Virtual Beach 3.0.6: User's Guide

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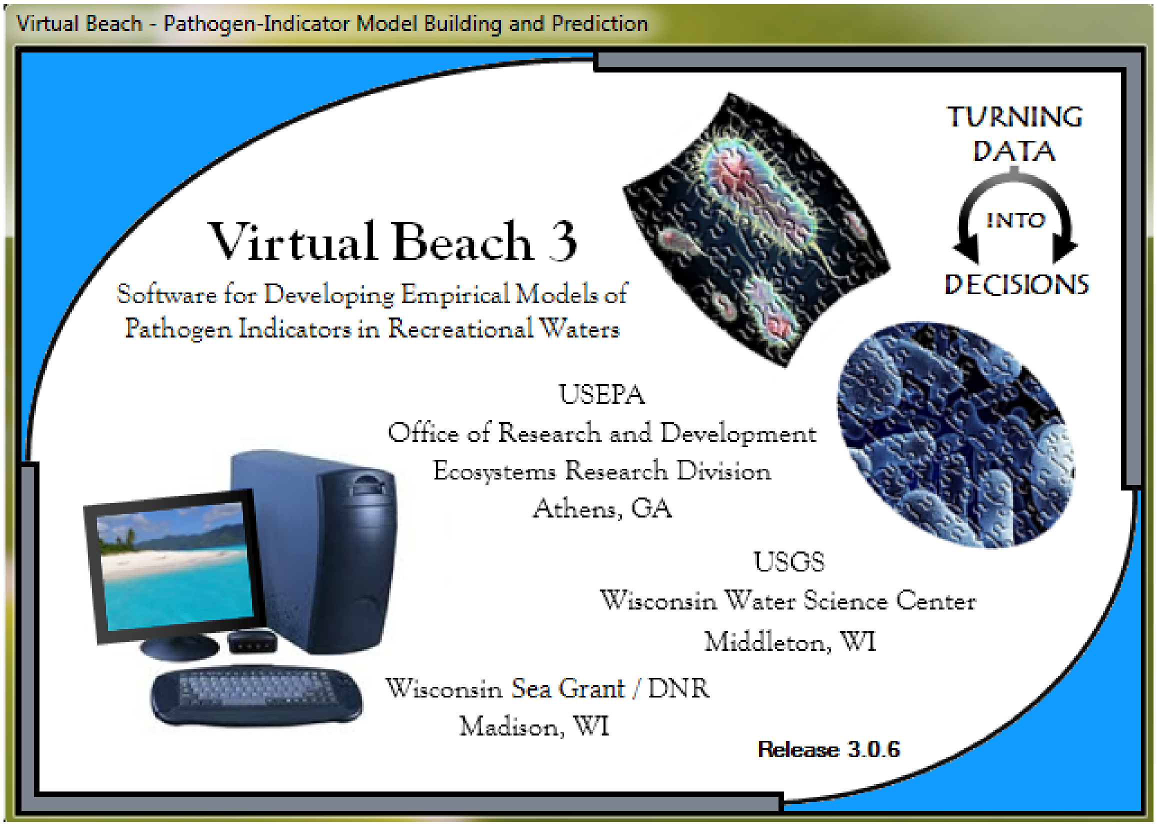

Virtual Beach - Pathogen-Indicator Model Building and Prediction

Virtual Beach 3

Software for Developing Empirical Models of Pathogen Indicators in Recreational Waters

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Release 3.0.6

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1. INTRODUCTION

Virtual Beach version 3 (VB_3) is a decision support tool that constructs site-specific statistical models to predict fecal indicator bacteria (FIB) concentrations at recreational beaches. VB_3 is primarily designed for beach managers responsible for making decisions regarding beach closures or the issuance of swimming advisories due to pathogen contamination. However, researchers, scientists, engineers, and students interested in studying relationships between water quality indicators and ambient environmental conditions will find VB_3 useful. VB_3 reads input data from a text file or Excel document, assists the user in preparing the data for analysis, enables automated model selection using a wide array of possible model evaluation criteria, and provides predictions using a chosen model parameterized with new data. With an integrated mapping component to determine the geographic orientation of the beach, the software can automatically decompose wind/current/wave speed and magnitude information into along-shore and onshore/offshore components for use in subsequent analyses. Data can be examined using simple scatter plots to evaluate relationships between the response and independent variables (IVs). VB_3 can produce interaction terms between the primary IVs, and it can also test an array of transformations to maximize the linearity of the relationship between the response variable and IVs. The software includes search routines for finding the "best" models from an array of possible choices. Automated censoring of statistical models with highly correlated IVs occurs during the selection process. Models can be constructed either using previously collected data or forecasted environmental information. VB_3 has residual diagnostics for regression models, including automated outlier identification and removal using DFFITs or Cook's Distances.

1.1 On Predictive Modeling

Empirical/statistical modeling outperforms persistence models (using the most recent FIB concentration as the sole predictor of the next FIB concentrations) at beaches where conditions such as weather, water characteristics, and human/animal density levels change significantly day to day (Frick et al. 2008, Brooks et al. 2013). Virtual Beach constructs models that can predict a dependent or response variable (i.e., FIB) by using variables to describe current environmental conditions that can be measured or estimated in a timely manner. These are referred to as independent variables (IVs) and often include beach water parameters such as turbidity, water temperature, specific conductance, or wave height; parameters monitored and made available via the web such as rainfall, stream flow, and stream water quality; and parameters estimated by environmental models such as water currents, wave height and direction, and radar rainfall.

In any predictive modeling endeavor, variability and uncertainty associated with model output arise for a variety of reasons that are impossible to eradicate completely. VB_3 attempts to examine this variability and uncertainty in a transparent manner using a probability of exceedance for any regulatory standard the user wishes to investigate. Even so, there is no guarantee than every model prediction will be correct, and a situation may arise in which the model predicts acceptable water quality for public recreation that could be erroneous. Decisions to allow or disallow swimming at beaches must be made, however, and in the best case scenarios, regression models developed with VB_3 will outperform traditional persistence models based on just the previous day's FIB concentrations.

1.2 Recommended User Background

For those using VB_3, some experience with spreadsheet data manipulation programs like Microsoft Excel is recommended, but not necessary. A familiarity with multiple linear regression analysis is also helpful, but again not mandatory. Without this background, VB_3 will take longer to master, but it should not prohibit users from producing and using models.

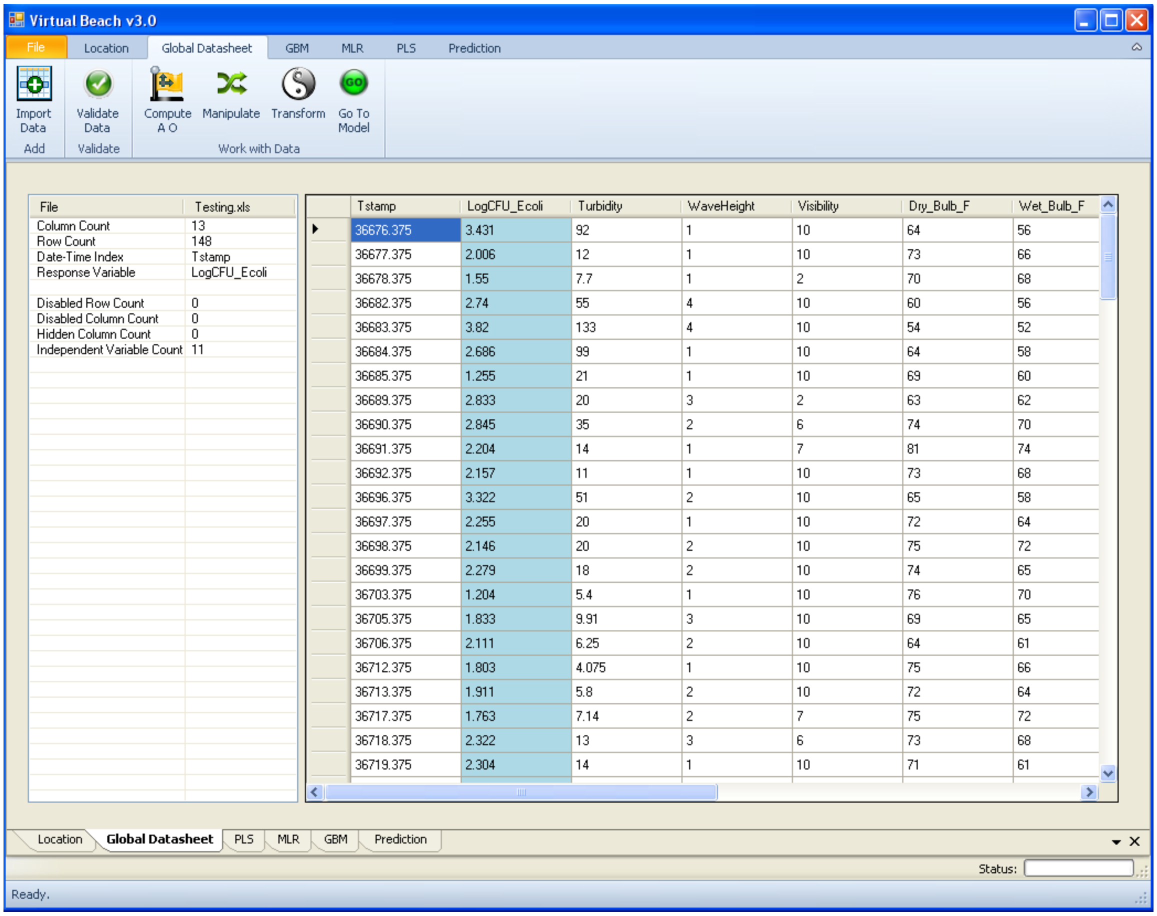
1.3 General Overview

VB_3 has four major components:

- Beach location map interface where users can define the orientation of the beach.
- Interface that facilitates initial import and manipulation of data.
- Multiple "method" tabs where the statistical modeling is done. Each tab has some features identical to those seen in other method tabs and some that are unique. For example, the multiple linear regression (MLR) tab allows examination of regression residuals, elimination of highly influential data records, and viewing of receiver operating characteristic (ROC) curves.
- Prediction interface allowing entry of new data and subsequent estimation of pathogen indicator concentrations with a selected model from any of the statistical methods.

Each component is accessible from the application's main window via tabs at the top and bottom of the main screen (Figure 1). The Location and Global Datasheet tabs are always visible, while the statistical method tabs only become visible once data pre-processing has been completed (i.e., clicking the "Go to Model" button on the Global Datasheet ribbon). The Prediction tab appears when model-building on any method tab is complete and a model is selected

Lastly, we note that statistical models are only as effective as the data used to develop them. No statistician, however skilled, can turn a dataset of low-quality independent variables (IVs) into a useful predictive device.



File	Testing.xls
Column Count	13
Row Count	148
Date-Time Index	Tstamp
Response Variable	LogCFU_Ecoli
Disabled Row Count	0
Disabled Column Count	0
Hidden Column Count	0
Independent Variable Count	11

Tstamp	LogCFU_Ecoli	Turbidity	WaveHeight	Visibility	Dry_Bulb_F	Wet_Bulb_F
36676.375	3.431	92	1	10	64	56
36677.375	2.006	12	1	10	73	66
36678.375	1.55	7.7	1	2	70	68
36682.375	2.74	55	4	10	60	56
36683.375	3.82	133	4	10	54	52
36684.375	2.686	99	1	10	64	58
36685.375	1.255	21	1	10	69	60
36689.375	2.833	20	3	2	63	62
36690.375	2.845	35	2	6	74	70
36691.375	2.204	14	1	7	81	74
36692.375	2.157	11	1	10	73	68
36696.375	3.322	51	2	10	65	58
36697.375	2.255	20	1	10	72	64
36698.375	2.146	20	2	10	75	72
36699.375	2.279	18	2	10	74	65
36703.375	1.204	5.4	1	10	76	70
36705.375	1.833	9.91	3	10	69	65
36706.375	2.111	6.25	2	10	64	61
36712.375	1.803	4.075	1	10	75	66
36713.375	1.911	5.8	2	10	72	64
36717.375	1.763	7.14	2	7	75	72
36718.375	2.322	13	3	6	73	68
36719.375	2.304	14	1	10	71	61

Figure 1. The major components of VB3: "Location," "Global Datasheet," three "Method" tabs (GBM, MLR, and PLS), and the "Prediction" interface. The Global Datasheet is currently active.

1.3 History of VB

VB3 is a direct descendant of Virtual Beach version 2, whose most recent release is VB2.4. The original Virtual Beach Model Builder application (Virtual Beach version 1) was developed by Walter Frick and Zhongfu Ge at the USEPA in Athens, Ga (Frick et al. 2008). VB1 can be characterized as a linear regression model-building tool that supports primarily manual analyses of datasets via visual inspection of data plots and manipulation of variables (e.g., transformations, creating interaction terms), followed by an iterative process of testing, comparing and evaluating models. The fitness of developed models is computed and tracked, allowing comparison and eventual selection of a "best" model for the dataset under consideration. This model then produces estimates of pathogen indicator concentrations using current or forecasted environmental data from the site.

VB2 (Cyterski et al. 2012) enhanced the functionality of its predecessor by performing similar functions (visual inspection of univariate data plots, manual transformations of individual variables, MLR model building, prediction, etc.), but also automated and extended functionality in several ways:

- The Map component provided a convenient method for defining beach orientation by overlaying the beach on current shoreline layers (satellite images, Google Maps, MS Virtual Earth, etc). Given the orientation, VB2 could calculate wind, wave, or current components (the A-component is parallel to shore and the O-component is perpendicular to shore) which can be important predictor variables.

- Although manual processing and analysis of imported data (visual inspection of univariate data plots and the transformations/interactions of variables) was retained, the data-processing component of VB_2 automated generation of all possible second-order interaction terms among a set of IVs, formed more complex functions of multiple columns, and automated testing of a suite of variable transformations that improved model linearity. This functionality increased the number of models to evaluate during later selection routines and removed the burden of manual assessment that users of VB_1 encountered.

- Within the linear regression analysis component, multi-collinearity among predictor variables was handled automatically. Any model containing an IV with a high degree of correlation with others (as measured by a large Variance Inflation Factor [VIF]) was removed from consideration during model selection.

- During MLR model selection, models were ranked by a user-selected evaluation criterion: R^2, Adjusted R^2, Akaike Information Criterion (AIC), Corrected AIC, Predicted Error Sum of Squares (PRESS), Bayesian Information Criterion (BIC), Accuracy, Sensitivity, Specificity, or the model's Root Mean Square Error (RMSE). See Section A.3 for definitions of these criteria. Regardless of which criterion is chosen, the software records the ten best models in terms of it. In comparison, VB_1 had a single criterion choice, Mallow's Cp.

- As the number of IVs in a dataset increases, possible MLR models increase exponentially (considering transforms/interactions), resulting in trillions of possible models from a modest number (12-13) of IVs. VB_2 implemented a genetic algorithm (GA) that efficiently searched for the best possible MLR model. Alternatively, VB_2 users could perform exhaustive calculations in which all possible combinations of IVs were tested if the number of possible models was reasonably small (< 500,000). Both the GA and exhaustive approaches greatly expanded the model-building capabilities of VB_2, compared to VB_1.

- Users no longer had to enter data values in transformed, interacted, or component-decomposed form to make a prediction with the selected MLR model. On the VB_2 MLR Prediction tab, a user-selected model is coded into an input grid with data entry columns matching main effects of the model. Any mathematical manipulation of these IVs is then performed automatically prior to making predictions.

VB_3 primarily builds on VB_2 by adding additional statistical methods that give users more flexibility in modeling their datasets. In addition to MLR, users can now use Partial Least Squares (PLS) regression and Generalized Boosted Regression Modeling (GBM) to fit their data and make predictions. The Prediction tab of VB_3 also has a button to allow direct interaction with the USGS's data acquisition system, EnDDaT (http://cida.usgs.gov/enddat/), for automated dataset construction and ease of FIB prediction from web-accessible data.

2. COMPOSITION AND INSTALLATION

VB$_3$ was developed with MS Visual Studio and written in C#, and uses multiple public domain system components:

- FLEE equation parser (http://flee.codeplex.com/)
- Accord.Net math libraries (http://accord-framework.net/)
- R statistical libraries (http://cran.r-project.org/web/packages/)
- DotSpatial mapping libraries (http://dotspatial.codeplex.com/)
- Weifen Luo Docking UI (http://sourceforge.net/projects/dockpanelsuite/)
- ZedGraph (http://sourceforge.net/projects/zedgraph/)
- GMap.Net (http://greatmaps.codeplex.com/)

No license or software purchase is required to install and run VB$_3$, but an internet connection is needed to display Geographical Information System (GIS) information. Users must have a Windows OS with DotNet Framework 4.0 to assure proper installation and operation. Old versions of Windows (e.g., Vista) have caused various errors to occur, thus are not recommended for use with VB$_3$. Certain VB$_3$ data manipulation and model-building operations are computationally intensive, so faster CPUs are better, but laptop or desktop systems with at least 2 GB RAM will be adequate. Disk space requirements are about 140 MB for VB$_3$ and 170 MB for the DotNet Framework 4. The VB$_3$ application installer will attempt to download and install the DotNet Framework 4.0 if it is not already installed on the target system; this also requires a network connection. If necessary, a user can obtain the DotNet Framework 4 installer at no cost at:

http://www.microsoft.com/download/en/details.aspx?id=17851

The EPA's Center for Exposure Assessment Modeling (CEAM) web site distributes VB at:

http://www2.epa.gov/exposure-assessment-models/virtual-beach-vb

Obtain and run the VB$_3$ application installer and follow the on-screen instructions. After installation, a shortcut will appear on the desktop.

3. OPERATIONAL OVERVIEW

To make VB_3 straightforward to operate, it has four functions, each with its own interface:

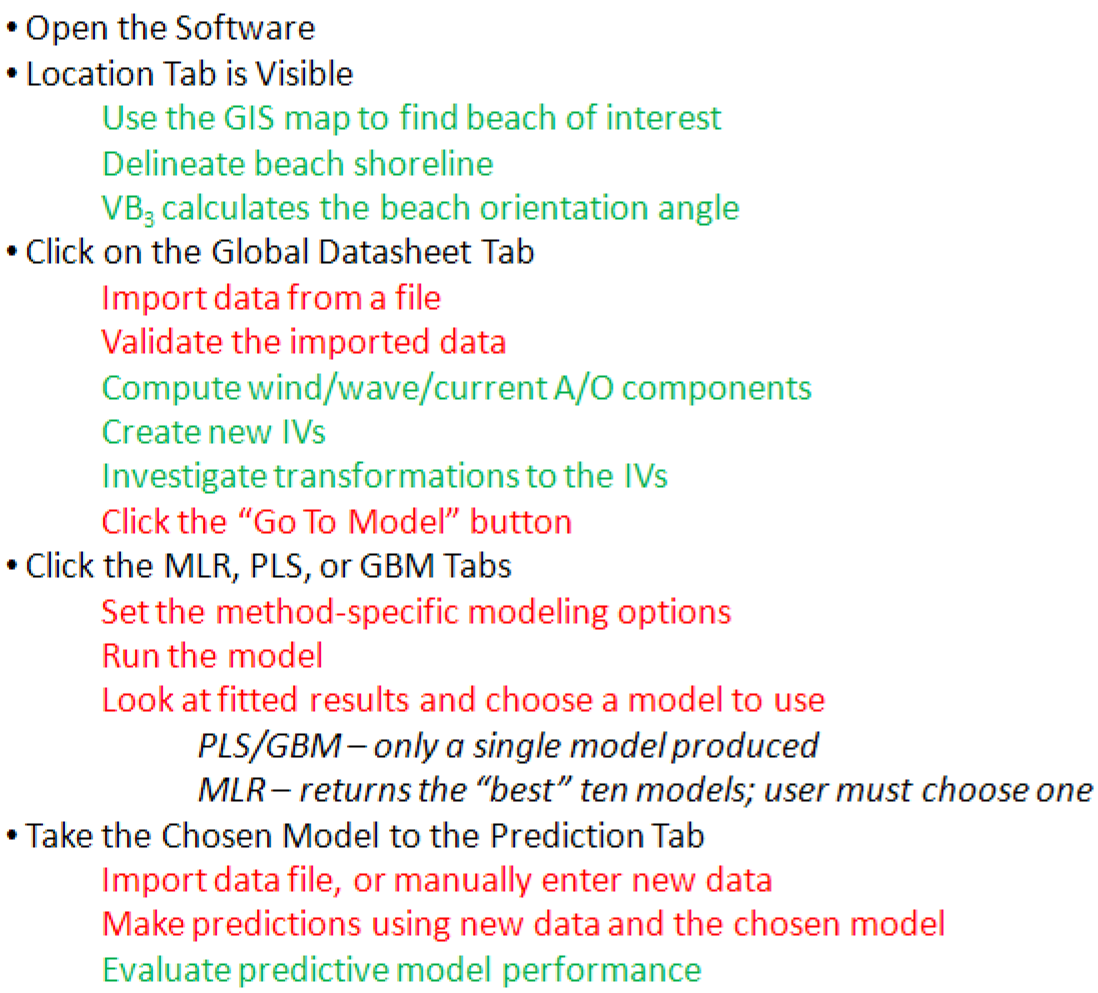
Location – an optional mapping/GIS screen for calculating a beach orientation used for later computation of orthogonal (alongshore and offshore/onshore) wind, current, and/or wave components for the beach under consideration. Such components can be powerful predictors of pathogen indicator concentrations at the beach, so defining the beach orientation is recommended if the dataset under consideration contains wind, wave or current data.

Global Datasheet – a way to support data manipulation on an imported dataset. In addition to wind/current/wave component generation, users can generate new independent variables that represent the products, means, sums, differences, minimums, and maximums of other IVs, as well as investigate data transformations for the IVs.

Methods – there are three Method tabs – Multiple Linear Regression (MLR), Partial Least Squares regression (PLS), and Generalized Boosted Regression Modeling (GBM). Each has its own unique interface, but shares common elements. One common element is a "variable selection" tab where the user chooses from a list of eligible IVs for consideration in model-building and model-generation. Another common element is a "Data Manipulation" tab which is initially populated with data from the Global Datasheet. After initialization, however, the user can then modify "local" data for the chosen statistical technique.

Prediction -- this tab is comprised of three spreadsheets/grids where users can enter or import the IVs needed for the chosen model (left grid), enter or import the values of the response/dependent variable that will be compared to model predictions (middle grid), and examine model predictions and exceedance probabilities (right grid). Time series and scatter plots of the measured dependent variable values versus predictions help users gauge model effectiveness.

The following list attempts to provide an overall context for how a general, basic modeling session using VB_3 would be conducted (optional actions in green, required actions in red):



- Open the Software
- Location Tab is Visible
  - Use the GIS map to find beach of interest
  - Delineate beach shoreline
  - VB$_3$ calculates the beach orientation angle
- Click on the Global Datasheet Tab
  - Import data from a file
  - Validate the imported data
  - Compute wind/wave/current A/O components
  - Create new IVs
  - Investigate transformations to the IVs
  - Click the "Go To Model" button
- Click the MLR, PLS, or GBM Tabs
  - Set the method-specific modeling options
  - Run the model
  - Look at fitted results and choose a model to use
    - *PLS/GBM – only a single model produced*
    - *MLR – returns the "best" ten models; user must choose one*
- Take the Chosen Model to the Prediction Tab
  - Import data file, or manually enter new data
  - Make predictions using new data and the chosen model
  - Evaluate predictive model performance

4. PROJECT MANAGEMENT

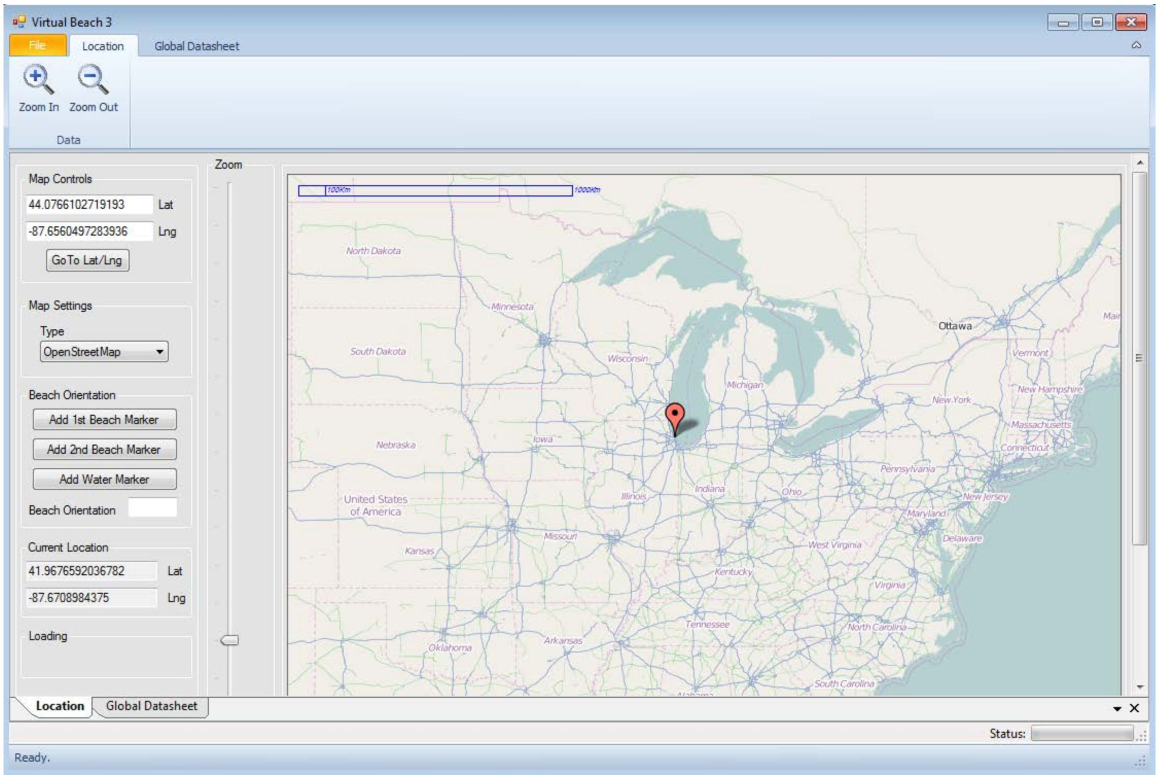
The user will often perform a number of pre-processing steps on an imported dataset to prepare it for analysis, and then develop models from the resulting data. To avoid repeating all of this work, a file can be saved (termed a "project" file) and re-opened via the File → Save and File → Open menu selection. Project files have a ".vb3p" extension. Opening a saved project file will load the saved data into the Global Datasheet and re-populate the methods tabs with the local data, as well as any modeling results generated prior to the save. The beach orientation defined by the user on the Location tab is also saved inside a project file. We suggest giving Project files a descriptive name of the beach/site being modeled for later easy identification.

In addition to project files, "model" files can be saved by using "Save As (prediction only)" under the "File" menu at the top of the VB_3 interface. These files have a ".vb3m" file extension. A model file contains information on the IVs, model parameters, and other metadata for the currently selected models on each method tab. When users open a saved model file within VB_3, they are taken directly to the Prediction tab (the only accessible tab) where they can use the model to generate predictions. Model files allow the user to construct models and choose a "best" one for a site, save a model file, and deliver this file to a beach manager. With this approach, a manager will not need VB_3 for full-scale model development, but only to input new data, generate predictions, and make decisions about issuing swimming advisories.

If the user clicks the red "X" in the upper-right corner of the main VB_3 window (Figure 1), a prompt will ask if they wish to save their project before closing.

5. LOCATION INTERFACE

On VB3 application startup, the “Location” tab is shown first (Figure 2). Because use of this tab is optional, users can go directly to the “Global Datasheet” interface by clicking that tab at the top or bottom of the screen.



Map Controls

44.0766102719193 Lat

-87.6560497283936 Lng

Map Settings

Type: OpenStreetMap

Current Location

41.9676592036782 Lat

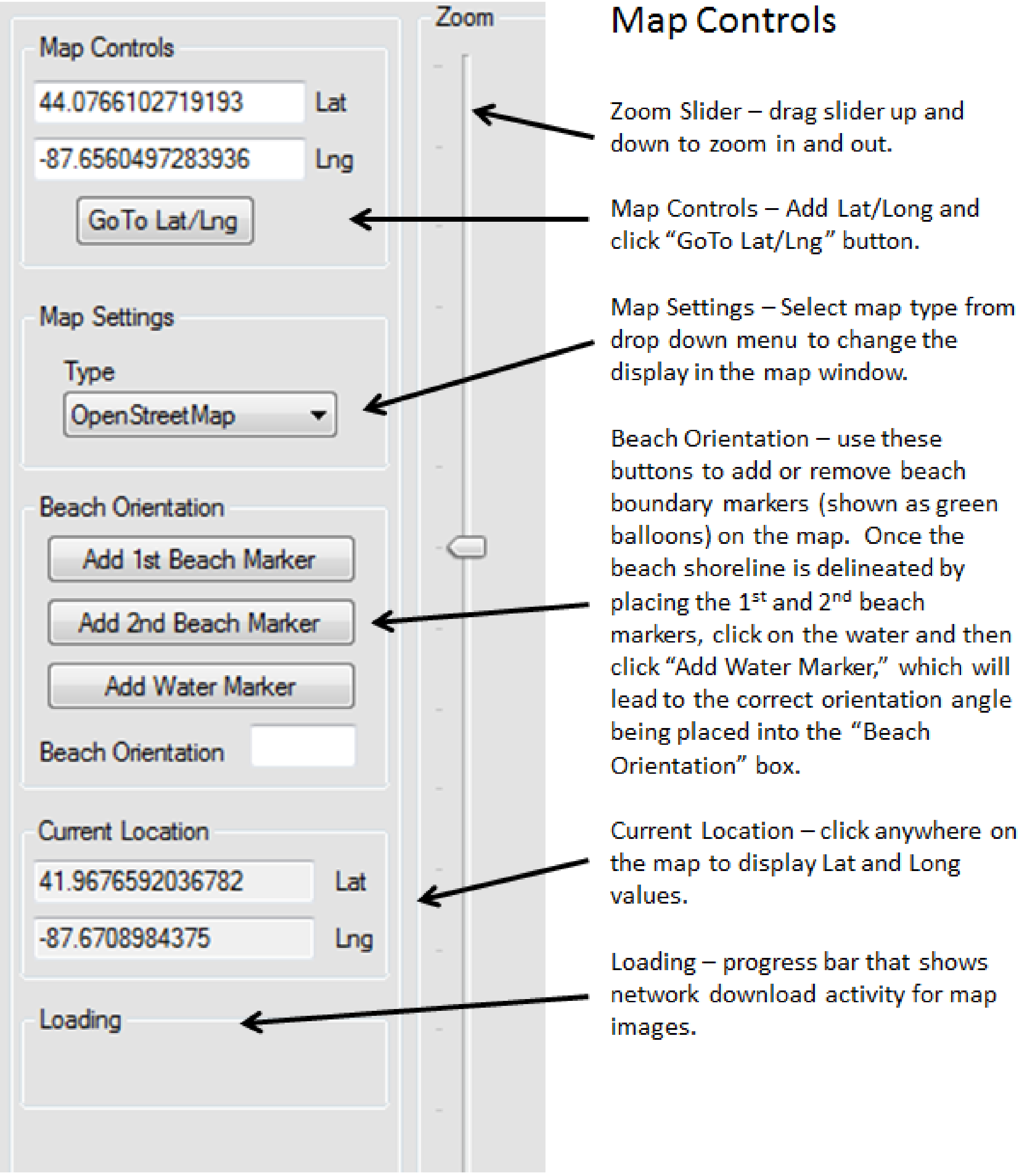
-87.6708984375 Lng

Ready.

Figure 2. Location interface; the default map type is OpenStreet, but users have several other options.

5.1 Finding a Beach

The location interface provides map controls (Figure 3) that let users navigate to a beach site by panning and zooming (right-click and drag mouse to pan; use mouse wheel, slider at the left of the map, or the two buttons in the top ribbon for zoom). Alternately, a latitude/longitude can be entered at the top left, followed by a click on “GoToLat/Lng” button.



