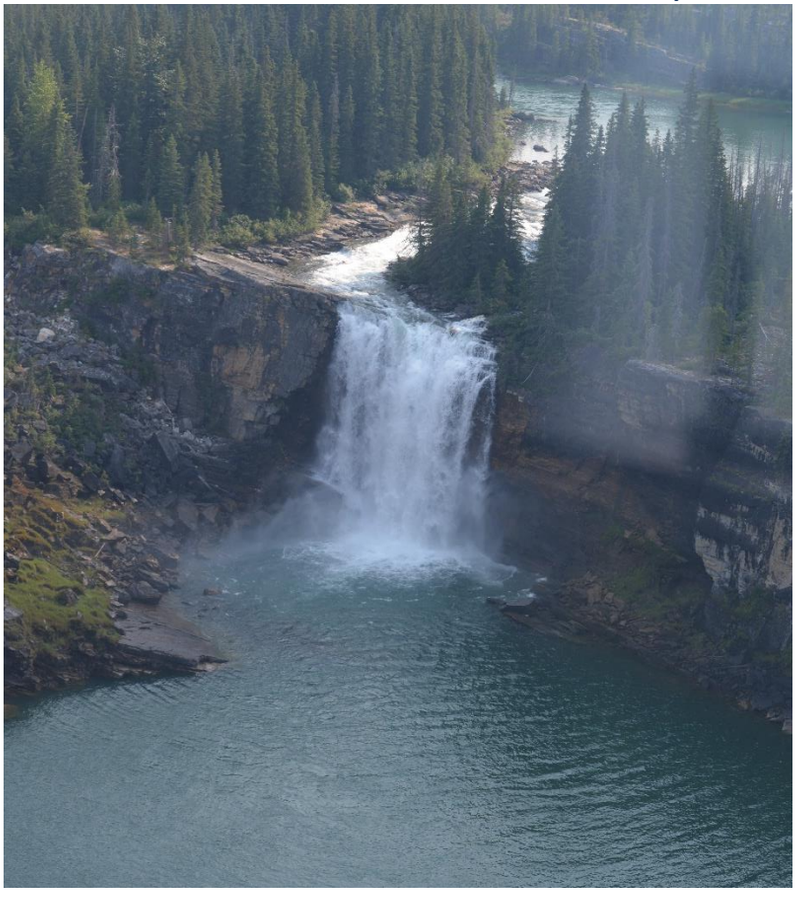
WATER QUALITY GUIDELINE SERIES

Nickel Water Quality Guideline for the Protection of Freshwater Aquatic Life
BC Ni BLM User's Manual

Ministry of Water, Land, and Resource Stewardship

Water Protection & Sustainability Branch



BRITISH COLUMBIA

No.WQG-22-2

The Water Quality Guideline Series is a collection of British Columbia (B.C.) Ministry of Water, Land, and Resource Stewardship water quality guidelines. Water quality guidelines are developed to protect a variety of water values and uses: aquatic life, drinking water sources, recreation, livestock watering, irrigation, and wildlife. The Water Quality Guideline Series focuses on publishing water quality guideline technical reports and guideline summaries using the best available science to aid in the management of B.C.'s water resources. For additional information on B.C.'s approved water quality parameter specific guidelines, visit:

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ISBN: XXX-X-XXXXXX-XX-X

Document citation:

B.C. Ministry of Water, Land, and Resources Stewardship 2022. Nickel Water Quality Guideline for the Protection of Freshwater Aquatic Life- BC Ni BLM User's Manual. Water Quality Guideline Series, WQG-22-2. Prov. B.C., Victoria B.C.

Cover Photograph:
Location: Brooks Falls, B.C.

Acknowledgements

The Ministry of Water, Land, and Resource Stewardship (WLRS) would like to thank Robert Santore and Kelly Croteau of Windward Environmental LLC. for their technical expertise and developing the BC Ni BLM software. WLRS would also like to thank the environmental impact assessment biologists in the regional offices for providing their expertise and knowledge on waterbodies across B.C. We would also like to thank those who provided comments during the internal and external review and editing of this document.

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1. INTRODUCTION

The British Columbia (B.C.) Ministry of Water, Land and Resource Stewardship (WLRS) Biotic Ligand Model (BLM) software (Version 0.08) automates the calculation of long-term chronic and short-term acute water quality guidelines (WQG) for nickel (Ni) for the protection of aquatic life. A full technical description of the toxicity data set and derivation procedure can be found in the Nickel Water Quality Guideline for the Protection of Freshwater Aquatic Life-Technical Report document. The software uses two separate toxicity databases for chronic and acute Ni exposures for a diverse mixture of aquatic organisms, including plants, invertebrates, fish, and amphibians. The BC Ni BLM software is used to normalize the toxicity database to site-specific water chemistry, which allows for consideration of the effects of certain water quality parameters on bioavailability. The BC Ni BLM software requires the input of site-specific water quality information to calculate guideline values. The user can choose to run either the full BLM model that requires 11 input parameters or the simplified model that requires 4 input parameters and estimates the others.

The BC Ni BLM software is based on the BLM software created by Windward Environmental (version 3.60.2.50). Note that BLM data files created using the older version of the BLM Windows® Interface can be used directly with BC Ni BLM.

This document describes the requirements for running the BC Ni BLM software, details the data requirements, and provides a step-by-step guide to using the various features using an example BLM data file.

2. SETUP AND INSTALLATION

2.1. SYSTEM REQUIREMENTS

The BC NI BLM software is designed for use with Microsoft Windows®. The minimum 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/Vista/Win7
  - ✓ 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 BC NI BLM software can be run on a system with the specified minimum requirements, the recommended system configuration or faster is recommended to minimize computation time.

2.2. INSTALLING THE BC Ni BLM SOFTWARE

Install the BC NI BLM software from the setup file "bc_ni_blm_setup.exe" and follow the prompts. The setup program will guide the user through a straightforward installation process, querying the user for information on where to install the necessary files (Figure 2.1). During the installation, a shortcut to the BC Ni BLM application will be added to the 'Programs' sub-menu within the 'Start' menu on the Microsoft Windows® desktop. In addition, the BC Ni BLM application will also be registered in the system registry so that the BLM data files created by the user can be accessed directly by just double-clicking on the file name.

