

**BIOTIC LIGAND MODEL WINDOWS[®] INTERFACE,
RESEARCH VERSION 3.1.2.37:
USER'S GUIDE AND REFERENCE MANUAL**

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Acronyms

Acronym	Definition
Ag	silver
BLM	Biotic Ligand Model
Ca	calcium
Ca²⁺	calcium ion
CaCO₃	calcium carbonate
CCC	Criterion continuous concentration
CHESS	Chemical Equilibria in Soils and Solutions
Cl	chloride
CMC	Criterion maximum concentration
CO₃	carbonate
Cu	copper
DIC	dissolved inorganic carbon
DOC	dissolved organic carbon
EPA	US Environmental Protection Agency
FAV	final acute value
FMB	fixed monitoring benchmarks
H₂CO₃	carbonic acid
HC5	Concentration corresponding to the 5 th percentile of the species sensitivity distribution (SSD)
HCO₃	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
SO₄	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 can be found In the User's Guide, or online at:

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

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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 functions 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 chemistry 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 (Paquin et al. 1999; Di Toro et al. 2001; 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 metal toxicity. Inorganic and organic ligands can also bind metal, thereby reducing accumulation at the biotic ligand. By incorporating the biotic ligand into a chemical equilibrium framework that includes aqueous metal complexation, the relationship 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 greater 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 concentrations 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 to 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 lethal biotic ligand accumulation (LA50) associated with the 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 LA50. While others have developed models capable of predicting metal bioaccumulation on the gill due to 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

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 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 greater than a critical threshold concentration leads to toxicity. This critical accumulation at the biotic ligand may be termed the LA50 for acute toxicity (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 accumulation 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 varies, 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?

In the most recent release of the BLM Windows® Interface, Version 2.2.3, there were some issues seen when installing onto a Windows® 7 or newer machine, all of which have been fixed in the current release. Also, a tab to enter site chemistry in a “simplified” way, with fewer necessary inputs, has been added. Finally, starting with Version 3.1.2.37, the version numbering system has been changed so that the first two numbers represent the major and minor version numbers of the user interface, and the last two numbers represent the major and minor version numbers of the newest BLM calculation engine being used (calculations such as the EPA Cu WQC may use an earlier version to be consistent with EPA standards).

Note that BLM data files created using the older version of the BLM Windows® Interface can be used directly with the new version.

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 is designed for use on computers running Microsoft Windows®. The memory requirements of the BLM software are modest and should not interfere with other resident programs. The minimum hardware and software requirements and the recommended system configurations are described below.

- ◆ Minimum system requirements
 - ◆ PC-compatible, Intel Pentium 233 MHz
 - ◆ Microsoft Windows® XP/Vista/Win7
 - ◆ 32 MB RAM
 - ◆ 30 MB free disk space (minimum) to 100 MB (recommended)

3.2 INSTALLING THE BLM WINDOWS® INTERFACE

- ◆ **Installing from a self-extracting executable file (BLM_3.1.2.37_setup.exe)** – Launch the installation program by simply double-clicking on the file name.

- ◆ **Installing from the compressed (.zip) file** – To install the BLM Windows® Interface from the compressed file “BLM_3.1.2.37.zip” double click on the file to extract its contents to a temporary folder. This temporary folder can be deleted once the installation is completed. To start the installation, locate and run the program ‘setup.exe’ located in the temporary folder by double-clicking on the file name.

Once the installation program is started it will require that the user accepts the license agreement. The installation program will guide the user through a fairly straightforward installation process, querying the user for information on where to install the program files, and a separate location for data 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.

4 Data Requirements

The BLM predicts metal toxicity and speciation for a particular site based on the ambient water quality. The BLM can also predict acute and chronic US EPA copper WQC for copper. 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
- ◆ Dissolved organic carbon (DOC)
- ◆ Major cations (calcium [Ca], magnesium [Mg], sodium [Na] and potassium [K])
- ◆ Major anions (sulfate [SO₄] and chloride [Cl])
- ◆ Alkalinity
- ◆ Sulfide

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 6.3), thereby allowing the model to run with only Temperature, pH, DOC, and hardness.

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.

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. 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.

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 freshwaters, SO_4 may be the dominant anion and is, therefore, important for determining charge balance and ionic strength. The chemistry of metals and NOM 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 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 Ag-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 Cu.

4.1.7 Alkalinity

Inorganic carbon species in the BLM include carbonate (CO_3), 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, including Cu, form carbonate complexes. Ag, on the other hand, does not form carbonate complexes, and so DIC is

not a critical input to BLM applications for Ag. 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.