Map Controls: 44.0766102719193 Lat, -87.6560497283936 Lng

Map Settings: Type OpenStreetMap

Beach Orientation:

Current Location: 41.9676592036782 Lat, -87.6708984375 Lng

Map Controls

Zoom Slider – drag slider up and down to zoom in and out.

Map Controls – Add Lat/Long and click "GoTo Lat/Lng" button.

Map Settings – Select map type from drop down menu to change the display in the map window.

Beach Orientation – use these buttons to add or remove beach boundary markers (shown as green balloons) on the map. Once the beach shoreline is delineated by placing the 1st and 2nd beach markers, click on the water and then click "Add Water Marker," which will lead to the correct orientation angle being placed into the "Beach Orientation" box.

Current Location – click anywhere on the map to display Lat and Long values.

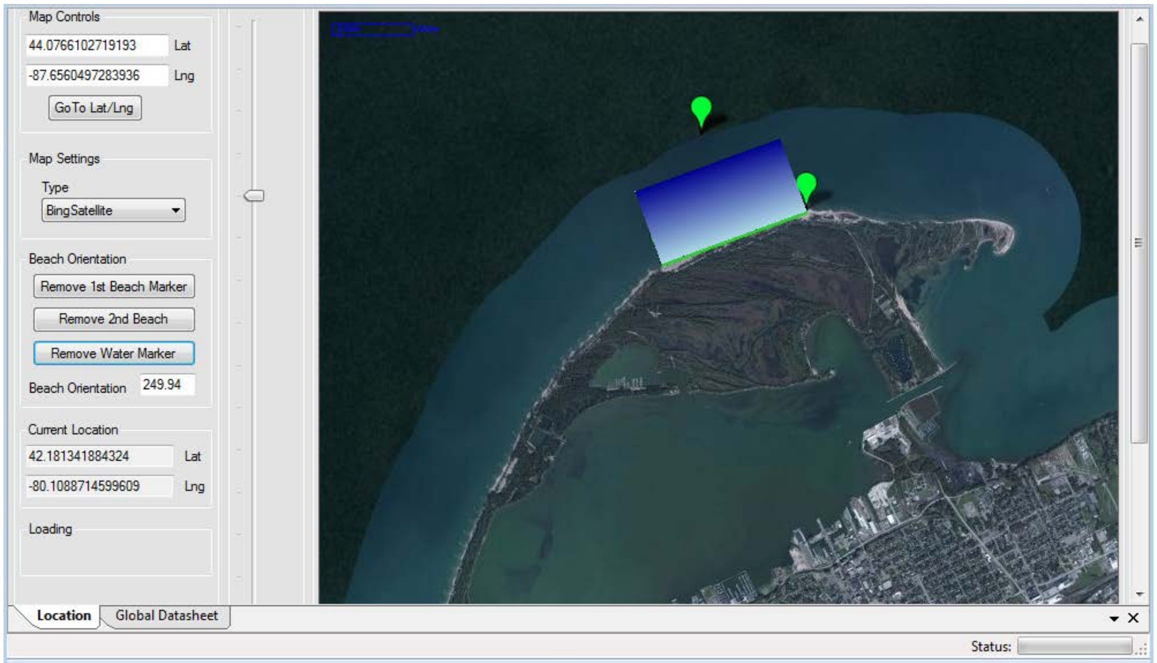
Loading – progress bar that shows network download activity for map images.

Figure 3. Location controls and their function.

5.2 Defining the Beach Boundaries for Orientation Calculation

The map control allows delineation of a beach's boundaries so that VB3 can calculate its orientation (Figure 4), which is useful if wind, wave, and/or current flow components are used in model-building. Maps provide less shoreline detail, so it is recommended that a hybrid or satellite image be selected prior to adding point locations that define beach boundaries. Once the beach of interest is found and the swimming area is located, left-click on the map (a red marker will appear) and click the "Add 1st Beach Marker" button; this represents one endpoint of the beach shoreline/swimming area. Now left-click the other end of the beach on the map and click the "Add 2nd Beach

Marker" button. Finally, left-click on the map to indicate where the water is, relative to the shoreline, and click the "Add Water Marker" button. Marker points will turn from red to green as they are identified. Once the water marker is added, a shaded box appears and the beach orientation angle is displayed to the left of the map at the bottom of the "Beach Orientation" box (Figure 4).


Map Controls

44.0766102719193 Lat

-87.6560497283936 Lng

Map Settings

Type: BingSatellite

Beach Orientation 249.94

Current Location

42.181341884324 Lat

-80.1088714599609 Lng

Figure 4. Adding shoreline and water markers to define beach orientation.

These boundary points can be added or removed until the user is satisfied with the beach representation. VB3 will pass the calculated beach orientation angle to the global datasheet for wind/current/wave component calculations.

5.3 Saving Beach Information

As covered in Section 4, the File→Save menu selection will open a window that allows the user to save the project information (such as placement of the beach/water boundary markers and the calculated beach orientation) inside a VB3 project file.

6. GLOBAL DATASHEET

6.1 Data Requirements and Considerations

VB3 can import .xls, .xlsx, and .csv files, but input data must conform to certain standards:

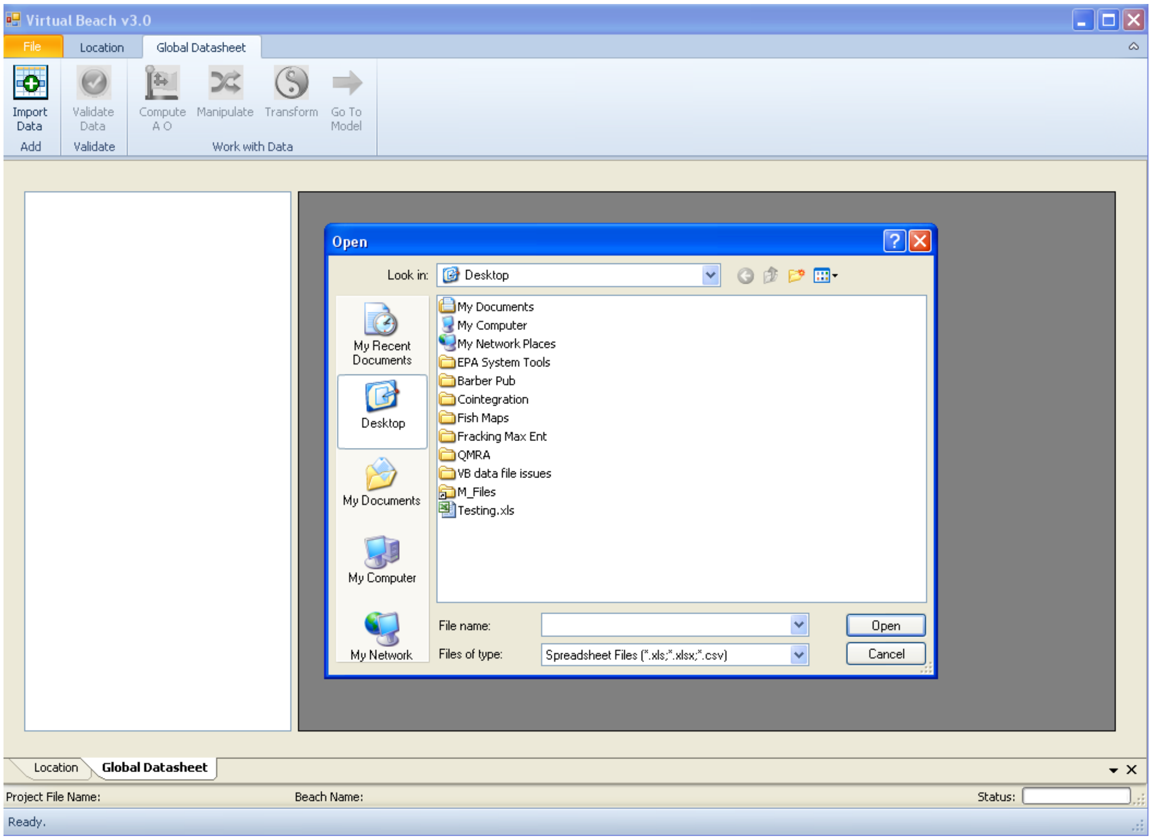
- The first row of any column must be a header specifying the column's name.
- For error-free operation of the software, column names should be composed only of letters, numbers, and/or underscores ("_").
- Do not begin a column name with a number.
- VB3 will issue an error statement if a dataset with spaces in a column name is imported.
- The left (first) column of the dataset must be an identifier for the observations -- typically a date, time, or serial number that indicates when or where that row of data was collected.
- Each row MUST have a unique ID value (left-most column). If VB3 finds duplicate IDs, it will issue an error statement.
- If the ID column specifies a collection date or time, time series plots in VB3 will be most interpretable if the rows are in chronological order, from the earliest to the most recent data. VB3 will not re-arrange the data in chronological order on its own.
- The second column of the dataset will initially be set as the response variable; however, this can be changed after data are imported. Other columns will be considered as IVs (besides the first ID column).
- Variable measurement units are not considered by VB3, but certainly affect predictions. Ensure that any data used for predictions are in the same units as those used to build the models; for example, do not build a model with water temperature in degrees Fahrenheit, then import water temperature in degrees Celsius for predictions. It is prudent to include unit information in the column names (e.g., "WaterTemp_C") to remind the user of the proper unit when entering data to make predictions.
- Missing data (blank cells) are permitted upon import, but must be dealt with (either deleted or values filled in) prior to modeling.
- If Excel data files are imported, cells with non-numeric values (i.e., symbols or text) are converted to empty cells. Exceptions are the column names and the first column of IDs. If such non-numeric characters are present in an imported .csv file, they will be imported into VB3's datasheet. However, they will be flagged as anomalous during the validation scan and they must be dealt with (deleted or populated) at that time.
- When the required validation scan is launched, VB3 will identify any column in the dataset containing only a single value and ask the user to delete the column (because such data columns are useless for predictive purposes).
- There is no hard-coded limit on the number of IVs one can import; however, the VB3 datasheet is designed for a maximum of 300 columns. Beyond that number, the application's performance will degrade significantly. Investigating 250+ IVs results in over $2*10^{20}$ possible IV combinations for MLR processing. The MLR genetic

algorithm can handle this modeling task, but choosing "Run all combinations" would likely take months or years to complete. Depending on how many additional IVs will be created by the user, importing a dataset with less than 100 IVs should be acceptable.

We note here that VB_3 can be used as a powerful exploratory research tool, allowing the user to investigate a great many IVs concurrently. However, this approach can lead to models with spurious response/IV relationships (i.e., the association is only a random statistical artifact, not a "real" phenomenon). To avoid this, the user could restrict their analyses to only those IVs for which they have a prior, process-based, theoretical expectation of influence on pathogen concentrations. A criticism of this approach is that the researcher will never discover a relationship between the response and a truly influential IV if they don't already expect it to exist. Discovery of unexpectedly influential IVs can lead to process insight and advancements in understanding of the physical system. If an exploratory approach is taken, there are mechanisms within the statistical modules of VB_3 (primarily cross-validation to ensure that predictions on future data points are nearly as good as the model fits) to protect against over-fitting a model using too many IVs and finding spurious correlations that don't hold up when the model is used for prediction of future events.

6.2 Importing a Dataset

When users first click on the Global Datasheet tab, they can import a data file using the "Import Data" button in the top ribbon (Figure 5). This opens a dialog screen where a directory explorer can be used to find the data file. If the file is an Excel workbook with multiple worksheets, the dialog box asks which worksheet to import.



Look in: Desktop

Files of type: Spreadsheet Files (*.xls;*.xlsx;*.csv)

Figure 5. Importing a dataset into the Data Processing tab.

Once imported, the data are shown in a datasheet. The second column of this datasheet will be highlighted in blue to indicate its status as the current response variable. Information about the dataset, such as number of rows and columns, name of the ID column and name of the response variable, appear at the left of the datasheet. At this point, the datasheet cannot be edited or interacted with in any manner; to access additional processing functionality, the data must be validated.

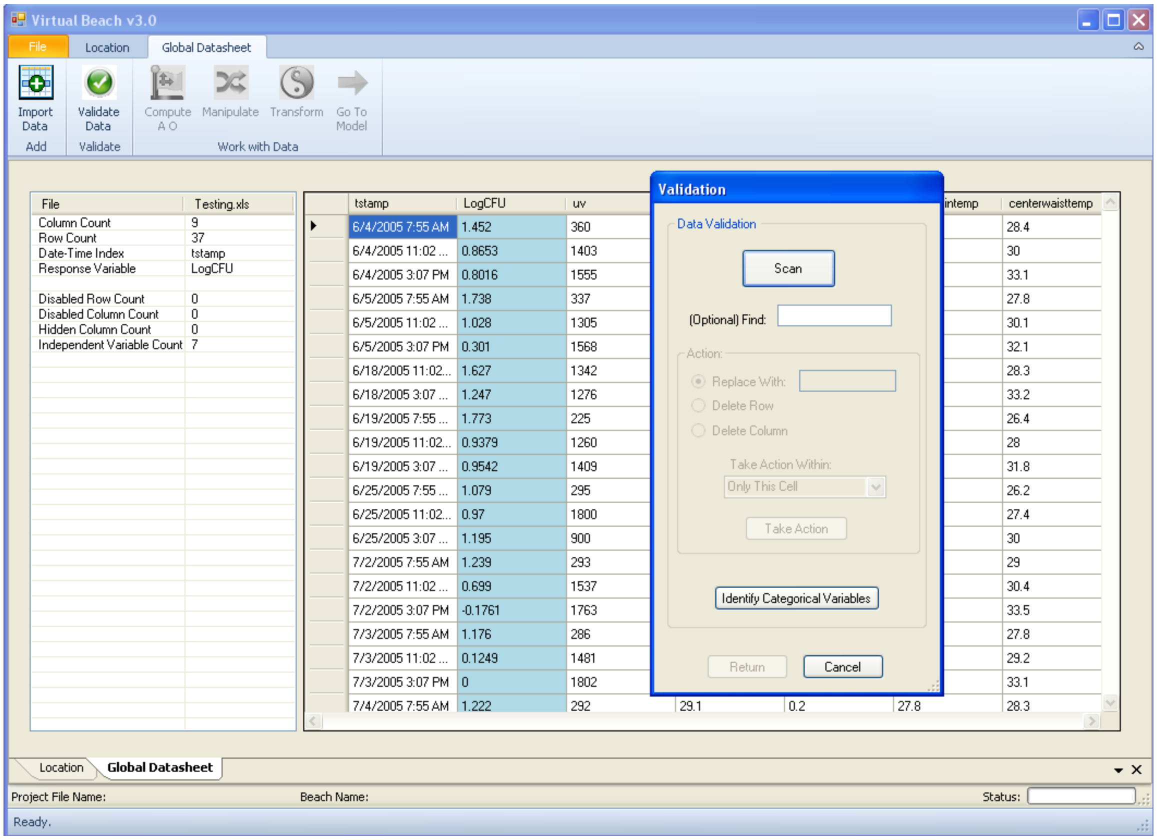
Note that proper importation of newer Excel files (.xlsx) may fail on some user's systems. If errors are encountered trying to import these .xlsx files, users can try installing Office 2007 System Driver Data Connectivity Components via the AccessDatabaseEngine program:

https://www.microsoft.com/en-us/download/details.aspx?id=23734

Alternatively, users can open these files in Excel and save as either .xls or csv format prior to importing into VB3.

6.3 Validating the Imported Data

Validation options can be accessed by clicking the "Validate Data" button in the top button ribbon. Validating the data launches a required scan to identify blank and non-numeric cells in the imported spreadsheet (Figure 6). One can also find and replace other specified values (e.g., a missing data tag like -999) in the dataset, using the "(Optional) Find:" input box.



File	Testing.xls
Column Count	9
Row Count	37
Date-Time Index	tstamp
Response Variable	LogCFU
Disabled Row Count	0
Disabled Column Count	0
Hidden Column Count	0
Independent Variable Count	7

tstamp	LogCFU	uv			intemp	centerwaisttemp
6/4/2005 7:55 AM	1.452	360				28.4
6/4/2005 11:02 ...	0.8653	1403				30
6/4/2005 3:07 PM	0.8016	1555				33.1
6/5/2005 7:55 AM	1.738	337				27.8
6/5/2005 11:02 ...	1.028	1305				30.1
6/5/2005 3:07 PM	0.301	1568				32.1
6/18/2005 11:02...	1.627	1342				28.3
6/18/2005 3:07 ...	1.247	1276				33.2
6/19/2005 7:55 ...	1.773	225				26.4
6/19/2005 11:02...	0.9379	1260				28
6/19/2005 3:07 ...	0.9542	1409				31.8
6/25/2005 7:55 ...	1.079	295				26.2
6/25/2005 11:02...	0.97	1800				27.4
6/25/2005 3:07 ...	1.195	900				30
7/2/2005 7:55 AM	1.239	293				29
7/2/2005 11:02 ...	0.699	1537				30.4
7/2/2005 3:07 PM	-0.1761	1763				33.5
7/3/2005 7:55 AM	1.176	286				27.8
7/3/2005 11:02 ...	0.1249	1481				29.2
7/3/2005 3:07 PM	0	1802				33.1
7/4/2005 7:55 AM	1.222	292	29.1	0.2	27.8	28.3

(Optional) Find:

○ Replace With:
○ Delete Row
○ Delete Column

Take Action Within: Only This Cell

Project File Name:

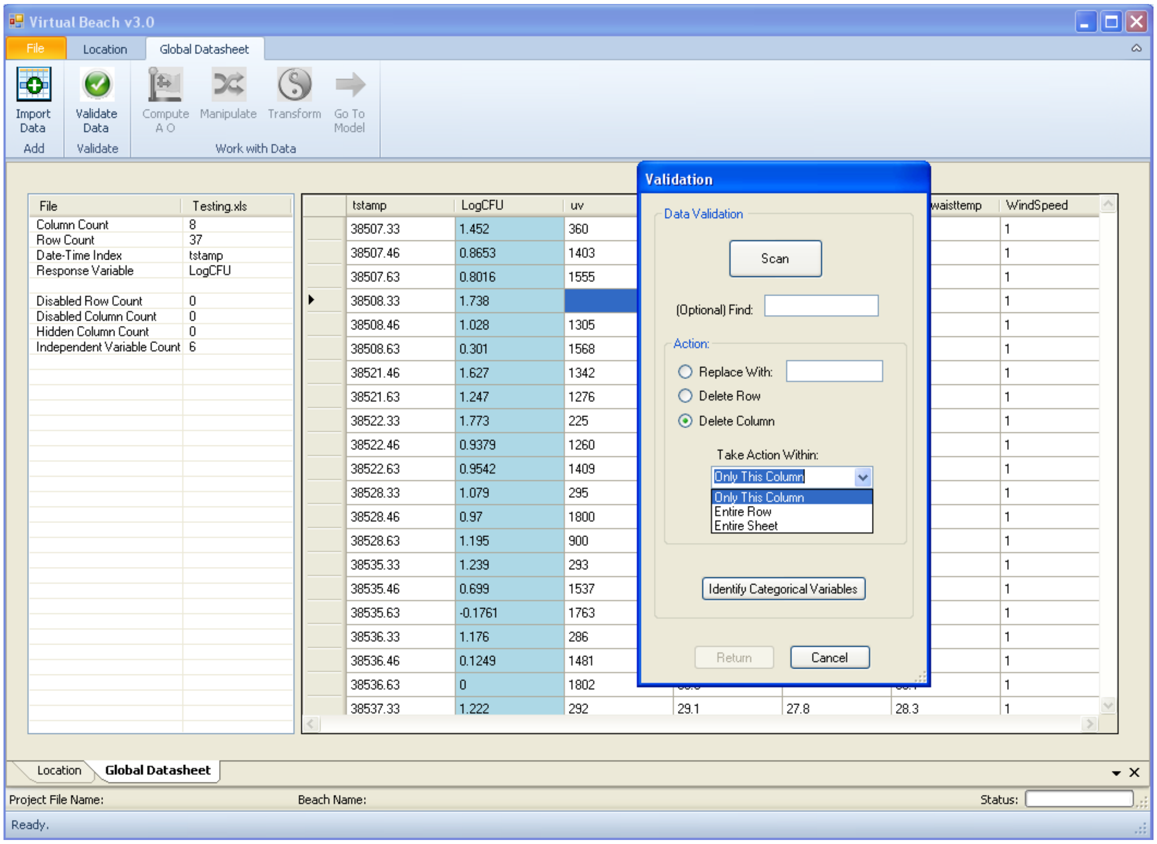
Beach Name:

Status:

Ready.

Figure 6. Data validation required to begin data processing.

Clicking "Scan" begins the validation process. VB3 goes through the datasheet, cell by cell, looking for blanks, non-numeric, or user-specified values entered in the "(Optional) Find:" input box. If such a cell is found, the scan will stop and highlight it. Users must then decide how to deal with that cell from choices in the "Action" section (Figure 7): replace the cell with a specified value, using the "Replace With:" input box, or delete the row or column containing the cell. The user must decide where to implement the chosen action with the "Take Action Within" dropdown menu. Possible choices are "Only this Cell," "Entire Row," "Entire Column," and "Entire Sheet." Items in this menu are context-sensitive, i.e., they change with the Action selected. After setting the "Take Action Within" menu, the user clicks the "Take Action" button, VB3 makes the specified changes to the datasheet, and the scan continues. Even if no cell errors are found, VB3 may still report that a "Column has no distinct values" and prompt the user to delete the column (see the second-to-last bulleted item in Section 6.1). When the entire datasheet has passed inspection, VB3 reports "no anomalous data values found" at the bottom of the Validation window.



File	Testing.xls
Column Count	8
Row Count	37
Date-Time Index	tstamp
Response Variable	LogCFU
Disabled Row Count	0
Disabled Column Count	0
Hidden Column Count	0
Independent Variable Count	6

tstamp	LogCFU	uv			waisttemp	WindSpeed
38507.33	1.452	360				1
38507.46	0.8653	1403				1
38507.63	0.8016	1555				1
38508.33	1.738					1
38508.46	1.028	1305				1
38508.63	0.301	1568				1
38521.46	1.627	1342				1
38521.63	1.247	1276				1
38522.33	1.773	225				1
38522.46	0.9379	1260				1
38522.63	0.9542	1409				1
38528.33	1.079	295				1
38528.46	0.97	1800				1
38528.63	1.195	900				1
38535.33	1.239	293				1
38535.46	0.699	1537				1
38535.63	-0.1761	1763				1
38536.33	1.176	286				1
38536.46	0.1249	1481				1
38536.63	0	1802				1
38537.33	1.222	292	29.1	27.8	28.3	1

Validation

Data Validation

(Optional) Find:

Action:

○ Replace With:

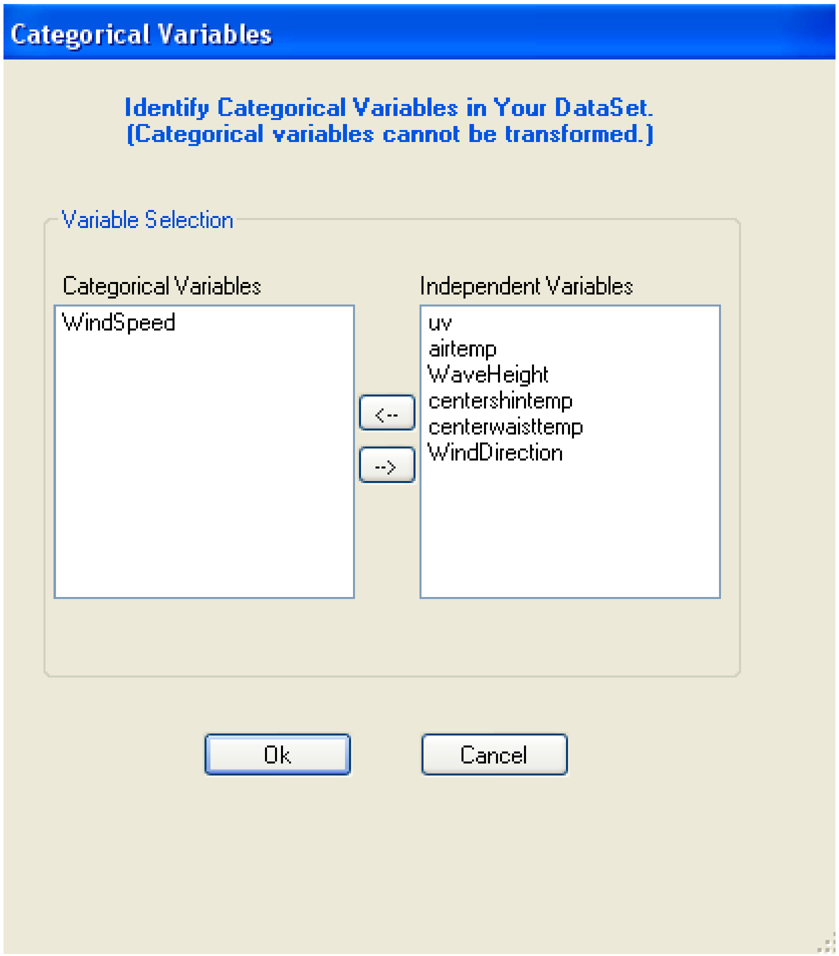
○ Delete Row

● Delete Column

Take Action Within: Only This Column

Figure 7. Context-sensitive choices for the "Take Action Within" drop-down menu.

After the data have been validated, but prior to clicking the "Return" button on the Validation window, the user has the option to specify which columns in the dataset are categorical variables. Why do this? VB3 will not attempt to transform categorical data columns (transformations discussed later), because it generally does not make sense to do so. Thus, identifying IV columns as categorical saves time later when transformations are investigated. If the user clicks on the "Identify Categorical Variables" button (Figure 7), a window pops up (Figure 8). A list of the datasheet's independent variables is shown in the right-hand section of this window. VB3 automatically identifies columns with only two unique values as categorical variables (i.e., they will already be in the left section of this window); if the user has other categorical IVs with more than two categories, those should be moved from the right to the left section using the <-- button. The user can also move any currently-identified categorical IV back to the right list using the --> button.



Categorical Variables

Identify Categorical Variables in Your DataSet.
(Categorical variables cannot be transformed.)

Variable Selection

Categorical Variables

WindSpeed

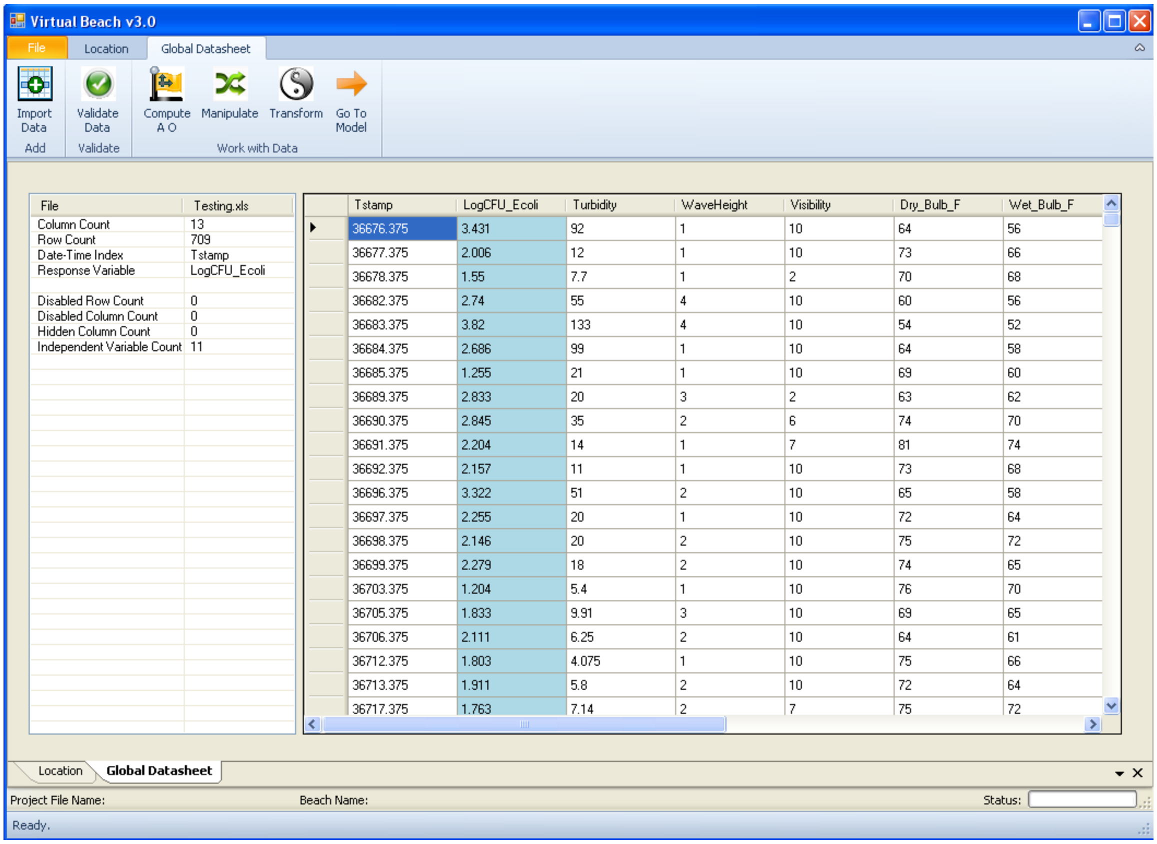
Independent Variables

uv
airtemp
WaveHeight
centershintemp
centerwaisttemp
WindDirection

Figure 8. Pop-up window for identifying categorical variables.

6.4 Working with a Dataset after Validation

After the dataset has passed the validation scan, the function buttons across the top of the Global Datasheet tab ribbon are enabled (Figure 9).



File	Testing.xls
Column Count	13
Row Count	709
Date-Time Index	Tstamp
Response Variable	LogCFU_Ecoli
Disabled Row Count	0
Disabled Column Count	0
Hidden Column Count	0
Independent Variable Count	11

Tstamp	LogCFU_Ecoli	Turbidity	WaveHeight	Visibility	Dry_Bulb_F	Wet_Bulb_F
36676.375	3.431	92	1	10	64	56
36677.375	2.006	12	1	10	73	66
36678.375	1.55	7.7	1	2	70	68
36682.375	2.74	55	4	10	60	56
36683.375	3.82	133	4	10	54	52
36684.375	2.686	99	1	10	64	58
36685.375	1.255	21	1	10	69	60
36689.375	2.833	20	3	2	63	62
36690.375	2.845	35	2	6	74	70
36691.375	2.204	14	1	7	81	74
36692.375	2.157	11	1	10	73	68
36696.375	3.322	51	2	10	65	58
36697.375	2.255	20	1	10	72	64
36698.375	2.146	20	2	10	75	72
36699.375	2.279	18	2	10	74	65
36703.375	1.204	5.4	1	10	76	70
36705.375	1.833	9.91	3	10	69	65
36706.375	2.111	6.25	2	10	64	61
36712.375	1.803	4.075	1	10	75	66
36713.375	1.911	5.8	2	10	72	64
36717.375	1.763	7.14	2	7	75	72

Figure 9. Post-validation enabling of the Global Datasheet functionality.