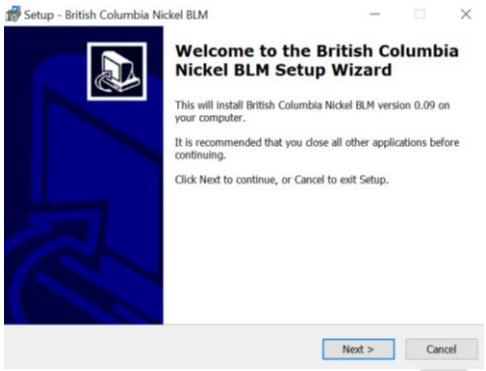


Figure 2.1. Installation directory screen for the BC NI BLM software setup program.

3. STARTING THE APPLICATION

To start the BC NI BLM, select 'Start -----> Programs -----> British Columbia Nickel BLM -----> British Columbia Nickel BLM' on the Microsoft Windows® desktop. The user will be presented with the screen shown in Figure 3.1., which contains the user input areas and the various functions of the BC NI BLM.

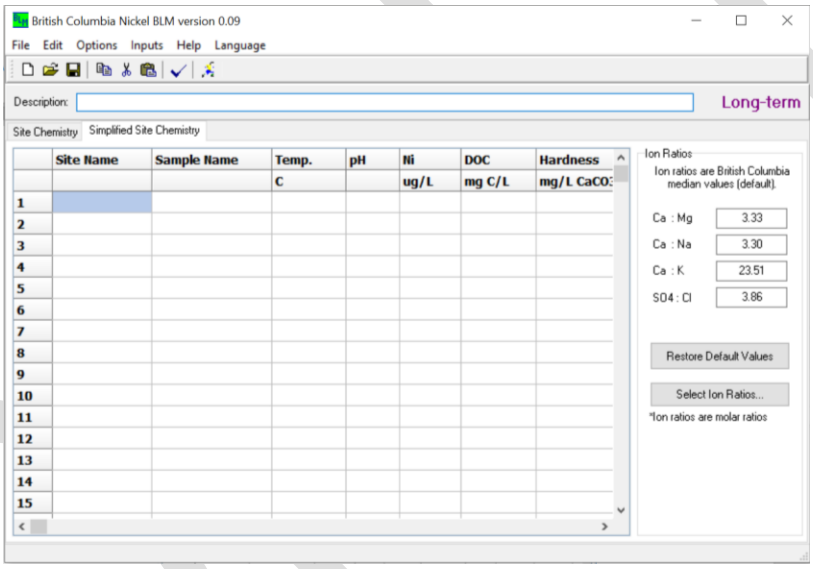


Figure 3.1. Opening screen for the BC NI BLM application.

Existing BLM data files created using other versions of the BLM Windows® Interface can be opened directly by double-clicking on the file name through a file system manager, such as Microsoft Windows® Explorer.

4. RUNNING THE APPLICATION

The following subsections describe the various functions and features available in the BC NI BLM Windows® Interface and its various predictive capabilities.

4.1. Quick Start Guide

Steps 1-7 provide an overview of the user's manual for quick application of the BC NI BLM. More details are provided in the following subsections.

Step 1: Enter water chemistry data or upload a saved '.blm' or '.blme' file (see sections 4.6 and 4.3.1);

Step 2: Save file on the desired destination on your computer (see Section 4.3.1);

Step 3: Select chronic/acute database (see Section 4.3.4);

Step 4: Step 5: Select run (see Section 4.4.4);

Step 5: Open the output directory suggested by the software (see Section 4.4.4);

Step 6: Obtain the acute/chronic WQG from the '.txt' file produced by the software (see Section 6).

4.2. Description of Interface

Figure 4.1 shows the BC NI BLM application. The interface provides an easy-to-use editor to construct input files for the BC NI BLM containing site-specific water chemistry data, checks and validates user input data to ensure the values entered for any given parameter are within the range for which the BC NI BLM has been calibrated, and runs the BC NI BLM to calculate WQGs. The interface window is divided into four areas based on their functionality. Each of these is described in the following subsections.

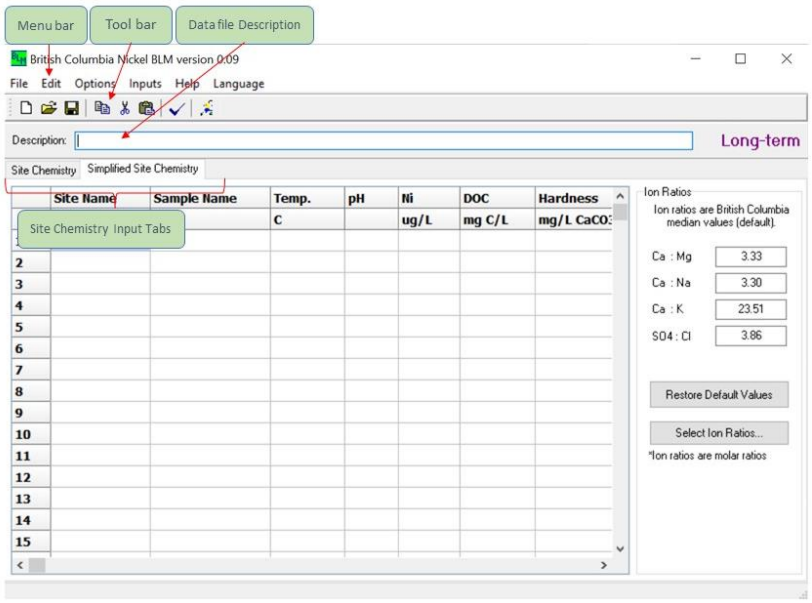


Figure 4.1. Opening screen for the BC NI BLM application.