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

where:

$$\begin{aligned} Alk &= \text{alkalinity in equivalents/L} \\ &= 2 \times 10^{-5} \times \text{alkalinity (as mg calcium carbonate [CaCO}_3\text{]/L)} \\ H &= 10^{-pH} \\ K_1 &= 10^{-6.352} \\ K_2 &= 10^{-10.329} \end{aligned}$$

The BLM Windows® Interface uses this expression to calculate the DIC internally, so only the alkalinity and the pH need to be specified. Alkalinity should be measured on filtered samples to eliminate potential contribution from suspended CaCO₃ and specified in units of mg/L of CaCO₃. However, depending on the inorganic carbon option selected, the user may also opt to specify DIC concentrations directly.

4.1.8 Sulfide

The presence of sulfide can strongly affect metal speciation and bioavailability of metals. However, in most well-aerated waters the concentration of sulfide is low and can be difficult to measure. Analytical challenges with sulfide can be problematic in BLM simulations since sulfide interactions are strong enough that poor quality sulfide data can have a large effect on model results. Since sulfide reactions are used in some applications of the BLM, we have retained a column for sulfide in the BLM input file to allow compatibility with BLM applications that include sulfide. However, for typical users we recommend that a near-zero concentration is entered as a default value (i.e., 1.0E-10 mg/L). Sulfide reactions have also been removed from the thermodynamic database to avoid any problems with potentially low quality sulfide data. 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.

4.2 SIMPLIFIED SITE CHEMISTRY

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)
- ◆ pCO₂ (defaults to atmospheric)

The requirements for temperature, pH, 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 CaCO₃.

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 Ca ions to Mg ions (in mol/L). These ions will vary among water samples depending on watershed geology and various inputs. If unknown for the region being considered, use the default values in the boxes.

4.2.3 pCO₂

Alkalinity is estimated from pH assuming an open system in equilibrium with CO₂ in the atmosphere. In most natural settings, it is a reasonable assumption that the CO₂ concentration will be 10^{-3.5} atmospheres (pCO₂ of 3.5), but for indoor settings, such as those where many toxicity tests are performed, this might not be the case. The relatively small differences between indoor and outdoor CO₂ concentrations may significantly affect the calculated alkalinity. For this reason, the user may adjust the pCO₂ value.

4.3 MINIMUM DATA REQUIREMENTS

The BLM can be run with any number of observations from 1 to 1,000; and for as many observations are input to the model, a corresponding number of instantaneous WQC values will be calculated.

5 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 3.1.2.37' 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.