At this point, grid cells (other than the ID column) are editable – that is, users can manually enter new numeric data with a left-double-click on a cell and typing in a new value. VB3 does not allow a cell to be made blank or non-numeric. A right-click on an IV column header presents additional options (Figure 10):

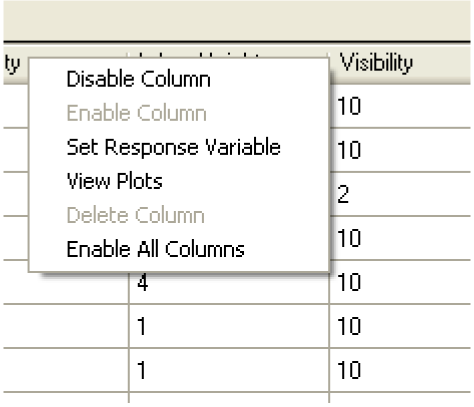
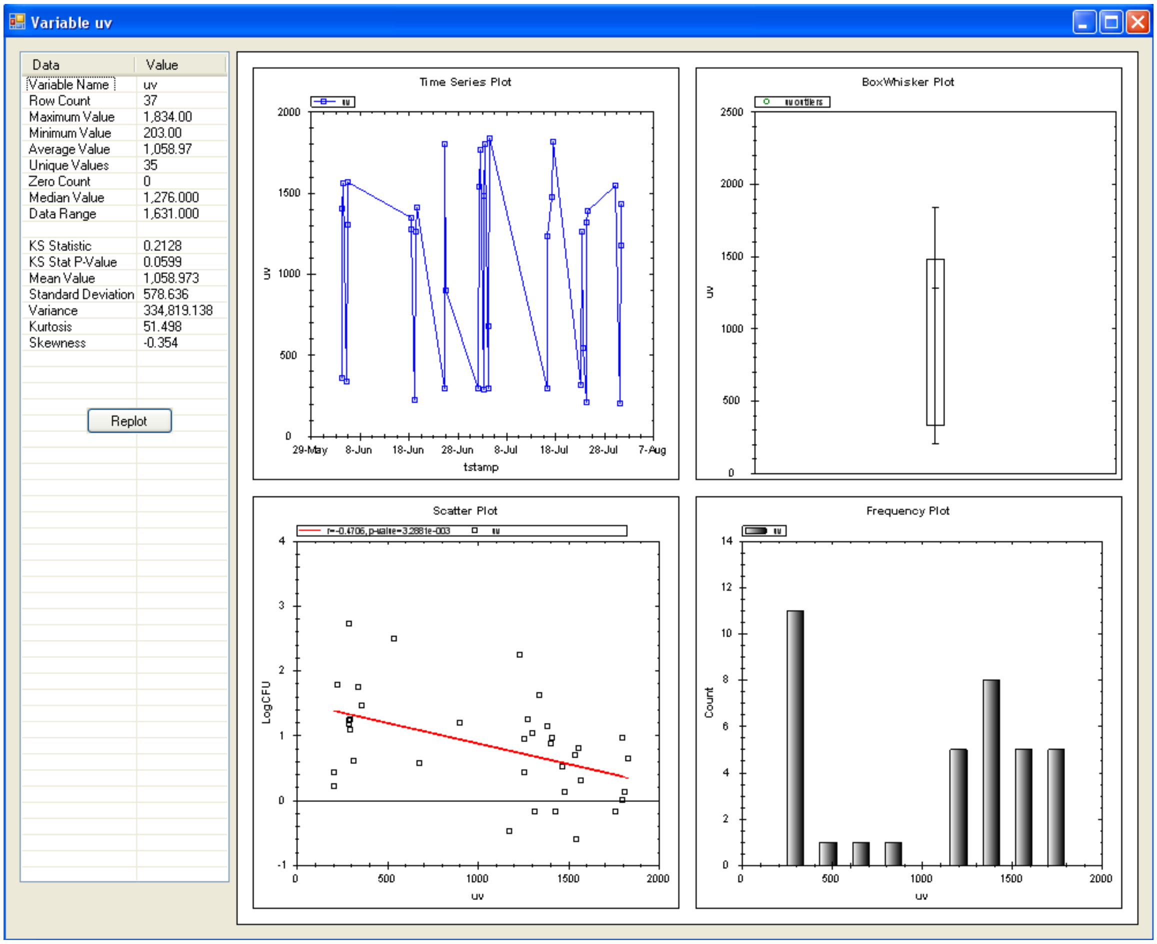


Figure 10. Right-click options on columns that are not the response variable.

"Disable Column" turns the text red and prevents the column from being passed to the method tabs. Previously-disabled columns can be activated with "Enable Column." "Set Response Variable" makes the chosen IV the new response variable (the column becomes blue to indicate this change). "View Plots" shows a new screen with column statistics at the far left and four plots for the chosen column (Figure 11): (1) a scatter plot of the IV versus the response variable in the lower left panel; (2) a plot of the IV values versus the ID column at the upper left (a time series plot if the ID is an observation date); (3) a box-and-whiskers plot at the top right; and (4) a histogram for IV values at the bottom right.



Variable uv

Data	Value
Variable Name	uv
Row Count	37
Maximum Value	1,834.00
Minimum Value	203.00
Average Value	1,058.97
Unique Values	35
Zero Count	0
Median Value	1,276.000
Data Range	1,631.000
KS Statistic	0.2128
KS Stat P-Value	0.0599
Mean Value	1,058.973
Standard Deviation	578.636
Variance	334,819.138
Kurtosis	51.498
Skewness	-0.354

Figure 11. Four different plots available for evaluation of IVs.

Scatter Plot Interpretation

Curvature in the scatter plot (lower left) can indicate a non-linear relationship between the IV and the response variable, problems with homogeneity of variance across the range of the IV, or outliers. Ensuring that the IVs are linearly related to the response variable raises the probability of producing a robust, meaningful MLR and PLS analysis (GBM does not need linearity). If the relationship between the response and the IV is not well-approximated by a straight line (a fundamental assumption of MLR and PLS), it may be beneficial to transform the IV. Using VB3 to accomplish this will be explained later (Section 6.7). The scatter plot also shows the best-fit linear regression line in red, along with the correlation coefficient (r) and the significance (p-value) of the correlation coefficient at the top of the plot. In general, p-values below 0.05 are considered statistically significant. While VB3 does not provide a plot of the residuals of the regression line depicted in the scatter plot, this important diagnostic is given much attention on the MLR tab (see Section 7.8).

Identifying odd values (potential outliers or bad data) of any IV can often be done by visual inspection. If users move the mouse cursor over a data point in any plot (other than the histogram), they will see the ID value of that observation (Figure 12). They can then go back to the datasheet, find the outlying observation (data row), and disable that row (described below) if justifiable.

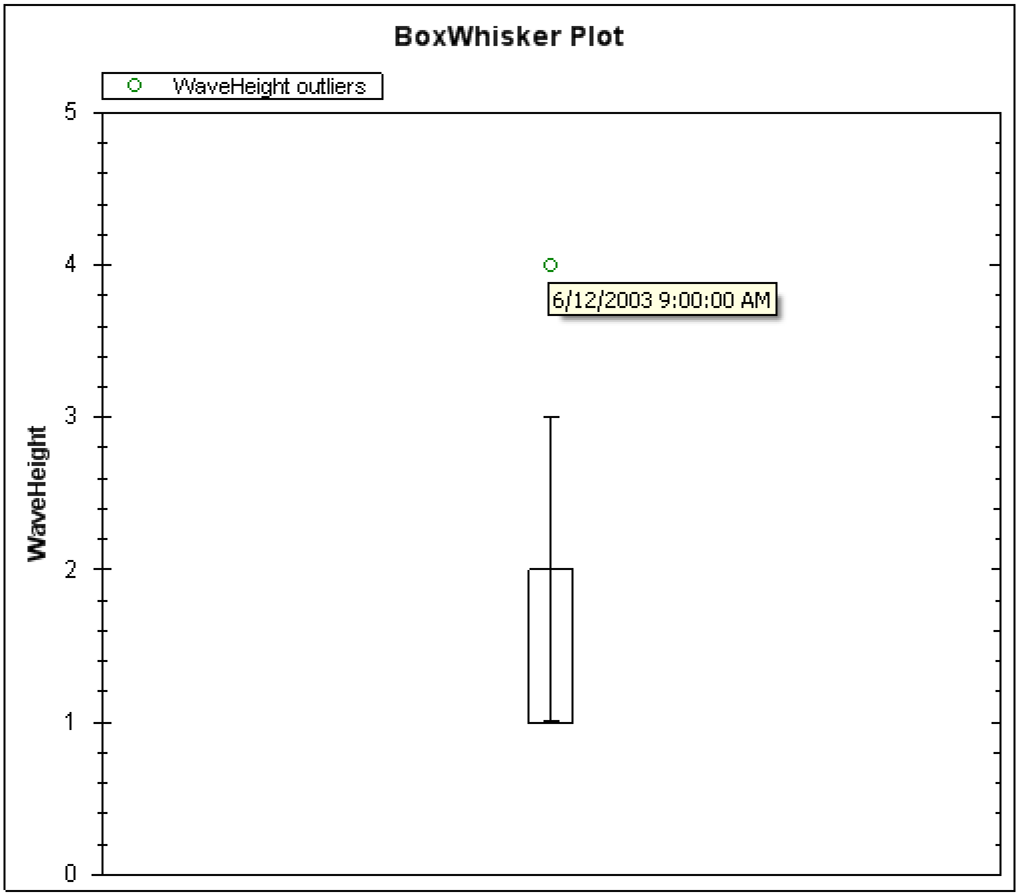
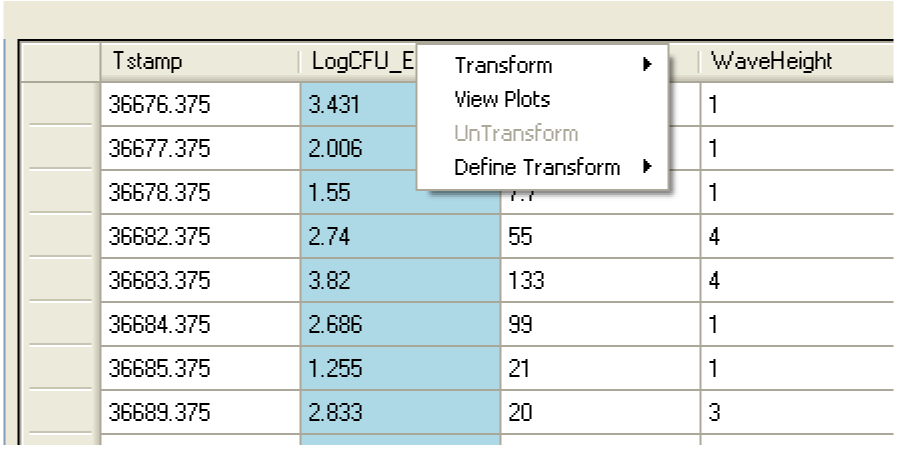


Figure 12. Identifying an observation from within the XY scatter plot.

The "Delete Column" right-click column header option deletes a column from the VB3 datasheet. Note that original columns of the imported data sheet (VB3 defines these as "main effects") cannot be deleted. Rows can be disabled and enabled, but not deleted, from the datasheet by right-clicking the row header (far left of each row) and making the desired choice. Changes that the user makes can be undone and redone using the "Undo" and "Redo" options under the VB3 "File" menu.

If the user right-clicks on the column header of the response variable, a different set of choices is shown (Figure 13).



Tstamp	LogCFU_E		WaveHeight
36676.375	3.431		1
36677.375	2.006		1
36678.375	1.55	7.7	1
36682.375	2.74	55	4
36683.375	3.82	133	4
36684.375	2.686	99	1
36685.375	1.255	21	1
36689.375	2.833	20	3

Figure 13. Available choices when right-clicking the response variable.

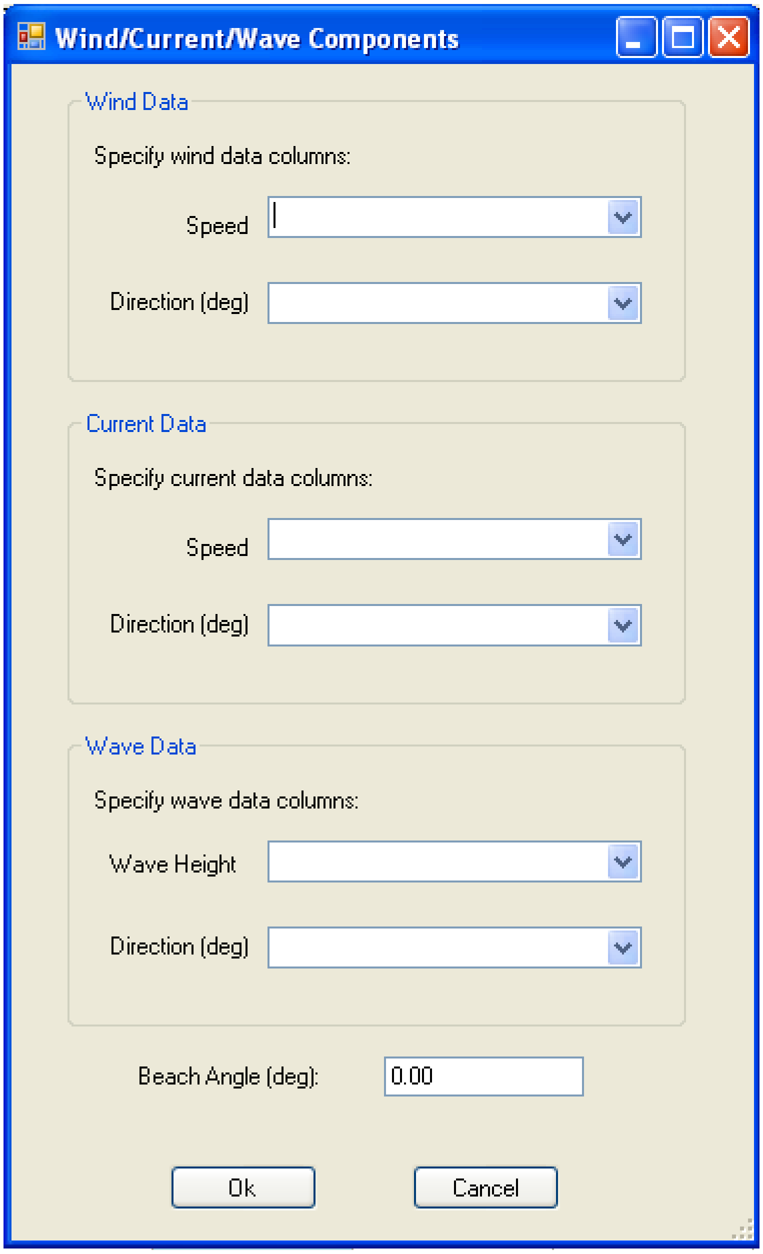
Users can transform the response variable in three ways: $\log_{10}$, $\log_e$, or a power transformation (raising the response to an exponent: y^λ). They can also un-transform the response, view the plots shown previously for the IVs, or define a transformation of the response variable. This last option is used when a datasheet is imported with an already-transformed response variable. For example, users could import a datasheet with $\log_{10}$-transformed fecal indicator bacteria concentrations and should define the response as $\log_{10}$-transformed. Doing this facilitates later comparisons with the fitted response variable values, decision criteria, and regulatory standards. If this is not done, then later plots and comparisons of model predictions to response variable values will be strange and misleading. When users transform the response variable within VB_3 using the "Transform" option, VB_3 automatically defines the response as having the chosen transformation and, in doing so, synchronizes the units of measurement for later comparisons.

6.5 Computing Wind, Wave and Current Components

Orthogonal wind, current, and wave components can be powerful predictors of beach bacterial concentrations. Depending on the orientation of the beach, wind and currents can influence the movement of bacteria from a nearby source to the beach, and wave action can re-suspend bacteria buried in beach sediment. To make more sense of this information, researchers typically decompose wind/current/wave magnitude and direction data into A (alongshore) and O (offshore/onshore) components for analysis (see equations at the end of this section).

If direction and magnitude (speed/height) data are available, A and O components can be calculated with the "Compute A O" button in the ribbon (Figure 9). Clicking it brings up a window with drop-down menus for users to specify which columns of the datasheet contain the relevant magnitude and directional data (Figure 14). There is also an input box at the bottom of the form for the beach orientation angle. If the user defined the beach angle on the "Location" tab, that value will be seen. After clicking "OK," new data columns are added to the far right of the grid, representing the A and O components of the specified wind, current, or wave data. Unlike the originally-imported IVs, these components can be deleted from the grid after creation. Names of these new columns are: WindA_comp(X,Y,Z), CurrentO_comp(X,Y,Z), WaveA_comp(X,Y,Z), etc., where

X is the name of the column of data used for direction, Y is the name of the column used for magnitude, and Z is the beach orientation angle. Note that the IVs used to create the A and O components are automatically disabled by VB3 once the components are created. These columns can be re-enabled by right-clicking on their column header in the datasheet and choosing “Enable Column.” The “Compute A O” function is repeatable as many times as the user wishes.


Wind/Current/Wave Components
Wind Data
Specify wind data columns:
Speed
Direction (deg)
Current Data
Specify current data columns:
Speed
Direction (deg)
Wave Data
Specify wave data columns:
Wave Height
Direction (deg)
Ok
Cancel

Beach Angle (deg): 0.00

Figure 14. Window for computation of alongshore and offshore/onshore components.

Notes on Component Calculations

Direction is an angular degree measure. Moving in a clockwise direction from north (0 degrees), values are positive, and negative while moving counter-clockwise. Wind and current speed (as well as wave height) can be measured in any unit. VB3 adheres to scientific convention: wind direction is specified as the direction from which the wind blows and current and wave directions are specified as the direction towards which the current or waves move. Thus, wind blowing west to east has a direction of 270 degrees (or equivalently -90) degrees, while a current/wave also moving west to east has a direction of 90 (or -270) degrees.

The A-component measures the force of the wind/current/wave moving parallel to the shoreline (Figure 15). A positive A-component means winds/currents/waves are moving from right to left as an observer looks out onto the water. A negative A-component means winds/currents/waves are moving left to right as an observer looks out onto the water. The O-component measures force perpendicular to the shoreline. A negative O value indicates movement from the land surface directly offshore (unlikely to be seen with wave action). A positive O indicates waves/wind/currents from the water to the shore. These relationships apply no matter how the beach is oriented (Figure 16).

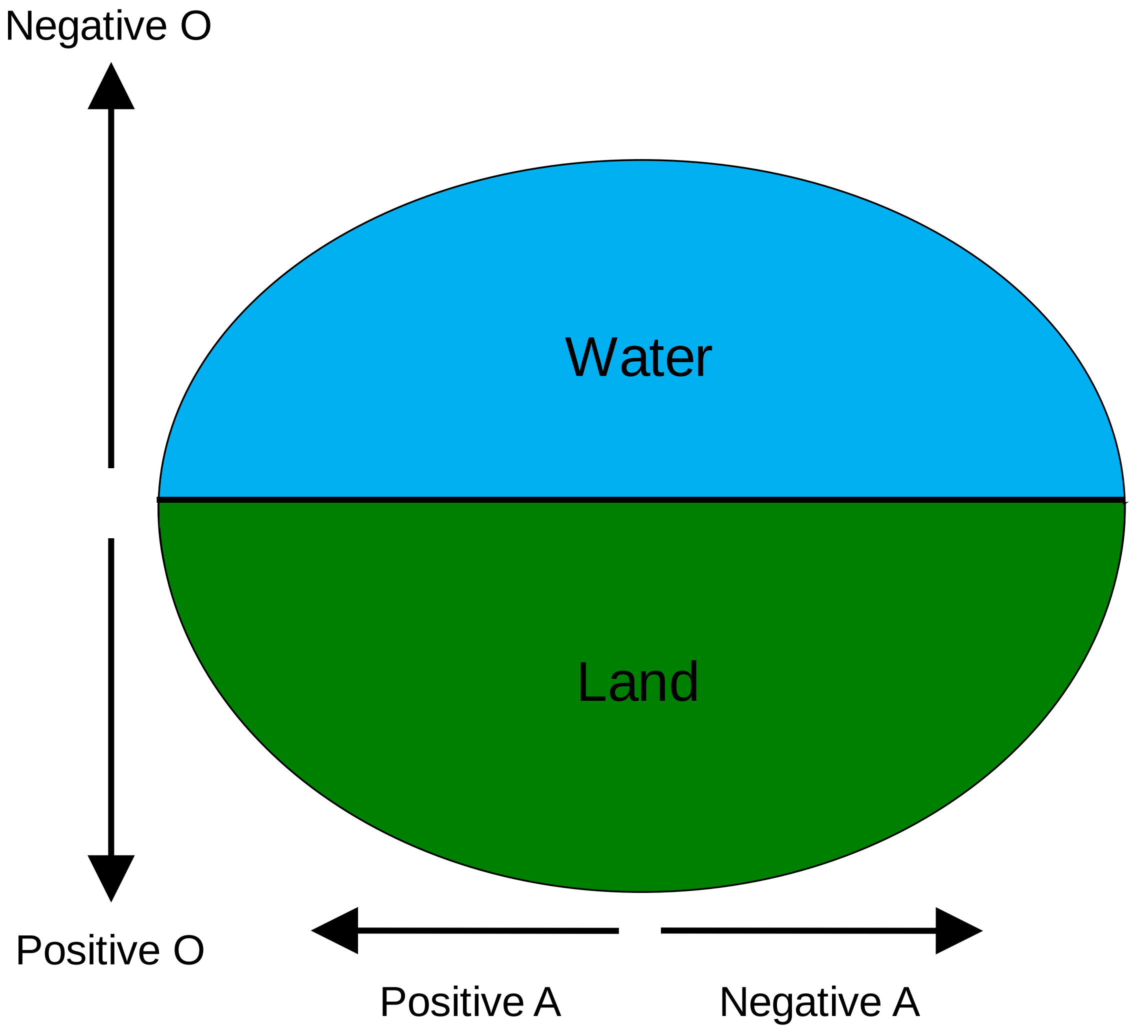


Figure 15. A- and O-component definitions for wind, current, and wave data.

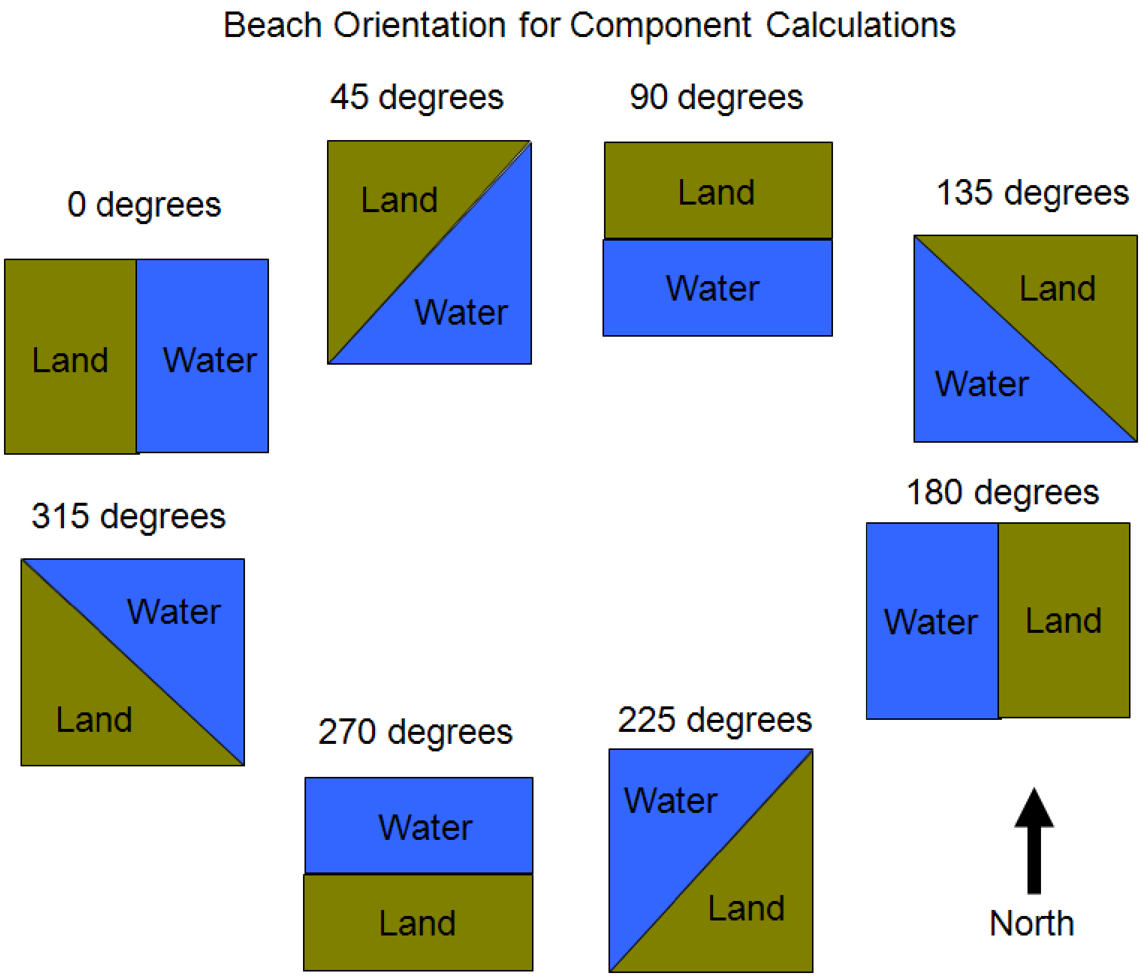


Figure 16. Principal beach orientations given in degrees.

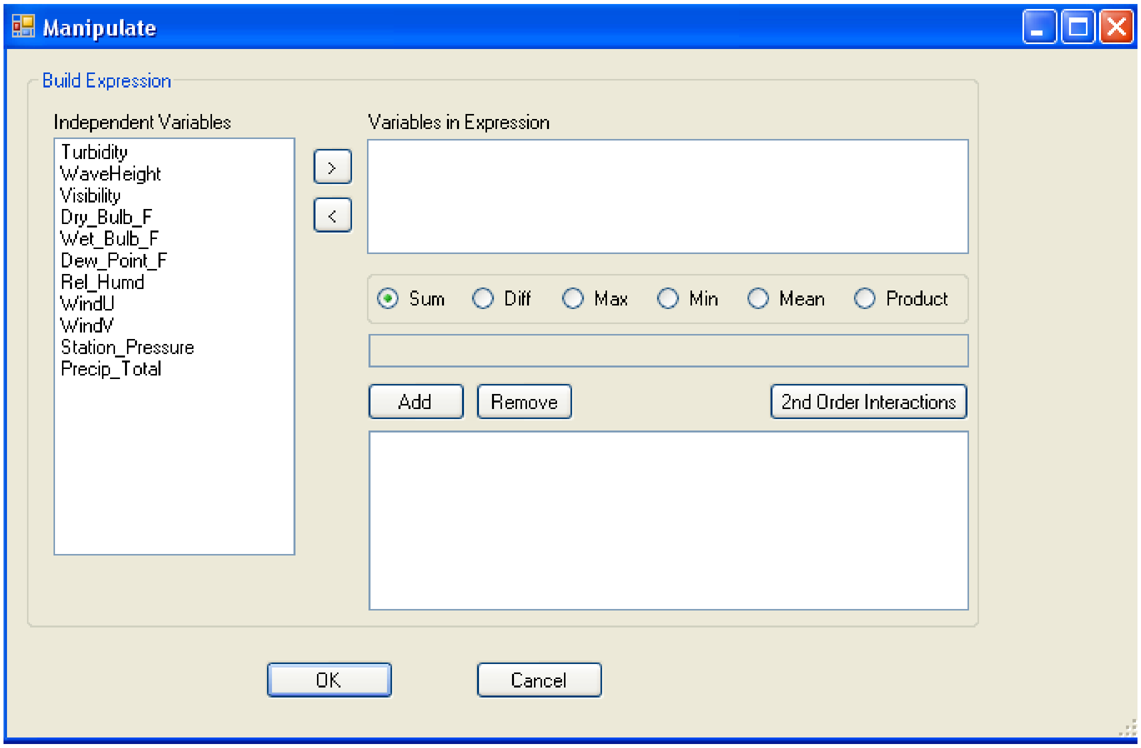
The equations for calculation of Wind A/O components:

$$\text{Wind A: } -S * \text{cosine } ((D-B) * \pi/180)$$
$$\text{Wind O: } S * \text{sine } ((D-B) * \pi/180)$$

where S is wind speed, D is wind direction, B is the beach orientation (in degrees) and $\pi \approx 3.1416$. Current A/O and Wave A/O are the same equations multiplied by -1 to account for the difference in how these data are measured.

6.6 Creation of New Independent Variables

Users may click the "Manipulate" button (Figure 9) to create new columns of data (as functions of existing IVs) that might be useful IVs. On the pop-up screen (Figure 17), there is a list (automatically populated by VB3 from the imported spreadsheet) of available IVs on the far left under "Independent Variables." If users wish to create a new term, they add the desired existing IVs to the "Variables in Expression" box by selecting the IV and clicking the ">" button. Clicking and dragging, shift-clicking and control-clicking in the "Independent Variables" list allow multiple IVs to be added at once.

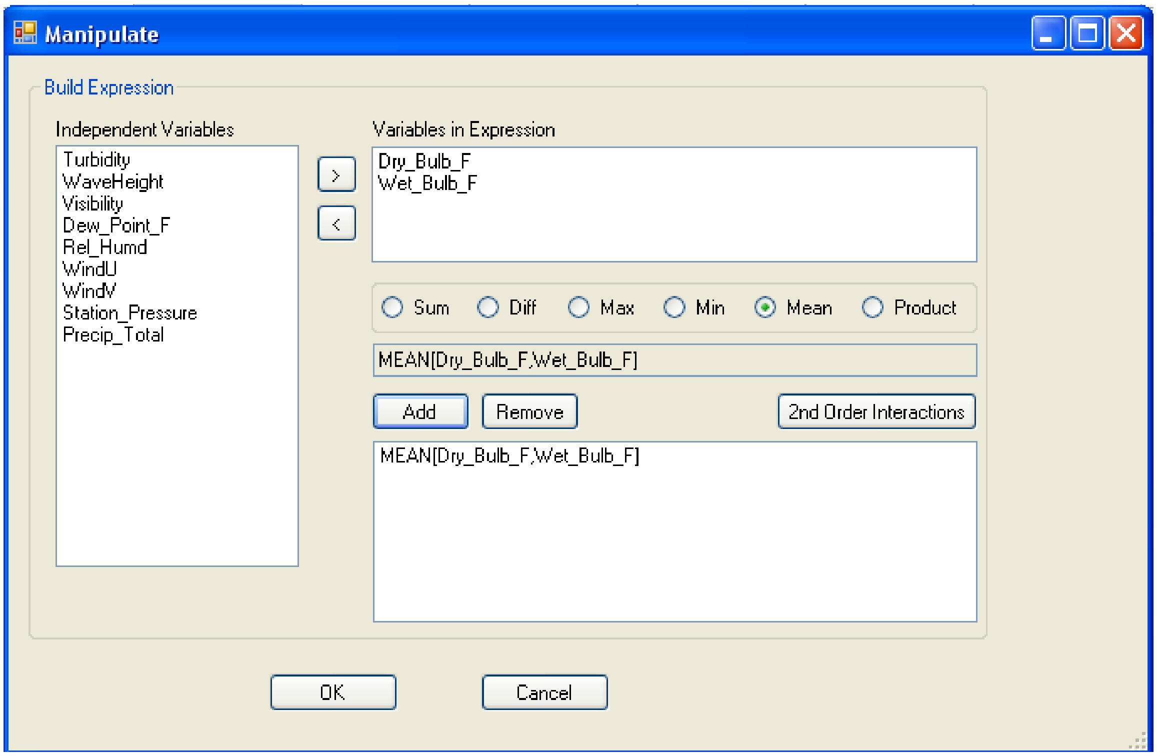


Turbidity
WaveHeight
Visibility
Dry_Bulb_F
Wet_Bulb_F
Dew_Point_F
Rel_Humd
WindU
WindV
Station_Pressure
Precip_Total

● Sum ○ Diff ○ Max ○ Min ○ Mean ○ Product

Figure 17. Window for the formulation of "Manipulates" - arithmetic combinations of existing columns within the datasheet.

For example, if users wish to create a new IV that is a row-by-row mean value of the "Dry_Bulb_F" and "Wet_Bulb_F" variables, they add those two IVs to the "Variables in Expression" box (Figure 18), choose the "Mean" function, "Add" that expression to the lower box, then click "OK." A new column of data representing a row-by-row average of those two IVs is then added to the end of the datasheet.