4.3. Menu Bar

The Menu Bar located at the top of the interface window provides the user with a range of functions and features described in the following sections.

4.3.1. File

The *File* menu (Figure 4.2) includes basic file management utilities to: create a new BLM data file (*New*); open an existing BLM data file (*Open…*); save a BLM data file (*Save*); and save a BLM data file under a different name or in a new location (*Save as…*). Shortcut keys (shown to the right of each item) are also available for the different functions in this menu item. Note that the BC NI BLM data files created by the interface application are given a '.blm' or 'blme' extension for full or simplified chemistry, respectively. Clicking the 'Open' icon while in the full or simplified site chemistry tabs will filter for files with the extension of '.blm' or '.blme', respectively.

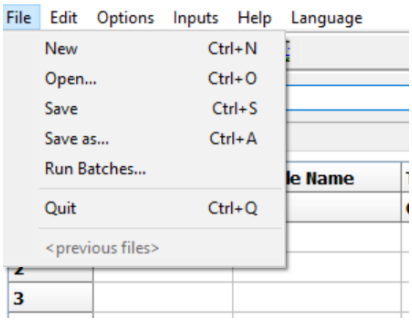


Figure 4.2. Snapshot of "File" menu item.

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

The *Run Batches…*function can be used to run several input files simultaneously.

The *Quit* function can be used to quit BC NI BLM application.

4.3.2. Edit

The *Edit* menu provides basic editing functions such as *Copy*, *Cut*, and *Paste* (Figure 4.3). These functions can be performed on a single cell or multiple cells by highlighting the cell with the cursor (left click and drag) or by using the Shift + Arrow functions on the keyboard. The editing functions can also be applied using the shortcut keys shown to the right of each function. Note that it is also possible to copy and paste data from external programs, such as spreadsheet applications, into the BC NI BLM.

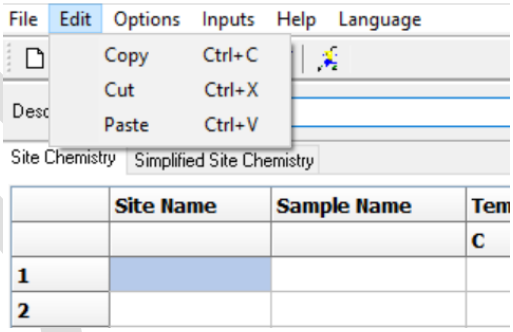


Figure 4.3. Snapshot of *Edit* menu item.

4.3.3. Options

Figure 4.4 shows the functions available under the *Options* menu.

Show Engine Runs

The run may take up to an hour when running several sites simultaneously, depending upon the computing power available. In these cases, it is recommended to select the *Show Engine Runs* option to show the software's progress allowing the user to ensure the software is working properly.

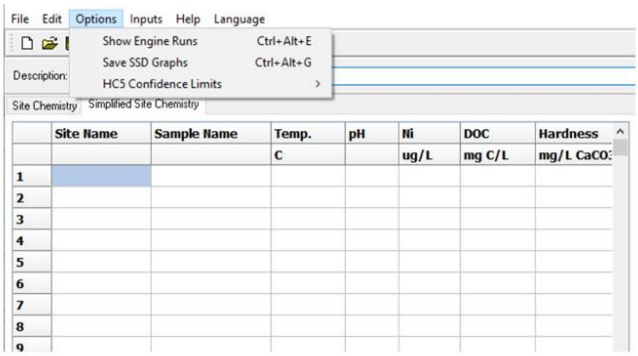


Figure 4.4. Snapshot of *Options* menu item.

Save SSD Graphs

The *Save SSD Graphs* feature allows the user to save a copy of the species sensitivity distribution (SSD) graph produced by the BLM software. The HC_5 of the SSD is the base of the WGQ for the intended water chemistry. For each site a separate SSD will be produced and saved.

HC5 Confidence Limits

The *HC5 Confidence Limits* options allows the user to select the number of bootstrap samples used to calculate confidence limits for the SSD. The recommended number of samples is 100. The higher number of samples will take more time to process but provides better confidence intervals of the SSD.

4.3.4. Inputs

Figure 4.5 shows the options available under the *Inputs* menu. The units for all parameters can be changed by selecting the *Set Units* function. For each component, the available units are displayed in the *Select Units* menu to the right. The Dissolved Inorganic Carbon (DIC) concentration is needed to run BC NI BLM. DIC can be calculated from alkalinity and since alkalinity is a more routinely measured, BC NI BLM requests for alkalinity data by default. However, the *Set Inorganic Carbon* function allows the user to input DIC instead of alkalinity in case of availability. If neither of measured DIC or Alkalinity data is available, DIC can be estimated from atmospheric CO_2.

Database Option allows the user to specify the calculation of either acute or chronic WQGs.

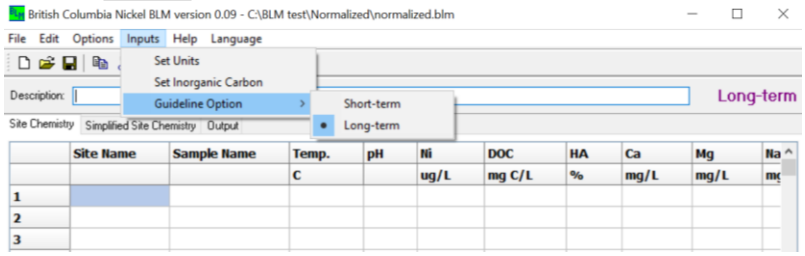


Figure 4.5. Snapshot of *Inputs* menu item.

4.3.5. *Help*

The User's Guide for the BC NI BLM can be accessed under the *Help* menu item (Figure 4.6). The *About BLM* option provides contact information for technical support. The *Create Debug Log* can be used to directly contact the developers of BC NI BLM (Windward Environmental) if the user faces a problem while working BC NI BLM.

