuck" on an observation, as it shows the progress through the observations. The BLM engine occasionally encounters a problem that it cannot overcome, and it will not proceed as normal. This is more likely with a toxicity mode run than a speciation run since the optimization may fail to converge, and it can usually be fixed by changing the order of the observations so that there is a different starting point for the optimization.
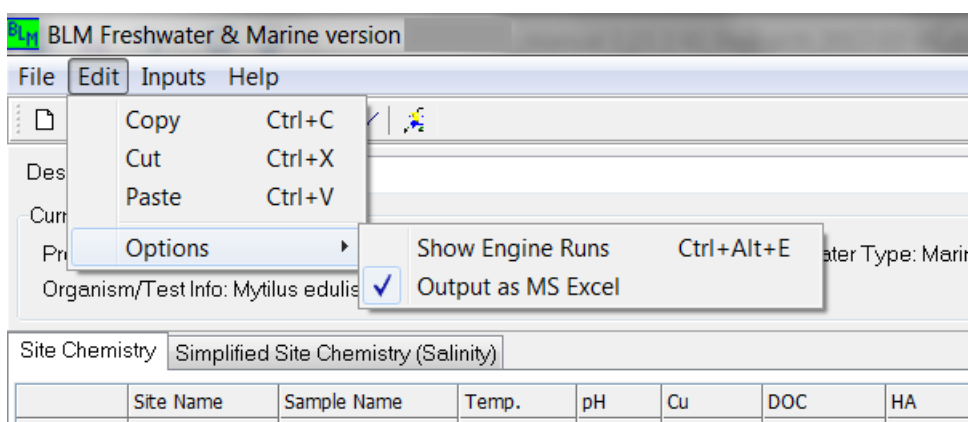

Figure 5-6. Snapshot of edit menu item

5.5.3 Inputs

Figure 5-7 shows the options available under the 'Inputs' menu item. The current input options 'Set Units' and 'Set Inorganic Carbon' are described in the following subsections.

The 'Water Type' submenu item lets the user toggle between freshwater and marine environments for the simulations. This will change some of the inputs that are needed, the format of the 'Simplified Site Chemistry' tab (hardness- or salinity-based, respectively), and will bring up the metal and organism selection screen for the user to choose an appropriate parameter file for their simulation. You should select the water type first, before entering data into the input grid, since the input grid will be cleared when switching to a new water type.
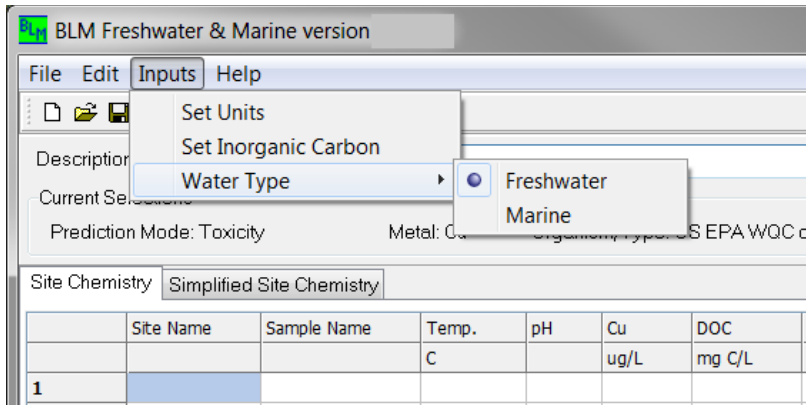
Figure 5-7. Snapshot of inputs menu item