Independent Variables

Turbidity
WaveHeight
Visibility
Dew_Point_F
Rel_Humd
WindU
WindV
Station_Pressure
Precip_Total

Variables in Expression

Dry_Bulb_F
Wet_Bulb_F

○ Sum ○ Diff ○ Max ○ Min ● Mean ○ Product

MEAN[Dry_Bulb_F,Wet_Bulb_F]

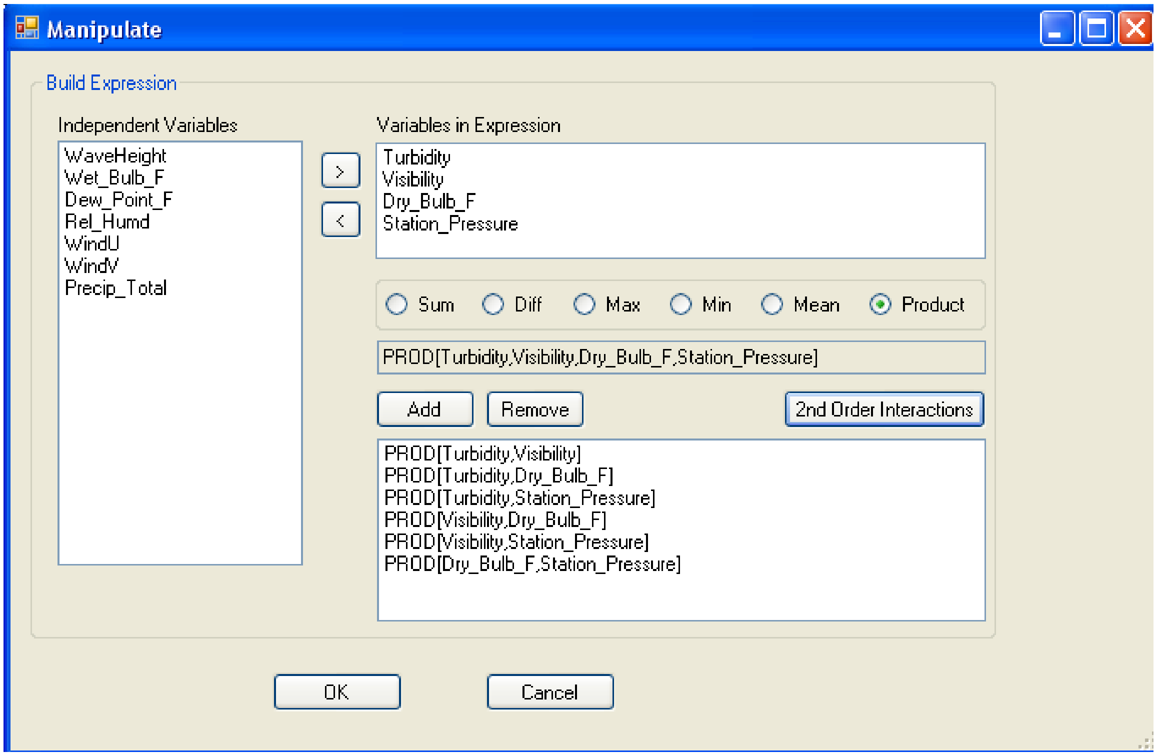
MEAN[Dry_Bulb_F,Wet_Bulb_F]

Figure 18. Creation of a new IV defined as the mean of two existent IVs.

Users can create a row-by-row sum, difference, maximum, minimum, mean, or product from any number of IVs added to the “Variables in Expression” box. More than one expression can be created before the “OK” button is clicked and IVs can be easily moved in and out of the “Variables in Expression” box using “<” and “>” keys. Note that creating a difference of more than two columns (e.g., X1, X2, X3, and X4) would lead to this quantity:

$$\mathrm{Diff}(X1,X2,X3,X4) = X1 - X2 - X3 - X4$$

Created expressions can be removed from the lower box with the “Remove” button. No matter how many IVs are added to the “Variables in Expression” box, clicking “2nd Order Interactions” will add the cross-products for all possible pairings of those IVs (Figure 19). Thus, four IVs in the “Variables in Expression” box will produce six 2nd second-order interactions; five IVs will produce ten interactions, and so on. Note that the names of the columns used to create any new data columns are inside the parentheses of those columns’ names.



Independent Variables

WaveHeight
Wet_Bulb_F
Dew_Point_F
Rel_Humd
WindU
WindV
Precip_Total

Variables in Expression

Turbidity
Visibility
Dry_Bulb_F
Station_Pressure

○ Sum ○ Diff ○ Max ○ Min ○ Mean ● Product

PROD[Turbidity,Visibility,Dry_Bulb_F,Station_Pressure]

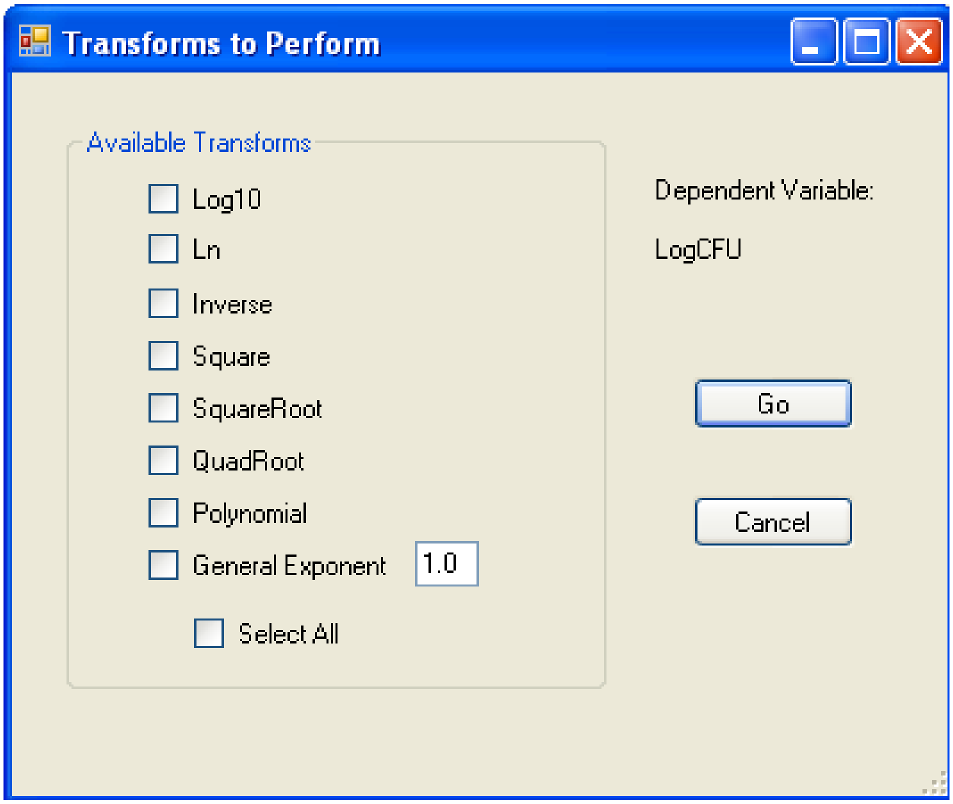
PROD[Turbidity,Visibility]
PROD[Turbidity,Dry_Bulb_F]
PROD[Turbidity,Station_Pressure]
PROD[Visibility,Dry_Bulb_F]
PROD[Visibility,Station_Pressure]
PROD[Dry_Bulb_F,Station_Pressure]

Figure 19. Formation of two-way cross-products of a set of four IVs.

VB3 does not allow previously created "manipulates" -- new columns of data created through the "Manipulate" button -- to be further manipulated. Previously created manipulates will not appear in the "Independent Variables" section at the left. They can, however, be chosen as the response variable or deleted from the datasheet, using the appropriate menu choices accessed by a right-click of the column header.

6.7 Transforming the Independent Variables

VB3 gives users the ability to transform non-categorical IVs to assist in linearizing the relationship between the IVs and the response variable, a fundamental assumption of an MLR/PLS analysis. VB3 transformations are described in section A.1. When users click the "Transform" button (Figure 9) in the Global Datasheet ribbon, they are presented with the window seen in Figure 20:



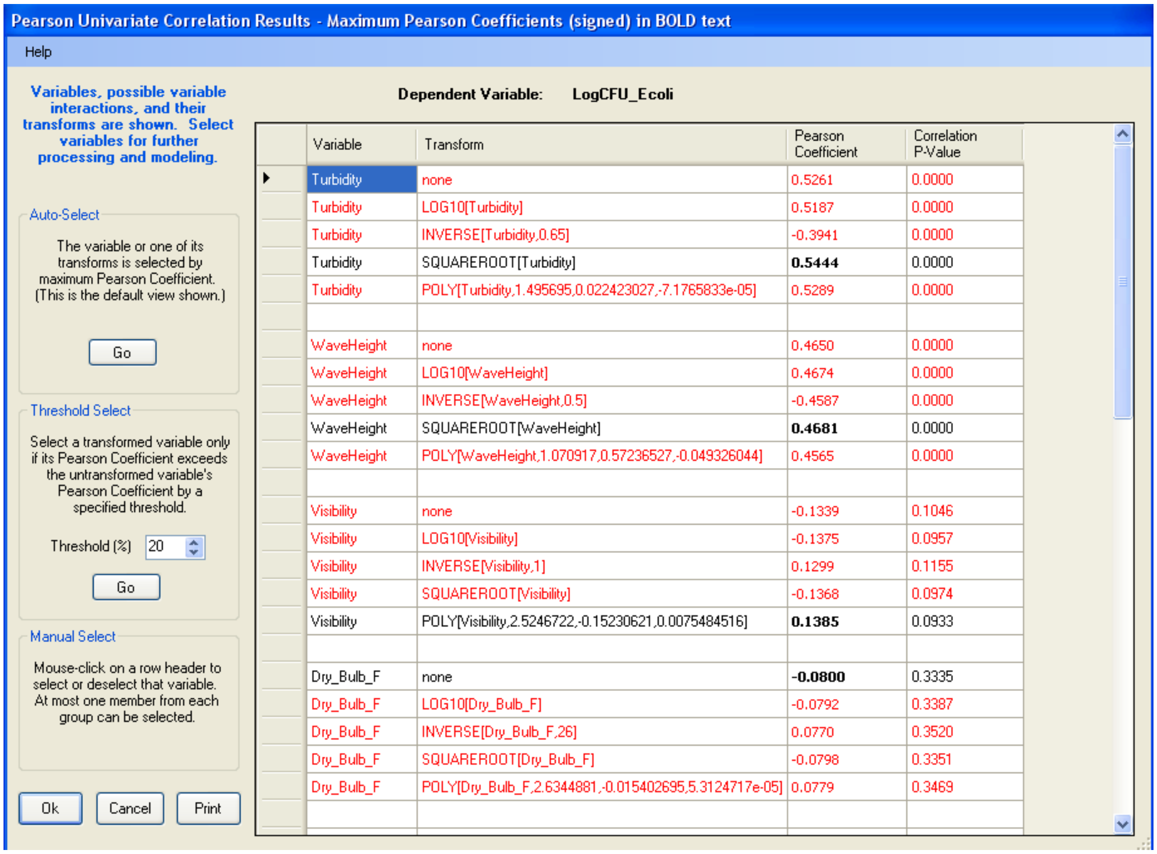
□ Log10
□ Ln
□ Inverse
□ Square
□ SquareRoot
□ QuadRoot
□ Polynomial
□ General Exponent 1.0
□ Select All

Dependent Variable:
LogCFU

Figure 20. The choices for IV transformations.

When users click "Go," the chosen transformations are applied to each and every non-categorical IV (there is not an option to ignore transformation for particular IVs). VB3 then opens a table (Figure 21) that compares the success of each transformation using a Pearson correlation coefficient which is a measure of linear dependence between the response variable and the IVs.

The table created byVB3 groups all transformed versions of each IV and specifies type of transformation, the Pearson coefficient, and its statistical significance (p-value). This includes the un-transformed version of the IV, denoted by "none." By default, the transformation with the largest absolute value of the Pearson coefficient is highlighted in black text. Users may override the default selection by left-clicking on the row header of a transformed IV. They may also override the default by setting a percentage and clicking "Go" under the "Threshold Select" box on the left side of the window. This will select the un-transformed version of every IV unless the transformed IV with the highest absolute value Pearson coefficient exceeds the un-transformed IV Pearson coefficient by the specified percentage. In essence, the user is saying, "Unless the Pearson coefficient of the transformed IV is some % greater than the Pearson coefficient of the un-transformed IV, use the un-transformed IV." This can be useful because transforming IVs makes interpreting model coefficients more difficult; unless a major improvement is seen, transformation simply may not be worth the trouble. Users can also revert to the default (selecting the transform with the largest absolute value Pearson coefficient) by clicking "Go" under "Auto Select."



Pearson Univariate Correlation Results - Maximum Pearson Coefficients (signed) in BOLD text

Variables, possible variable interactions, and their transforms are shown. Select variables for further processing and modeling.

Auto-Select

The variable or one of its transforms is selected by maximum Pearson Coefficient. (This is the default view shown.)

Threshold Select

Select a transformed variable only if its Pearson Coefficient exceeds the untransformed variable's Pearson Coefficient by a specified threshold.

Threshold (%) 20

Manual Select

Mouse-click on a row header to select or deselect that variable. At most one member from each group can be selected.

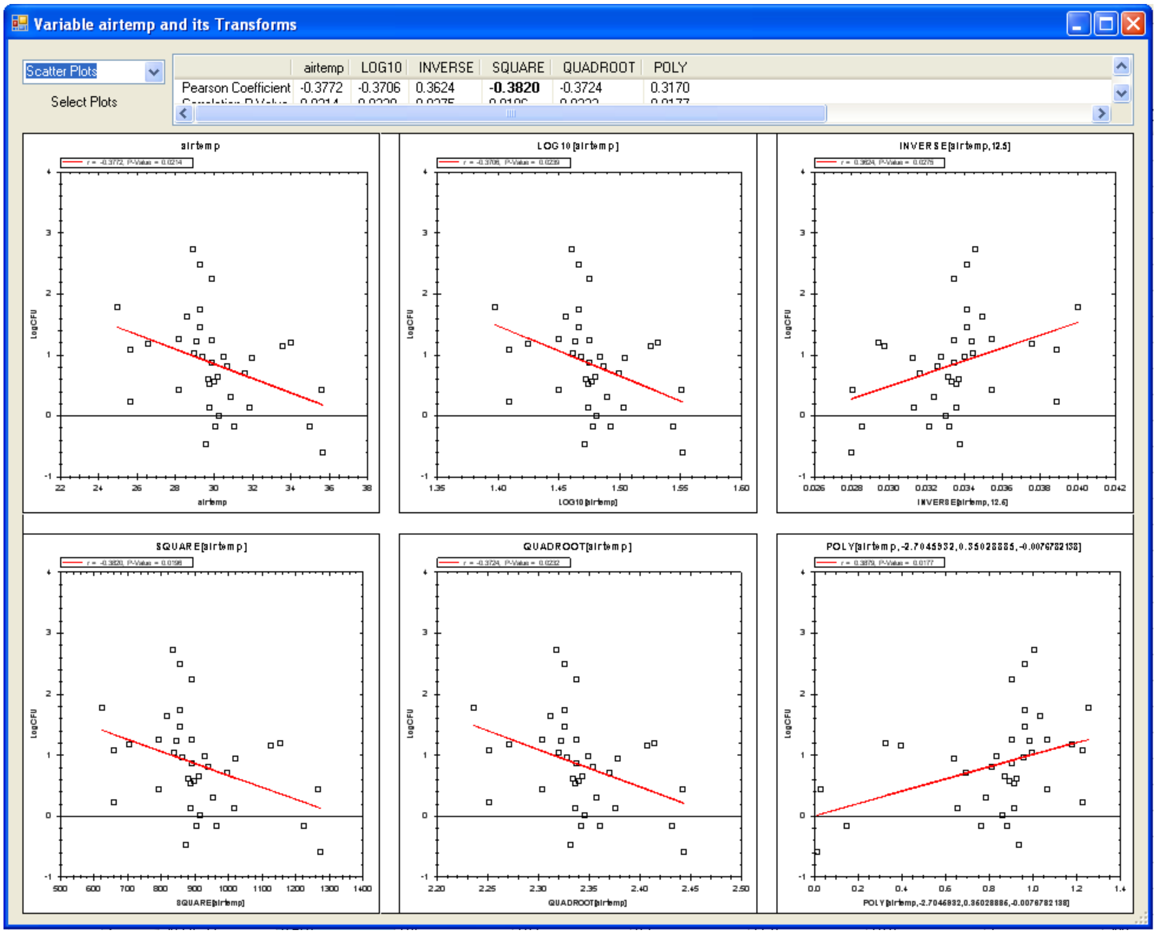
Dependent Variable: LogCFU_Ecoli

Variable	Transform	Pearson Coefficient	Correlation P-Value
Turbidity	none	0.5261	0.0000
Turbidity	LOG10[Turbidity]	0.5187	0.0000
Turbidity	INVERSE[Turbidity,0.65]	-0.3941	0.0000
Turbidity	SQUAREROOT[Turbidity]	**0.5444**	0.0000
Turbidity	POLY[Turbidity,1.495695,0.022423027,-7.1765833e-05]	0.5289	0.0000
WaveHeight	none	0.4650	0.0000
WaveHeight	LOG10[WaveHeight]	0.4674	0.0000
WaveHeight	INVERSE[WaveHeight,0.5]	-0.4587	0.0000
WaveHeight	SQUAREROOT[WaveHeight]	**0.4681**	0.0000
WaveHeight	POLY[WaveHeight,1.070917,0.57236527,-0.049326044]	0.4565	0.0000
Visibility	none	-0.1339	0.1046
Visibility	LOG10[Visibility]	-0.1375	0.0957
Visibility	INVERSE[Visibility,1]	0.1299	0.1155
Visibility	SQUAREROOT[Visibility]	-0.1368	0.0974
Visibility	POLY[Visibility,2.5246722,-0.15230621,0.0075484516]	**0.1385**	0.0933
Dry_Bulb_F	none	**-0.0800**	0.3335
Dry_Bulb_F	LOG10[Dry_Bulb_F]	-0.0792	0.3387
Dry_Bulb_F	INVERSE[Dry_Bulb_F,26]	0.0770	0.3520
Dry_Bulb_F	SQUAREROOT[Dry_Bulb_F]	-0.0798	0.3351
Dry_Bulb_F	POLY[Dry_Bulb_F,2.6344881,-0.015402695,5.3124717e-05]	0.0779	0.3469

Figure 21. Pearson correlation coefficient scores for judging the efficacy of IV transformations.

Plotting Transformed IVs

Users may prefer to examine plots visually in determining which transformation of IV to choose. Right-clicking on a row header in the correlation table provides an array of scatter plots, time series plots, or frequency plots for each transformation of that IV (Figure 22). Scatter plots show the best-fit regression line. In the table at the top of this window, users are shown the correlation coefficient and its p-value, as well as the Anderson-Darling test statistic for normality, and its p-value.



Variable airtemp and its Transforms

Scatter Plots

Select Plots

	airtemp	LOG10	INVERSE	SQUARE	QUADROOT	POLY
Pearson Coefficient	-0.3772	-0.3706	0.3624	**-0.3820**	-0.3724	0.3170

airtemp
r = -0.3772, P-Value = 0.0214
LOG10[airtemp]
r = -0.3706, P-Value = 0.0239
INVERSE[airtemp, 12.5]
r = 0.3624, P-Value = 0.0275
SQUARE[airtemp]
r = -0.3820, P-Value = 0.0196
QUADROOT[airtemp]
r = -0.3724, P-Value = 0.0232
POLY[airtemp, -2.7045932, 0.35028885, -0.0076782138]
r = 0.3879, P-Value = 0.0177
logCFU
airtemp
LOG10[airtemp]
INVERSE[airtemp, 12.6]
SQUARE[airtemp]
QUADROOT[airtemp]
POLY[airtemp, -2.7045932, 0.35028885, -0.0076782138]

Figure 22. Scatter plots (Response vs. IV) for six different data transformations of a single IV.

After choosing a transformation for each IV, users click "OK." This populates the datasheet with new columns representing transformed versions of the IVs. Notice two things: if a transformation was chosen for an IV, the column representing the untransformed version of that IV is disabled in the datasheet (it can be re-enabled by using the right-click column header menu option) and the transformed versions of an IV are put into the datasheet immediately after the original, un-transformed IV. Any transformations put into the datasheet can be deleted with the "Delete Column" choice (right-click on their column header). Transformed IVs will appear in the list of IVs on the "Manipulate" screen, however, transformed IVs cannot be further transformed and will not appear in the transform table if the user returns to the "Transform" window. Also, transformed IVs cannot be the response variable. Finally, because transformations are determined from the current response variable, all transformed IVs in the datasheet are erased (a warning appears) when users change the response variable in the datasheet. For the interested reader, further discussion of VB3 transformations can be found in section A.1.

6.8 Singular Matrices and Nominal Variables

Advice on avoiding singularities within the data matrix and handling nominal categorical variables can be found in section A.2.

6.9 Saving Processed Data

Changes made to the imported spreadsheet can be saved in a project file (File→Save). When it is re-opened, the datasheet will appear as it did when the project was saved. Users also may highlight the entire datasheet or sections of the datasheet and use Control-C and Control-V to copy and paste it into a word processing or spreadsheet application.

6.10 Proceeding to Modeling

After data processing is complete, users must click the “Go to Model” button to open the statistical method tabs. If they have already done some modeling and return to the global datasheet to make changes, they will receive a message that the datasheet has changed and any prior modeling results will be erased.

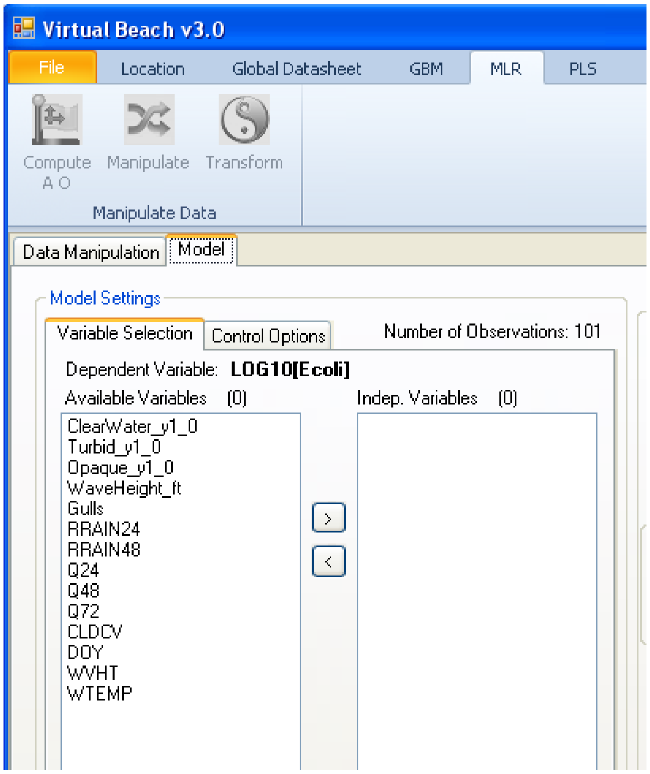
7. MULTIPLE LINEAR REGRESSION MODELING

The MLR tab finds the best multiple linear regression model based on criteria selected by the user. As the number of IVs increases, the number of possible models in the solution space increases exponentially. Users may select all or a subset of the IVs for consideration in the model to reduce the size of the solution space.

Notice that the MLR tab (as well as the PLS and GBM tabs) has its own datasheet on the "Data Manipulation" sub-tab. When the user first moves over to the MLR tab from the Global Datasheet, the data in the MLR Data Manipulation sub-tab is identical to the data on the Global Datasheet. Once inside the MLR tab, the user can change the "local" data to suit the MLR analysis. The local datasheet has all of the functionality of the Global Datasheet discussed in Section 6. Changing the local data has no effect on the Global Datasheet, however, going back to the Global Datasheet and making changes causes local datasheets on the MLR, PLS, and GBM tabs to be overwritten.

7.1 Selecting Variables for Model Building

Under the "Model" sub-tab, two additional sub-tabs are found (Figure 23). On the "Variable Selection" sub-tab, all eligible IVs are listed in the left column ("Available Variables"). Any variable users wish to consider for model inclusion must be moved to the right column list ("Indep. Variables") by highlighting the IV and clicking the ">" button. IVs currently under consideration (in the right list) can be ignored by highlighting them and clicking the "<" button. The user can hold down shift while left-clicking or control while left-clicking to select multiple IVs at once.



Number of Observations: 101

Dependent Variable: LOG10[Ecoli]

Available Variables (0)

ClearWater_y1_0
Turbid_y1_0
Opaque_y1_0
WaveHeight_ft
Gulls
RRAIN24
RRAIN48
Q24
Q48
Q72
CLDCV
DOY
WVHT
WTEMP

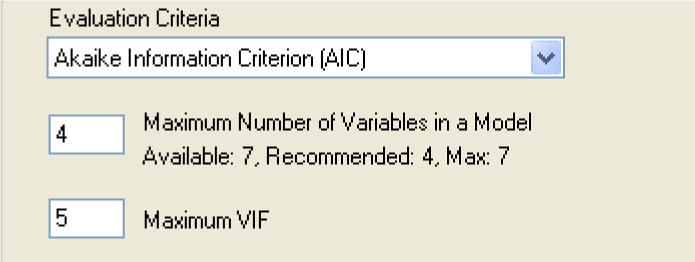
Indep. Variables (0)

Figure 23. Selecting variables for MLR processing within the Modeling tab.

7.2 Modeling Control Options

After choosing the set of IVs to investigate, the user should click the “Control Options” sub-tab. The first decision to be made involves which evaluation criterion will be used to judge model fitness (Figure 24). There are ten choices in the drop-down menu:

- Akaike Information Criterion (AIC)
- Corrected Akaike Information Criterion (AICC)
- R^2
- Adjusted R^2
- Predicted Error Sum of Squares (PRESS)
- Bayesian Information Criterion (BIC)
- RMSE
- Sensitivity
- Specificity
- Accuracy



Evaluation Criteria

Akaike Information Criterion (AIC)

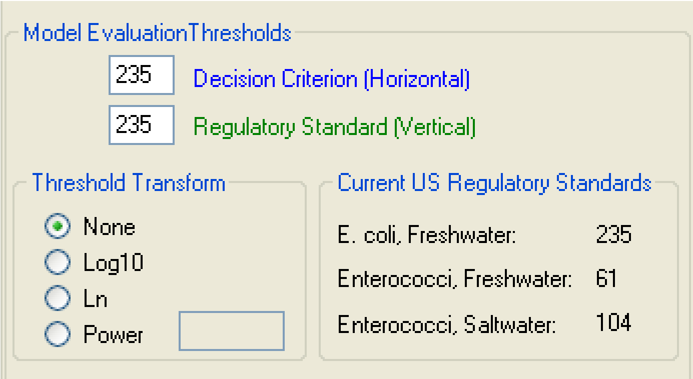
4 Maximum Number of Variables in a Model
Available: 7, Recommended: 4, Max: 7

5 Maximum VIF

Figure 24. Setting modeling options within the modeling interface.

Depending on the evaluation criteria, VB$_3$ searches for a minimum or maximum value. The minimum value for AIC, AICC, BIC, RMSE, and PRESS is used to choose a model, while the maximum is used for R^2, Adjusted R^2, accuracy, specificity, and sensitivity. A more detailed description of each criterion can be found in section A.3.

Sensitivity, specificity and accuracy are special cases requiring users to enter both a Decision Criterion (DC) and Regulatory Standard (RS) so that true/false positives and true/false negatives can be defined (Figure 25). The user chooses the DC value. Model predictions above this threshold are considered exceedances/positives, and model predictions below this value are considered non-exceedances/negatives. The RS is typically a safety limit on fecal indicator bacteria (FIB) concentrations set by a state or federal agency. The “Threshold Transform” radio buttons tell VB$_3$ the units of DC and RS to ensure a proper comparison to model predictions and observations. For example, if “235” is entered into the DC box (representing the EPA standard for freshwater *E.coli)*, then “none” should be chosen. If 2.371 (= log$_{10}$(235)) is entered as the DC, then “Log10” is used. The DC and RS should always use the same units. Improper setting of this button choice will lead to problems later when comparing modeling predictions to observations.



Model EvaluationThresholds

235 Decision Criterion (Horizontal)

235 Regulatory Standard (Vertical)

Threshold Transform

- ● None
- ○ Log10
- ○ Ln
- ○ Power

Current US Regulatory Standards

E. coli, Freshwater: 235

Enterococci, Freshwater: 61

Enterococci, Saltwater: 104

Figure 25. Setting evaluation thresholds and threshold transformation information within the modeling interface.

The “Maximum Number of Variables in a Model” parameter tells VB3 the maximum allowable size for any tested models. In general, one should have about 10-20 observations per estimated parameter in a model, otherwise model over-fitting and poor estimation of regression parameters can occur. VB3 recommends this limit be set to (1 + n/10) parameters, where n is the number of observations in the dataset. The maximum allowable limit is n/5. The total number of available parameters is also shown.

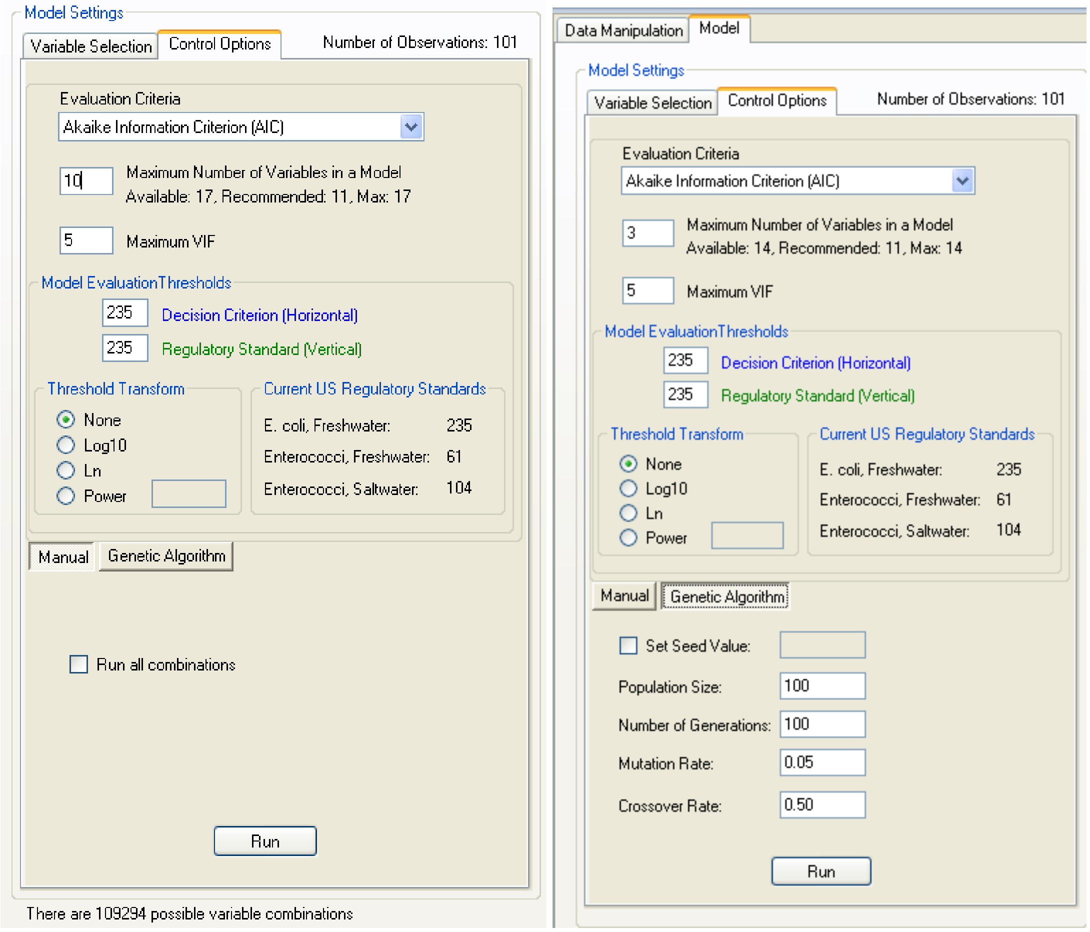
The “Maximum VIF” (Variance Inflation Factor) is used to discard models containing variables with a high degree of multi-collinearity, i.e., IVs that are highly correlated with other IVs in the model. If any IV in a model has a VIF exceeding the VIF threshold, that model will be ignored. The default VIF is 5, which means that 80% (1 – 1/VIF = 1 – 1/5 = 4/5) of the variability in an IV can be explained by the other IVs in the model. A VIF of 10 means that 90% (1 - 1/10 = 9/10) of the IVs variability can be explained, and so on. Raising the Maximum VIF means a higher degree of multi-collinearity will be tolerated, but this can lead to poorly estimated regression coefficients (i.e., large standard deviations of these coefficients).