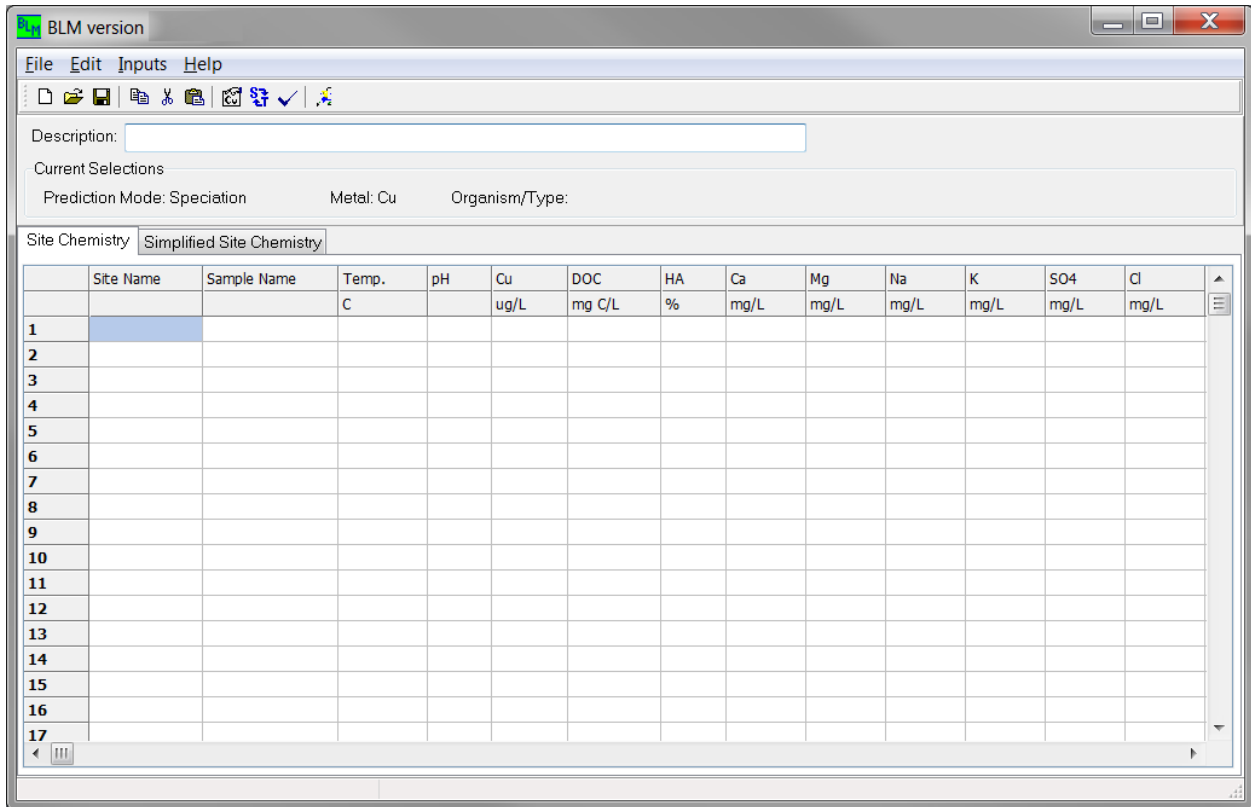


Figure 5-1. Opening screen for the BLM Windows® Interface application

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

6 Running the Application

The BLM Windows® Interface provides access to the full suite of capabilities in the BLM (e.g., predicting metal speciation and toxicity, predicting water effect ratios [WERs], comparison to laboratory measurements of toxicity, and calibration to new metals and organisms). By providing an easy-to-use interface and environment for developing datasets of water chemistry information and applying the BLM for predictions of metal speciation and toxicity, the Windows® Interface streamlines and makes the process of BLM development more efficient and productive.

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.

6.1 DESCRIPTION OF INTERFACE

Figure 6-1 shows a snapshot of the BLM Windows® Interface application. The main purposes of this section of the interface application are 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.

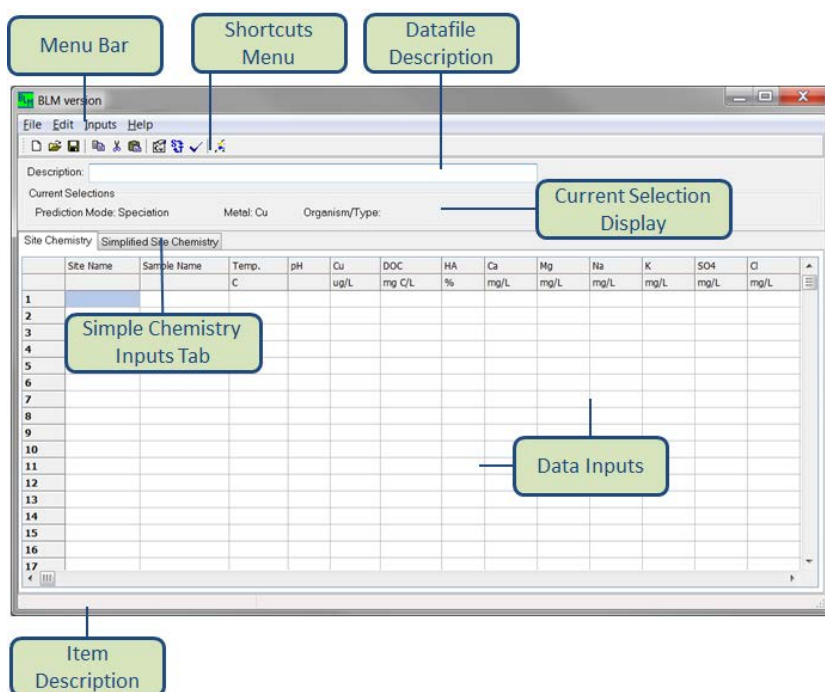


Figure 6-1. Snapshot of the BLM Windows® Interface

As shown in Figure 6-1, the interface window is divided into seven areas broadly based on their functionality. Each of these is described in the subsections that follow.

6.2 DATA 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 naming the sites and the samples described in a given BLM data file. Figure 6-2 shows the various columns typically available for user input.