5.5.3.1 Units

The first option 'Set Units' allows the user to select the units for the various BLM input parameters, as shown in Figure 5-8. For each parameter, the currently selected unit is highlighted by default, and the user can select the desired unit from the list of options shown. When changing a unit for a given parameter, data already input for that parameter can be converted to the new unit to prevent any loss of data.
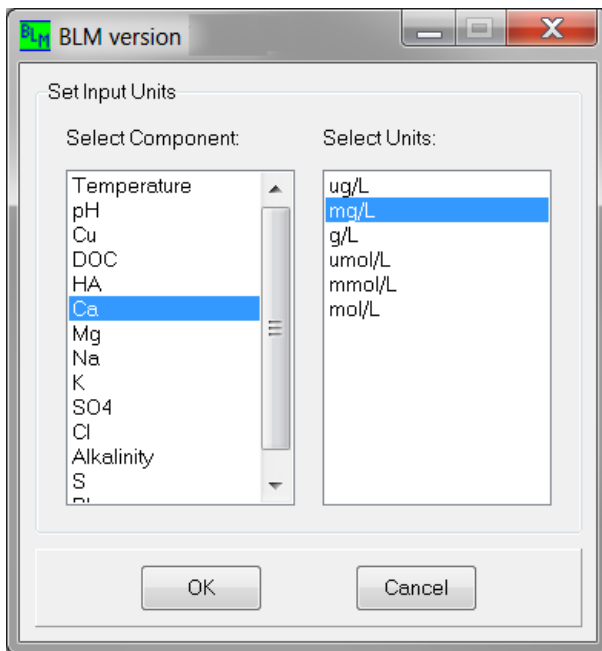

Figure 5-8. View of typical 'Set Units' screen

5.5.3.2 Inorganic carbon

The second option, 'Inorganic Carbon,' gives the user the opportunity to select an option for specifying the inorganic carbon in the system. As mentioned previously, the BLM simulates the formation of metal-carbonate complexes; therefore, inorganic

carbon is a required input for BLM simulations. Inorganic carbon in the system can be specified in one of two ways: alkalinity or DIC. Accordingly, the user can select between these two options by means of the 'Inorganic Carbon' feature, as shown in Figure 5-9. The third option, using an open system, has been described previously. It instructs the engine to disregard any inorganic carbon inputs and instead calculate DIC based on chemical equilibria and atmospheric CO_2 inputs.
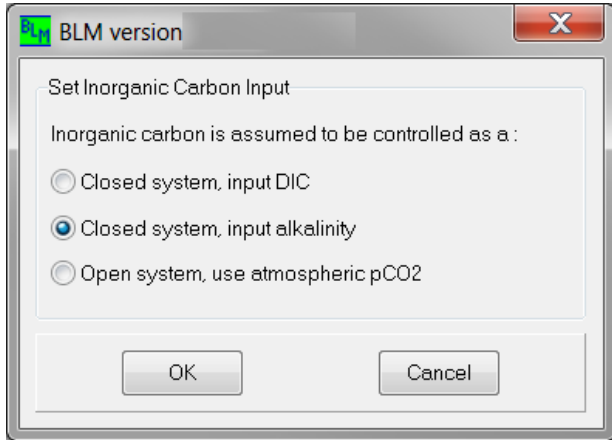
Figure 5-9.   View of inorganic carbon input options screen

5.5.4 Help

Figure 5-10 shows the various features available under the 'Help' menu item.
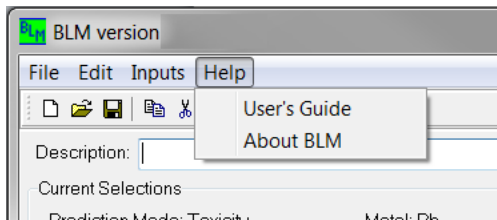
Figure 5-10. Snapshot of help menu item

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.

5.6   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 5-11 shows the various icons and their functions; brief descriptions are provided in the subsections that follow.
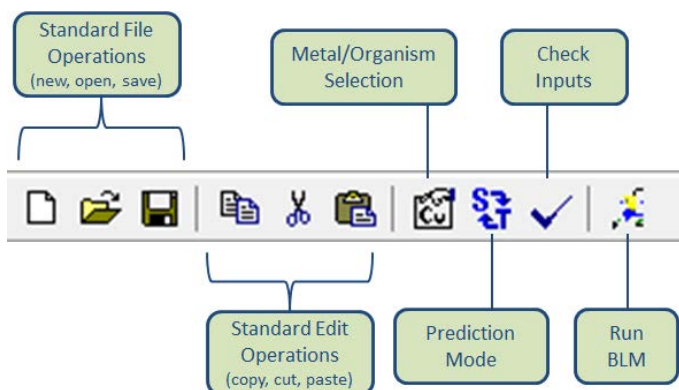
Figure 5-11. Shortcut menu icons

5.6.1 Open file

This is a shortcut to the menu bar item under 'File -----> Open' and 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.