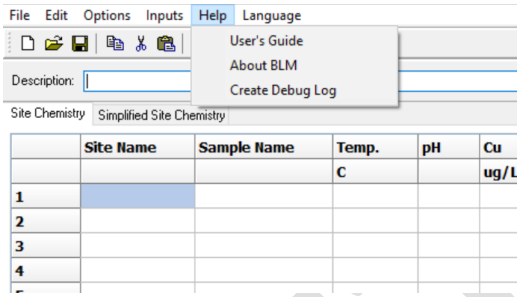


Figure 4.6. Snapshot of *Help* menu item.

4.3.6. *Language*

The user can select either English or French from the *Language* menu item.

4.4. Tool Bar

The *Tool Bar* provides shortcuts to some BC NI BLM functions (Figure 4.7).

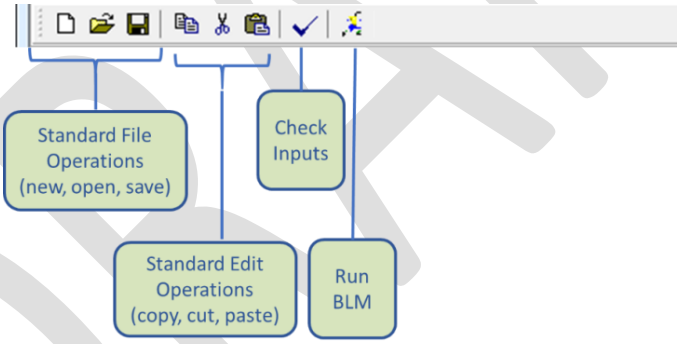


Figure 4.7. *Tool Bar* menu icons.

4.4.1. *Standard File Operations*

New File: this shortcut allows the user to create a new file for water chemistry input (Section 4.3.1).

Open File: this shortcut provides quick access to the BC NI BLM data files (Section 4.3.1). If the BC NI 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 asked if the current data file should be saved prior to opening another.

Save File: this shortcut allows quick saving of the BC NI BLM data file (Section 4.3.1). The data file will be saved with the same, existing name. If the user wishes to save the file under a different file name, the menu bar item *File* → *Save As* should be chosen.

4.4.2. *Standard Edit Operations*

Shortcuts for basic editing functions such as *Copy*, *Cut*, and *Paste* are provided and can be used to edit the water chemistry data at any point (Section 4.3.2).

4.4.3. Check Inputs

The range of parameter values used to develop and calibrate the BC NI BLM are listed in Table 4.1. These ranges were taken from chronic and acute toxicity studies that considered the effects of water chemistry (e.g., pH, DOC, or hardness cations) on Ni bioavailability. The BC NI BLM is only valid within these data ranges. After creating a BC NI 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 BC NI BLM has been calibrated, and to see whether data for all the parameters necessary for a BC NI 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 BC NI BLM has been calibrated) and which parameters are missing for any given input row. Figure 4.8 shows an example of an input check report.

If water quality input values are greater or less than these ranges, the BC NI BLM software automatically applies the upper or lower bounds while calculating WQGs.

Table 4.1. Ranges of values for BLM input parameters.

Parameter	Lower Bound	Upper Bound
Temperature (°C)	4	27
pH	3.5	8.9
DOC (mg/L)	0.032	25
Humic acid content (%)	0.01	99
Calcium (mg/L)	5.428	392
Magnesium (mg/L)	1.547	115
Sodium (mg/L)	0.00751	322
Potassium (mg/L)	3.91e-6	166.86
Sulfate (mg/L)	0.51	890
Chloride (mg/L)	0.0414	550
Alkalinity (mg/L)	0.01	728
Hardness (mg/L)	20	1100

Figure 4.8. Example of an "Input Check Report" generated by the *Check Inputs* function.

4.4.4. Run BLM

The *Run BLM* icon is used to launch the BC NI BLM program to calculate WQGs for the user-specified water chemistry in the data file currently open. If the data file has unsaved changes, the user is given the option of saving the changes prior to running the BC NI BLM. The program will use either the chronic or acute database, depending on which guideline was selected from the *Inputs Menu* (see Section 4.3.4), and calculates the WQG for each row in the database. The runtime for BC NI BLM calculations can vary from a few seconds to a few hours depending on the number of input rows in the data file and the database selected (chronic or acute). Upon completion, the user is informed of the names and the locations of the output files, and given the option to open the directory, as shown in Figure 4.9.

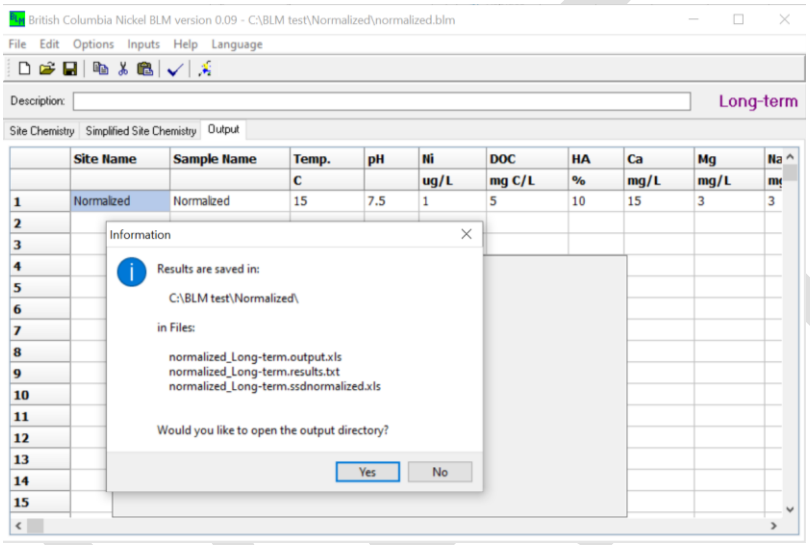


Figure 4.9. Example of the notification window shown at completion of BC NI BLM run.

4.5. Data File Description

The *Data File Description* field (Figure 4.10) allows the user to insert comments describing the BC NI BLM data file which will be saved with the water chemistry data entered by the user. Although this function is not critical to the function of the BC NI BLM, it is useful for record-keeping and quality assurance/quality control purposes.