7.3 Linear Regression Modeling Methods

Two buttons are at the bottom of the “Control Options” sub-tab to provide different ways of exploring the regression solution space (Figure 26).

- The Manual button is for a directed model search. If the ‘Run all combinations’ box is not checked, only a single model that includes every IV that was added to the “Indep. Variables” column will be evaluated. If the number of available IVs exceeds the “Maximum Number of Variables in a Model” value, however, VB3 will show an error. If ‘Run all combinations’ is checked, an exhaustive search is performed, testing every model that can be constructed with the selected IVs, but does not evaluate models with more parameters than the “Maximum Number of Variables in a Model.” For example, if there are 24 available IVs and the maximum number of IVs is 8, the exhaustive routine will examine every 1-, 2-, 3-, 4-, 5-, 6-, 7- and 8-parameter model. VB3 shows the total possible number of combinations below the “Model Settings” box. As the number of IVs rises, the number of possible models gets so large that the time needed to compute regression fits for each of them becomes unreasonable. We advise switching to the genetic algorithm in this case.

- The genetic algorithm (GA) button explores solution spaces too large to handle exhaustively. Genetic algorithms are loosely based on natural evolution in which individuals in a population reproduce and mutate (Fogel 1998). Individuals with high fitness (regression models that produce small residuals) are more likely to reproduce and pass their genes (IVs) to the next generation. The goal is to find a good solution without having to examine every possible option. The GA balances random and directed searching.



Number of Observations: 101

Evaluation Criteria: Akaike Information Criterion (AIC)

10 Maximum Number of Variables in a Model
Available: 17, Recommended: 11, Max: 17

5 Maximum VIF

235 Decision Criterion (Horizontal)
235 Regulatory Standard (Vertical)

● None
○ Log10
○ Ln
○ Power

E. coli, Freshwater:	235
Enterococci, Freshwater:	61
Enterococci, Saltwater:	104

□ Run all combinations

There are 109294 possible variable combinations

Number of Observations: 101

Evaluation Criteria: Akaike Information Criterion (AIC)

3 Maximum Number of Variables in a Model
Available: 14, Recommended: 11, Max: 14

5 Maximum VIF

235 Decision Criterion (Horizontal)
235 Regulatory Standard (Vertical)

● None
○ Log10
○ Ln
○ Power

E. coli, Freshwater:	235
Enterococci, Freshwater:	61
Enterococci, Saltwater:	104

□ Set Seed Value:

Population Size: 100
Number of Generations: 100
Mutation Rate: 0.05
Crossover Rate: 0.50

Figure 26. Model building interface using a manual search (left panel) or the genetic algorithm (right panel).

Choosing between the exhaustive and the GA searches depends on the dataset, the computer's available random access memory (RAM), and time constraints. On a dataset of 101 observations and ten IVs, the exhaustive search was completed in approximately 6 seconds, using a Dell Precision T5400 (WinXP; dual Xeon 2.66 GHz processors; 4 GB RAM). Every additional IV doubles the number of models to examine and, thus, approximately doubles necessary computational time (Table 1).

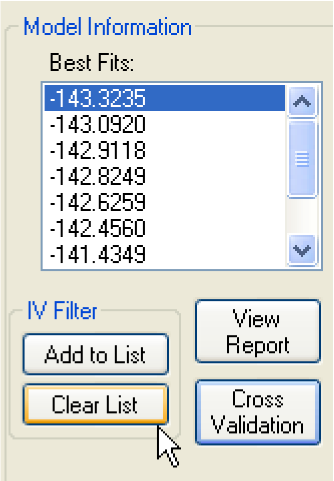
Table 1. Relationship between the number of IVs, number of possible models, and time required to execute an exhaustive search using VB3.

Exhaustive Search – Run All Combinations

Number of IVs	Number of MLR models	Approximate Time Required to Generate and Filter Models (seconds)
10	1023	6
11	2047	13
12	4095	27

In contrast, running the GA with 10 IVs, using a population of 100 for 100 generations, took 90 seconds to complete (90/6 = 15 times slower than the exhaustive routine for this number of IVs); the GA with 12 IVs takes about the same amount of time: 90 seconds. So, as computational time of the exhaustive routine doubles every time an IV is added, the time required to run the GA stays approximately the same. As the number of IVs rises (here, to 14 or 15), the GA would be expected to save time and provide a solution very close to optimal.

An alternative modeling strategy with a large number of IVs would be to run the GA on the entire list of IVs initially, then switch to the exhaustive search on a subset of initial IVs – any IV that appears in one of the best ten models found by the GA. This two-step process is facilitated with the “IV Filter” list control (Figure 27).



Model Information

Best Fits:

-143.3235
-143.0920
-142.9118
-142.8249
-142.6259
-142.4560
-141.4349

Figure 27. Using the IV filter to select a subset of variables from the best-fit models.

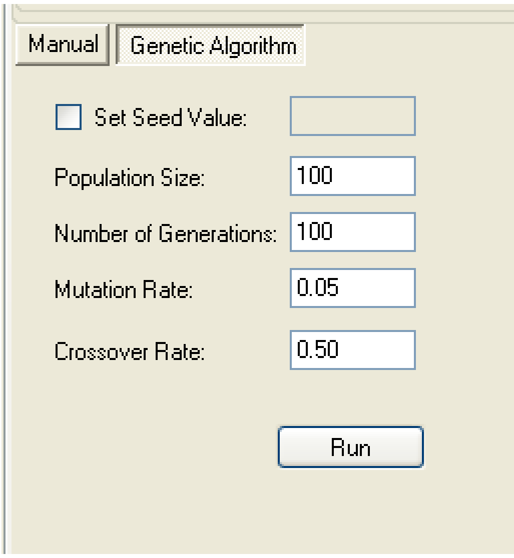
When the GA finishes and the 10 best models are shown in the Model Information box “Best Fits” window, clicking the “Clear List” button removes all IVs from the selection list. Select a model from the “Best Fits” list and click “Add to List” which adds any IVs in the selected model to the “Indep. Variable” list in the Model Settings box. After doing this for each of the ten best models, users will have a more manageable IV list and can run an exhaustive search to find the best combination of IVs. Regardless of the method chosen to build models, the “Best Fits” window shows the top ten models found, based on user-specified evaluation criterion.

7.4 Using the Genetic Algorithm

Several parameters are used to adjust the performance of the GA (Figure 28):

- Seed value: VB3 uses an internal random number generator to produce random values. Setting the seed to a previously-used value will produce results identical to that earlier run, allowing the analysis to be reproduced by other parties. Changing the seed creates a new series of random values, possibly returning a different set of identified regression models.
- Population size: number of individuals in the population of each generation. A larger population broadens the search at each generation, but slows processing time.
- Number of generations: because individuals can reproduce and mutate once each generation, the question is how long to run the search. Fitness of every individual in the population is evaluated at the end of each generation.
- Mutation rate: chance each individual has of undergoing random mutation in each generation. The higher the mutation rate, the more random (less directed) the search of parameter space is.
- Crossover rate: the percent of each parent's genome that children receive. For example, if crossover = 0.5, child 1 and child 2 each receive 50% of the genome of parent 1 and parent 2. If crossover = 0.3, child 1 receives 30% of the parent 1 genome and 70% of the parent 2 genome, while child 2 receives 70% of the parent 1 genome and 30% of the parent 2 genome.

The best GA parameter values depend on the dataset being investigated, but typical values of the mutation rate are between 0.001-0.1 and typical values of the crossover rate are 0.25-0.5. For small datasets, a population size and generation number of 100 are sufficient. Larger datasets may require increased numbers for optimal solutions. The user must invoke an experimental approach for changing these parameters and examining the results.



☐ Set Seed Value:

Population Size: 100

Number of Generations: 100

Mutation Rate: 0.05

Crossover Rate: 0.50

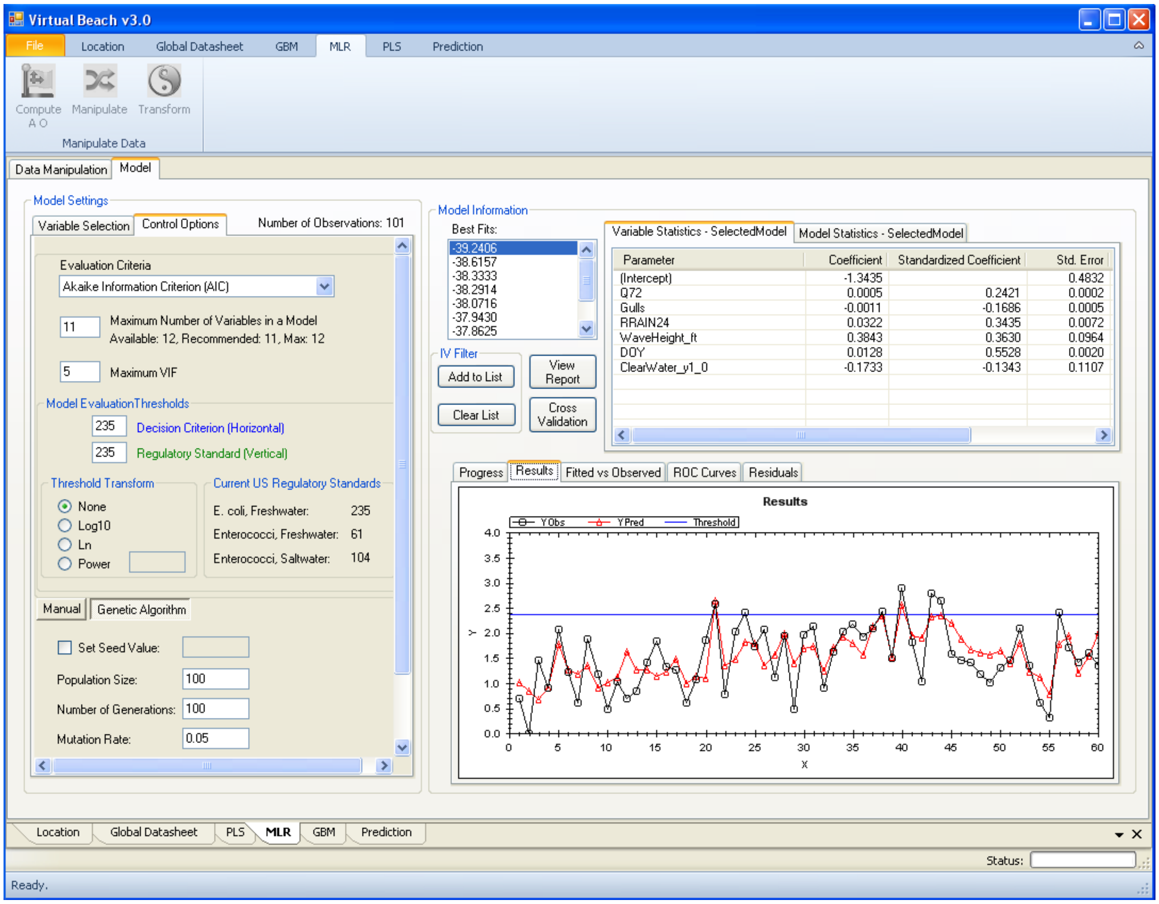
Figure 28. Genetic algorithm options within the modeling interface.

7.5 Evaluating Model Output

After selecting a method to build models (GA or Exhaustive) and an evaluation criterion, click the "Run" button at the bottom of the "Control Options" sub-tab (Figure 25). Progress is displayed on the "Progress" sub-tab at the lower left of the MLR screen. Note that the "Run" button changes to "Cancel" if the user desires to terminate the process. Once model-building is completed, the ten best models are displayed in the "Best Fits" window (Figure 29). Selecting a model from the list results in:

- A list of selected IVs for the model, with associated regression coefficients and statistics displayed on the "Variable Statistics" sub-tab (Figure 30).
- A list of evaluation metrics for the selected model shown on the "Model Statistics" sub-tab (Figure 31).
- The "Results" sub-tab shows two data series - model fits and observations versus observations (Figure 32). Observations that are chronologically ordered are similar to a time series plot of the two data series, but ignore the possibility that time steps between data points are not equally spaced.
- The "Fitted vs Observed" sub-tab shows plots and tables based on fitted model values versus the observations (Figure 33).
- The "ROC Curves" sub-tab shows a plot of the Receiver Operating Characteristic curve of each "Best Fits" model (Figure 34), as well as a table showing the computed AUC (area-under-the-curve) for each ROC curve (see Section 7.7).
- The "View Report" generates a text report of model and variable statistics for the selected model.
- The "Residuals" sub-tab allows access to residual analysis functions in VB3 (see Section 7.8).
- The "Prediction" tab appears at the top and bottom of the VB3 screen, allowing users to proceed to the prediction component (Figure 29).

Note that selecting a different model from the "Best Fits" list will update the Variable and Model Statistics tables, as well as the information displayed on the "Results," "Fitted vs Observed," "ROC Curves," and "Residuals" sub-tabs.



Number of Observations: 101

Evaluation Criteria

Akaike Information Criterion (AIC)

11 Maximum Number of Variables in a Model
Available: 12, Recommended: 11, Max: 12

5 Maximum VIF

235 Decision Criterion (Horizontal)

235 Regulatory Standard (Vertical)

- ● None
- ○ Log10
- ○ Ln
- ○ Power

E. coli, Freshwater:	235
Enterococci, Freshwater:	61
Enterococci, Saltwater:	104

□ Set Seed Value:

Population Size: 100

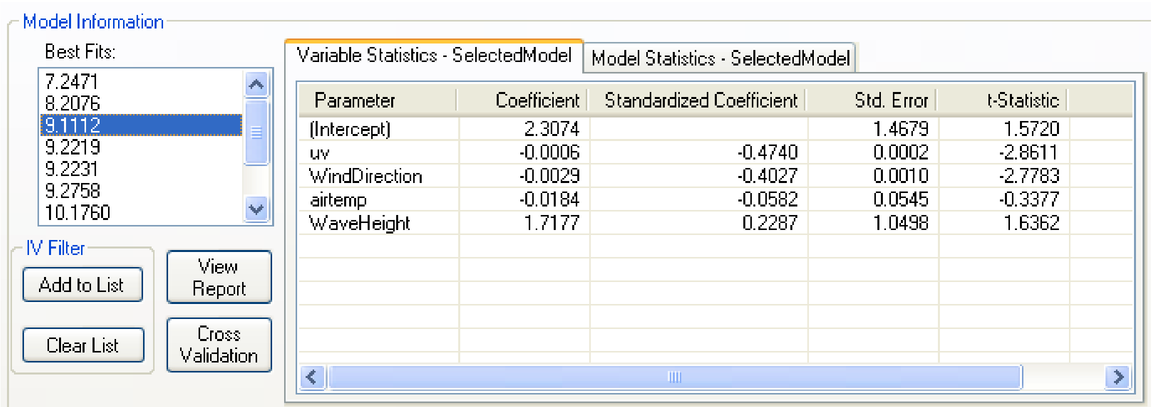
Number of Generations: 100

Mutation Rate: 0.05

Best Fits:
-39.2406
-38.6157
-38.3333
-38.2914
-38.0716
-37.9430
-37.8625

Parameter	Coefficient	Standardized Coefficient	Std. Error
(Intercept)	-1.3435		0.4832
Q72	0.0005	0.2421	0.0002
Gulls	-0.0011	-0.1686	0.0005
RRAIN24	0.0322	0.3435	0.0072
WaveHeight_ft	0.3843	0.3630	0.0964
DOY	0.0128	0.5528	0.0020
ClearWater_y1_0	-0.1733	-0.1343	0.1107

Figure 29. Modeling results after completion of a run using the genetic algorithm.

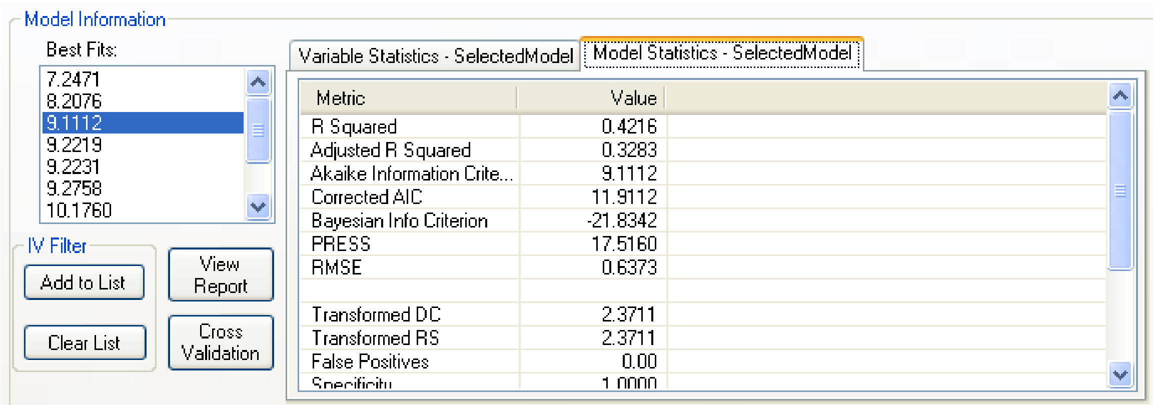


Best Fits:

7.2471
8.2076
9.1112
9.2219
9.2231
9.2758
10.1760

Parameter	Coefficient	Standardized Coefficient	Std. Error	t-Statistic
(Intercept)	2.3074		1.4679	1.5720
uv	-0.0006	-0.4740	0.0002	-2.8611
WindDirection	-0.0029	-0.4027	0.0010	-2.7783
airtemp	-0.0184	-0.0582	0.0545	-0.3377
WaveHeight	1.7177	0.2287	1.0498	1.6362

Figure 30. Modeling Interface showing variable statistics for the selected model.



Best Fits:

7.2471
8.2076
9.1112
9.2219
9.2231
9.2758
10.1760

Metric	Value
R Squared	0.4216
Adjusted R Squared	0.3283
Akaike Information Crite...	9.1112
Corrected AIC	11.9112
Bayesian Info Criterion	-21.8342
PRESS	17.5160
RMSE	0.6373
Transformed DC	2.3711
Transformed RS	2.3711
False Positives	0.00
Specificity	1.0000

Figure 31. Modeling interface showing model evaluation metrics for the selected model.

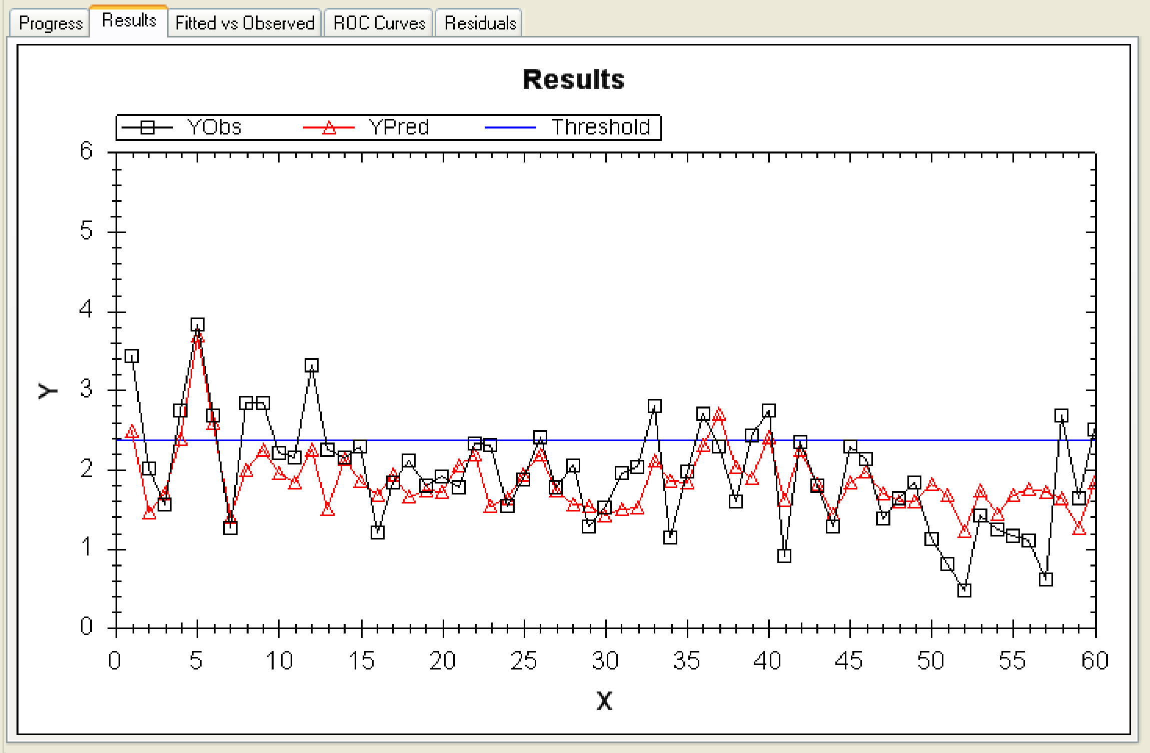
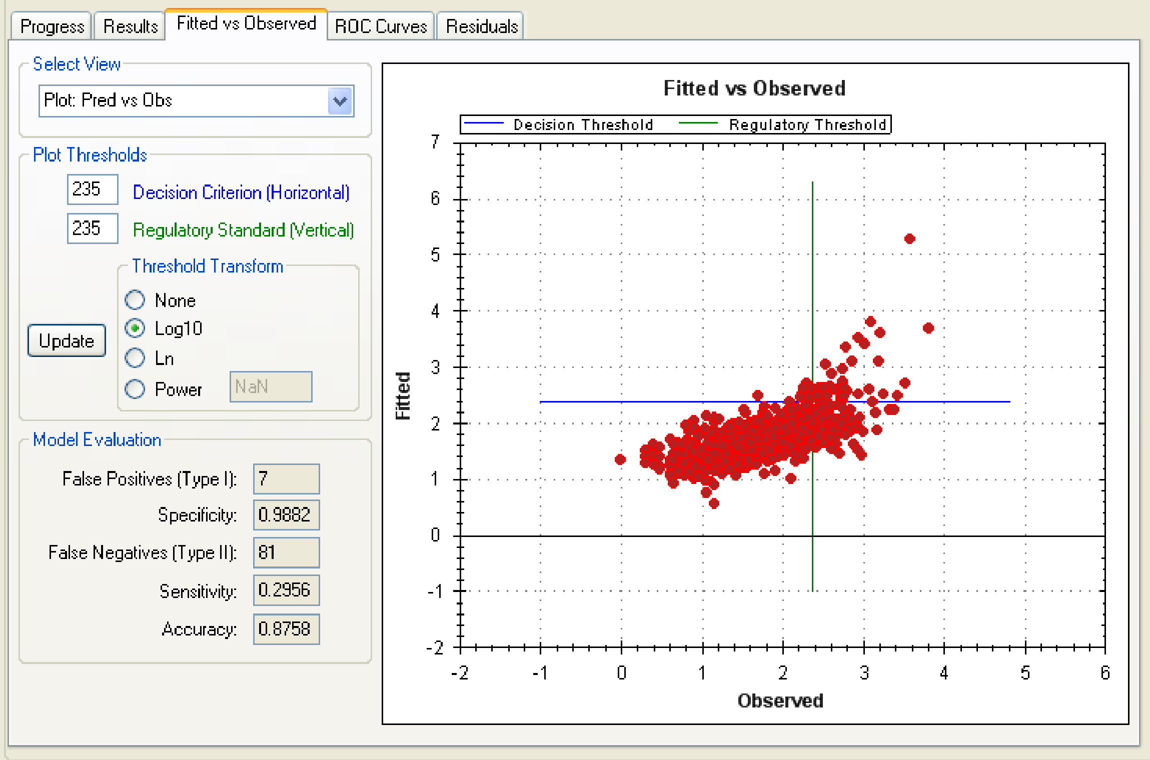


Figure 32. Modeling interface showing a time series plot for the selected model.



Select View

Plot: Pred vs Obs

Plot Thresholds

235 Decision Criterion (Horizontal)

235 Regulatory Standard (Vertical)

Threshold Transform

○ None

● Log10

○ Ln

○ Power NaN

Model Evaluation

False Positives (Type I): 7

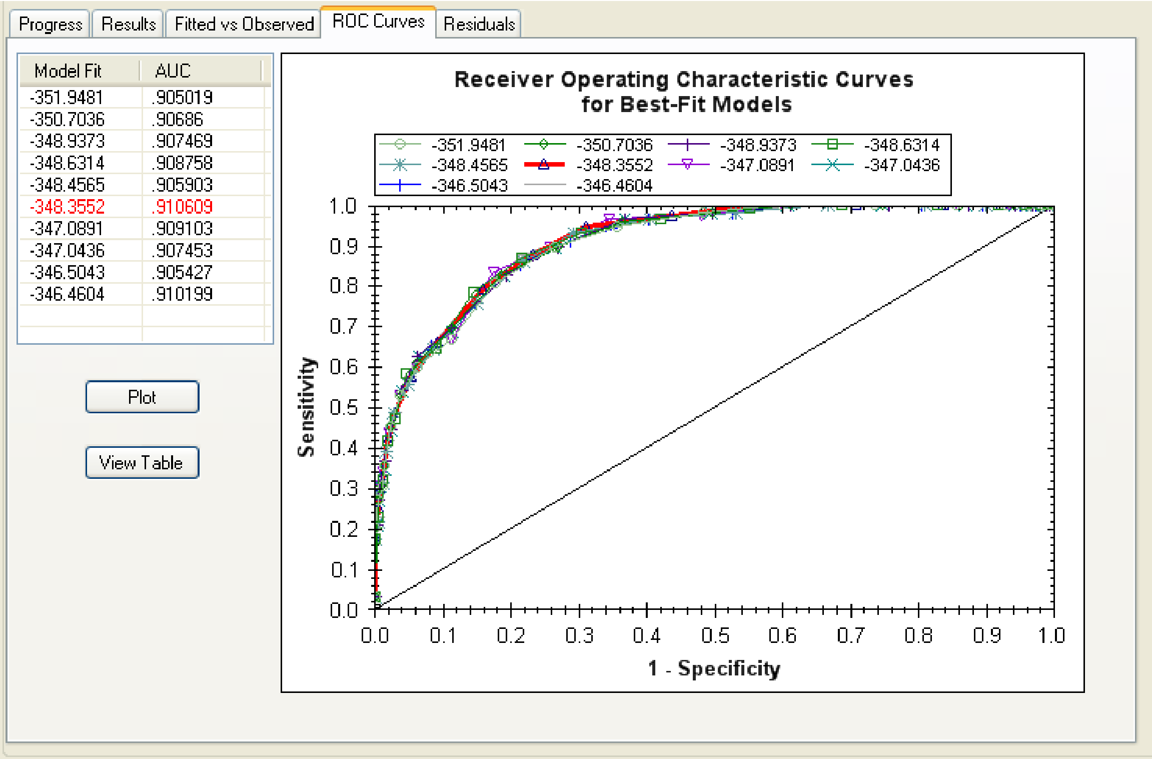
Specificity: 0.9882

False Negatives (Type II): 81

Sensitivity: 0.2956

Accuracy: 0.8758

Figure 33. A scatter plot of fitted values versus observations of the selected model.



Model Fit	AUC
-351.9481	.905019
-350.7036	.90686
-348.9373	.907469
-348.6314	.908758
-348.4565	.905903
-348.3552	.910609
-347.0891	.909103
-347.0436	.907453
-346.5043	.905427
-346.4604	.910199

Figure 34. The ROC curves and AUC table for the model chosen from the “Best Fits” window.

7.6 Viewing X-Y Scatter plots

On the MLR “Fitted vs Observed” and the MLR “Residuals” sub-tabs in the Model Information box, users are shown a graph to compare observations to fitted values from the model (Figure 33). Users can view different results from the pull-down tab from the “Select View” box:

- A plot of fitted values versus observations: “Pred vs. Obs”
- A table summarizing model errors (false negatives/false positives) as the decision criterion (DC) varies across the range of the response variable: “Error Table: DC as CFU”
- A plot of the percent of probability of exceedance (based on the current DC) versus observations: “% Exc vs. Obs”
- A table summarizing model errors as the percent of probability of exceedance is varied: “Error Table: DC as % Exc”

On the two plots, a right-click in the plot area shows a menu of functions for saving, copying, printing or manipulating the plot view. The plot area can be zoomed and un-zoomed: the left-click on the mouse drags an area for zooming in; the right-click selects “Un-Zoom” or “Set Scale to Default” to see the entire data set. To pan to a plot area not in view, hold the Shift key down and use the left mouse button to drag the view. Hovering the cursor over a data point shows the ID of the selected data point; if the information does not appear, right-click on the graph and select “Show Point Values.”

Regarding interpretation of these plots, the green (Regulatory Standard or RS) and blue (Decision Criterion or DC) lines allow model evaluation and provide information for choosing a DC for later predictive purposes. On the plots, false positives represent data points in the upper left quadrant of the graph, where the model fits/predictions exceed the DC, but observations are below the RS. In such cases, a beach advisory would be incorrectly issued based on the model's prediction, potentially leading to, for example, economic losses. False negatives (points in the lower right quadrant) represent a more serious scenario: model fits/predictions below the DC and observations that exceed the RS. In other words, swimming at the beach may have been allowed when it should have been prohibited due to elevated FIB concentrations.

A model that produces no false positives or false negatives would be an ideal decision tool, but this is often unattainable with real data. Examining the two tables from the "Fitted vs Observed" select view tab should allow users to set a robust DC, by using units of the actual response variable or a percentage probability of exceedance that minimizes both errors. In most cases, the RS is set by federal or state law and should not be adjusted by the user; however, users are free to adjust the DC to minimize false negatives and false positives.

7.7 ROC Curves

In addition to time series and scatter plots which show results for an individual model, users may also compare all the "Best Fits" models using the ROC Curves tab (Figure 34). A Receiver Operating Characteristic curve shows the true positive rate (sensitivity) plotted against its false positive rate (1 - specificity) for a model, as the Decision Criterion (DC) varies between its minimum and maximum predicted values. Models can then be compared using the area under their ROC curves (AUC). Models having the largest AUC values perform best over the entire decision space.

