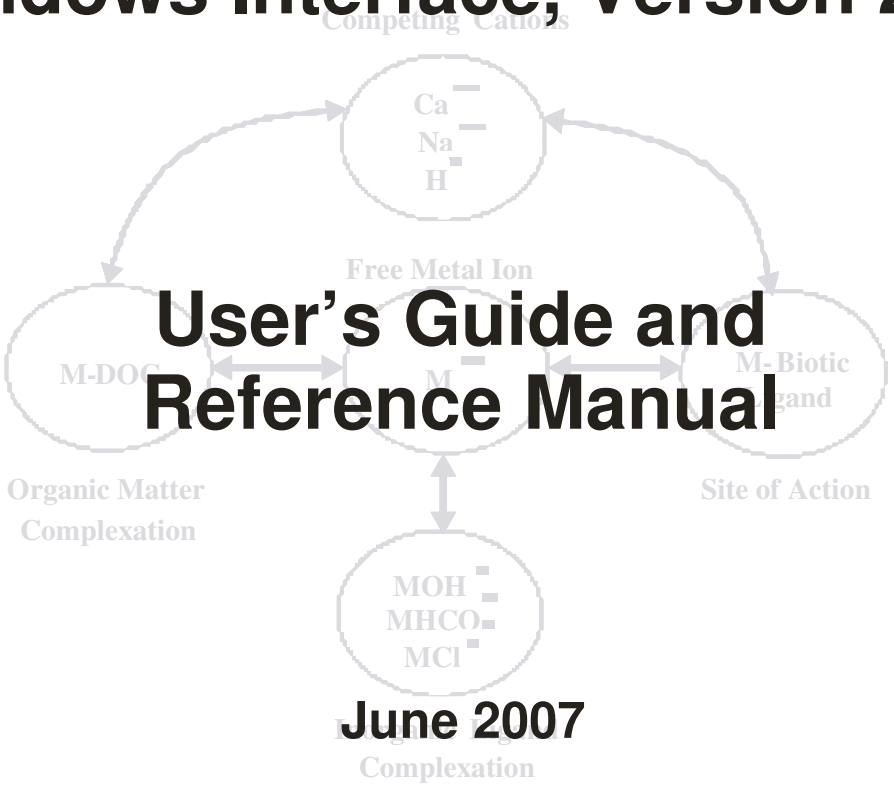
Biotic Ligand Model
Windows Interface, Version 2.2.3



User's Guide and Reference Manual

June 2007

HydroQual, Inc.
1200 MacArthur Blvd.
Mahwah, NJ 07430
(201) 529-5151

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OBTAINING THE BLM

The BLM can be downloaded from http://www.hydroqual.com/blm

Additional information including support details can also be found online or in the User's Guide.

CITATIONS

This report was prepared by:

HydroQual, Inc.
1200 MacArthur Blvd.
Mahwah, New Jersey 07430

Principal Investigators:

Paul Paquin

Robert Santore

Rooni Mathew

The report is a corporate document that should be cited in the literature in the following manner:

The Biotic Ligand Model Windows Interface, Version 2.2.3: User's Guide and Reference Manual, HydroQual, Inc, Mahwah, NJ, April 2005.

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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, 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 concentration. 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 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). The BLM is based on a conceptual model similar to the gill site interaction model proposed by Pagenkopf (1983). 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 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 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 copper toxicity to fathead minnows (*Pimephales promelas*). The "biotic ligand" or site of acute copper toxicity for fathead minnow has been identified as Na ion uptake channels in the gill membrane (Playle et al., 1993a). Copper 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 copper on gill surfaces in the BLM has been calibrated to measurements of copper accumulation on the gill over a wide range of water quality conditions (Playle et al., 1992 and 1993b). Additionally, MacRae (1994) established a dose response relationship necessary to determine the biotic ligand LC50 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, 1993b), 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, 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 Lethal Accumulation of metal on the biotic ligand that results in 50% mortality in a toxicological exposure. 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 acute toxicity within a given aquatic system.

2
OVERVIEW AND HELP FILE LAYOUT

2.1 What's New In This Distribution?

Originally, the BLM was developed as a MS-DOS based program, with the user developing the BLM input files using an external spreadsheet program, such as Microsoft Excel, running the BLM in the MS-DOS environment and then analyzing the BLM output using a different set of software tools. In order to facilitate data-entry; however, model simulations, and the analysis of model output in a common application environment and in a more efficient and user-friendly fashion, a graphical user interface was developed for the BLM and first distributed as BLM, Windows Interface Version 1.0.0. The current distribution, Version 2.2.3, is an updated version that offers additional options for data inputs and model simulations. The new functionalities are further described in the subsequent sections. The BLM, Windows Interface Version 2.2.3 incorporates the most current version of the BLM, Version 223.

Note that BLM datafiles 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, the data requirements of the BLM, a step-by-step guide to using the various functionalities of the BLM Windows Interface and a walk-through of the application using a example BLM datafile.

3
SETUP AND INSTALLATION

3.1 System Requirements

The BLM Windows Interface is designed for use on the IBM compatible PC family of microcomputers running Microsoft Windows. The memory requirements of the BLM Windows Interface 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 95/98/2000/ME/XP
- 32 MB RAM
- 30 MB free disk space

Recommended System Configuration

- Intel Pentium 3, 500 MHz
- 64 MB RAM
- 100 MB free disk space

Even though the BLM Windows Interface can be run on a system with the specified minimum requirements, in the interest of computation time, the recommended system configuration or a faster one would be ideal.