	Site Name	Sample Name	Temp.	pH	Cu	DOC	HA	Ca	Mg	Na	K	SO4	Cl	Alkalinity	S
			C		ug/L	mg C/L	%	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L CaCO3	mg/L
1															
2															
3															
4															

Figure 6-2. Columns for data input in the BLM Windows® Interface

6.2.1 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 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 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.

6.2.2 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. For predictions of metal speciation (including the WQC calculation), 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.

6.3 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 6-3. Additionally, there is a side bar with boxes where the ion ratios and pCO₂ 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 default 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 optionally lists the ion ratios and pCO₂ at the top and leaves fewer empty lines (10 rather than 20) before the data. An example file is included with the software download.

After the simplified site chemistry data has been inserted into this grid, simply select the 'Site Chemistry' tab again to have the full site chemistry estimated for you, and run the BLM as normal (see section 6.5.6 for information on running the model).

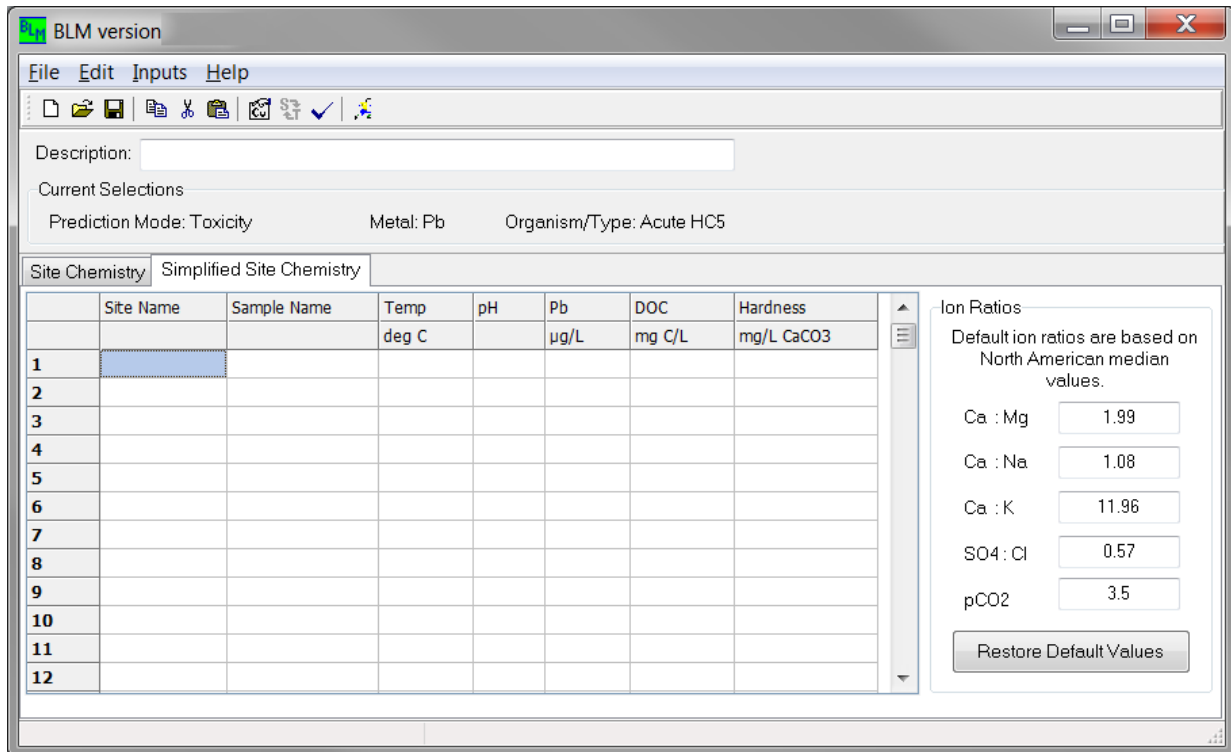


Figure 6-3. Snapshot of Simplified Site Chemistry inputs and ion ratios

6.4 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 among various units for data inputs
- ◆ A help function

These features are described below.

6.4.1 File

Figure 6-4 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.

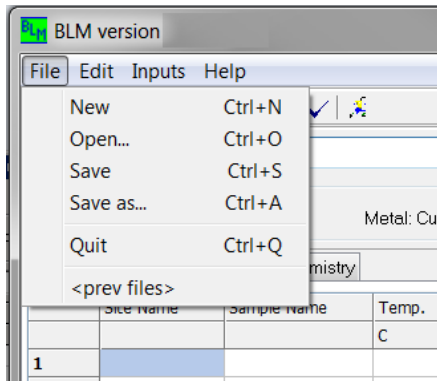


Figure 6-4. Snapshot of file menu item

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 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.