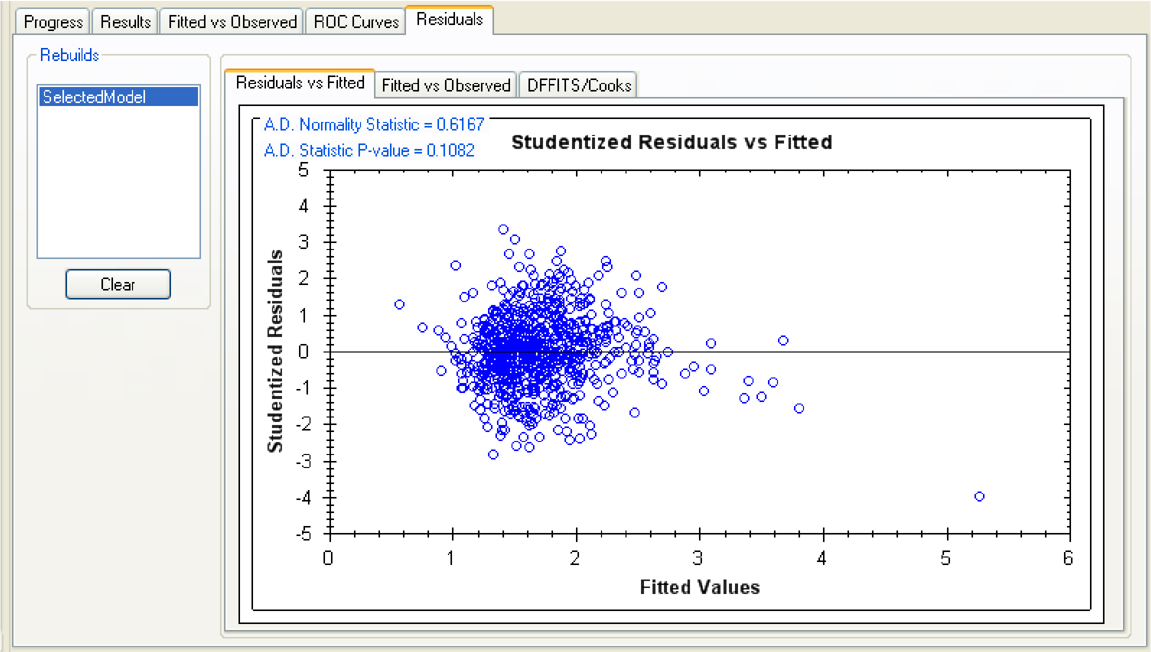
The model with the largest AUC appears in red text in the ROC tab's model list. A single ROC may be plotted by selecting a model in the list and clicking the "Plot" button. Multiple models can be selected in the usual Windows fashion with Shift-Click (select all items between the first and second selection) or Control-Click (select only the clicked items). The background cell color of models *not* selected for plot display will be gray after "Plot" button is clicked.

Clicking the "View Table" button will replace the ROC plot with a table showing false positives, false negatives, sensitivity, and specificity at every evaluated value of the Decision Criterion for a single model. Users need only click on a model in the list at the left of this table to see its results. The ROC plot returns to view after clicking the "View Plot" button.

AUC calculations are performed and curves are plotted when the "ROC Curve" sub-tab is selected. If this tab is active and new models are subsequently built, leaving this tab and returning will generate the new plots and AUC values.

7.8 Residual Analysis

Users may click the "Residuals" sub-tab to view information about the residuals of the selected model (Figure 35). There are three additional tabs on Residuals: "Residuals vs Fitted," "Fitted vs Observed," and "DFFITS/Cooks" (DF/C).

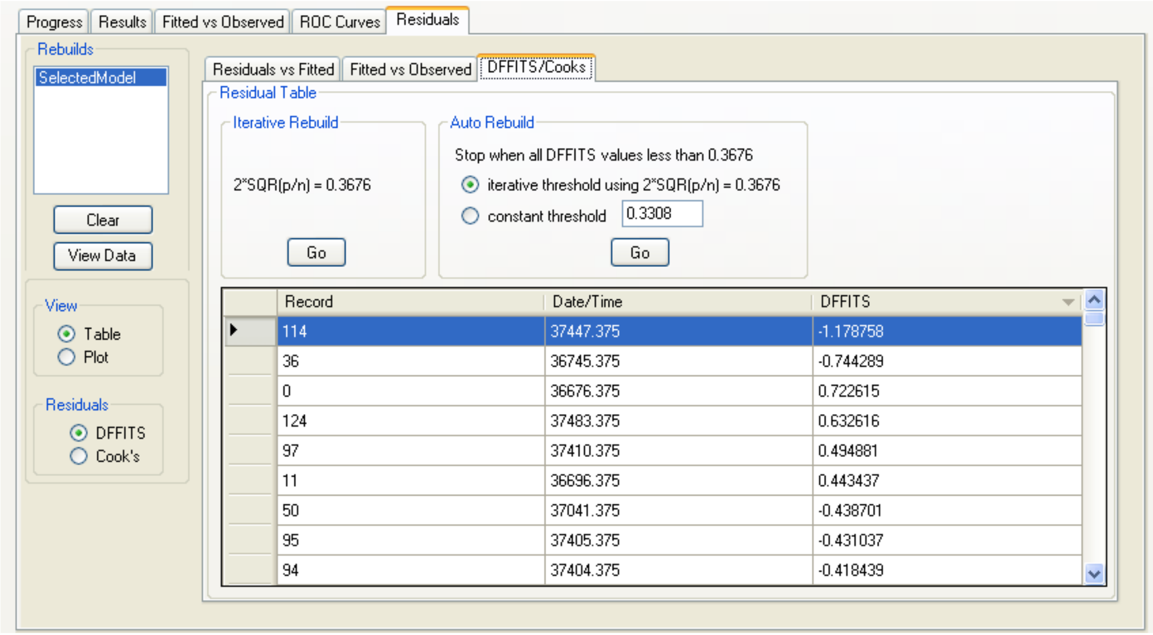


A.D. Normality Statistic = 0.6167
A.D. Statistic P-value = 0.1082

Figure 35. Information available on the Residuals sub-tab, including a plot of externally-studentized residuals versus model fits that shows results of the Anderson-Darling normality test.

The Residuals vs Fitted tab shows a plot of externally-studentized residuals (Cook and Weisberg 1982) versus their fitted model values (Figure 35). In the upper-left corner of the plot, the Anderson-Darling normality statistic (Anderson and Darling 1952) is shown with its statistical significance (p-value). Linear regression assumes normally-distributed residuals, so that if this A-D normality test fails (i.e., the p-value is less than 0.05), the user can transform the response variable, transform some of the IVs, or delete high leverage observations, using the DF/C tab.

On the DF/C tab, observations are sorted by the largest (absolute value) measure in a table (Figure 36). At the lower left, radio buttons can be used to toggle between DFFITS and Cook's values, as well as change the view from a table of sorted values to a plot of the DF/C values versus the Record ID (Figure 37). Data points with very large DF/C values (i.e., lying outside the horizontal red boundaries on the plot) distort the estimates and standard deviations of the regression coefficients. They are essentially "outliers" and some thought to their removal from the dataset should be given.



2*SQR(p/n) = 0.3676

Stop when all DFFITS values less than 0.3676

● iterative threshold using 2*SQR(p/n) = 0.3676

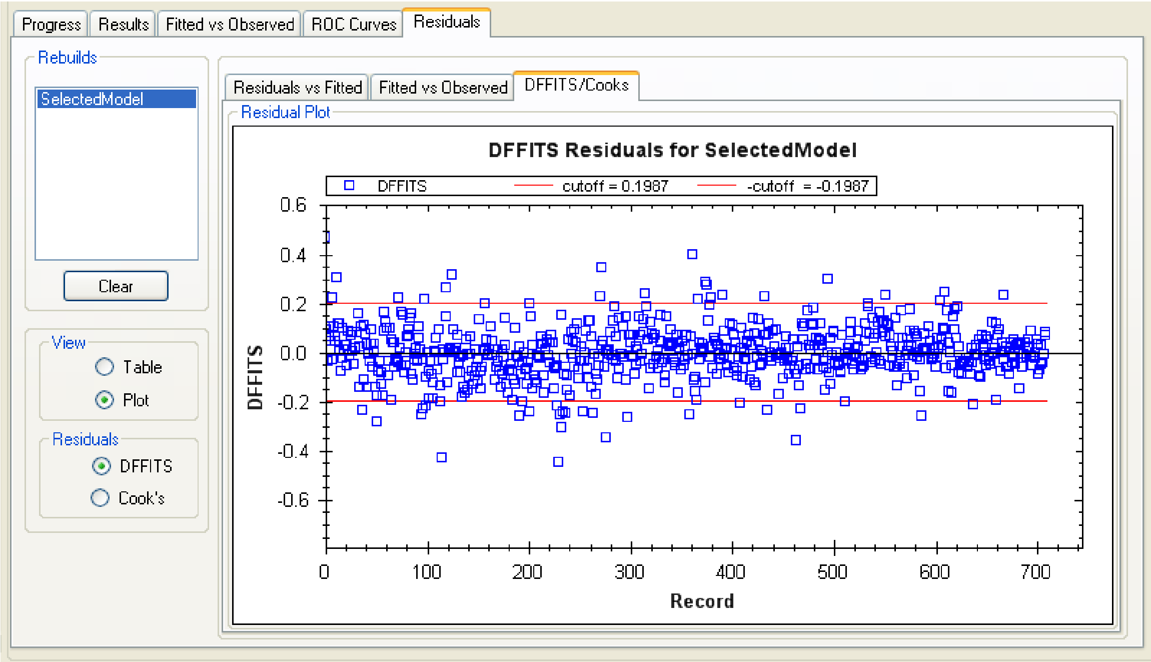
○ constant threshold 0.3308

View: ● Table ○ Plot

Residuals: ● DFFITS ○ Cook's

Record	Date/Time	DFFITS
114	37447.375	-1.178758
36	36745.375	-0.744289
0	36676.375	0.722615
124	37483.375	0.632616
97	37410.375	0.494881
11	36696.375	0.443437
50	37041.375	-0.438701
95	37405.375	-0.431037
94	37404.375	-0.418439

Figure 36. A table of the DFFITS scores of the residuals.



View: ○ Table ● Plot

Residuals: ● DFFITS ○ Cook's

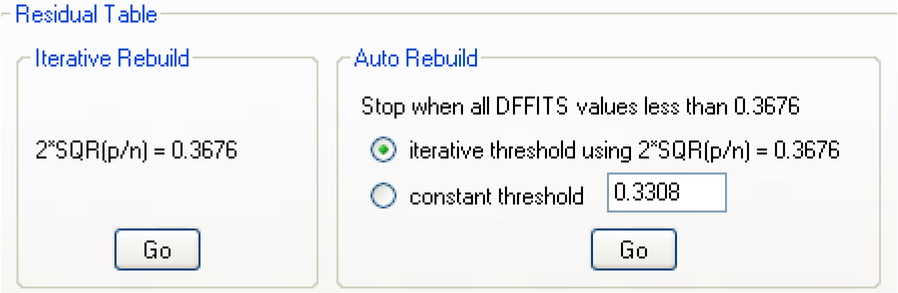
Figure 37. A plot of the DFFITS scores of the residuals.

When the grid of DF/C values is visible, clicking the “Go” button in the Iterative Rebuild section removes the observation with the largest absolute value DF/C, re-fits the regression, and calculates new DF/C values for the remaining observations (Figure 38). This model is named Rebuild1 and added to the “Rebuilds” window at the top left of the sub-screen. Clicking the Iterative Rebuild “Go” button again produces a model called Rebuild2 which is calculated after removing the observation with the largest absolute value DF/C remaining in the dataset. The user can continue to click “Go” and remove observations with the largest remaining DF/C, creating Rebuild3, Rebuild4, Rebuild5, etc. VB3 will not allow users to delete any observations if 10 or fewer remain in the dataset.

Whenever a rebuild model is created by pressing the “Go” button, the information displayed in the Variable and Model Statistics tables, as well as the plots and information on the “Residuals” sub-tab, is automatically updated to reflect it, even if another model is highlighted in the “Best Fits” window. The user can select any model in the “Best Fits” window list, however, to view its associated data and plots.

The user has freedom to remove outliers while toggling between DF/C measures. For example, the first removal can be based on a DFFITS value, the next removal on a Cook’s Distance, the next two removals on DFFITS, etc. Users may clear models from the “Rebuilds” window by clicking the “Clear” button.

Rather than using Iterative Rebuild, there are two other choices under the “Auto Rebuild” box, both of which remove all observations above some threshold. The “iterative threshold” radio button bases removals on a threshold that is updated whenever an observation is deleted. For DFFITS, this threshold is $2*(p/n)^{0.5}$, where p is the number of IVs in the model and n is the current number of observations in the dataset. For Cook’s Distance, the threshold is 4/n.



2*SQR(p/n) = 0.3676

Stop when all DFFITS values less than 0.3676

● iterative threshold using 2*SQR(p/n) = 0.3676

○ constant threshold 0.3308

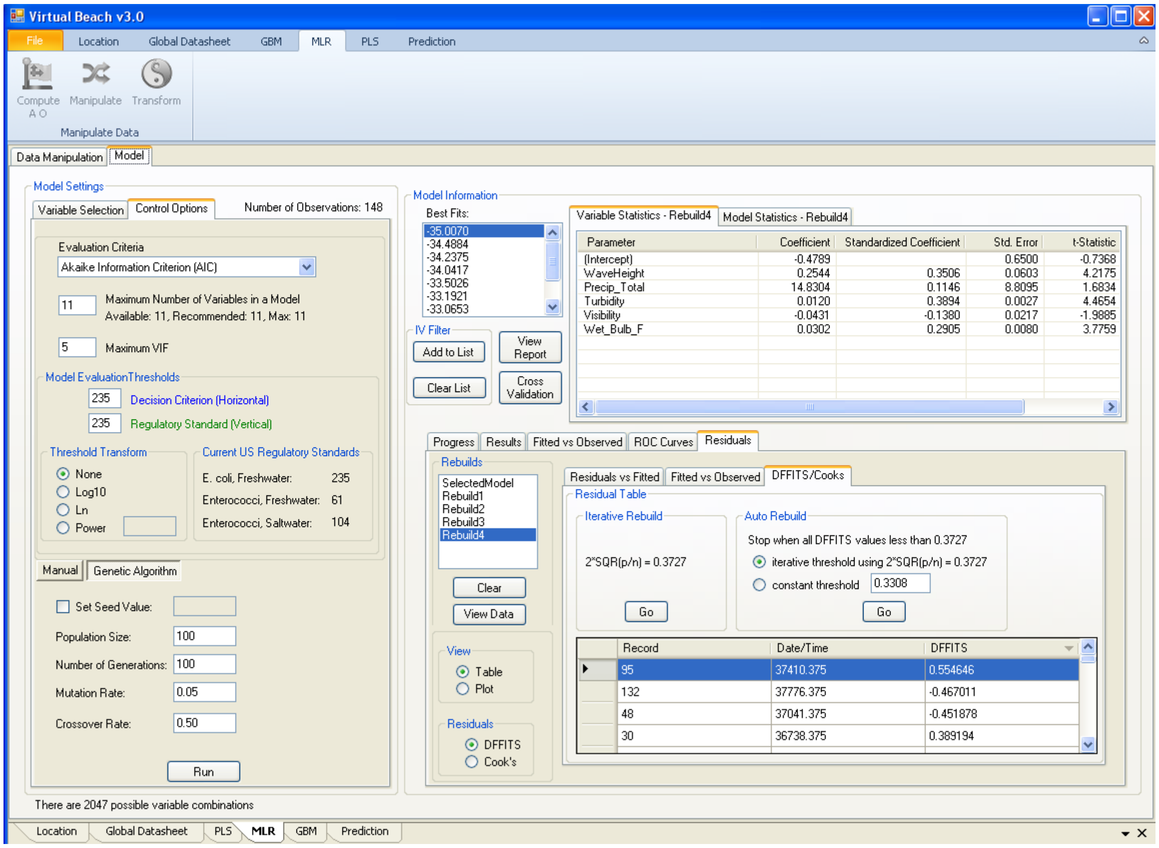
Figure 38. DFFITS/Cook’s Distance controls for removing highly influential data points.

When the “iterative threshold” radio button is invoked inside the “Auto Rebuild” box, VB3 first checks if any DF/C values are above the threshold; if so, VB3 removes the observation with the largest absolute DF/C and recalculates the regression model, the DF/C values, and the threshold because n has been reduced by 1. VB3 then checks if any of these new DF/C values are above the recalculated threshold. If so, the process repeats. VB3 continues until no remaining DF/C values exceed the current threshold or until half of the dataset has been removed, whichever comes first. For example, if a dataset has 100 observations, VB3 will allow 50 to be removed before it breaks the Auto Rebuild removal loop. The user can then click the Auto Rebuild “Go” button again to remove another 25 observations of the remaining 50. In practice, one should not remove more than about 5% of the original dataset as outliers; removing more observations than this indicates a poor regression fit and warrants a different analytical technique. Indeed, under the assumption of normally distributed data, we expect 5% of the observations to fit relatively poorly.

The “constant threshold” radio button option differs from the “iterative threshold” only in that the threshold entered by the user to the input box remains the same regardless of how many observations are deleted. Updated DF/C values are still calculated after every removal. VB3 will also stop this process if half the number of starting observations has been deleted. There is an upper limit to the number that can be entered into the "constant threshold" input box (DFFITS = 3; Cook's Distance = 16/n).

Upon completion of the Auto Rebuild process, multiple models may have been added to the "Rebuilds" window (Figure 39). For example, if 10 observations were removed, Rebuild1 through Rebuild10 will appear in that window.

When the user wants to move from the MLR tab to the Prediction tab, the model carried forward is the one highlighted blue in the "Best Fits" window or "Rebuilds" window. It is easy to confirm that the model selected will be carried forward by checking the numbers shown within the "Variable Statistics" and "Model Statistics" sub-tabs (Figures 30 and 31). Note that observations removed from the dataset using the "Residuals" sub-tab are not removed from the local dataset shown on the MLR "Data Manipulation" tab.



Number of Observations: 148

Evaluation Criteria: Akaike Information Criterion (AIC)

11 Maximum Number of Variables in a Model
Available: 11, Recommended: 11, Max: 11

5 Maximum VIF

235 Decision Criterion (Horizontal)
235 Regulatory Standard (Vertical)

Threshold Transform: ● None ○ Log10 ○ Ln ○ Power

Current US Regulatory Standards	
E. coli, Freshwater:	235
Enterococci, Freshwater:	61
Enterococci, Saltwater:	104

□ Set Seed Value:
Population Size: 100
Number of Generations: 100
Mutation Rate: 0.05
Crossover Rate: 0.50

There are 2047 possible variable combinations

Best Fits:
-35.0070
-34.4884
-34.2375
-34.0417
-33.5026
-33.1921
-33.0653

Parameter	Coefficient	Standardized Coefficient	Std. Error	t-Statistic
(Intercept)	-0.4789		0.6500	-0.7368
WaveHeight	0.2544	0.3506	0.0603	4.2175
Precip_Total	14.8304	0.1146	8.8095	1.6834
Turbidity	0.0120	0.3894	0.0027	4.4654
Visibility	-0.0431	-0.1380	0.0217	-1.9885
Wet_Bulb_F	0.0302	0.2905	0.0080	3.7759

Rebuilds:
SelectedModel
Rebuild1
Rebuild2
Rebuild3
Rebuild4

View: ● Table ○ Plot

Residuals: ● DFFITS ○ Cook's

Iterative Rebuild: 2*SQR(p/n) = 0.3727

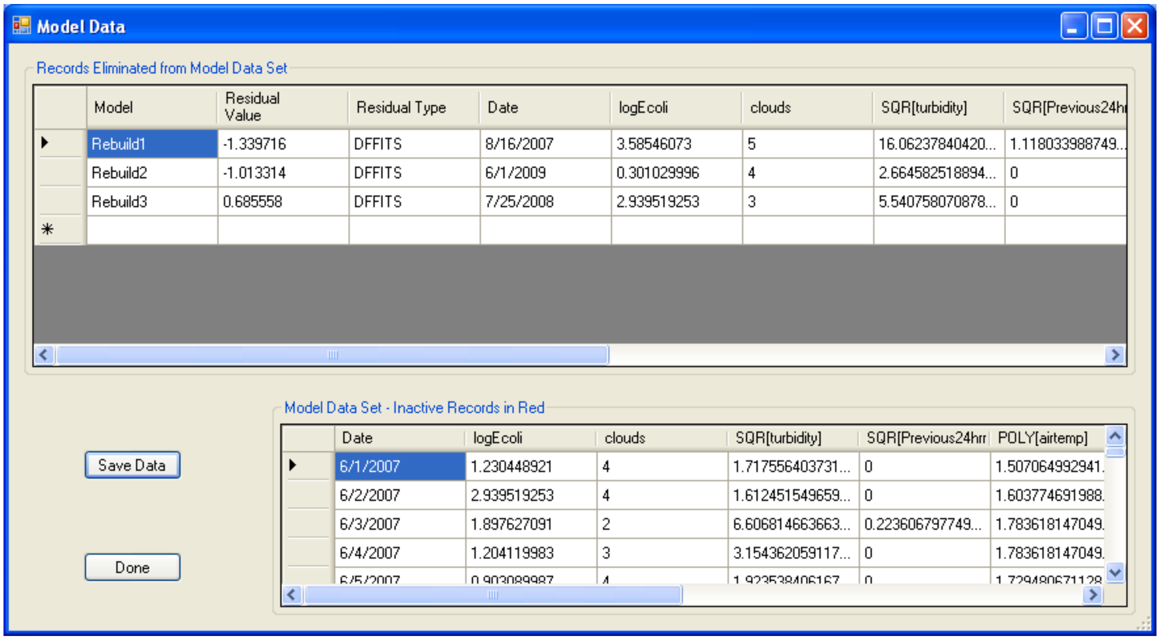
Auto Rebuild: Stop when all DFFITS values less than 0.3727
● iterative threshold using 2*SQR(p/n) = 0.3727
○ constant threshold 0.3308

Record	Date/Time	DFFITS
95	37410.375	0.554646
132	37776.375	-0.467011
48	37041.375	-0.451878
30	36738.375	0.389194

Figure 39. Residuals interface showing a list of rebuilt models resulting from observation deletions, and their associated statistics and residual plots.

Viewing the Data Table

From the DFFITS/Cooks sub-tab, users can click the "View Data" button to display a history of observation removal for the selected model. From this window, users may export the dataset for external use or re-importation into VB3 (Figure 40).



Records Eliminated from Model Data Set

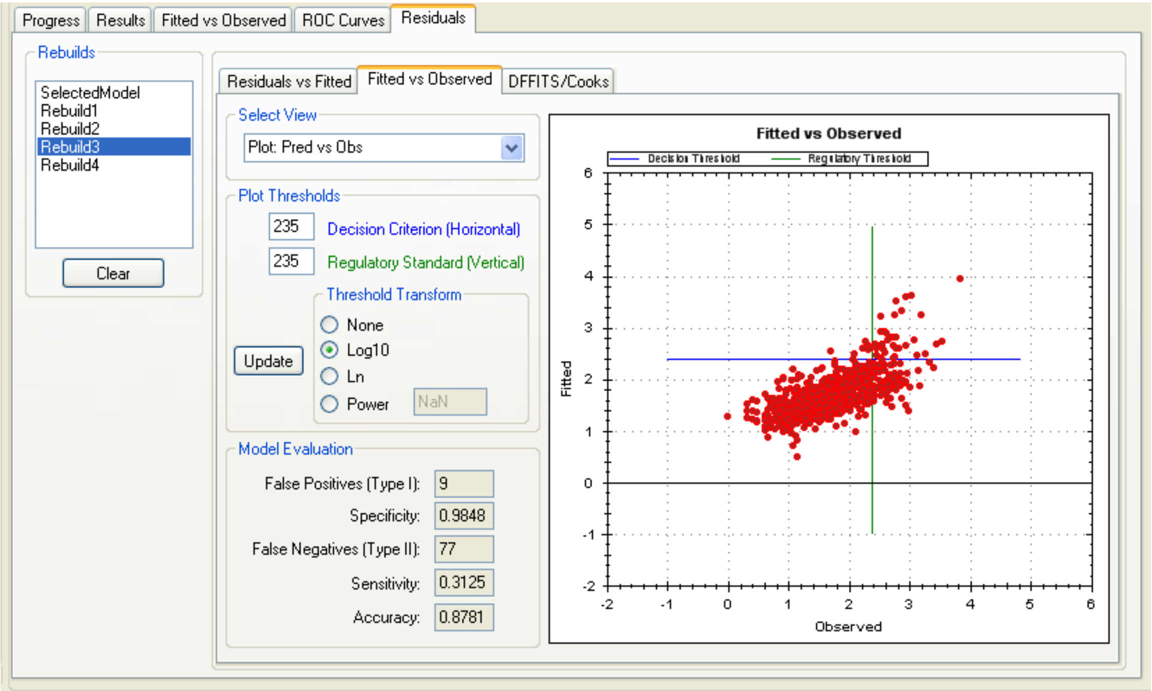
	Model	Residual Value	Residual Type	Date	logEcoli	clouds	SQR[turbidity]	SQR[Previous24h
▶	Rebuild1	-1.339716	DFFITS	8/16/2007	3.58546073	5	16.06237840420...	1.118033988749...
	Rebuild2	-1.013314	DFFITS	6/1/2009	0.301029996	4	2.664582518894...	0
	Rebuild3	0.685558	DFFITS	7/25/2008	2.939519253	3	5.540758070878...	0
*								

Model Data Set - Inactive Records in Red

	Date	logEcoli	clouds	SQR[turbidity]	SQR[Previous24hr	POLY[airtemp]
▶	6/1/2007	1.230448921	4	1.717556403731...	0	1.507064992941.
	6/2/2007	2.939519253	4	1.612451549659...	0	1.603774691988.
	6/3/2007	1.897627091	2	6.606814663663...	0.223606797749...	1.783618147049.
	6/4/2007	1.204119983	3	3.154362059117...	0	1.783618147049.
	6/5/2007	0.903089987	4	1.923538406167	0	1.729480671128

Figure 40. "View Data Table" window for examining the dataset after removal of influential data points.

The "Fitted vs Observed" plot on the "Residuals" sub-tab is the same as that introduced in Section 7.6 (Figure 41). There are two plots and two tables to examine, along with controls to modify the Decision Criterion (blue horizontal line) and Regulatory Standard (green vertical line).



Select View

Plot: Pred vs Obs

Plot Thresholds

235 Decision Criterion (Horizontal)

235 Regulatory Standard (Vertical)

Threshold Transform

○ None
● Log10
○ Ln
○ Power NaN

Model Evaluation

False Positives (Type I): 9

Specificity: 0.9848

False Negatives (Type II): 77

Sensitivity: 0.3125

Accuracy: 0.8781

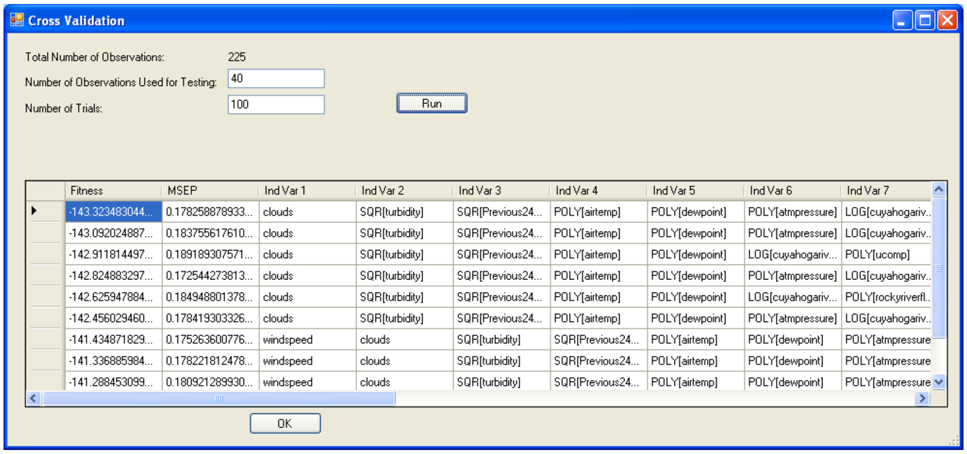
Figure 41. Fitted vs Observed plot on the Residual sub-tab with model evaluation threshold control and model evaluation statistics.

7.9 Cross-Validation

Clicking the "Cross-Validation" button in the "Model Information" box brings up another window where the user can set two parameters: sample size for the *testing* data (N_E) and number of random samples (N_R) taken (Figure 42). When the "Run" button is clicked, a random sample of size N_E is taken from the modeling dataset and set aside. Each "Best Fits" model is then re-fit to the remaining *training* data. The IVs in each model stay the same, but the regression coefficients are adjusted to reflect the least-squares fit to the *training* data. The Mean Squared Error of Prediction (MSEP) is then calculated based on the N_E *testing* data points for each candidate model. This process is done N_R times. A table then appears to show the average MSEP values for each of the 10 "Best-Fit" models.

Cross-validation is useful for examining the predictive power of models, i.e., ability to make predictions for data they have not seen before. For users wishing to emphasize predictive ability of a potential model, cross-validation allows evaluation of which candidate model consistently makes the best predictions, i.e., has the lowest MSEP. Note that the PRESS statistic VB3 provides as a model evaluation criterion is a cross-validation statistic with N_E, set to 1. The PRESS algorithm removes one observation at a time from the dataset, re-fits the model regression coefficients, and calculates the squared residual for the removed observation. It does this once for every observation in the dataset to compute the model's PRESS value -- a somewhat cursory look at a model's predictive potential.

We recommend that approximately 25% of the total number of observations be used for testing, and that at least 1000 trials be performed.



Total Number of Observations: 225

Number of Observations Used for Testing: 40

Number of Trials: 100

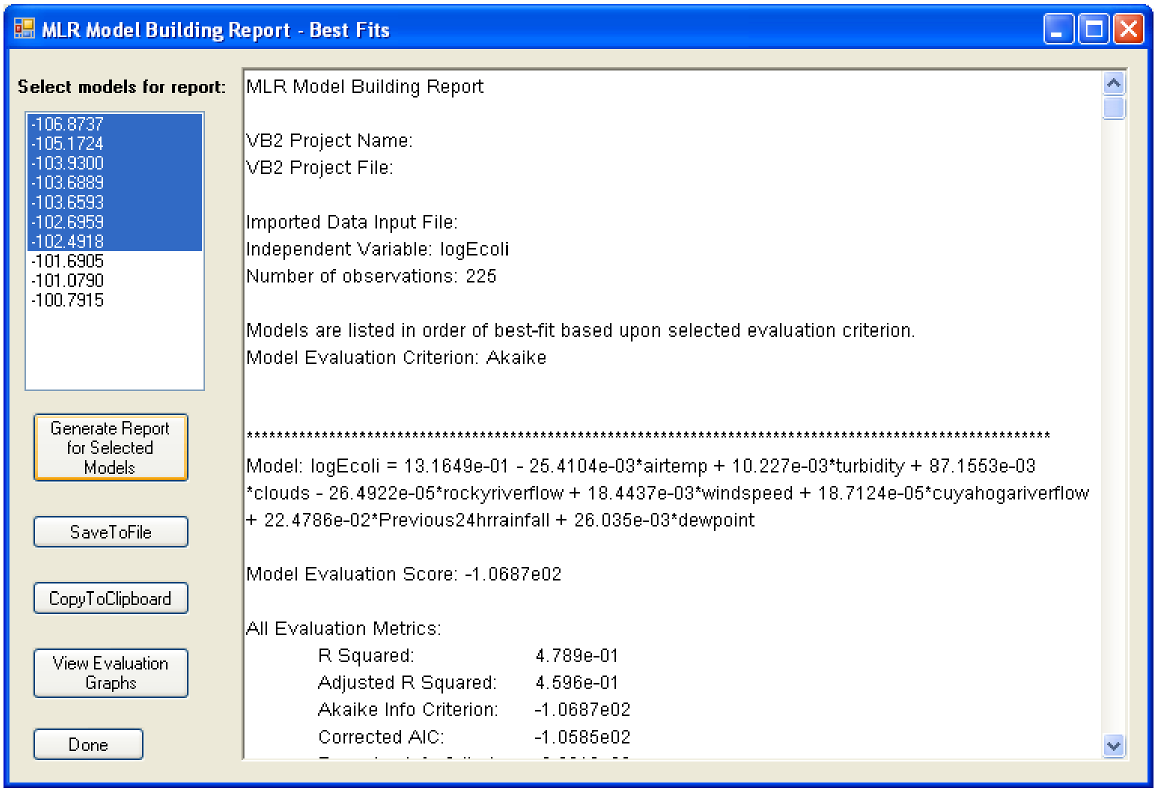
Fitness	MSEP	Ind Var 1	Ind Var 2	Ind Var 3	Ind Var 4	Ind Var 5	Ind Var 6	Ind Var 7
-143.323483044...	0.178258878933...	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	POLY[atmpressure]	LOG[cuyahogariv...
-143.092024887...	0.183755617610...	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	POLY[atmpressure]	LOG[cuyahogariv...
-142.911814497...	0.189189307571...	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	LOG[cuyahogariv...	POLY[ucomp]
-142.824883297...	0.172544273813...	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	POLY[atmpressure]	LOG[cuyahogariv...
-142.625947884...	0.184948801378...	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	LOG[cuyahogariv...	POLY[rockyriverfl...
-142.456029460...	0.178419303326...	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	POLY[atmpressure]	LOG[cuyahogariv...
-141.434871829...	0.175263600776...	windspeed	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	POLY[atmpressure
-141.336885984...	0.178221812478...	windspeed	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	POLY[atmpressure
-141.288453099...	0.180921289930...	windspeed	clouds	SQR[turbidity]	SQR[Previous24...	POLY[airtemp]	POLY[dewpoint]	POLY[atmpressure

Figure 42. Cross-validation results for each of the 10 best-fit models.