5.6.2 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.

5.6.3 Metal/organism selection

As mentioned previously, the BLM can be used to study the toxicity and speciation for a variety of metals and organisms. This action button is provided to allow the user to select the metal and the organism for which toxicity or speciation needs to be predicted. Clicking on this icon will present the user with the window shown in Figure 5-12. The user can then choose the desired metal and organism for the BLM predictions. The current metal and organism selections are displayed in the 'Current Selection' display area (see Section 5.7).

Acute and chronic parameter files have been developed for several metals in freshwater and marine environments, and they will be added to the package over time as they are finalized. Unless otherwise specified, the available parameter files are currently for acute effects.
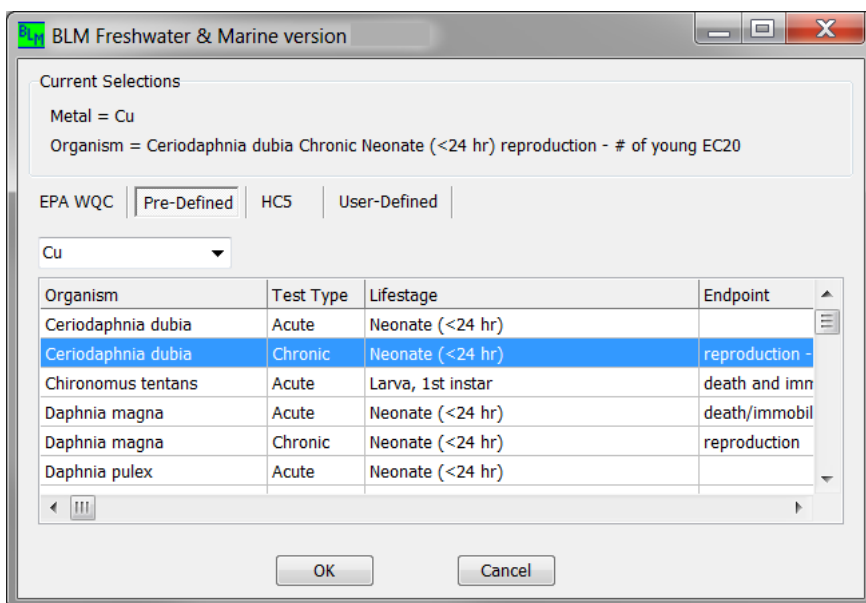
Figure 5-12. Metal and organism selection options

5.6.3.1 Metal and organism options available

The metal- and organism-specific parameter files that are included in the current distribution of the BLM Windows® Interface are available by selecting the 'Pre-defined' tab button, then selecting first the metal and then a row from the table, as shown in Figure 5-12. The user can resize the column widths by clicking and draging between two column headers. The user can sort the table by any of the columns by clicking on the column header (sorting will cycle through original-, descending-, and ascending-order sorting). Note that these organism-, lifestage-, and endpoint-specific options available in the table are subject to change as part of the ongoing refinement of the calibration and application of the BLM, and may therefore undergo revisions from time to time.

In order to provide enough information to accommodate chronic endpoints, a new parameter file format was created for starting in this distribution. Old parameter files only contained information about the organism, and nothing about the lifestage, endpoint, references, or methods were in any format that could be interpreted by the BLM Interface program. We still would like to make the old parameter files available to users, so many of the columns in the table will be blank for some metals and organisms until we have converted everything to the new parameter file format.

It is recommended that the user develop separate BLM data files for separate metals, even though the application of the BLM may be for the same set of observations. The current distribution of the BLM can be applied to only one metal at a time. Because the input metal concentrations in the BLM Interface Site Chemistry grid are specified in

units of μg/L, the interface application internally converts these to moles/L using the molecular weight for the metal selected by the user when saving the input file. Changing the metal for the BLM application within an existing data file developed for a different metal may result in an erroneous conversion from μg/L to moles/L when the user saves and opens the data file the next time.