6.4.2 Edit

Figure 6-5 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. Additionally, there are the options to have output saved as Microsoft® Excel (as opposed to an ASCII text file).

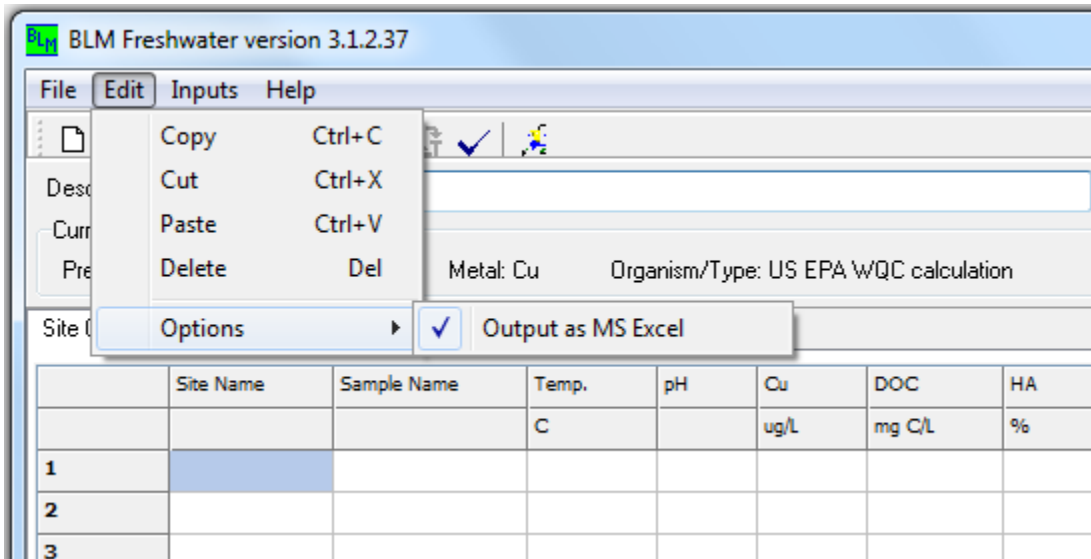


Figure 6-5. Snapshot of edit menu item

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 using the shortcut keys shown to the right of each item. Note that it is also possible to copy and paste data from external programs, such as a spreadsheet application, into the BLM Windows® Interface.

6.4.3 Inputs

Measurements of the water quality parameters required for using the BLM are often reported in varying units. In order to provide the user with a greater degree of flexibility in creating BLM input files, the BLM interface 'Inputs' menu item allows data inputs in several different units, as shown in Figure 6-6.

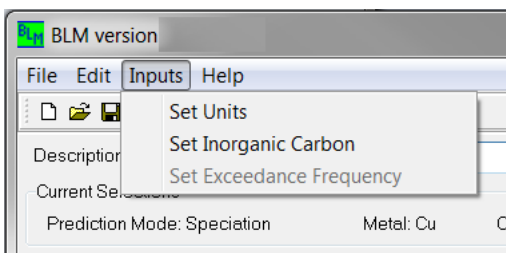


Figure 6-6. Snapshot of inputs menu item

6.4.3.1 Units

The first option 'Set Units' allows the user to select the units for the various BLM input parameters, as shown in Figure 6-7. 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.