3.2 Installing the BLM Windows Interface

- **Installing from a disk -** To install the BLM Windows Interface from a CD-ROM, insert the installation disk into the CD-ROM drive. In case the installation does not start up automatically, locate and run the program 'setup.exe' located in the main directory in the installation disk by simply double-clicking on the file name.
- **Installing from the compressed (.zip) file -** To install the BLM Windows Interface from the compressed file "BLMWindowsInterface_Version2.2.3.zip" simply 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 simply double-clicking on the file name.

Note that on PCs running Microsoft Windows 2000/ME/XP, the user may need to be logged on as the "Administrator" or have the relevant permissions to modify the 'System' directory in order to install the necessary files.

The setup program will guide the user through a fairly straightforward installation process, querying the user for information on where to install the necessary files. During the installation, a shortcut to the BLM Windows Interface application will be added to the 'Programs' sub-menu within the 'Start' menu on the Microsoft Windows desktop. In addition, the BLM Windows Interface application will also be registered in the system registry so that the BLM datafiles 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. Therefore, the user will be expected to provide data describing the physical and chemical properties of the site water. The data requirements of the BLM are conventional physical and chemical parameters that are easily measurable in the laboratory. This section describes the general physical and chemical data requirements for an application of the BLM to predict metal speciation and toxicity in aquatic systems.

4.1 Water Quality Parameters Required

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

- Temperature
- pH
- Dissolved Organic Carbon
- Major cations (Ca, Mg, Na and K)
- Major anions (SO_4 and Cl)
- Alkalinity
- Sulfide

For a given metal some of these chemical inputs have an important effect on determining 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 sections may be helpful in that assessment.

Each water sample has to be fully described in terms of the above water quality inputs before the BLM can be used. If some of the parameters are known to be absent in the water sample; however, a nominal, negligible concentration should be input (a value on the order of 1E-10 mg/L should suffice typically) rather than a zero concentration.

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. Since the BLM is based on a thermodynamic chemical equilibrium modeling framework, temperature measurements are important in determining the relevant thermodynamic reaction rates.

4.1.2 pH

Accurate pH values are important to BLM results for most metals. The chemical speciation of many metals, such as copper, is directly affected by pH. pH is; however, 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 to laboratory measurements of metal toxicity, then it is preferable that the pH is measured within the test chamber during the exposure.

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 dissolved organic carbon (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 the Windermere Humic Aqueous Model (WHAM, Version 1.0), 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 found to be an especially critical parameter and little benefit is achieved by characterizing NOM beyond DOC concentrations.

4.1.4 Metal Concentrations

The BLM can be used to predict the speciation and bioaccumulation of metals when a metal concentration is provided as an input. When the model is used in metal speciation mode, metal concentrations are a required input. The BLM model; however, is probably most useful as a means of predicting metal toxicity (i.e., a concentration associated with a specific toxicological effect). When used in metal toxicity mode, there is no need to input metal concentrations.

4.1.5 Major Cations

The cations Ca, Mg, Na, and K are all necessary inputs to the BLM. For copper and silver, Ca and Na can directly compete with the metal at biotic ligand sites and 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, it is discussed separately subsequently). 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 of 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 copper simulations, Cl is only important as a contribution to ionic strength, but for silver simulations Cl can have an additional importance due to the formation of silver-chloride complexes. Therefore, it is preferable that only measured Cl concentrations are used for BLM applications involving silver, while estimates can be used for applications involving copper.

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 called dissolved inorganic carbon (DIC). Bicarbonate is usually the most important DIC species in natural waters since it is the dominant species between pH 6.35 and 10.33. Inorganic carbon is a critical input to the BLM since many metals, including copper, form carbonate complexes. Silver, on the other hand, does not form carbonate complexes, and so DIC is not a critical input to BLM applications for silver. Unfortunately, measurements of DIC are not often made in natural water samples. It can be estimated; however, from alkalinity and pH measurements as in the equation below.

$$DIC = Alk \cdot \frac{\frac{H}{K1} + 1 + \frac{K2}{H}}{1 + \frac{2 \cdot K2}{H}}$$

where Alk. = alkalinity in equivalents/L

= 2 x 10^{-5} x alkalinity (as mg $CaCO_3$ / 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 $CaCO_3$. Depending on the inorganic carbon option selected; however, the user may also opt to specify DIC concentrations directly.

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 freshwaters. 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. If it is present, therefore, 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; however, 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 which 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.

5
STARTING THE APPLICATION

To start using the BLM Windows Interface, select the application using 'Start -----> Programs ----> Biotic Ligand Model -----> Biotic Ligand Model, Version 2.2.3' on the Microsoft Windows desktop. The user will be presented with the following screen, which contains the user input areas, and the various functions implemented in this version of the BLM Windows Interface.