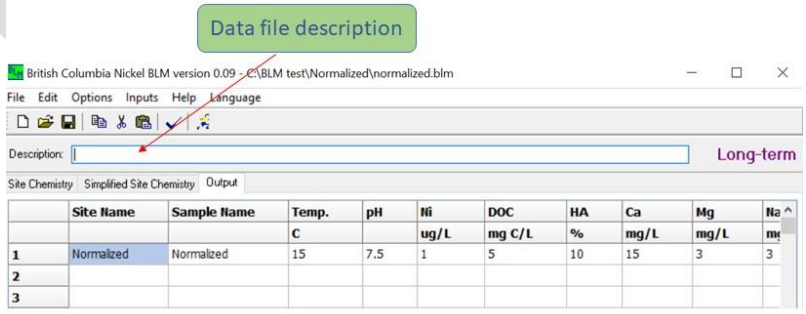


Figure 4.10. Snapshot of BC NI BLM application

Item Description

Located at the very bottom of the interface window, this area displays a brief description of the feature over which the cursor is currently positioned.

4.6. Site Chemistry Input Tabs

There are two options for entering the water chemistry data depending on the parameters available: *Site Chemistry* (i.e., full site chemistry) and *Simplified Site Chemistry*.

4.6.1. Site Chemistry

This region of the interface window contains a spreadsheet-based editor, which organizes the various BC NI BLM input data in a columnar format such that the chemistry for each discrete water sample can be specified in a separate row. Two additional columns are provided for labeling the sites and samples in a given BC NI BLM data file. Figure 4.11 shows the columns available for user input.

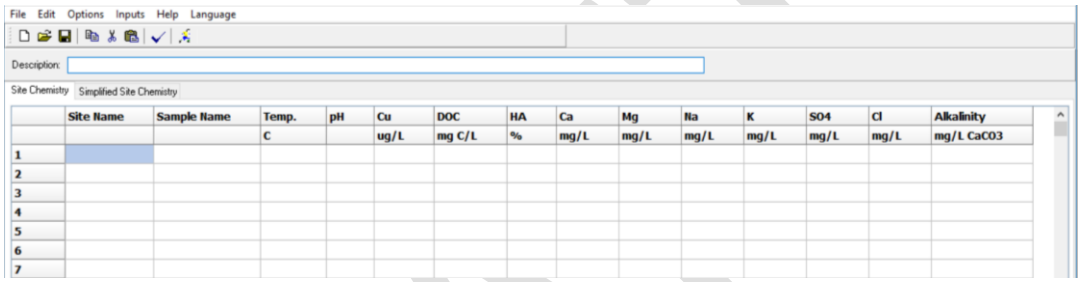


Figure 4.11. Columns for data input in the BC NI BLM.

The BC NI BLM predicts Ni toxicity in aquatic systems and calculates WQGs for a site based on ambient water chemistry. The user is required 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 listed in Table 4.2. Some of these parameters have an important effect on BC NI BLM predictions, while others have only minor effects.

Table 4.2. Water chemistry factors necessary to run the BC NI BLM, their unit and relative importance in calculation of WQGs.

Factor	Unit	Importance
Temperature	°C	Low
pH	NA	High
Dissolved organic carbon (DOC)	mg/L	High
Humic acid fraction of DOC	%	Low
Calcium	mg/L	High
Magnesium	mg/L	High
Sodium	mg/L	High
Potassium	mg/L	Low
Sulfate	mg/L	Low
Chloride	mg/L	Low
Alkalinity	mg/L	High

Nickel concentrations are not required for the model to calculate WQGs, however, this field is retained to allow compatibility with other BLM versions. Nickel concentrations entered will not affect the WQG calculations but are included in the output text file for comparison with the WQG.

4.6.2. Simplified Site Chemistry

The *Simplified Site Chemistry* tab provides an option when all the water chemistry factors are not available. It differs from the *Site Chemistry* tab in that it only requires data for temperature, pH, DOC and hardness (mg/L as $CaCO_3$) to run the BC NI BLM. Selecting the *Simplified Site Chemistry* tab provides a simpler site chemistry data input spreadsheet (Figure 4.12).

Additionally, there is a side bar where the ion ratios can be set. The ion ratios will vary depending on watershed geology. The default values provided are the median ion ratios for B.C. and can be used if the ratios are unknown. These values can be changed to match the conditions of the site or test and can be reset to the default values at any time by clicking the *Restore Default Values* button at the bottom of the box. The *Select Ion Ratios* button allows the user to select default ion ratios for other regions of North America. Note that this is not recommended for calculating WQGs in B.C.; this option is included only to make the BC NI BLM compatible with other versions of BLM Windows® Interface.

After the simplified site chemistry data has been entered, the BC NI BLM estimates the missing water chemistry information while calculating WQGs. Due to the uncertainty in estimating the absent water chemistry data, a cautious strategy was employed to guarantee that the WQGs generated by the simplified BC BLM do not surpass the values generated by the complete BC BLM. For this purpose, a correction factor was introduced to reduce the guideline values derived from the simplified chemistry BLM, ensuring that they do not exceed the corresponding values based on the full chemistry data.

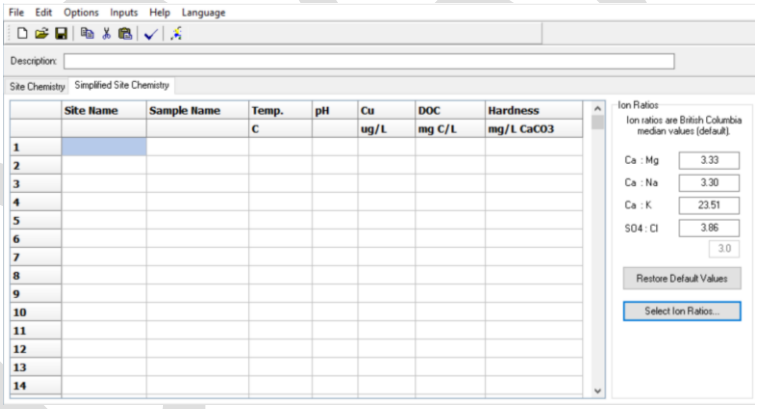


Figure 4.12. Snapshot of *Simplified Site Chemistry* inputs and ion ratios.