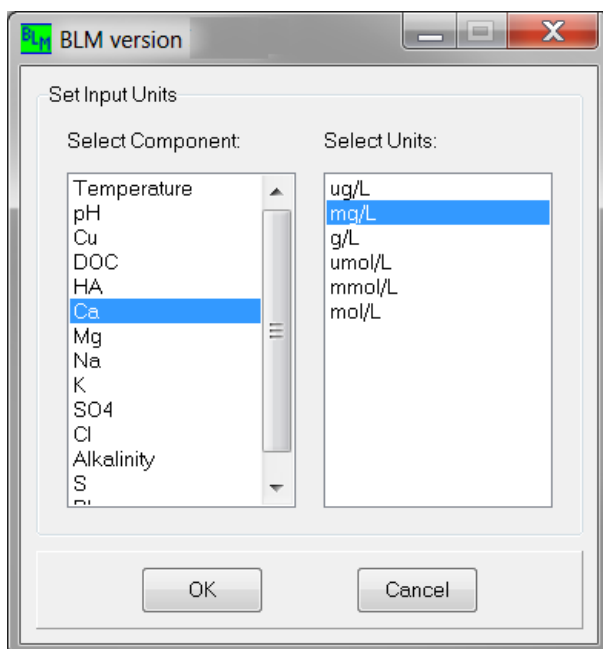


Figure 6-7. View of typical 'Set Units' screen

6.4.3.2 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 6-8

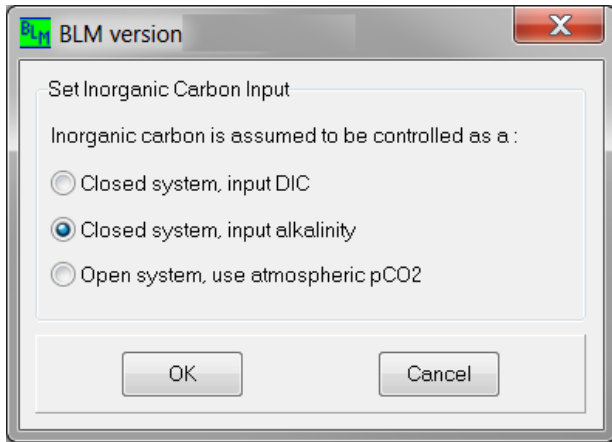


Figure 6-8. View of inorganic carbon input options screen

6.4.4 Help

Figure 6-10 shows the various features available under the 'Help' menu item.

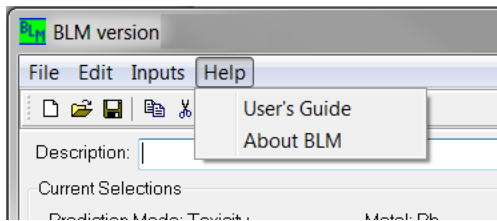


Figure 6-10. Snapshot of help menu item

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 information on contacts for technical support and the version information. The license agreement for use of the BLM can be accessed in the first few pages of the User's Guide.

6.5 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 6-11 shows the various icons and their functions; brief descriptions are provided in the subsections that follow.

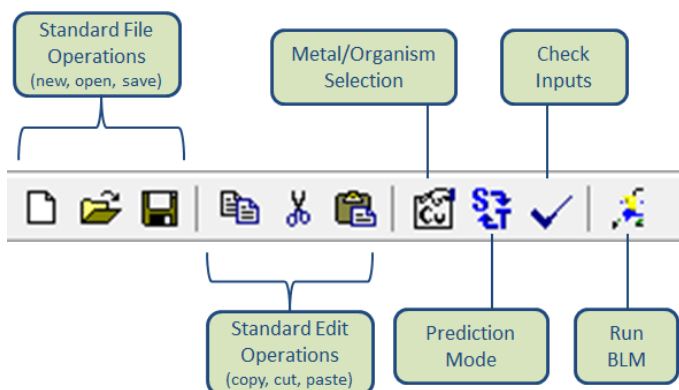


Figure 6-11. Shortcut menu icons

6.5.1 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.

6.5.2 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.

6.5.3 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 6-12, and the user can 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 6.6).

Acute and chronic parameter files for the metals shown in figure 6-12 have been developed and will be added to the package over time as they are finalized. Unless otherwise specified, the available parameter files are currently for acute effects.