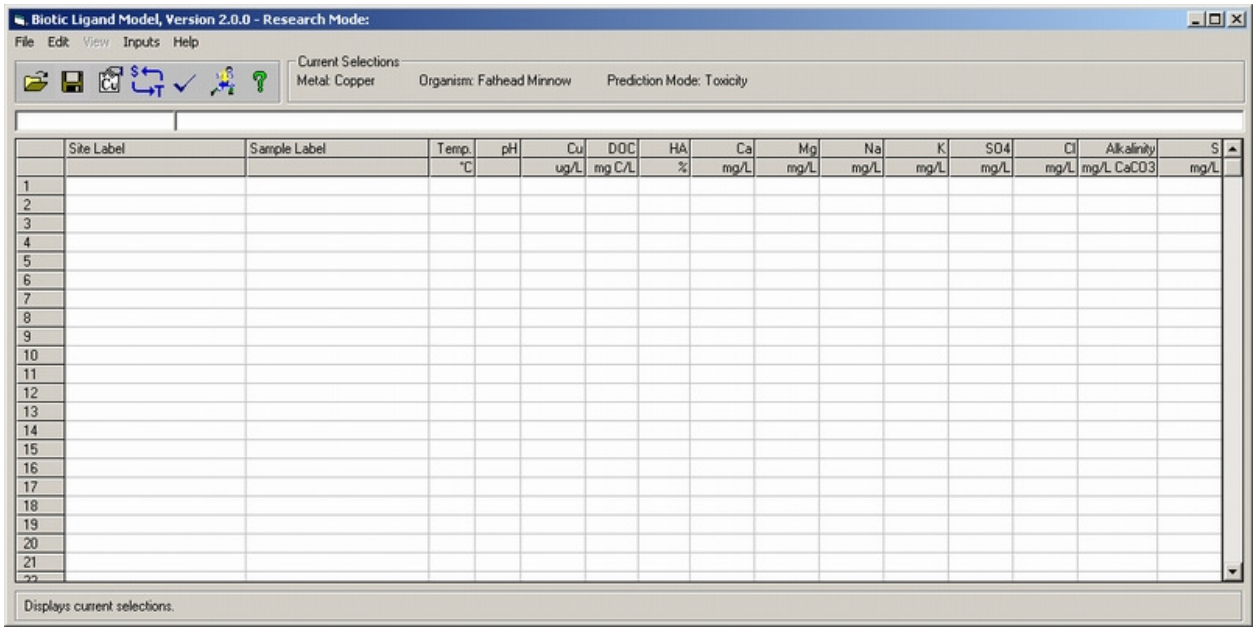


Figure 5-1. Opening Screen for the BLM Windows Interface Application

In case the user already has a BLM datafile 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.

6
RUNNING THE APPLICATION

The BLM Windows Interface provides access to the BLM in its full suite of capabilities, i.e., predicting metal speciation and toxicity, predicting Water Effect Ratios (WER), comparison to laboratory measurements of toxicity, calibration to new metals and organisms, etc. 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, it streamlines and makes the process of BLM development more efficient and productive.

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

6.1 Description of Interface

Figure 6-1 shows a snapshot of the BLM Windows Interface application. The main purpose of this section of the interface application is to provide an easy to use editor to develop input files containing water chemistry information for the BLM, to facilitate checks and validate the user inputs for the various parameters, to perform checks on whether the values entered for any given parameter is within the range for which the BLM has been calibrated, and to run the BLM for predictions of aquatic speciation or toxicity for a variety of metals and organisms.

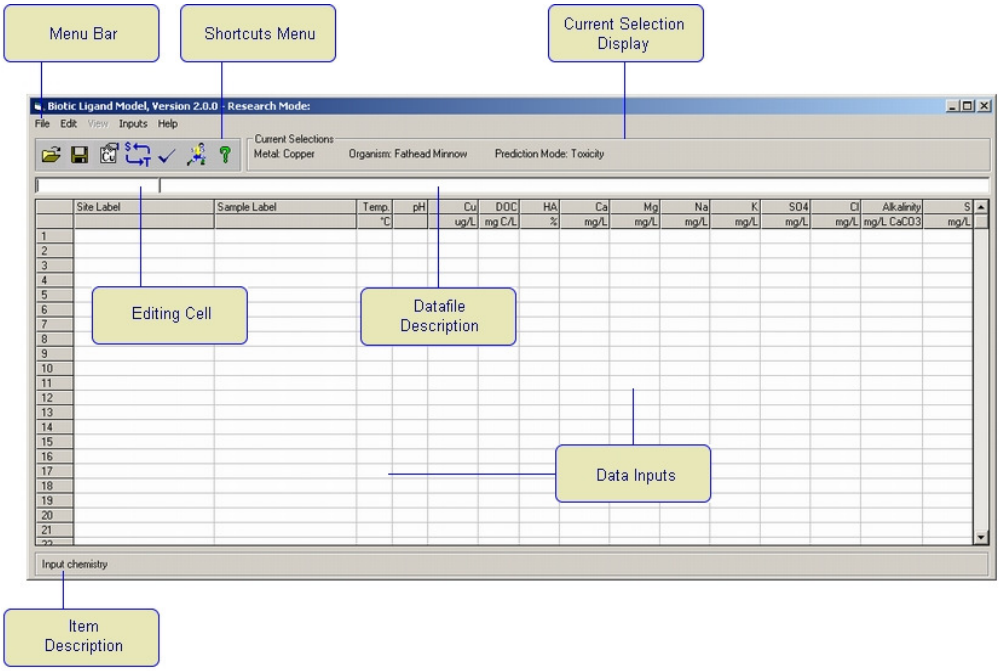


Figure 6-1. Snapshot of the BLM Windows Interface

As shown in Figure 6-1, the interface window is divided into 7 areas broadly based on their functionality. Each of these is described in the subsequent sections.

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 labeling the sites and the samples described in a given BLM datafile. Figure 6-2 shows the various columns typically available for user input.

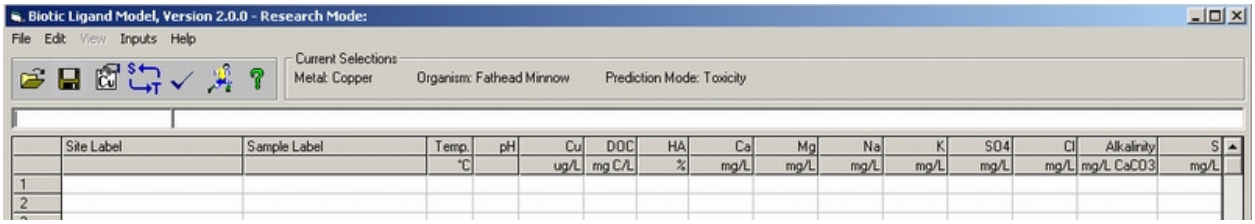


Figure 6-2. Columns for Data Input in the BLM Windows Interface

6.2.1 Site Label and Sample Descriptor

The very first column, the 'Site Label', 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 information contained within the 'Sample Label' 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; however, there is an upper limit of 20 characters that are allowed in each field.