7.10 Report Generation

A text report of modeling results can be generated, copied to the system clipboard, or saved to a text file using the "View Report" button in the middle of the MLR-Model screen. From here (Figure 43), users can view the report by selecting the desired models and clicking the "Generate Report for Selected Models" button. The report contains descriptive statistics for each model variable and model evaluation statistics. Any number of best-fit models can be selected for reporting.

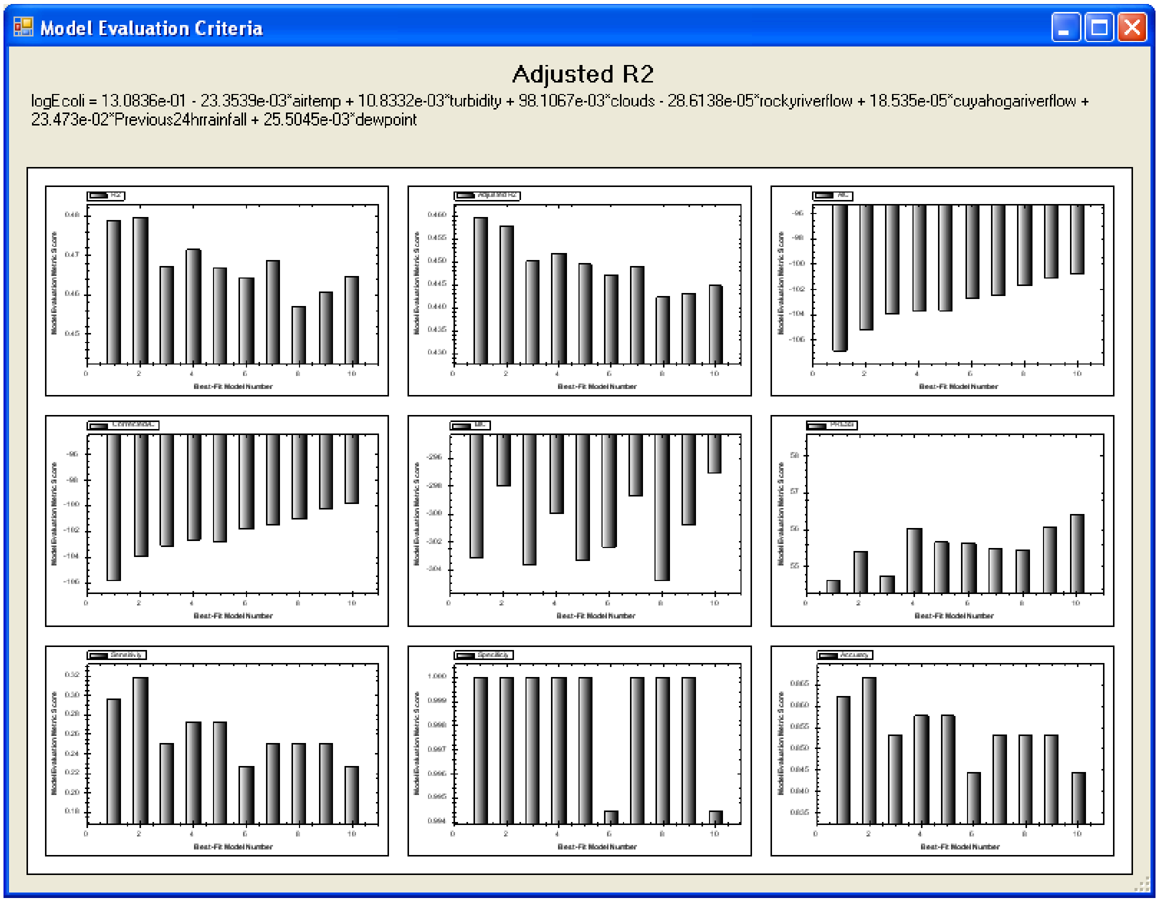
A recommended approach to saving the information in an external application is to copy the report to the clipboard with the “CopytoClipboard” button and paste it into an application such as Microsoft Word or WordPad. NotePad or other simple text editors will also work, but column formats will likely be lost, making the report difficult to interpret.



```
MLR Model Building Report

VB2 Project Name:
VB2 Project File:

Imported Data Input File:
Independent Variable: logEcoli
Number of observations: 225

Models are listed in order of best-fit based upon selected evaluation criterion.
Model Evaluation Criterion: Akaike


**************************************************************************************************************
Model: logEcoli = 13.1649e-01 - 25.4104e-03*airtemp + 10.227e-03*turbidity + 87.1553e-03
*clouds - 26.4922e-05*rockyriverflow + 18.4437e-03*windspeed + 18.7124e-05*cuyahogariverflow
+ 22.4786e-02*Previous24hrrainfall + 26.035e-03*dewpoint

Model Evaluation Score: -1.0687e02

All Evaluation Metrics:
          R Squared:             4.789e-01
          Adjusted R Squared:    4.596e-01
          Akaike Info Criterion: -1.0687e02
          Corrected AIC:         -1.0585e02
```

Figure 43. A text report generated on the modeling results.

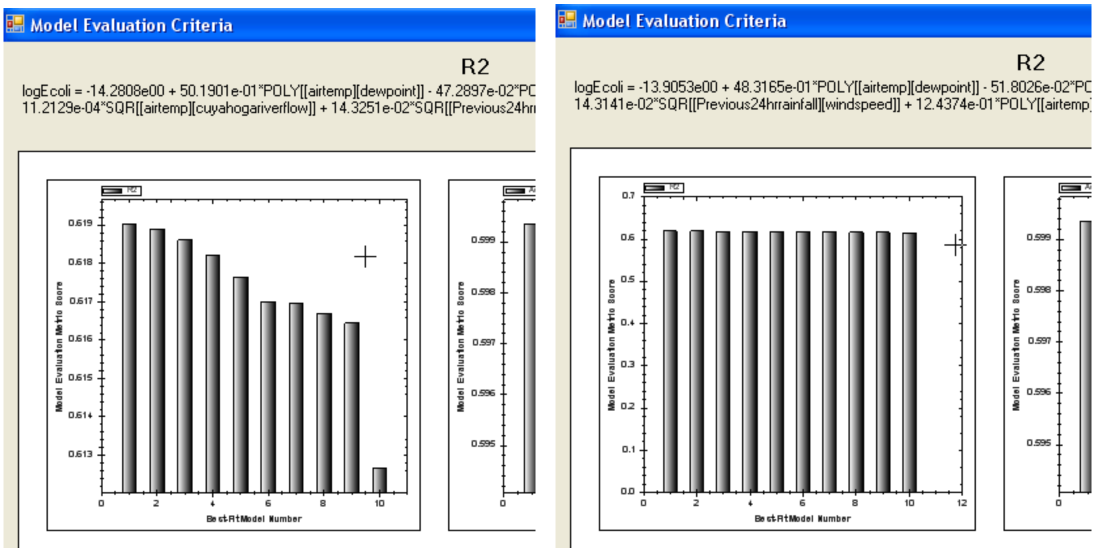
Comparative bar graphs can be displayed (Figure 44) to view evaluation criteria for all top models by left-clicking and dragging the mouse to highlight selection and clicking the “View Evaluation Graphs” button (Figure 43). Hover the mouse over any plot to display the model evaluation criteria at the very top of the screen. Moving the mouse over a bar on a plot will show that model’s coefficients under the title at the top, and a label will appear with that same information. Note that evaluation criteria graphs are initially scaled to emphasize differences between model scores although those differences may, in fact, be quite small on an absolute scale (Figure 45). With the cursor over any graph, right-click the mouse and select “Set Scale to Default” to view the un-scaled graph.



Adjusted R2

logEcoli = 13.0836e-01 - 23.3539e-03*airtemp + 10.8332e-03*turbidity + 98.1067e-03*clouds - 28.6138e-05*rockyriverflow + 18.535e-05*cuyahogariverflow + 23.473e-02*Previous24hrrainfall + 25.5045e-03*dewpoint

Figure 44. Plots of various model evaluation metrics for the 10 best-fit models.



R2

logEcoli = -14.2808e00 + 50.1901e-01*POLY[[airtemp][dewpoint]] - 47.2897e-02*PC
11.2129e-04*SQR[[airtemp][cuyahogariverflow]] + 14.3251e-02*SQR[[Previous24hr

R2

logEcoli = -13.9053e00 + 48.3165e-01*POLY[[airtemp][dewpoint]] - 51.8026e-02*PC
14.3141e-02*SQR[[Previous24hrrainfall][windspeed]] + 12.4374e-01*POLY[[airtemp]

Figure 45. Scaled versus un-scaled views of selected model evaluation criteria.

8. PARTIAL LEAST SQUARES

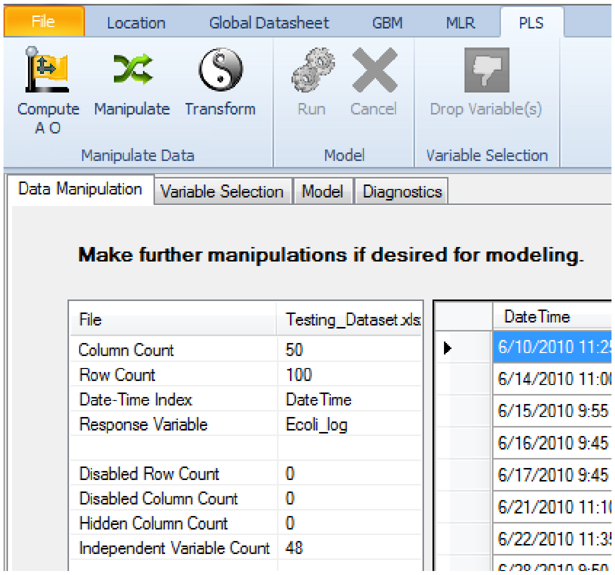
Partial Least Squares (PLS) regression minimizes a problem that can arise in MLR modeling: over-fitting in the presence of correlated predictors. To over-fit is to match past data more closely than the real-world process being modeled. MLR is prone to over-fitting because it makes the closest possible linear match to past data, even at the cost of accuracy in predicting future observations.

As opposed to requiring the MLR user to be vigilant and proactive, PLS regression (Brooks et al. 2013) inherently accounts for collinearity to suppress over-fitting, and ranks the IVs by their influence in variable selection. Using PLS regression, the user can include all available IVs in the model and let the algorithm sort out which IVs are most useful, simplifying the sometimes laborious processes of variable selection and comparing interactions.

A key feature of PLS (and GBM) modeling is the use of cross-validation to assess real-world prediction accuracy. Model selection and threshold setting (section 8.4) are done with reference to the true positive, true negative, false positive and false negative counts, which are calculated by 5-fold cross validation. This means that the data are split randomly and evenly into five subsets and five models are built to predict exceedances on each of the five subsets. For each of these models, the subset predicted is left out of model building, so the counts reflect prediction of novel observations, not accuracy in fitting past observations. Greater detail about the PLS modeling method is available in Brooks et al., 2013 and Hastie et al. 2009.

8.1 Data Manipulation

The MLR, PLS, and GBM modules all have "Data Manipulation" sub-tabs (Figure 46). When the user first clicks on the PLS tab from the Global Datasheet, data in the PLS Data Manipulation sub-tab is identical to data on the Global Datasheet. From the PLS data tab, the user can change the "local" data to suit the PLS analysis. The local datasheet has all of the functionality of the Global Datasheet discussed in Section 6. Changing local data has no effect on the Global Datasheet; however, going back to the Global Datasheet and making changes will overwrite local datasheets on each of the modeling tabs.



Make further manipulations if desired for modeling.

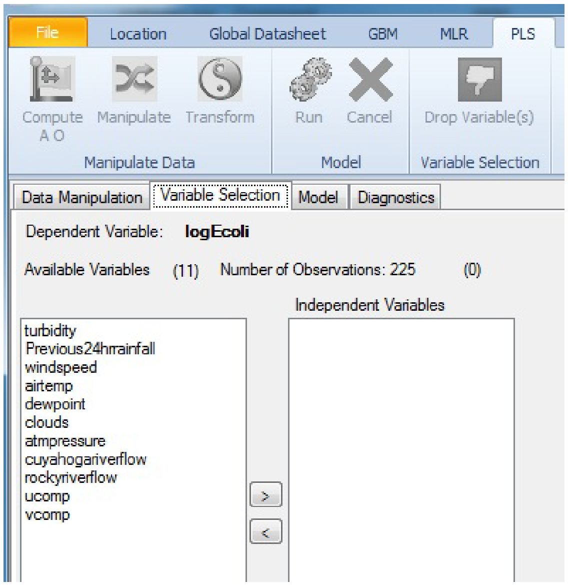
File	Testing_Dataset.xls
Column Count	50
Row Count	100
Date-Time Index	DateTime
Response Variable	Ecoli_log
Disabled Row Count	0
Disabled Column Count	0
Hidden Column Count	0
Independent Variable Count	48

DateTime
6/10/2010 11:2
6/14/2010 11:0
6/15/2010 9:55
6/16/2010 9:45
6/17/2010 9:45
6/21/2010 11:1
6/22/2010 11:3

Figure 46. Data Manipulation: the first sub-tab on each of the method tabs.

8.2 Selecting Variables for Model Building

The “Variable Selection” tab is where IVs for model development are chosen (Figure 47). Users may select all or a subset of the IVs for consideration in the model. All eligible IVs are listed in the “Available Variables” window (left column). Any IVs that users wish to include in the model must then be moved to the “Independent Variables” window by highlighting the IV and clicking the “>” key. Any number of IVs can be added or removed from this list. Once the desired IVs have been selected, click the “Model” sub-tab.



Dependent Variable: logEcoli

Available Variables (11) Number of Observations: 225 (0)

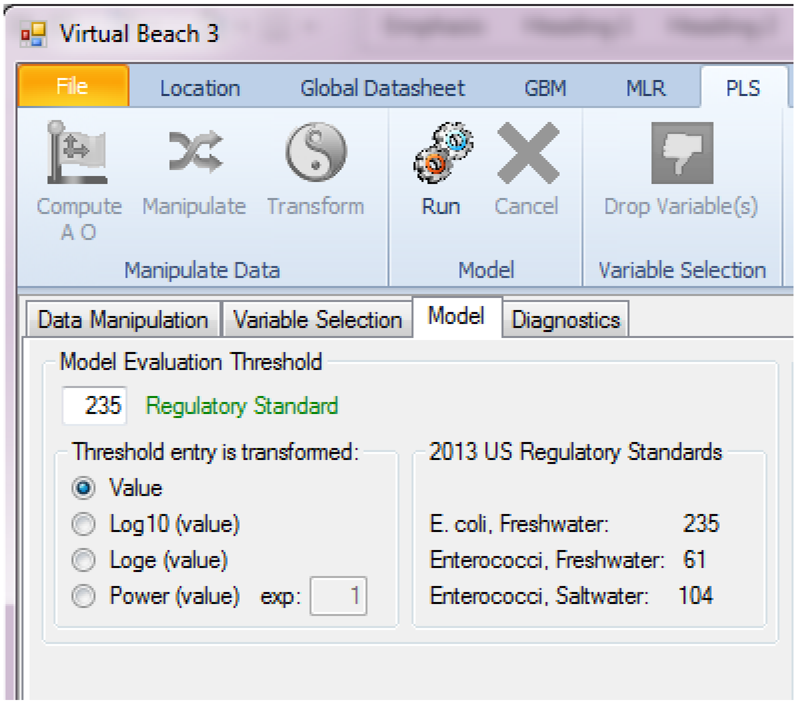
Independent Variables

turbidity
Previous24hrrainfall
windspeed
airtemp
dewpoint
clouds
atmpressure
cuyahogariverflow
rockyriverflow
ucomp
vcomp

Figure 47. Selecting variables for PLS processing within the modeling module.

8.3 The Regulatory Standard

To build a PLS ribbon, observations must be defined as exceedances or non-exceedances; PLS and GBM models will not run if the dataset has no exceedances. This is done by setting the Regulatory Standard (RS) at the top of the "Model" tab and then specifying, using the radio buttons, units to enter into the RS. The default RS is the USEPA's federal standard for *E. coli* in freshwater, 235 CFU per 100 mL. Because these are raw units of measurement, the radio button transformation choice should be set to "Value." However, users may be thinking of bacteria concentrations in logarithmic units; if so, the RS is 2.371 (= $\log_{10}(235)$). To communicate this to VB_3, enter 2.371 in the "Regulatory Standard" box and click the "Log10 (value)" radio button (Figure 48).



Model Evaluation Threshold

235 Regulatory Standard

Threshold entry is transformed:

● Value
○ Log10 (value)
○ Loge (value)
○ Power (value) exp: 1

2013 US Regulatory Standards

E. coli, Freshwater:	235
Enterococci, Freshwater:	61
Enterococci, Saltwater:	104

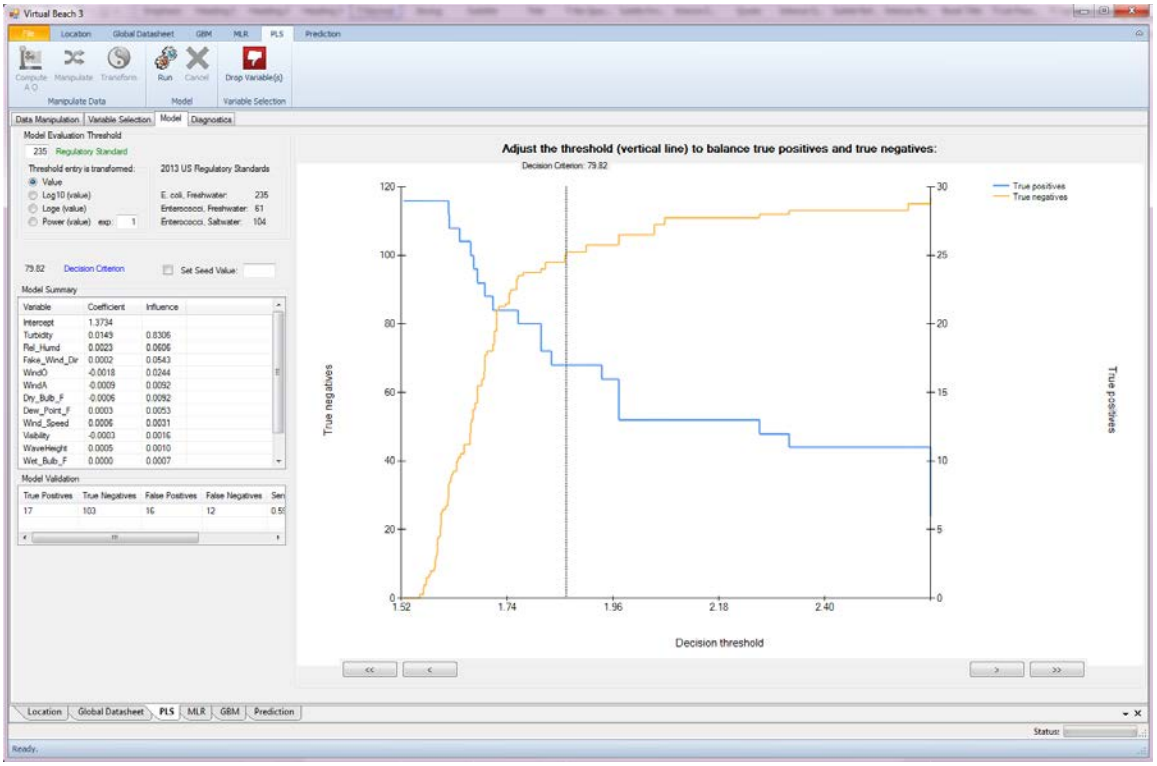
Figure 48. Setting the Regulatory Standard and running models for PLS.

8.4 Modeling Control Options

Clicking "Run" on the PLS Model tab (Figure 48) will start model development. There is some randomness built into the PLS/GBM solver (due to the aforementioned randomly-created data folds), so running the PLS/GBM multiple times on the same dataset will likely produce slightly different solutions. If the user wishes to later replicate a given PLS/GBM modeling result, they should check the "Set Seed Value" box and put some positive integer into the input box (Figure 49). If that seed is input again, the PLS/GBM solver will return a solution identical to the previous solution using that seed value. After a solution is reached, the "Drop Variable(s)" option on the PLS ribbon becomes enabled and a Decision Criterion (DC) for the model can be chosen.

Dropping Unimportant Variables

The “Model Summary” window (left side of Figure 49) lists IVs in descending order of influence. For a PLS model, a variable’s influence is its model coefficient multiplied by its standard deviation. The influence measurements are then adjusted to sum to one. The larger the influence of a variable (global sensitivity), the more its variation drives the response. Low-influence variables can be dropped from the model by clicking on the variable’s name in the list, then clicking the “Drop Variable(s)” button on the ribbon. If any variables are dropped at this stage, the model must be rebuilt by clicking the “Run” button.



Model Evaluation Threshold

235 Regulatory Standard

Threshold entry is transformed:

● Value
○ Log10 (value)
○ Loge (value)
○ Power (value) exp: 1

2013 US Regulatory Standards

E. coli, Freshwater:	235
Enterococci, Freshwater:	61
Enterococci, Saltwater:	104

79.82 Decision Criterion

□ Set Seed Value:

Model Summary

Variable	Coefficient	Influence
Intercept	1.3734	
Turbidity	0.0149	0.8306
Rel_Humd	0.0023	0.0606
Fake_Wind_Dir	0.0002	0.0543
WindO	-0.0018	0.0244
WindA	-0.0009	0.0092
Dry_Bulb_F	-0.0006	0.0092
Dew_Point_F	0.0003	0.0053
Wind_Speed	0.0006	0.0031
Visibility	-0.0003	0.0016
WaveHeight	0.0005	0.0010
Wet_Bulb_F	0.0000	0.0007

Model Validation

True Positives	True Negatives	False Positives	False Negatives	Sen
17	103	16	12	0.5

Figure 49. Results after completion of a PLS model run.

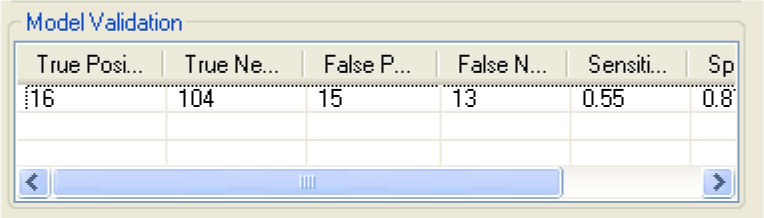
Setting the Decision Threshold

Once the user has selected a model, the Decision Criterion (DC) is chosen (see Section 7.2 for a description of the DC). The graph on the right side of the “Model” tab is used for this purpose (Figure 49). To understand the plot, consider that a lower DC will correctly identify more exceedances of the RS threshold, but also produce more “false positives” by flagging predicted values when the actual water quality is below the RS. Raising the DC has the opposite tradeoff: reducing false positives at the expense of identifying fewer true exceedances.

The blue line on the graph indicates true positives and the yellow line indicates true negatives. Current model performance is indicated by the following:

- The vertical dotted line indicates the current location of the DC. The arrow buttons at the bottom are used to lower/raise the threshold by a small (< , >) or large (<< , >>) amount.
- The "Model Validation" window (Figure 50) indicates the number of true positives, true negatives, false positives, false negatives, sensitivity, specificity, and total accuracy of the model using the current DC. These results are based on cross-validation of the training data. These numbers will change after a short computational delay as the DC is moved. Care should be taken when comparing PLS/GBM model performance (in terms of false/true positives/negatives) with MLR models. MLR model performance is based on fitted, not cross-validated results. Cross-validation results are commonly thought to be more realistic in how well the model will do in future predictions, while fitted values better indicate how well the model fits previously-collected data. Cross-validation results are generated by developing models with partial data sets and making predictions for data left out of model development. For example, 5-fold cross validation would result in five different sets of IV coefficients for a single model by using 4/5 of the data to develop each set of IV coefficients, then predicting the remaining 1/5 of the data using those coefficients. MLR, on the other hand, uses all available data points to fit the model coefficients and then predicts the same data points. Look at cross-validated performance of MLR models using the "Cross-Validation" button described in Section 7.9.
- The current numeric value of the DC is shown above the "Model Summary" window (Figure 49).

The user can change the DC, drop variables, and re-run the model to fine-tune it. After the model and DC have been chosen, the user can advance to the Prediction tab (Section 10) to make predictions with the most recently computed model.



Model Validation

True Posi...	True Ne...	False P...	False N...	Sensiti...	Sp
16	104	15	13	0.55	0.8

Figure 50. Summary of PLS model performance metrics.

8.5 Diagnostics

There are four plots are offered on the "Diagnostics" sub-tab (Figure 51):

- The Time Series plot (upper left) displays predicted and observed values of the response variable. This is a time-series plot if the ID values for the observations are chronologically-ordered dates/times. If they are not, then this plot will look rather messy and strange, and be of little interest to the user.

- The Residuals vs. Fitted plot (upper right) shows the externally-studentized residuals versus model-fitted values. The externally-studentized residuals are a way to flag influential outliers. A common benchmark for a data point with undue influence on the regression model is an externally-studentized residual (absolute value) greater than 3.0.
- The Residuals vs. Observed plot (lower left) graphs the externally-studentized residuals against the observations.
- The Fitted vs. Observed plot (lower right) shows observations versus model fits and depicts the RS (green horizontal line) and current DC (blue vertical line).

Note that the fitted values plotted here are not cross-validated fits; rather they are the model fits based on all the data. For this reason, model performance in this plot (numbers of true negatives/positives) will likely be better than the model performance metrics given in the "Model Validation" window on the "Model" tab. A perfect model will fall along the 1:1 line. The more scatter in this plot, the worse the model fit.

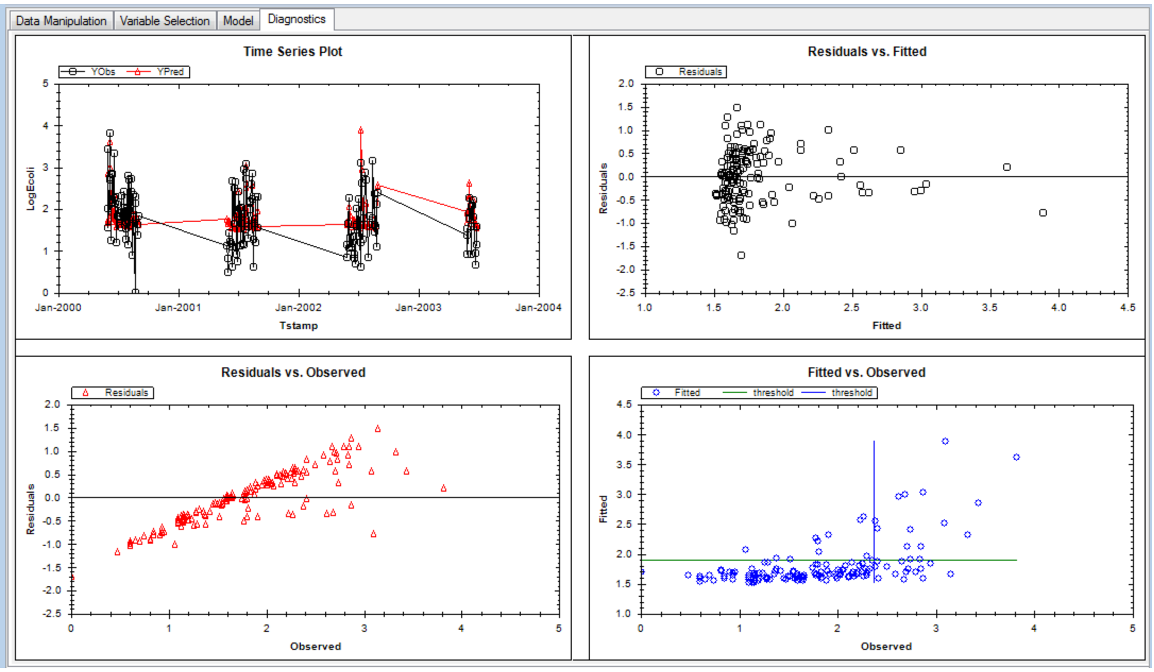


Figure 51. PLS Diagnostic plots to help evaluate model fit and influential outliers.

9. GENERALIZED BOOSTED REGRESSION MODELING

The Generalized Boosted Regression Model (GBM, also known as a gradient boosting machine) is a machine learning method that uses decision/regression trees instead of linear equations (Friedman, 2001). A decision/regression tree is a set of binary decision rules. For example, "if turbidity is less than 15 NTU, go down the right branch, otherwise go left." A "node" is the end of any branch and designates a continuous or categorical predictive value for the response variable. The innovative aspect of GBM is that it doesn't build a single, complex tree: it builds a hierarchical set of many simple trees, with each subsequent tree fit to the remaining residual error in the data after previous trees have all been fit. The default maximum number of trees in VB_3 is 10,000. Each tree is determined using a random set of the residual values from the dataset. This, along with the fact that it sensibly weights the data to learn more about the most difficult-to-predict cases, means GBM can make accurate predictions for new observations without over-fitting the training data.

While each tree is a simple structure, the long, linear combination of regression trees is more complicated. A negative aspect of a GBM model is that the model cannot easily be inspected graphically or expressed mathematically – it's something of a "black box." But what it lacks in interpretability and transparency can often be made up in terms of prediction accuracy. Another noted aspect of GBM, unlike MLR and PLS, is that it handles non-linear relationships between the response and IVs without having to transform the IVs. However, GBM is best used on larger datasets (> 100 observations), and odd results can occur if using GBM on small datasets.