5.6.3.2 User-defined files

In addition to the metal- and organism-specific parameter files that are included with the current distribution, users may opt to develop and use their own versions of these files for BLM predictions. This is achieved by selecting the 'User-defined' tab button shown in Figure 5-12 and clicking 'Select Parameter File…' to browse for the desired parameter file. New parameter files can be developed by the user along the lines of the parameter files supplied with this distribution (i.e., files with the extension '.dat' located in the 'Model' sub-directory within the BLM directory in Program Files). Note that the user should first select the appropriate parameter file when opening a BLM input file that was previously developed for a user-selected parameter file.

5.6.3.3 EPA WQC & HC5 Calculations

The US Environmental Protection Agency's (EPA's) nationally recommended AWQC for Cu are based on the BLM (EPA 2007). The ability to calculate criteria has been available in previous publicly available BLM software versions (2.2.1, 2.2.3) and continues to be available in this version of the BLM Windows® Interface. The freshwater Cu AWQC can be generated by selecting the 'EPA WQC' tab button shown in Figure 5-12, and then selecting 'Cu' in the 'Select Metal' drop-down menu. When the BLM is run in the Cu WQC mode, it generates the EPA 2007 freshwater dissolved copper WQC (acute and chronic) for each row of input and provides these results in the "WQC" report (see Section 5.10). The report provides the BLM-based final acute value (FAV) and the acute IWQC (which is calculated as the FAV divided by two; see EPA 2007). The acute and chronic criteria are also known as the criterion maximum concentration (CMC) and criterion continuous concentration (CCC), respectively. If dissolved Cu input data are provided by the user in the BLM input data file, the values are tabulated in the criteria output file and used to calculate acute and chronic toxic units (TUs). These TUs are computed as the ratio of the input dissolved Cu concentration to the IWQC output for each input row, with TU values >1 indicating a potential exceedance of the particular Cu IWQC. Given the basis of EPA's aquatic life WQC derivations (Stephan et al. 1985), a TU > 1 does not explicitly mean actual toxicity would be expected to occur. Rather, it simply indicates an exceedance of the particular magnitude of the criterion.

The acute and chronic HC5 option is available for other metals for which we have used BLM-normalized toxicity data to construct a SSD, and then used this SSD to calculate the 5th percentile of organism sensitivity. The BLM-predicted HC5 can be

interpreted in a manner similar to the way EPA derives aquatic life WQC, but HC5 calculations have not been reviewed and adopted by EPA.

Figure 5-13. Instantaneous copper criteria report

For additional information on the terminology and the exact workings of the WQC calculation, the user is advised to refer to EPA (2007). The criteria report shown in Figure 5-13, being a Microsoft® Excel file format, can also be copied for pasting onto any external application or report.

5.6.4 Prediction mode

The BLM interface application allows the user to run the BLM either in toxicity mode or in speciation mode. When run in toxicity mode, for the metal and organism specified by the user, the BLM will predict the amount of metal required to cause acute or chronic toxicity in each observation/line in the input file. However, when the BLM is run in speciation mode, for the metal concentration specified by the user, the BLM will predict the organic and the inorganic chemical speciation in the water column and the metal accumulation on the biotic ligand that would result.

The 'Prediction Mode' button allows the user to toggle between the speciation and toxicity prediction modes in the BLM. The current prediction mode is also displayed in the Current Selection Display area (see Section 5.7). The current prediction mode setting is saved when the application is closed, and the application will default to the last prediction mode used.