6.2.2 Water Chemistry Inputs

The subsequent columns contain the data input area for the water quality parameters described under 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, the metal concentration is a required input and if no metal concentration is specified; however, 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 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:

- Managing the BLM datafiles
- Text editing functions
- Functions to select between various units for data inputs
- A help function.

These features are described below in further detail.

6.3.1 File

Figure 6-3 shows the functions available under this menu item. Basic file management utilities to create a new BLM datafile, to open an existing BLM datafile and to save a BLM datafile are provided.

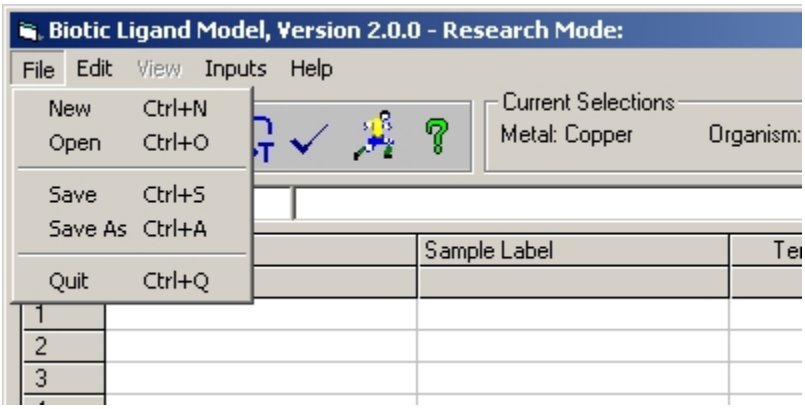


Figure 6-3. Snapshot of File Menu Item

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

For ease of access, BLM datafiles can also be opened directly by double-clicking on the BLM datafile 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 datafile of interest.

Note that the BLM datafiles created by the interface application are given a '.BLM' extension by default. Even though the BLM datafile 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 datafile getting corrupted and if this happens, the next time the user tries to edit that BLM datafile using the BLM Windows Interface, the file may not be read correctly by the BLM interface application.

6.3.2 Edit

Figure 6-4 shows the editing functions available in the BLM Windows Interface. Basic editing functions such as 'Cut', 'Copy', 'Paste' and 'Delete' as well as a couple of different output file format options are implemented in the interface application.

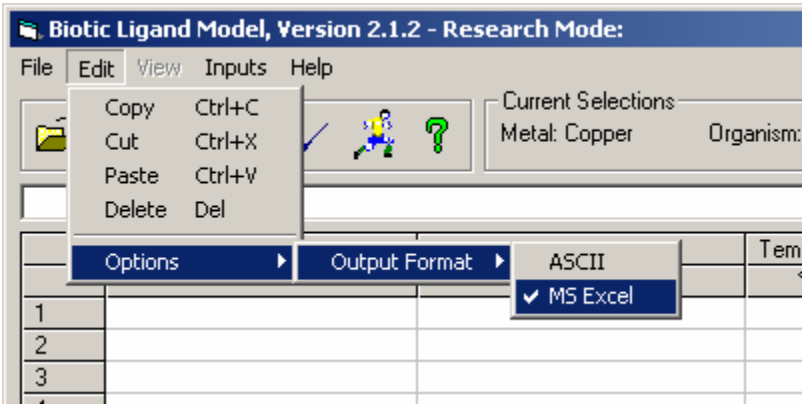


Figure 6-4. Snapshot of Edit Menu Item

The editing functions can be performed on a single cell or multiple cells selected by highlighting the cells with a mouse click and drag operation 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 item or by clicking the right mouse over the selected data cells and then selecting the editing operation from the editing menu that is displayed. Note that it is also possible to copy and paste data from external programs, such as a spreadsheet application into the BLM Windows Interface.

Previous versions of the BLM and the BLM Windows Interface provided model output (i.e. the predictions of speciation or toxicity) in only ASCII format. However, BLM Windows Interface Version 2.2.3 allows the flexibility to select between ASCII or Microsoft Excel formats for the BLM output files simply by selecting the format under 'Edit -----> Options -----> Output Format'.

6.3.3 View

This feature is not implemented in the current distribution of the BLM Windows Interface and may be available only in subsequent versions.

6.3.4 Inputs

Measurements of the water quality parameters required for using the BLM are often reported with varying units. In order to provide the user with a higher degree of flexibility in developing BLM input files, the BLM interface allows data-inputs in several different units by means of this menu item, as shown in Figure 6-5.

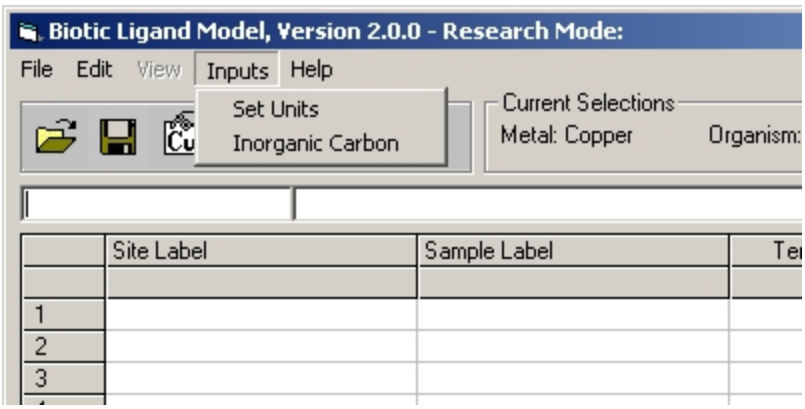


Figure 6-5. Snapshot of Inputs Menu Item

Units

The first option 'Set Units' allows the user to select the units for the various BLM input parameters, as shown in Figure 6-6. For each parameter, the current selected units are highlighted by default and the user can select the desired units from the list of options shown. When changing units for a given parameter, data already input for that parameter is converted to the new units to prevent any loss of data.