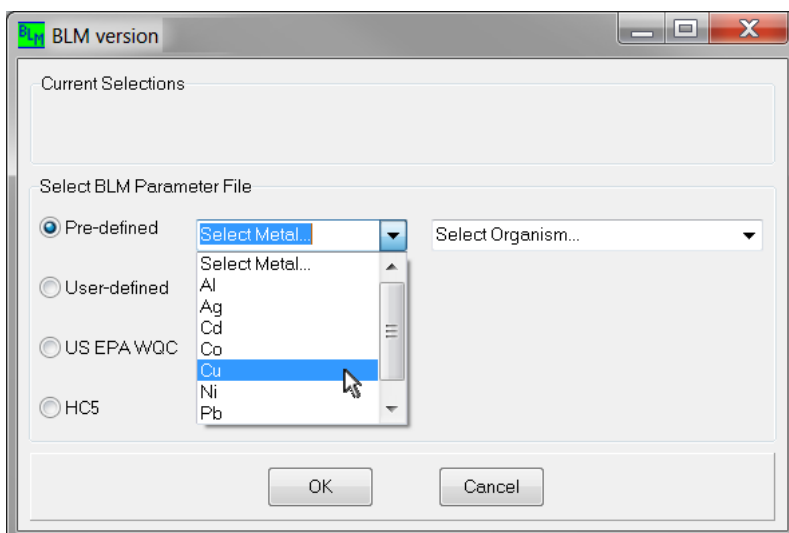


Figure 6-12. Metal and organism selection options

6.5.3.1 Metal and organism options available

The metal- and organism-specific parameter files that are included in the current distribution of the BLM Windows® Interface, Version 3.1.2.37, are available by selecting the 'Pre-defined' radio button, then selecting first the metal and then an organism from the drop-down menus, as shown in Figure 6-12. Note that these metal- and organism-specific options 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.

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 are specified in units of $\mu\text{g}/\text{L}$, the interface application internally converts these to moles/L using the molecular weight for the metal selected by the user. Changing the metal for the BLM application within an existing data file developed for a different metal may result in an erroneous conversion from $\mu\text{g}/\text{L}$ to moles/L when the user saves and opens the data file the next time.

6.5.3.2 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' radio button shown in Figure 6-12 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 will be asked to identify the appropriate parameter file when opening a BLM input file that was previously developed for a user-selected parameter file.

6.5.3.3 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 ‘US EPA WQC’ option radio button shown in Figure 6-12, 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 6.9). 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.

Site Label	Sample Label	Final Acute Value (FAV), ug/L	CMC (CMC=FAV/2), ug/L	CCC (CCC=FAV/ACR), ug/L	Cu ug/L	Acute Toxic Units (Acute TU=Cu/CMC)	Chronic Toxic Censored Flag (Chronic TU= (0 = quantified, 1 = BDL)
"Kansas River 6892350" *7/22/1987	"	212.10	106.05	65.87	6.00	0.06	0.09 0.00
"Kansas River 6892350" *10/20/1987	"	173.43	86.71	53.86	2.50	0.03	0.05 0.00
"Kansas River 6892350" *11/23/1987	"	116.44	58.22	36.16	1.20	0.02	0.03 0.00

Figure 6-13. 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 6-13 can also be copied for pasting onto any external application by simply highlighting the cells of interest and either using shortcut keys Control-C or right-clicking the highlighted area and selecting Copy from the resulting option(s). The same information can be found in the WQC output file.

6.5.4 Prediction mode

The BLM interface application allows the user to run the BLM either in toxicity mode or in the speciation mode. When run in the 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 the speciation mode, for the metal concentration specified by the user, the BLM will predict the organic and the inorganic speciation in the water column.

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 6.6). By default, the BLM interface application assumes that the BLM prediction mode is the toxicity mode unless the user specifies otherwise. The current prediction mode is also saved in the BLM data file, and the next time the user opens up the BLM data file, the application will default to the prediction mode used at the time the file was saved.

6.5.5 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 to check 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 7, Input Check Range. Figure 6-14 shows an example of an input check report.

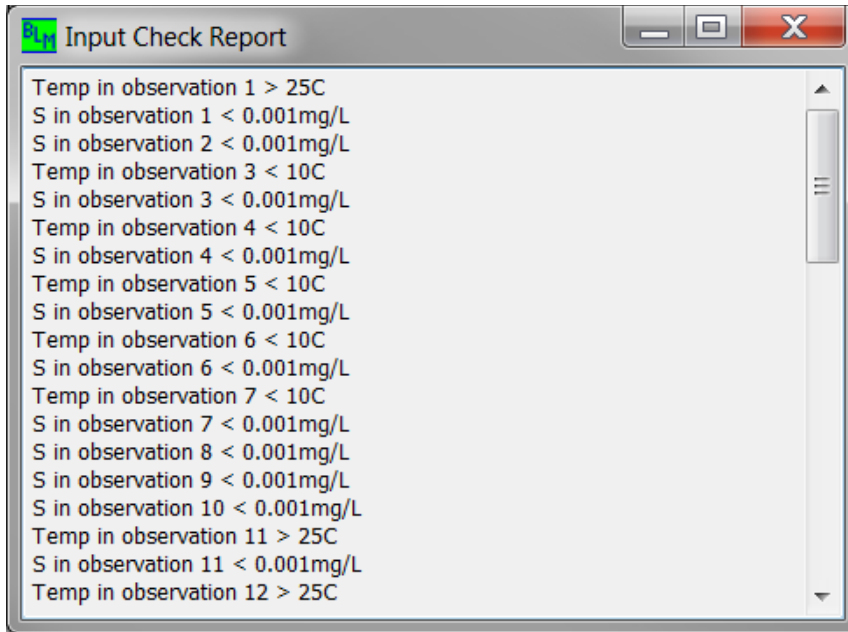


Figure 6-14. Example of an input check report generated by the check inputs function

6.5.6 Run BLM

This icon (see Figure 6-11) is used to launch the BLM program 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.