5.6.5 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 range of parameter values for which the BLM has been calibrated is described in Section 6, Input Check Range. Figure 5-14 shows an example of an input check report.
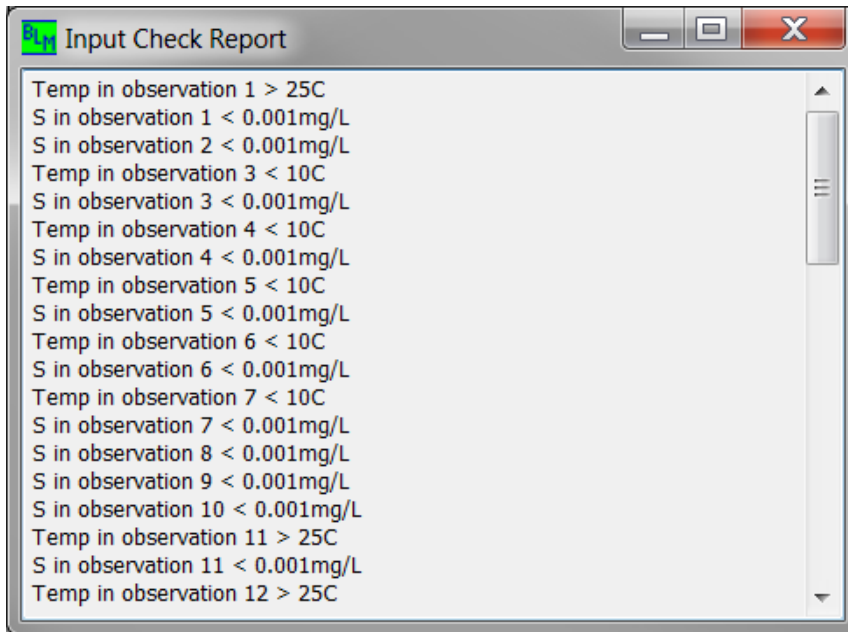
Figure 5-14. Example of an input check report generated by the check inputs function

5.6.6 Run BLM

This icon (see Figure 5-11) is used to launch the BLM calculation engine to predict either metal toxicity or speciation 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.

5.7   CURRENT SELECTION DISPLAY

This area of the interface window displays the current water type, metal, organism, and prediction mode selections made by the user. For the example shown in Figure 5-1, the user has opted to predict the toxicity of Cu for the EPA WQC calculation in freshwater. The options selected by the user are saved in the BLM data file and by the program when it closes. When opening the program, it will default to the set of options selected when it last closed. When opening a BLM input file, the application switches to the selections made by the user when the input file was last saved, or asks the user to select the input file they would like to use.

5.8   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.

5.9   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 5-1, the cursor is positioned over the 'Data Inputs' area. Similar messages are displayed when the cursor is moved over other areas of the interface window.

5.10   DESCRIPTION OF OUTPUT FILES

The BLM creates three output files within the directory containing the BLM input file. The file extensions are ".sim," ".det," and ".wqc," with filenames based on the name of the input file. For example, using the input file 'test.blm' would create output files: 'test.sim.txt' or 'test.sim.xls' (the simple version of the model output), 'test.det.txt' or 'test.det.xls' (the detailed version), and 'test.wqc.xls' (the water quality report, only when running the model for an EPA WQC). The format of the output files, as either text or Microsoft Excel® files, is selected under the 'Edit' menu (see Section 5.5.2).

The ".det" report file contains all the chemical species accounted for in the BLM. Because this file can be quite large, the ".sim" report contains the following selected output results that may be of interest:

- ◆ Site and sample names
- ◆ BLM mode chosen (Speciation, Toxicity, LC50, etc.)
- ◆ pH
- ◆ Dissolved metal concentration in mol/L (this is the predicted FAV for Cu)
- ◆ Free metal concentration in mol/L
- ◆ Concentration of metal and metal hydroxide bound to DOC in mol/L
- ◆ Concentration of metal on the biotic ligand in nmol/g_{wet}
- ◆ DOC in mg/L
- ◆ Percent humic acid
- ◆ The rest of the input water chemistry in units of mg/L

6　Input Check Range

In order to provide users with an idea of the range of water chemistry to which the BLM can be applied, the range of parameter values to which the BLM has been developed and calibrated is defined in the BLM interface application. Users can check to verify that the user input water chemistry parameter values are within this range to which the BLM has been calibrated. This is done by clicking the check icon on the menu for the 'Check Inputs' function. The ranges prescribed for each of the BLM input parameters are shown in Table 6-1. The BLM will still run when input data are outside of these ranges and it is up to the user to evaluate whether chemistry in these cases is relevant for the organism they wish to consider.