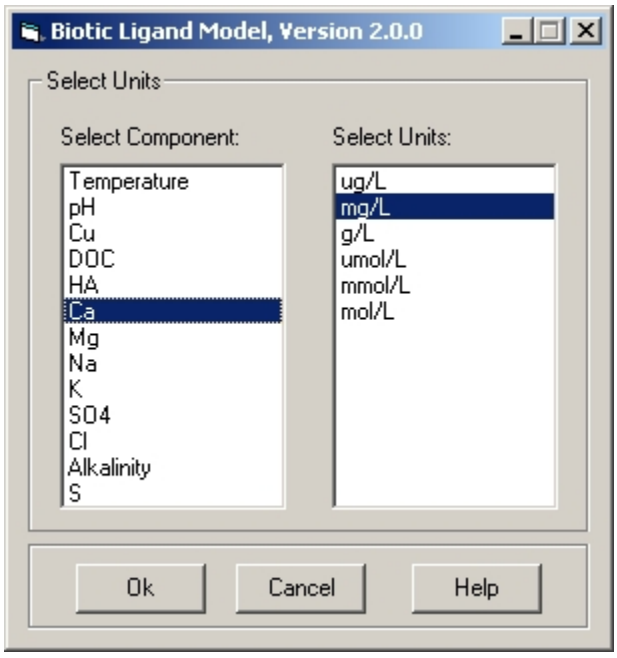


Figure 6-6. View of Typical 'Set Units' Screen

Inorganic Carbon

The second option 'Inorganic carbon' gives the user the option to select between various options for specifying the inorganic carbon in the system. As mentioned previously, the BLM simulates the formation of metal-carbonate complexes and 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 dissolved inorganic carbon. Accordingly, the user can select between these two options by means of the 'Inorganic carbon' feature, as shown in Figure 6-7.

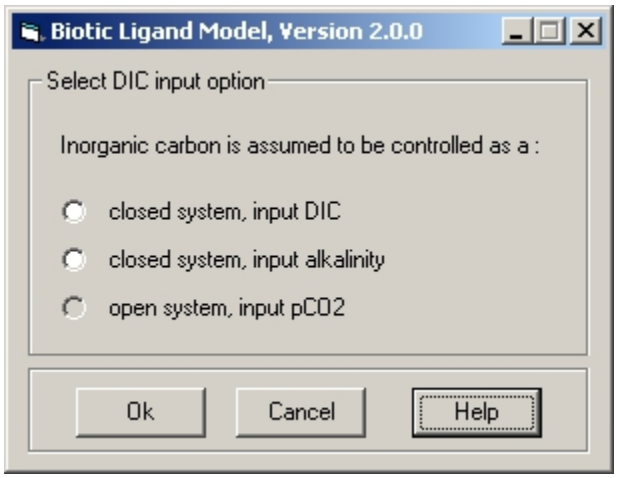


Figure 6-7. View of Inorganic Carbon Input Options Screen

6.3.5 Help

Figure 6-8 shows the various features available under the Help menu item.

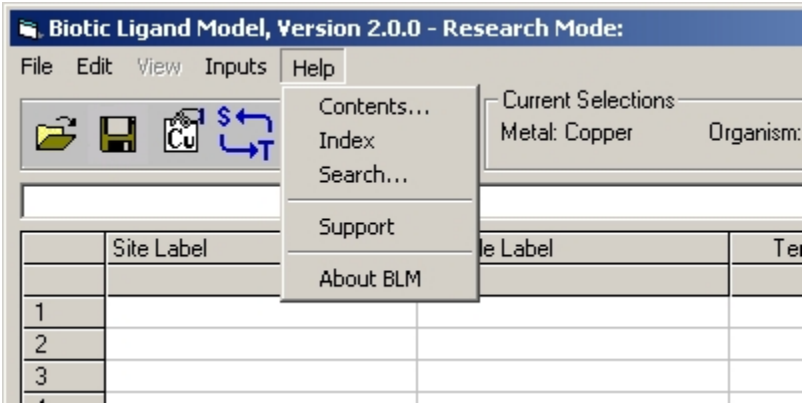


Figure 6-8. Snapshot of Help Menu Item

The help file for the BLM Windows Interface can be accessed via this menu item and can be browsed by its contents, by a keyword index or by searching for a particular word or phrase. In addition, under the 'Support' sub-item, there is also information on whom to contact for technical support and sending bug reports, etc. A short description of the BLM can be found under the sub-item 'About BLM.'

6.4 Shortcuts Menu

This group of icons contains shortcuts to some of the menu bar items and some additional functions that are not available on the menu bar. Figure 6-9 shows the various icons and their functions.