When additional water chemistry data for the simplified option are available (e.g., major ions), but insufficient for the full BC NI BLM, the following steps should be taken:

- Enter the parameters in the S*implified Site Chemistry* tab;
- Switch to the full *Site Chemistry* tab and replace the estimates for parameters with the available measured values;
- If alkalinity data are available, the *Set Inorganic Carbon* option should be selected from the *Inputs* menu and then *Closed System, Input Alkalinity* should be selected (Figure 4.13). An additional column for alkalinity will appear and the data are entered there.

- If the user is missing calcium, magnesium, or alkalinity from the full chemistry, but is using the full chemistry tab in the software, then the correction factor needs to be added manually. The correction factor can be used from the below equation (the equation is presented as an Excel function):

$$CF_{long-term} = \min\left(0.8371, \max(0.5446, -0.1067 * log_{10}(Hardness, mg/L) + 0.7846)\right)$$

Note that if you switch back to the *Simplified Site Chemistry* tab without saving the data, the water chemistry data will be deleted.

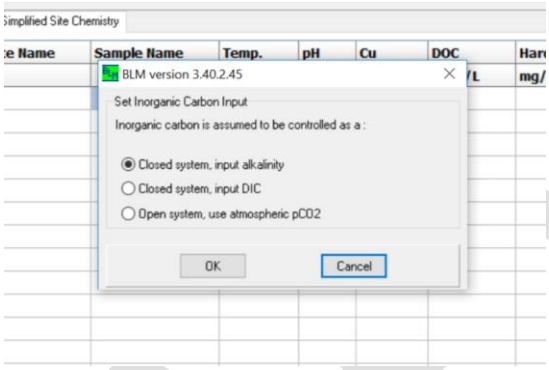


Figure 4.13. Snapshot of *Set Inorganic Carbon* menu item.

5. EXAMPLE APPLICATION

The BC NI BLM features an example application for demonstration purposes. This file, named 'Lake Superior.blm,' is installed along with the BC NI BLM and is in the "My Documents → British Columbia Nickel Biotic Ligand Model" folder. The file can be opened directly, by double-clicking on the file name through a file-system manager such as Microsoft Windows® Explorer or by first starting the BC NI BLM and selecting the file through the 'File → Open' action. This data file 'Lake Superior.blm' can be used to calculate a Ni WQG example produced by the BC NI BLM.

6. DESCRIPTION OF OUTPUT FILES

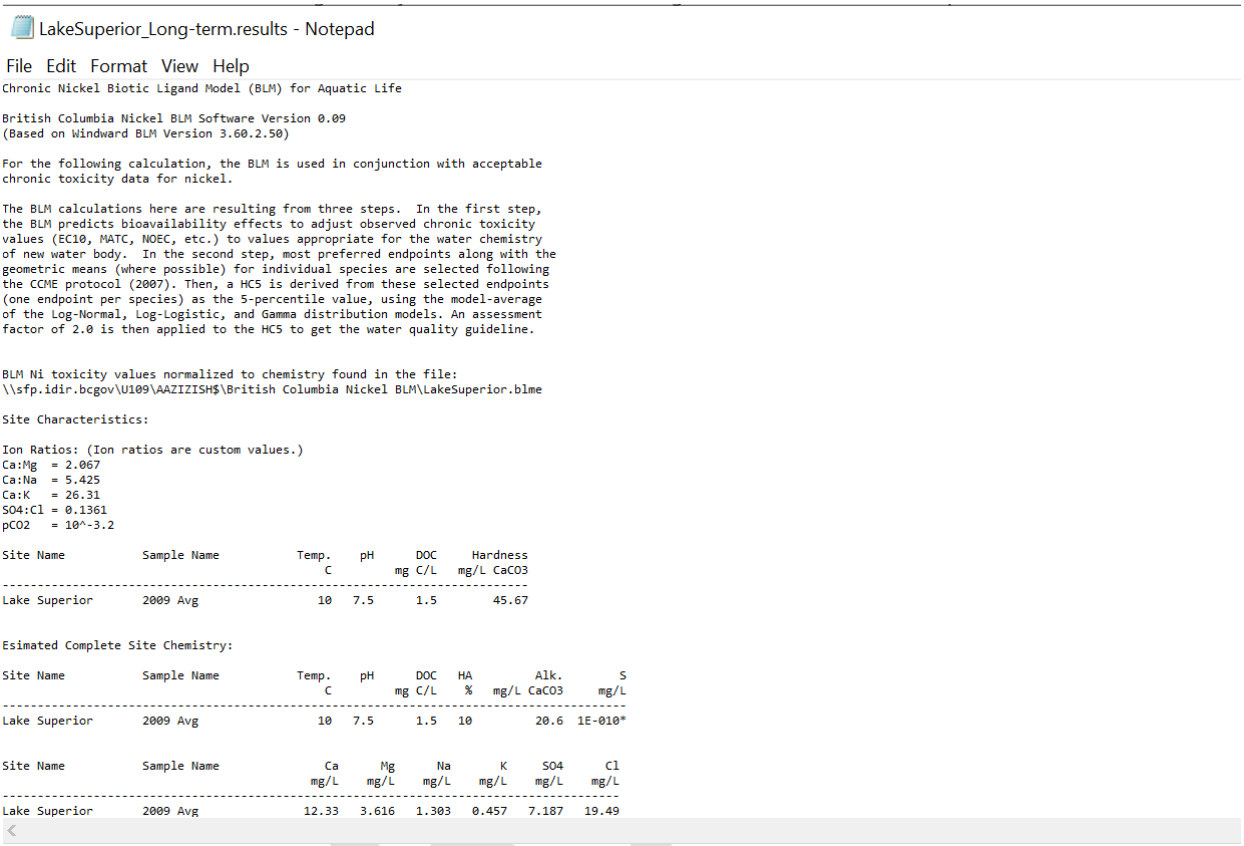
The contents of the output files will appear in an *Output* tab in the BC NI BLM User Interface once the model has finished running. The main output is written to a text file and saved to the same location as the input file, with the same name as the input file but with '.results' appended (Figure 6.1). For example, using the input file 'LakeSuperior.blm' would create an output file titled 'LakeSuperior_Chronic.results.txt' or 'LakeSuperior_Acute.results.txt' depending on the selection of *Acute* or *Chronic* databases (see Section 4.3.4). The output file includes the site chemistry used, and the WQG value calculated for each site.