Table 6-1.　Prescribed ranges for BLM input parameters

Parameter	Lower Bound	Upper Bound
Temperature (^oC)	10	25
pH	4.9	9.2
DOC (mg/L)	0.05	29.65
Humic acid content (%)	10	60
Calcium (mg/L)	0.204	120.24
Magnesium (mg/L)	0.024	51.9
Sodium (mg/L)	0.16	236.9
Potassium (mg/L)	0.039	156
Sulfate (mg/L)	0.096	278.4
Chloride (mg/L)	0.32	279.72
Alkalinity (mg/L)	1.99	360
DIC (mmol/L)	0.056	44.92
Sulfide (mg/L)	0.001	0.006

DIC – dissolved inorganic carbon
DOC – dissolved organic carbon

7   Example Application

The BLM Windows® Interface installation also features an example application for demonstration purposes. This file, named 'LakeSuperior.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 2009 average water quality observation from Lake Superior, as reported in Chapra et al. (2012).

The data file 'LakeSuperior.blm' can be used to predict metal speciation using the input metal concentration, or to predict the LC50 for a variety of metals and organisms. It is recommended that separate BLM data files always be maintained for each metal. In this case, the data file contains dissolved Cu concentrations; the BLM can be used to predict the inorganic, organic, and biotic speciation by setting the BLM prediction mode to 'Speciation' using the shortcut Menu button 'Prediction Mode.' Metal toxicity for the specified site water chemistry can also be predicted by setting the prediction mode to 'Toxicity' and selecting the metal and organism for which toxicity is to be predicted using the shortcut Menu button 'Metal/Organism Selection.'

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, the runtime for the BLM predictions can vary from a few seconds to several minutes. Upon completion of the BLM run, the user is informed of the names and locations of the output files, and given the option to open the directory, as shown in Figure 7-1.
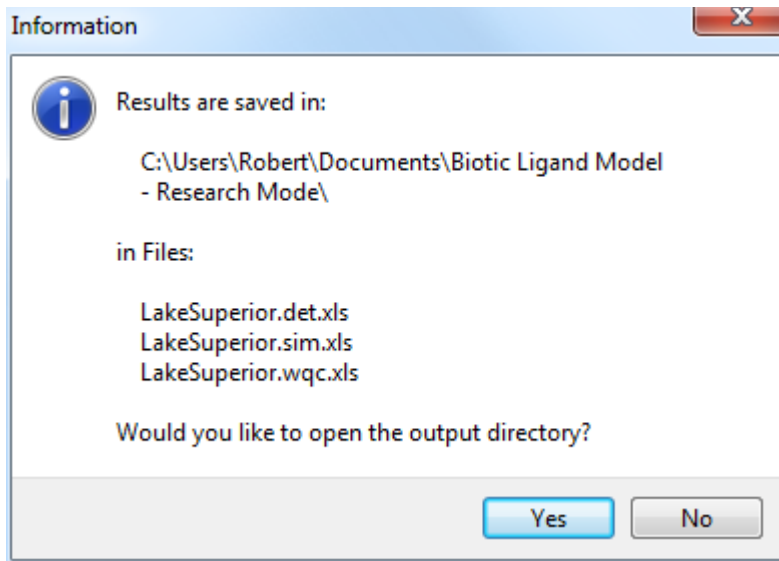
Figure 7-1.   Example of notification window shown at completion of BLM run

The contents of the output files have been described in Section 5.10, Description of Output Files.

8   Uninstalling the BLM

To uninstall the BLM Windows® Interface, select the uninstall utility using 'Start ----->
Programs -----> Biotic Ligand Model -----> Uninstall.' All 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 uninstall. These will
have to be deleted manually by the user, if so desired.

9 Ion Ratio Tables

Monitoring data were gathered from across the United States and Canada. Data from the U.S. were collected using the dataRetrieval package in R statistical software, and total 21,685 observations from 47 states (Hirsch and De Cicco, 2015). The Canadian data were collected from mostly publicly available monitoring data, and total 40498 observations from 13 provinces and territories.