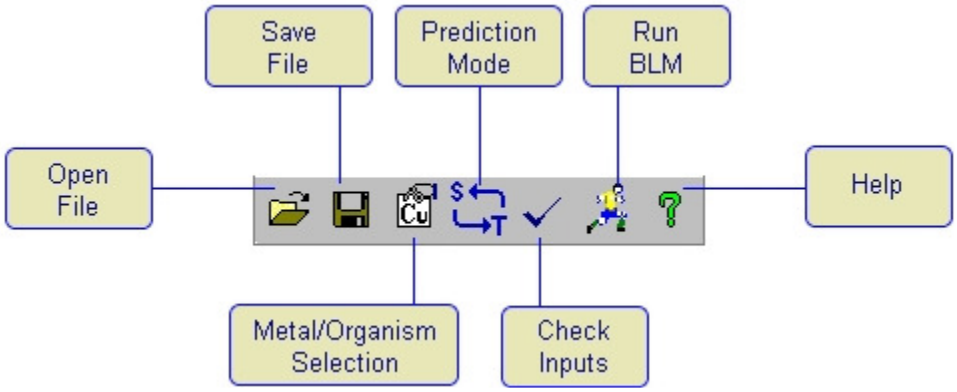


Figure 6-9. Shortcut Menu Icons

6.4.1 Open File

This is a shortcut to the menu bar item under 'File -----> Open' and is provided for a quick mode of access to the BLM datafiles. In case the BLM datafile being edited by the user has changed since the last time it was saved, the user will be queried for a confirmation on whether to proceed to open another datafile with or without saving the current datafile.

6.4.2 Save File

This is a shortcut to the menu bar item under 'File -----> Save' and is provided for a quick mode of saving the BLM datafiles. The datafile will be saved under the same name as it was last saved as. In case the user wishes to save the file under a different file name, the menu bar item 'File -----> Save As' should be chosen.

6.4.3 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 has to be predicted. Clicking on this icon will present the

user with the window shown in Figure 6-10 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.

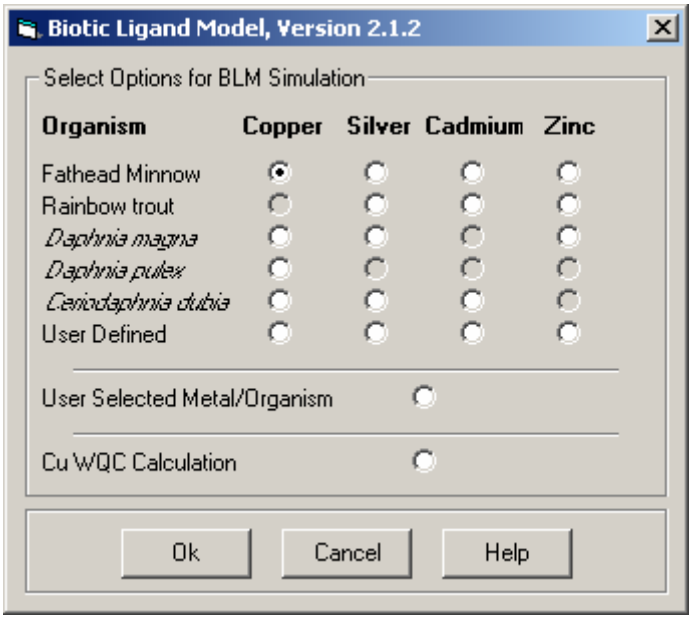


Figure 6-10. Metal and Organism Selection Options

Metal and Organism Options Available

The metal and organism specific parameter files that are distributed along with the current distribution of the BLM Windows Interface, Version 2.2.3 are indicated by the options that are not grayed out in Figure 6-10, i.e., the combinations available for the user to choose from. Note that these metal and organism specific parameter files are part of an ongoing task of refining the calibration and application of the BLM and may therefore undergo revisions from time to time as the case may be. The metal and organism selections made by the user are also saved in the BLM datafile and the next time the user opens the BLM datafile, the application will default to the selections made by the user at the time the file was saved.

It is advisable to develop separate BLM datafiles 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. Since the input metal concentrations are specified in units of µg/L, the interface application internally converts these to units of moles/L using the molecular weight for the metal selected by the user. Changing the metal for the BLM application within an existing datafile developed for a different metal, may result in an erroneous conversion from units of µg/L to moles/L when the user saves and opens the datafile the next time.

User Defined

Normally, when run in the toxicity prediction mode for a given organism and metal, the BLM interface application will derive the LA50 for the user selected organism from the parameter file specific to that particular metal and organism. The BLM will then predict the LC50 of the selected metal to the selected organism for all the observations with a complete set of BLM input parameters. In order to provide additional flexibility in operation; however, the BLM can be run for a given metal with different LA50s for different rows of input. That is, the BLM will predict LC50s corresponding to different LA50s for each row. This is accomplished by selecting the 'User Defined' option shown in Figure 6-10 and selecting 'Ok.' This will add an extra column to the spreadsheet editor in the application window in the very last column position, to the extreme right. The user is expected to populate this column for each row of input, with the desired LA50. Note that leaving this column blank for any line of input can result in the BLM treating that line of input as a incomplete input and will result in failure to predict toxicity.