In addition, a bitmap image is produced for each site that illustrates the SSD for the different species in the toxicity database, normalized to the specified site chemistry (Figure 6.2). Solid lines on the graphic indicate the confidence intervals and the dotted line denotes the HC_5. The bitmap file will not be produced if the "Save SSD Graphs" option is not selected.

Two Microsoft Excel® files will also be produced:

1. *.output: shows the water chemistry, HC_5, confidence intervals, and guidelines values (Figure 6.3).

2. *.ssdnormalized: shows the data associated with the toxicity datapoints for different species such as water chemistry, life stage, endpoint, and endpoint quantifiers it also shows the effect concentration normalized to the site water chemistry ().



LakeSuperior_Long-term.results - Notepad

File Edit Format View Help

```
Chronic Nickel Biotic Ligand Model (BLM) for Aquatic Life

British Columbia Nickel BLM Software Version 0.09
(Based on Windward BLM Version 3.60.2.50)

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

The BLM calculations here are resulting from three steps.  In the first step,
the BLM predicts bioavailability effects to adjust observed chronic toxicity
values (EC10, MATC, NOEC, etc.) to values appropriate for the water chemistry
of new water body.  In the second step, most preferred endpoints along with the
geometric means (where possible) for individual species are selected following
the CCME protocol (2007). Then, a HC5 is derived from these selected endpoints
(one endpoint per species) as the 5-percentile value, using the model-average
of the Log-Normal, Log-Logistic, and Gamma distribution models. An assessment
factor of 2.0 is then applied to the HC5 to get the water quality guideline.


BLM Ni toxicity values normalized to chemistry found in the file:
\\sfp.idir.bcgov\U109\AAZIZISH$\British Columbia Nickel BLM\LakeSuperior.blme

Site Characteristics:

Ion Ratios: (Ion ratios are custom values.)
Ca:Mg  = 2.067
Ca:Na  = 5.425
Ca:K   = 26.31
SO4:Cl = 0.1361
pCO2   = 10^-3.2

Site Name           Sample Name           Temp.    pH      DOC     Hardness
                                             C           mg C/L   mg/L CaCO3
-------------------------------------------------------------------------
Lake Superior       2009 Avg                10   7.5      1.5        45.67


Esimated Complete Site Chemistry:

Site Name           Sample Name           Temp.    pH      DOC   HA         Alk.        S
                                             C           mg C/L    %   mg/L CaCO3     mg/L
-------------------------------------------------------------------------------------------
Lake Superior       2009 Avg                10   7.5      1.5   10         20.6  1E-010*


Site Name           Sample Name             Ca      Mg      Na       K     SO4      Cl
                                          mg/L    mg/L    mg/L    mg/L    mg/L    mg/L
-------------------------------------------------------------------------------------
Lake Superior       2009 Avg             12.33   3.616   1.303   0.457   7.187   19.49
```

Figure 6.1. Example of a text file produced by BC NI BLM.