6.6 CURRENT SELECTION DISPLAY

This area of the interface window displays the current metal, organism, and prediction mode selections made by the user. For the example shown in Figure 6-1, the user has opted to predict the toxicity of Cu to fathead minnows by using the 'Shortcuts Menu' buttons 'Prediction Mode' and 'Metal/Organism Selection'. The options selected by the user are saved in the BLM data file; the next time the user opens the BLM data file, the application defaults to the selections made by the user at the time of the previous file save.

6.7 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.

6.8 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 6-1, 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.

6.9 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). The format of the output files, as either text or Microsoft Excel® files, is selected under the 'Edit' menu (see Section 6.4.2).

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 (WQC, HC5, LC50, etc)
- ◆ Input datasets
- ◆ 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} of the gill
- ◆ DOC in mg/L
- ◆ Percent humic acid
- ◆ The rest of the input water chemistry in units of mg/L

7 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 provided in the BLM interface application. Users can check to verify that the input dataset values fall within the ranges for which the BLM has been calibrated. This check is done by clicking the check icon on the menu for the 'Check Inputs' function. The calibration and ranges for each of the BLM input parameters are shown in Table 7-1. 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 7-1. Prescribed ranges for BLM input parameters

Parameter	Lower Bound	Upper Bound
Temperature (°C)	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

BLM – Biotic Ligand Model

DIC – dissolved inorganic carbon

DOC – dissolved organic carbon

8 Example Application

The BLM Windows® Interface installation also features an example application for demonstration purposes. This file, named 'Kansas River.BLM,' is installed along with the BLM interface application and is located in the 'Data' directory within the BLM home directory on the user's hard drive. The file can be opened either by double-clicking on the file name through a file system manager (e.g., Microsoft Windows® Explorer), or by first starting the BLM Windows® Interface application and then selecting the file through the 'File ----> Open' action. This example data file contains the water quality observations for US Geological Survey (USGS) Station 6892350 on the Kansas River at Desoto, Kansas. Although in this case, only observations with a complete characterization of all the BLM input parameters are included in the BLM data file, it is recommended that all the available water quality measurements (including ones without a complete characterization of the BLM input parameters) be included in the BLM data file.

The data file 'Kansas River.BLM' can be used to predict metal speciation using the input metal concentrations, 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, as shown in Figure 8-1.

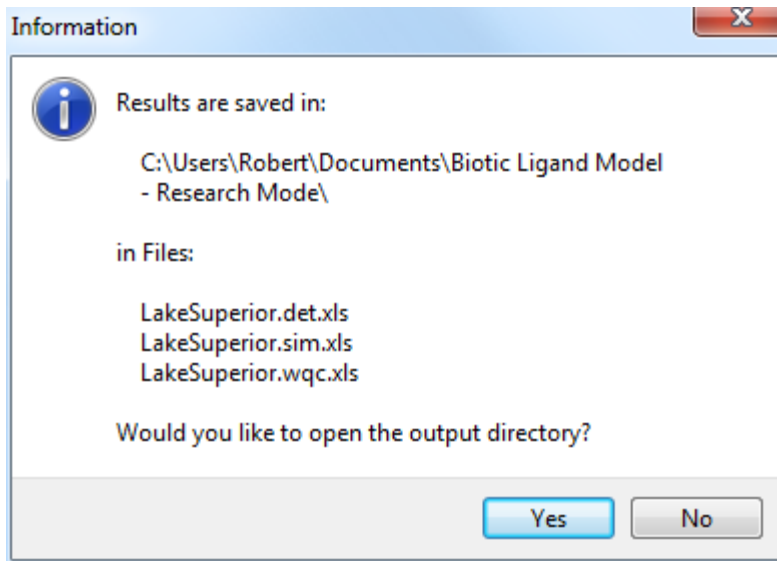


Figure 8-1. Example of notification window shown at completion of BLM run

The formats of the output files have been described in Section 6.9, Description of Output Files.

9 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.

10 References

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