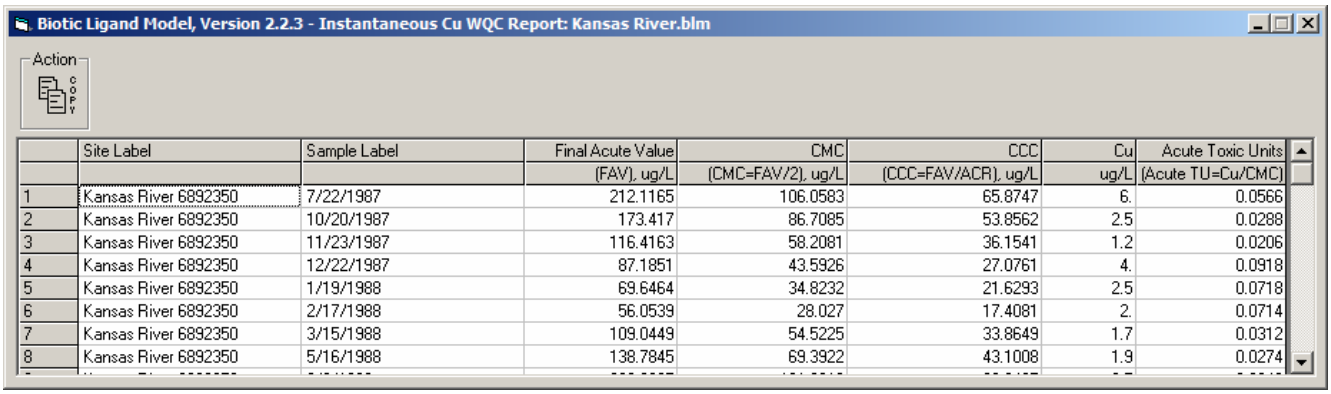
User Selected

In addition to the metal and organism specific parameter files that are distributed along with the current distribution, the user may also opt to develop and use their own versions of these files for BLM predictions. This is achieved by selecting the 'User Selected' option shown in Figure 11 and selecting 'Ok'. The user will then be queried for the location of the desired parameter file. New parameter files can be developed by the user along the lines of the parameter files supplied with this distribution (files with the extension '.DAT' located in the 'Model' sub-directory within the BLM home directory). Note that the user will be asked to indicate the appropriate parameter file when opening up a BLM input file that was previously developed for a user selected parameter file.

Cu WQC Calculation

The US EPA's proposed BLM based Water Quality Criteria (WQC) for copper (USEPA, 2003) has been implemented in Version 2.2.3 of the BLM Windows Interface and can be accessed by selecting this option. When run in this mode, the BLM predicts the site-specific WQC for each row of input and displays a criteria report as shown in Figure 12. In addition to the BLM predicted Final Acute Value (FAV) and the Instantaneous WQC (calculated as the FAV divided by 2), if dissolved copper inputs are present in the BLM datafile, it is tabulated on the criteria report screen and used to calculate toxic units (TU). TUs are computed as the ratio of the copper in the water to the instantaneous WQC for that water sample, with TU values greater than 1 indicating a violation of the instantaneous copper WQC.

For additional information on the terminology and the exact mechanistics of the WQC calculation, the user is advised to refer to USEPA, 2003. The criteria report shown in Figure 12 can also be copied for pasting onto any external applications simply by highlighting the cells of interest and either using shortcut keys Control-C or by a mouse right-click followed by selecting Copy from the resulting option(s).



	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)
1	Kansas River 6892350	7/22/1987	212.1165	106.0583	65.8747	6.	0.0566
2	Kansas River 6892350	10/20/1987	173.417	86.7085	53.8562	2.5	0.0288
3	Kansas River 6892350	11/23/1987	116.4163	58.2081	36.1541	1.2	0.0206
4	Kansas River 6892350	12/22/1987	87.1851	43.5926	27.0761	4.	0.0918
5	Kansas River 6892350	1/19/1988	69.6464	34.8232	21.6293	2.5	0.0718
6	Kansas River 6892350	2/17/1988	56.0539	28.027	17.4081	2.	0.0714
7	Kansas River 6892350	3/15/1988	109.0449	54.5225	33.8649	1.7	0.0312
8	Kansas River 6892350	5/16/1988	138.7845	69.3922	43.1008	1.9	0.0274

Figure 6-11. Instantaneous Copper Criteria Report

6.4.4 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 mortality in the water specified by the user. When the BLM is run in the speciation mode; however, 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. 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 datafile and the next time the user opens up the BLM datafile, the application will default to the prediction mode at the time the file was saved.

6.4.5 Check Inputs

After creating a BLM datafile, the user may wish to check the water chemistry inputs to verify if the parameter values are within the overall range for which the BLM has been calibrated and to check to see if all the parameters necessary for a BLM prediction have been specified. Clicking on this icon serves to generate an input check report which contains information on what parameters are out of range (too high or too low when compared to range for which the BLM has been calibrated) and what parameters are missing for any given row of input. The range of parameter values for which the BLM has been calibrated is described in Input Check Range. Figure 6-11 shows an example of such an input check report.

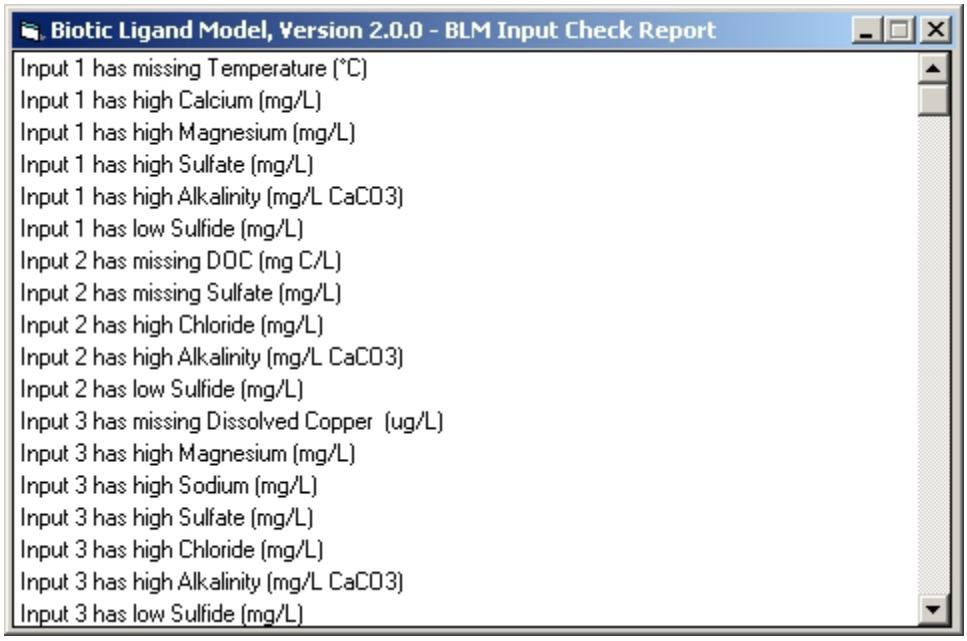


Figure 6-12. An Example of an Input Check Report Generated by the Check Inputs Function

Note that a similar check is also done every time the user edits the contents of any cell in the water chemistry input section. In this case; however, an input check report is not generated. Instead, the out of range parameter value is highlighted in red as opposed to the normal text color of black.