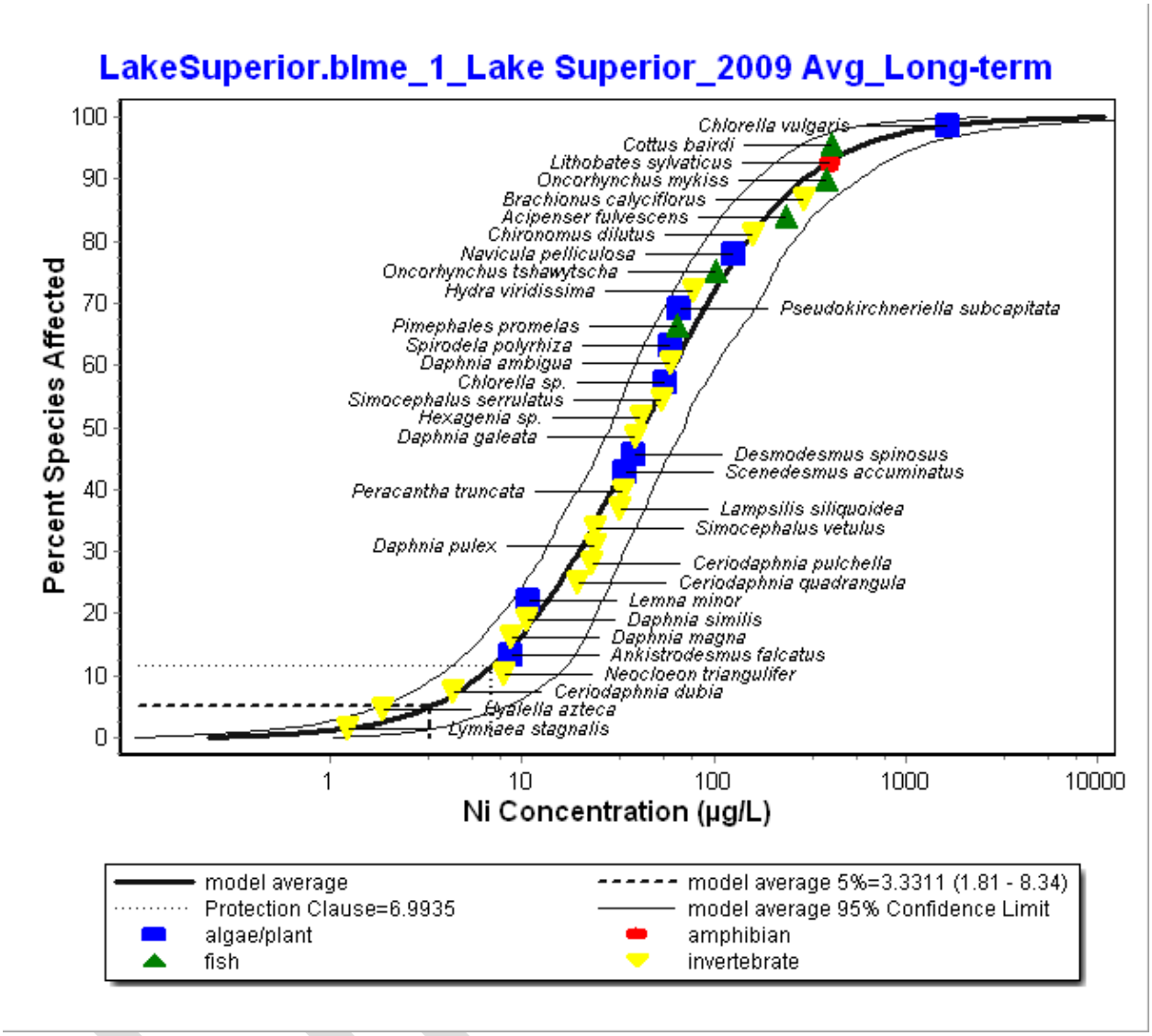


Figure 6.2. Example of the BC NI BLM SSD output file.

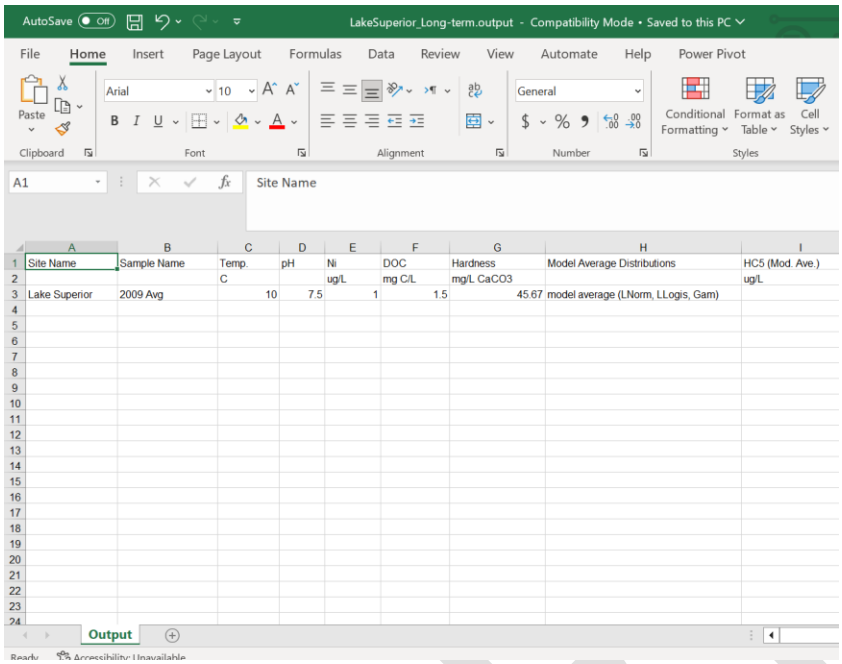


Figure 6.3. Example of the Microsoft Excel® file (*.output) produced by BC NI BLM.

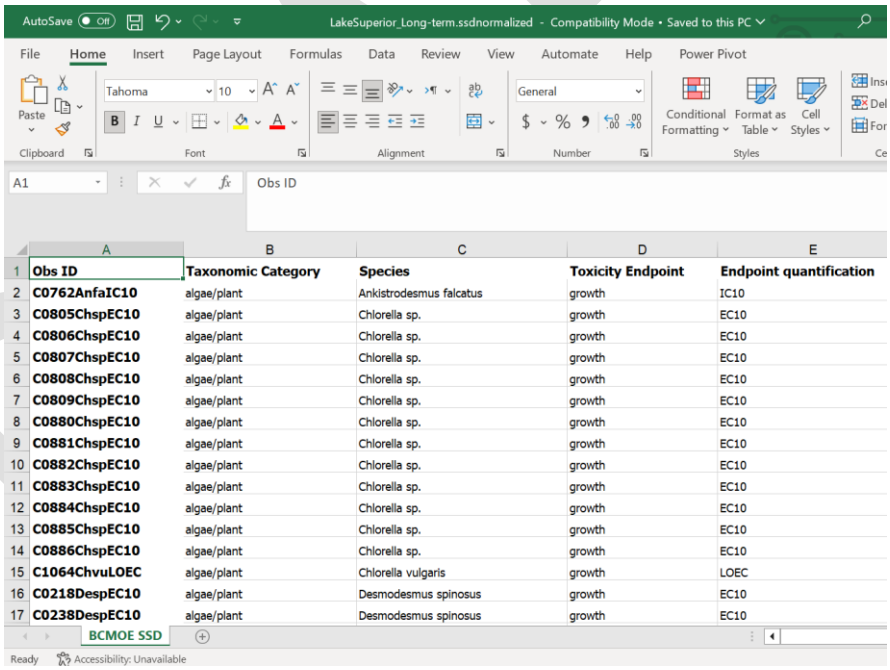


Figure 6.4. Example of the Microsoft Excel® file (*.ssdnormalized) produced by BC NI BLM.

7. UNINSTALLING THE BC NI BLM

To uninstall the BC NI BLM, select the Uninstall Utility using 'Microsoft Windows® Start Menu → Programs → British Columbia Nickel Biotic Ligand Model → Uninstall.' All files installed by the BC NI BLM during setup will be uninstalled. None of the files created by the user and saved in the BC NI BLM installation directory will be deleted during this process. These need to be manually deleted by the user, if so desired.