Table 9-1.   Median ion ratios in North America

Geographic Unit	Ca:Mg	Ca:Na	Ca:K	SO4:Cl
North America	2.04	1.33	12.61	0.79
Canada	2.14	1.47	13.94	1.70
United States	2.11	1.19	12.21	0.65

Table 9-2.   Median ion ratios in Canadian provinces

Geographic Unit	Ca:Mg	Ca:Na	Ca:K	SO4:Cl
Alberta	1.82	1.96	29.27	4.70
British Columbia	3.33	3.30	23.51	3.86
Manitoba	1.28	1.29	8.69	1.52
New Brunswick	4.15	1.35	16.92	0.48
Newfoundland and Labrador	2.49	0.42	6.79	0.10
Northwest Territories	1.87	2.15	7.32	1.23
Nova Scotia	1.28	0.15	3.49	0.12
Nunavut	2.61	3.58	6.66	4.92
Ontario	2.27	1.34	13.19	1.41
Prince Edward Island	1.53	2.51	31.86	0.16
Quebec	2.48	1.41	16.26	0.56
Saskatchewan	0.83	0.48	4.61	3.29
Yukon	3.35	8.07	37.53	22.14

Table 9-3.   Median ion ratios in U.S. States

Geographic Unit	Ca:Mg	Ca:Na	Ca:K	SO4:Cl
Alabama	2.81	0.89	8.26	0.81
Alaska	2.87	5.26	25.22	5.87
Arizona	1.76	0.54	18.93	0.95
Arkansas	2.84	0.79	11.38	0.29
California	2.20	0.54	9.73	0.41
Colorado	2.81	1.23	12.68	1.81

Geographic Unit	Ca:Mg	Ca:Na	Ca:K	SO4:Cl
Connecticut	2.05	0.47	8.13	0.08
Delaware	1.70	0.67	6.26	0.19
Florida	4.83	1.68	5.75	0.48
Georgia	2.39	0.57	3.17	0.35
Hawaii	0.86	0.38	5.35	0.08
Idaho	1.67	1.04	11.56	0.76
Illinois	1.73	1.80	13.68	0.75
Indiana	1.99	1.95	16.93	0.64
Iowa	1.56	2.60	17.31	0.53
Kansas	3.04	0.71	9.11	0.36
Kentucky	3.40	2.59	11.55	0.58
Louisiana	1.97	1.13	10.85	0.63
Maryland	2.31	1.19	11.59	0.47
Massachusetts	3.70	0.23	6.22	0.07
Michigan	2.11	0.90	21.53	0.10
Minnesota	0.89	1.31	18.91	0.73
Mississippi	1.89	1.34	6.60	0.74
Missouri	1.76	1.19	10.65	1.62
Montana	2.01	1.02	13.58	5.09
Nebraska	1.88	0.75	10.04	2.23
Nevada	1.65	0.46	15.07	1.01
New Hampshire	2.39	0.12	5.39	0.05
New Jersey	1.76	0.60	10.64	0.21
New Mexico	3.64	1.19	12.76	2.51
New York	2.86	1.42	20.94	0.47
North Carolina	1.62	0.57	1.84	0.24
North Dakota	1.49	0.54	12.09	5.68
Ohio	2.02	1.52	11.41	0.51
Oklahoma	1.86	0.53	7.68	0.34
Oregon	1.90	1.32	11.45	0.38
Pennsylvania	2.10	1.48	13.61	0.53
South Carolina	1.38	0.45	2.12	0.23
South Dakota	1.55	0.48	10.90	7.59
Tennessee	2.18	2.06	11.08	1.04
Texas	2.67	0.46	14.99	0.49
Utah	1.46	0.51	19.04	1.12
Virginia	1.39	0.70	4.13	0.18
Washington	1.83	1.06	10.09	1.28
West Virginia	1.12	1.20	11.46	4.29
Wisconsin	1.34	0.89	20.05	0.21
Wyoming	2.12	0.62	14.15	2.35

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