6.4.6 Run BLM

This icon 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 datafile currently open in the BLM Windows Interface. In case the BLM datafile has been edited since its last save, the user is queried for confirmation on whether to save the file or not and the BLM predictions proceed subsequently.

6.4.7 Help

This feature provides a point-and-click help functionality for several features of the interface application. To use this feature, simply click on this icon and point and click on the icon or area for which the user is interested in finding help/additional information.

6.5 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 copper 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 datafile and the next

time the user opens the BLM datafile, the application defaults to the selections made by the user at the time of the previous file save.

6.6 Editing Cell

This area shows the value of the parameter in the current cell as it is being edited.

6.7 Datafile Description

This area is provided for the user to insert comments describing the BLM datafile which will then be saved along with the water chemistry parameters input by the user. Though it is not of critical importance to the use of the BLM, for record keeping and possibly QA/QC purposes, it is a desirable input.

6.8 Item Description

Located at the very bottom of the interface window, this area is designed to show a brief description of the icon/image/area the mouse cursor is currently positioned over. For the case shown in Figure 6-1, the mouse cursor is positioned over the 'Data Inputs' area. Similar messages are displayed when the mouse cursor is moved over other areas of the interface window.

6.9 Description of Output Files

When run in the metal speciation or metal toxicity mode, the BLM creates two output files within the directory containing the BLM input file. The names of the output files are based on the name of the input file. For example, using the input file 'TEST.BLM' would create two output files, 'TEST.SIM.TXT' or 'TEST.SIM. XLS' (the simple version of the model output), and 'TEST.DET.TXT' or 'TEST.DET. XLS' (the detailed version). The text of MS Excel versions of the output files will depend on the output file format selected under the options menu (see Section 4.2.3).

The detailed version of the model output contains all the chemical species in the simulation. Since this file can grow quite large, the more useful information is summarized in the simple version of output. The simple version of the model output contains the most relevant information for most users. Included are the site and sample labels, the mode of operation (i.e., did the BLM use an input dissolved metal concentration to predict metal speciation or was it predicting the LC50?), the pH, the total dissolved metal in mol/L (this is the input metal concentration in the speciation mode and the predicted LC50 in the toxicity prediction mode), the free metal concentration in mol/L, the activity corrected free metal concentration in mol/L, concentration of metal bound to DOC in mol/L, concentration of metal and metal hydroxide bound to DOC in mol/L, the concentration of metal on the biotic ligand in nmol/g_{wet} of the gill, the DOC in mg/L, the percent humic acid and the rest of the input water chemistry in units of mol/L.

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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. The users can check to verify if the user input water chemistry parameter values are within this range to which the BLM has been calibrated. This is done by using the 'Check Inputs' function. The ranges prescribed for each of the BLM input parameters are shown below.

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	0

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EXAMPLE APPLICATION

The BLM Windows Interface installation also contains an example application for demonstration purposes. This file is named 'Kansas River.BLM' and 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-disk. 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 datafile contains the water quality observations for USGS Station 6892350 on the Kansas River at Desoto, KS. Although in this case, only observations with a complete characterization of all the BLM input parameters are included in the BLM datafile, it is recommended that all the available water quality measurements (including the ones without a complete characterization of the BLM input parameters) be included in the BLM datafile.

This datafile 'Kansas River.BLM' can be used to predict metal speciation using the input metal concentrations or to predict the LC50 to a variety of metals and organisms. However, it is recommended that separate BLM datafiles be maintained for each metal. In this case, the datafile contains dissolved copper concentrations and 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 has 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 datafile, the runtime for the BLM predictions can vary from a few seconds to minutes. Upon completion of the BLM run, the user is informed of the names and the locations of the output files as shown in Figure 8-1.

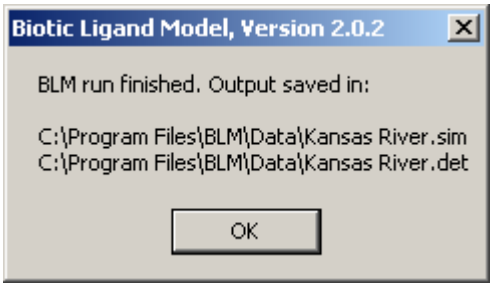

Figure 8-1. Example of notification window shown at completion of BLM run

The formats of the output files have been described in a previous section (see Description of Output Files).

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UNINSTALLING THE BLM

To uninstall the BLM Windows Interface, select the uninstall utility using 'Start -----> Programs -----> Biotic Ligand Model -----> Uninstall' on the Microsoft Windows desktop. 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.

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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:

Robert Santore

HydroQual, Inc.

4914 West Genesee St.

Camillus, NY 13031

Phone: (315) 484-6220

E-mail: rsantore@hydroqual.com

or:

Rooni Mathew

HydroQual, Inc.

1200 MacArthur Blvd.

Mahwah, NJ 07430

Phone: (201) 529-5151

E-mail: rmathew@hydroqual.com

Additional information including support details can be found online at http://www.hydroqual.com/blm.