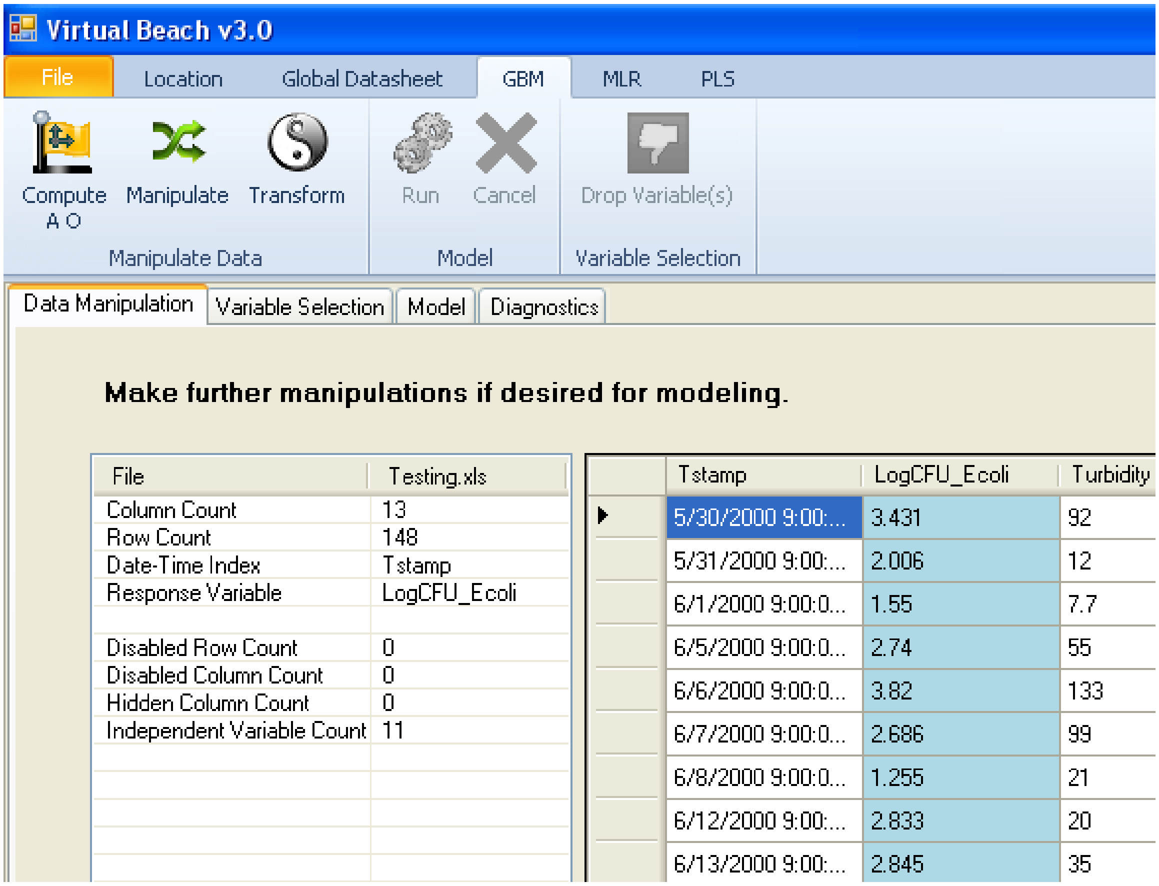
In a GBM, variable selection (identifying and dropping unimportant IV's from the model) is less important, compared to MLR. Even so, the "Drop Variables" button (Figure 52) performs as described in Section 8.4. For a GBM model, an IV's influence is the percentage of branches across all of the decision trees involving that variable, i.e., the most important variables are those that are most often used to create the branches.

For the GBM analysis, VB_3 implements the "gbm" package in R. Details of the algorithm are provided in Hastie (2009). Despite very different underlying mathematics, the GBM modeling interface in VB_3 is almost identical to the PLS interface (Section 8).

A key feature of GBM and PLS modeling is the use of cross-validation to assess real-world prediction accuracy. Model selection and threshold setting (Section 8.4) are done with reference to true positive, true negative, false positive and false negative counts which are calculated by 5-fold cross-validation. This means the data are split randomly and evenly into five sections and five models are built to predict exceedances on each of the five sections. For each, the section being predicted is left out of model building, so the counts reflect prediction of novel observations, not accuracy in fitting to past observations.

9.1 Data Manipulation

The MLR, PLS, and GBM modules all have "Data Manipulation" sub-tabs (Figure 52). When the user first clicks the GBM tab, the data in the GBM Data Manipulation sub-tab are identical to data on the Global Datasheet. From here, the user can change the "local" data to suit the GBM analysis. The local datasheet has all of the functionality of the Global Datasheet discussed in Section 6. Changing the local data has no effect on the Global Datasheet; however, going back to the Global Datasheet and making changes will overwrite the local datasheets on each of the modeling tabs.



Make further manipulations if desired for modeling.

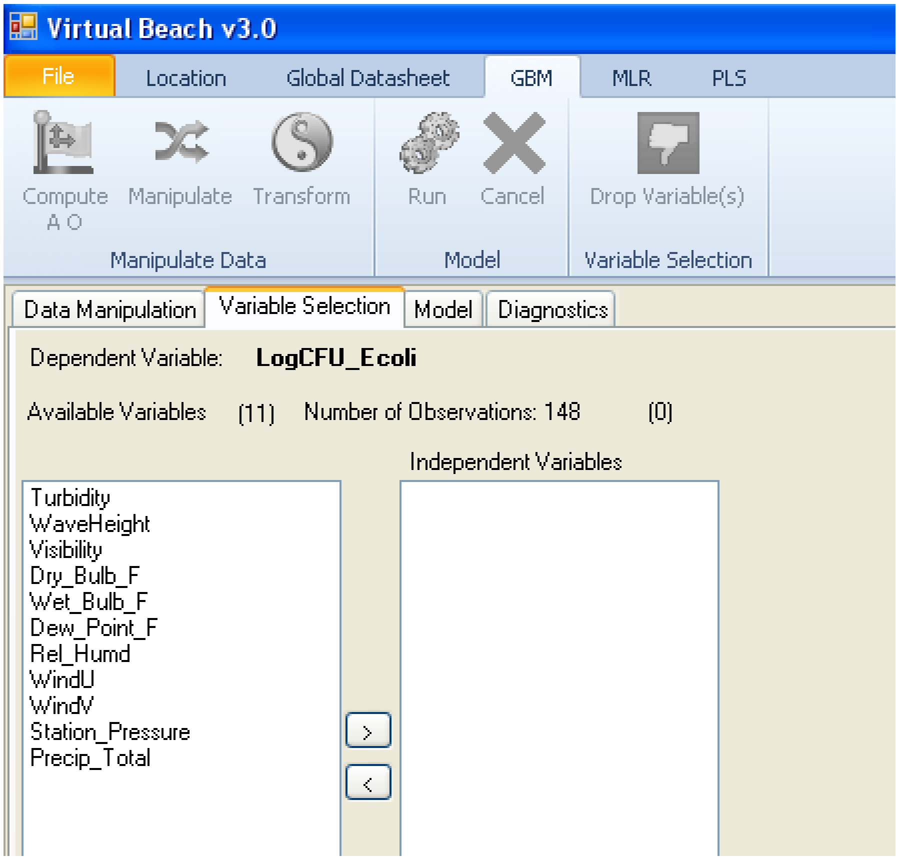
File	Testing.xls
Column Count	13
Row Count	148
Date-Time Index	Tstamp
Response Variable	LogCFU_Ecoli
Disabled Row Count	0
Disabled Column Count	0
Hidden Column Count	0
Independent Variable Count	11

Tstamp	LogCFU_Ecoli	Turbidity
5/30/2000 9:00:...	3.431	92
5/31/2000 9:00:...	2.006	12
6/1/2000 9:00:0...	1.55	7.7
6/5/2000 9:00:0...	2.74	55
6/6/2000 9:00:0...	3.82	133
6/7/2000 9:00:0...	2.686	99
6/8/2000 9:00:0...	1.255	21
6/12/2000 9:00:...	2.833	20
6/13/2000 9:00:...	2.845	35

Figure 52. Data Manipulation: the first sub-tab on each of the Method tabs.

9.2 Selecting Variables for Model Building

The "Variable Selection" sub-tab is where IVs for model development are chosen (Figure 53). Users may select all or a subset of IVs for the model. All eligible IVs are listed in the "Available Variables" window (left column). Any IVs that users wish to include in the model must be moved to the "Independent Variables" window by highlighting the IV and clicking the ">" key. Any number of IVs can be added or removed from this list. Once the desired IVs have been selected, click the "Model" sub-tab.



Dependent Variable: **LogCFU_Ecoli**

Available Variables (11) Number of Observations: 148 (0)

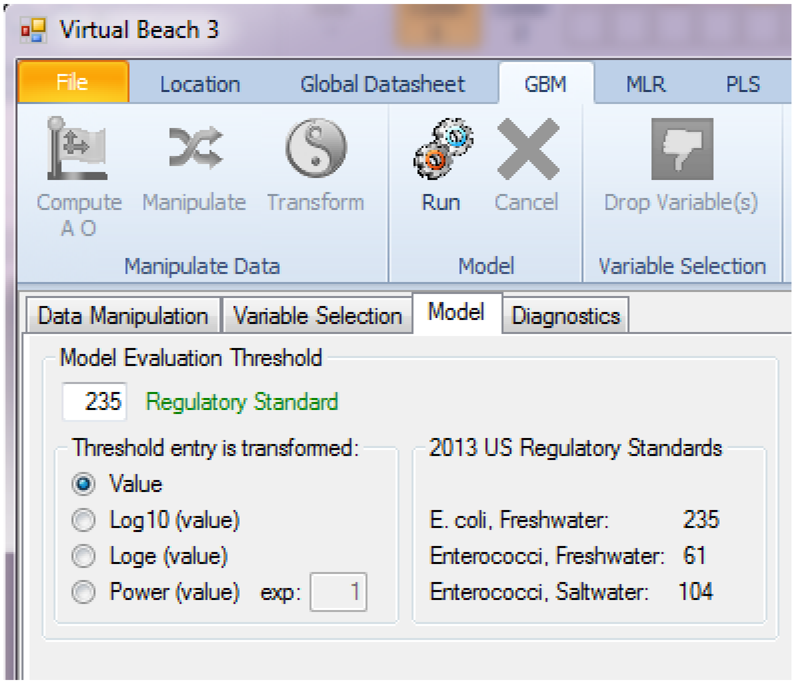
Turbidity
WaveHeight
Visibility
Dry_Bulb_F
Wet_Bulb_F
Dew_Point_F
Rel_Humd
WindU
WindV
Station_Pressure
Precip_Total

Independent Variables

Figure 53. Selecting variables for GBM processing within the modeling module.

9.3 The Regulatory Standard

To build a GBM model, observations must be defined as exceedances or non-exceedances; GBM and PLS models will not run if the dataset has no exceedances. This is done by setting the Regulatory Standard (RS) at the top of the “Model” sub-tab (Figure 54) and then specifying with the radio buttons units to enter for the RS. The default RS is the USEPA’s federal standard for *E. coli* in freshwater, 235 CFU per 100 mL. Because these are the raw units of measurement, the radio button transformation choice should be set to “Value.” When thinking of bacteria concentrations in logarithmic units, think of the RS as 2.371 [= $\log_{10}(235)$]. To communicate this to VB_3, enter 2.371 in the “Regulatory Standard” box and click the “Log10 (value)” radio button (Figure 54).



Model Evaluation Threshold

235 Regulatory Standard

Threshold entry is transformed:

● Value
○ Log10 (value)
○ Loge (value)
○ Power (value) exp: 1

2013 US Regulatory Standards

E. coli, Freshwater:	235
Enterococci, Freshwater:	61
Enterococci, Saltwater:	104

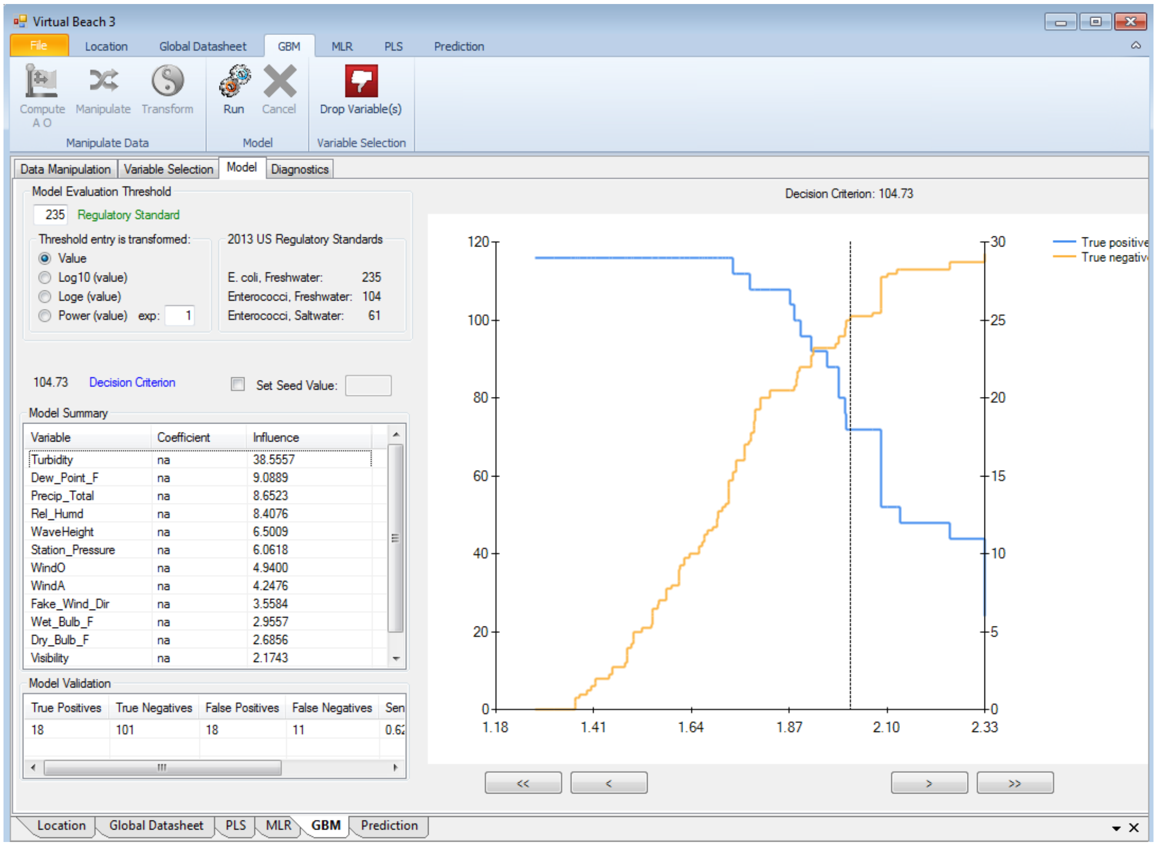
Figure 54. Setting the Regulatory Standard and running models for GBM.

9.4 Modeling Control Options

Clicking the "Run" button on the GBM ribbon (Figure 54) will start model development. When modeling is finished, results are displayed (Figure 55). The "Drop Variable(s)" option is now available on the ribbon and a Decision Criterion (DC) for the model can be chosen. As described in Section 8.4, a GBM model solution can be replicated using the "Set Seed Value" check and input box. After a solution is reached, the "Drop Variable(s)" option on the PLS ribbon becomes enabled and a Decision Criterion (DC) for the model can be chosen.

Dropping Unimportant Variables

The "Model Summary" window (left side of Figure 55) lists the IVs in descending order of influence. For a GBM model, a variable's influence is the percentage of the model's total branches based on the given variable. The larger the influence of a variable (global sensitivity), the more its variation drives the response. Low-influence variables can be dropped from the model by clicking on the variable's name in the list, then clicking the "Drop Variable(s)" button. If any variables are dropped at this stage, the model must be rebuilt by clicking the "Run" button.



Model Evaluation Threshold

235 Regulatory Standard

Threshold entry is transformed:

● Value
○ Log10 (value)
○ Loge (value)
○ Power (value) exp: 1

2013 US Regulatory Standards

E. coli, Freshwater:	235
Enterococci, Freshwater:	104
Enterococci, Saltwater:	61

104.73 Decision Criterion

□ Set Seed Value:

Model Summary

Variable	Coefficient	Influence
Turbidity	na	38.5557
Dew_Point_F	na	9.0889
Precip_Total	na	8.6523
Rel_Humd	na	8.4076
WaveHeight	na	6.5009
Station_Pressure	na	6.0618
WindO	na	4.9400
WindA	na	4.2476
Fake_Wind_Dir	na	3.5584
Wet_Bulb_F	na	2.9557
Dry_Bulb_F	na	2.6856
Visibility	na	2.1743

Model Validation

True Positives	True Negatives	False Positives	False Negatives	Sen
18	101	18	11	0.62

Figure 55. Results after completion of a GBM model run.

Setting the Decision Threshold

Once the user selects a model, the Decision Criterion (DC) can be chosen (see Section 7.2 for a description of the DC). The graph on the right side of the Model tab is used for this purpose (Figure 55). To understand the plot, consider that a lower DC correctly identifies more exceedances of the RS threshold, but also produces more "false positives" by flagging predicted values when the actual water quality is below the RS. Raising the DC has the opposite tradeoff: reducing false positives at the expense of identifying fewer true exceedances.

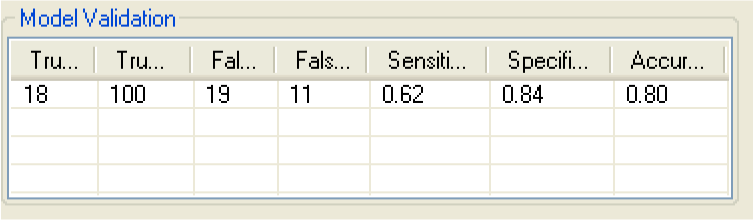
The blue line on the graph indicates true positives and the yellow line indicates true negatives. Current model performance is indicated by the following:

- The vertical dotted line indicates the current location of the DC. The arrow buttons at the bottom are used to lower/raise the threshold by a small (< , >) or large (<< , >>) amount.
- The "Model Validation" window (Figure 56) indicates the number of true positives, true negatives, false positives, false negatives, sensitivity, specificity, and total accuracy of the model using the current DC. These results are based on cross-validation of the training data. These numbers will change after a short computational delay as the DC is moved. Comparing GBM (and PLS) model

performance, in terms of false/true positives/negatives, with MLR models must be done carefully. MLR model performance is based on fitted results, not cross-validated results. Cross-validation results are commonly thought to indicate more realistically how well the model will do in future predictions and fitted values better indicate how well the model fits previously collected data. Cross-validation results are generated by developing models with partial data sets and subsequently making predictions for data that were left out. For example, 5-fold cross validation would result in 5 different sets of IV coefficients for a single model by using 4/5 of the data to develop each set of IV coefficients, and then predicting the remaining 1/5 of the data using those coefficients. MLR, on the other hand, uses all available data points to fit the model coefficients and then predicts the same data points. Look at cross-validated performance of MLR models using the "Cross-Validation" button described in Section 7.9.

- The current numeric value of the DC is shown above the "Model Summary" window (Figure 55).

The user can change the DC, drop variables and re-run the model to fine-tune it. After the model and DC have been chosen, the user can advance to the Prediction tab (Section 10) to make predictions with the most recently computed model.



Model Validation

Tru...	Tru...	Fal...	Fals...	Sensiti...	Specifi...	Accur...
18	100	19	11	0.62	0.84	0.80

Figure 56. Summary of GBM model performance metrics.

9.5 Diagnostics

There are four plots offered on the "Diagnostics" sub-tab (Figure 57):

- The Time Series plot (upper left) displays predicted and observed values of the response variable over time if the ID values for the observations are dates/times.
- The Residuals vs. Fitted plot (upper right) shows the externally-studentized residuals versus model-fitted values. The externally-studentized residuals are a way to flag influential outliers. A common benchmark for a data point with undue influence on the regression model is an externally-studentized residual (absolute value) greater than 3.0. Certain patterns seen in this residual plot can indicate the need for a transformation of the response variable or model IVs. Refer to Meyers (1990) for details.
- The Residuals vs. Observed plot (lower left) graphs the externally-studentized residuals against the observations.

- The Fitted vs. Observed plot (lower right) shows observations versus model fits and depicts the RS (green horizontal line) and current DC (blue vertical line).

Note that the fitted values plotted here are not cross-validated fits; rather they are the model fits based on all the data. For this reason, model performance in this plot (numbers of true negatives/positives) will likely be better than the model performance metrics given in the Model Validation table on the Model tab. A perfect model will fall along the 1:1 line. The more scatter in this plot, the worse the model fit.

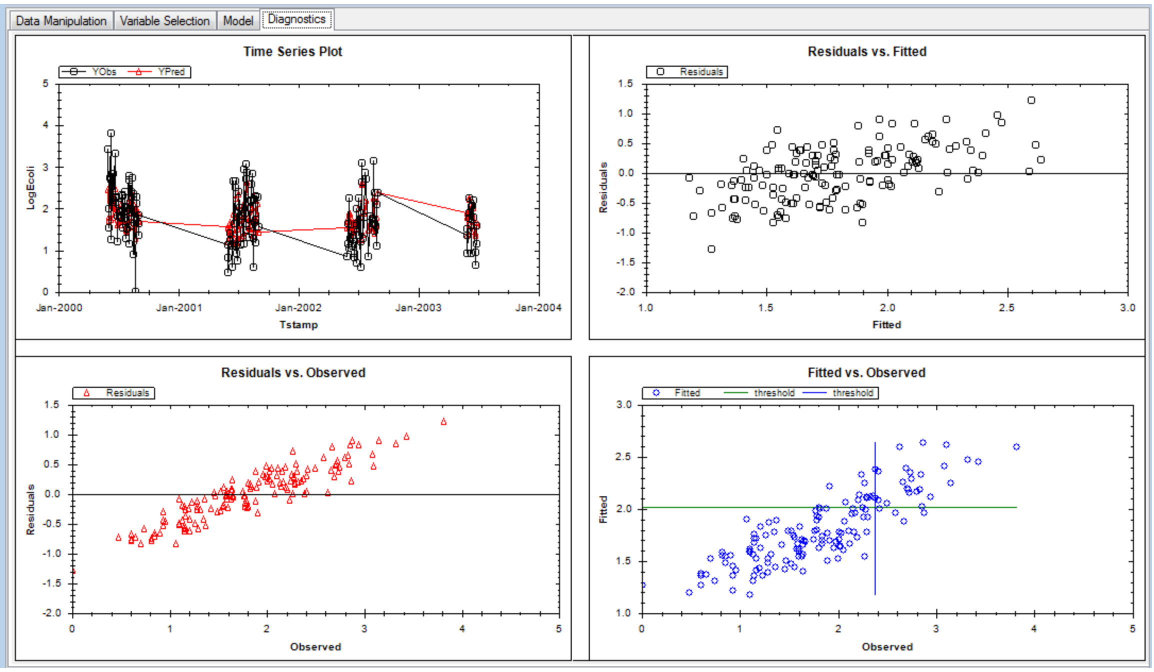


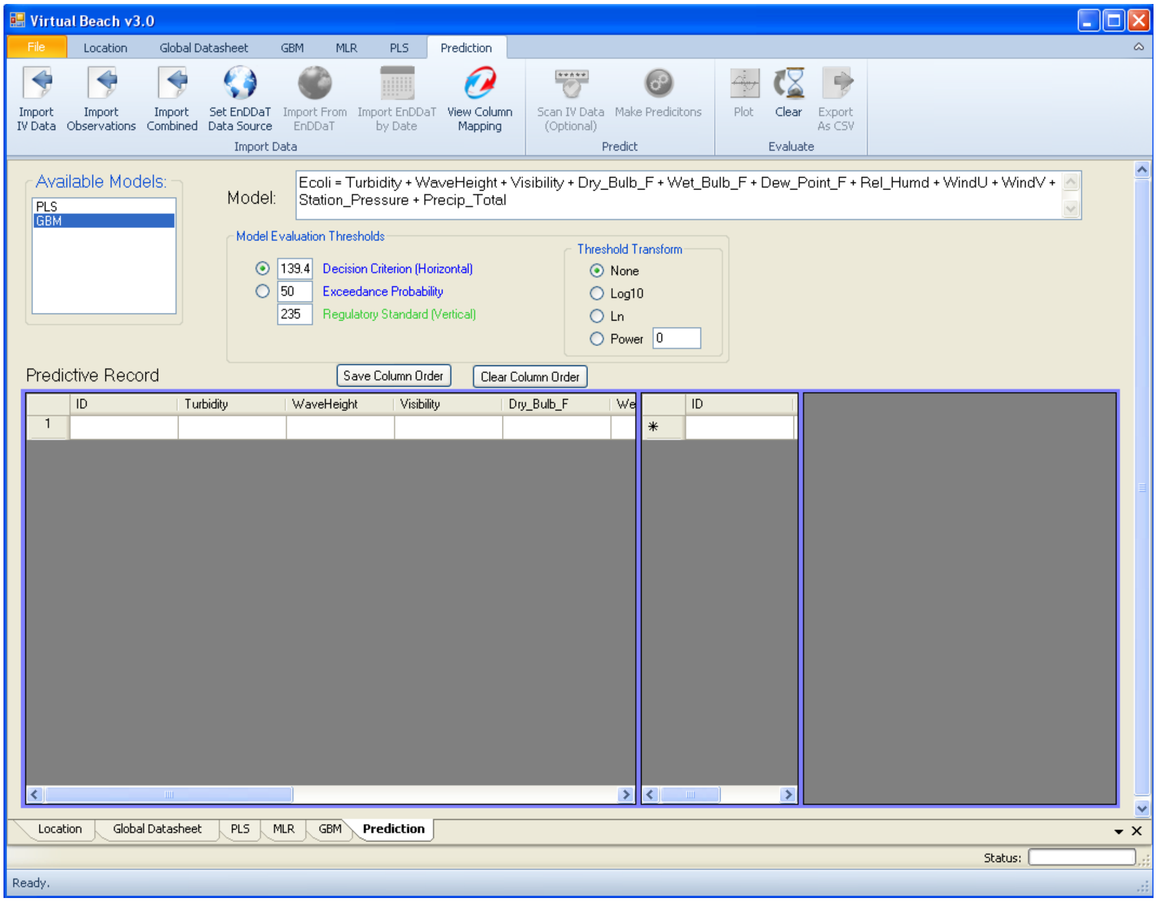
Figure 57. GBM diagnostic plots to help evaluate model fit and influential outliers.

10. PREDICTION

VB3's Prediction interface allows users to select a model from the PLS, GBM, or MLR tabs and make predictions with it, but the prediction tab is hidden until a model is chosen.

10.1 Model Statement

At the top left of the Prediction tab is the "Available Models" window. Depending on how many statistical methods were performed on the data, the user could see "MLR," "PLS," and/or "GBM" in this area. Once a model is chosen, an expression with the IVs and coefficients in that model is shown in the "Model" window to the right (Figure 58).



Available Models:
PLS
GBM

Model: Ecoli = Turbidity + WaveHeight + Visibility + Dry_Bulb_F + Wet_Bulb_F + Dew_Point_F + Rel_Humd + WindU + WindV + Station_Pressure + Precip_Total

Model Evaluation Thresholds

● 139.4 Decision Criterion (Horizontal)
○ 50 Exceedance Probability
235 Regulatory Standard (Vertical)

Threshold Transform

● None
○ Log10
○ Ln
○ Power 0

Predictive Record

	ID	Turbidity	WaveHeight	Visibility	Dry_Bulb_F	We
1						

	ID
*	

Figure 58. The VB3 Prediction interface.

10.2 Model Evaluation Thresholds

In the "Model Evaluation Thresholds" box, there are input boxes for the Decision Criterion (DC), Exceedance Probability, and Regulatory Standard (RS). Setting these allows model predictions to be evaluated and model specificity, sensitivity, and accuracy to be calculated. The radio buttons inside the "Threshold Transform" box tells VB3 how to transform the DC and RS to compare to model predictions and observations (see Section 7.2 for further guidance). Note that we define the "observations" as the measured values of the model's response variable (e.g., *E.coli* CFU measurements). If the threshold transform definition is set improperly, there can be problems when comparing modeling predictions to observations, so exercise caution.

10.3 Prediction Form

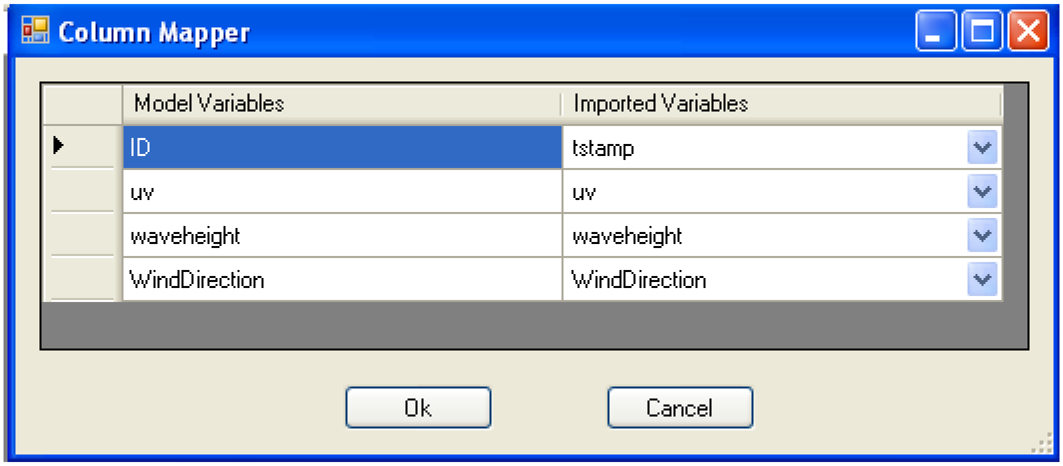
The bottom half of the Prediction interface is occupied by three data panels (the empty gray sections separated by blue vertical bars at the bottom of Figure 58): the left holds IV data; the middle is for observations; and the right shows model predictions and evaluation metrics. Each panel also contains a column for a unique ID for each row of data, e.g., the date that data were collected. The panels have separate horizontal and vertical scroll bars that become visible if the number of rows or columns exceeds the viewable area. The three panels independently scroll horizontally, but as a group vertically. Panels can be re-sized by clicking and dragging the blue vertical partitions. The order of the columns in the left (IV) and right (Model Predictions) panels can be changed by clicking and dragging the column headers left or right. If it is important to save a re-arranged column order for the selected model, click on the "Save Column Order" button just above the IV panel.

Users can import data from files using the "Import IV Data," "Import Observations" and "Import Combined" (both IVs and observations) buttons on the top ribbon, or type data directly into the left and middle grids. It is the user's responsibility to ensure that IV data are in the same units as those used to construct the model. Depending on the model selected for prediction, the left panel will contain one column for every unique model IV plus a column for an ID. The middle panel has two columns: one for the ID and one for the observations (note that the name of the observation column is identical to the name of the model's response variable).

10.4 Column Mapping of Imported Data

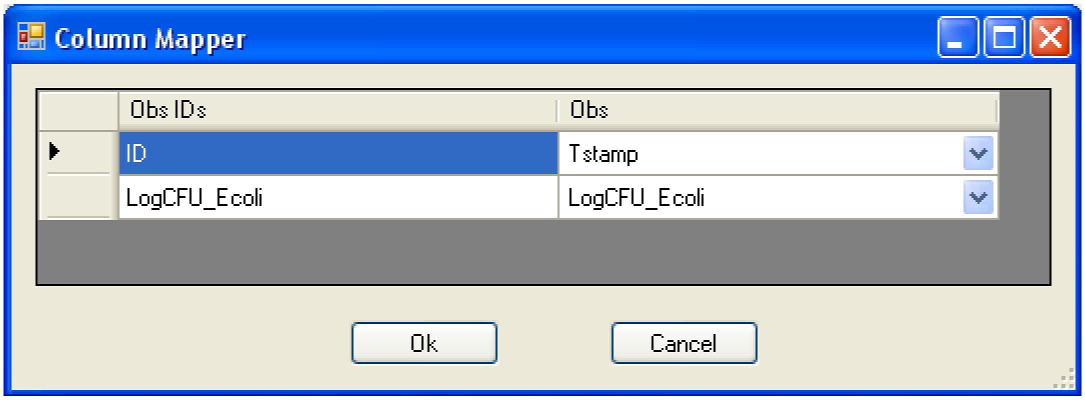
When data are imported via one of the three import buttons (Figure 58), a "Column Mapper" window opens (Figure 59). This allows users to tell VB_3 which columns in the imported datasheet should be used to fill in the row IDs, IVs and the observations. By default, the first column of the imported file is mapped to the ID field, but this can be overridden. If a column in the imported spreadsheet has a name identical to a model IV or the response variable, VB_3 will select it as the appropriate column for that IV or the observations. If no identically-named column is found, the user must specify which column of the imported file should be used for the IV and observations.

Once a user has gone through the mapping process for a model, that configuration is saved. If another data file with the same column names is imported, the column mapper will not appear. If a model has a saved mapping configuration, it can be viewed and cleared by clicking "View Column Mapping" on the ribbon (Figure 58).



	Model Variables	Imported Variables
▶	ID	tstamp
	uv	uv
	waveheight	waveheight
	WindDirection	WindDirection

Figure 59. Importation of IV data using the "Column Mapper" window.

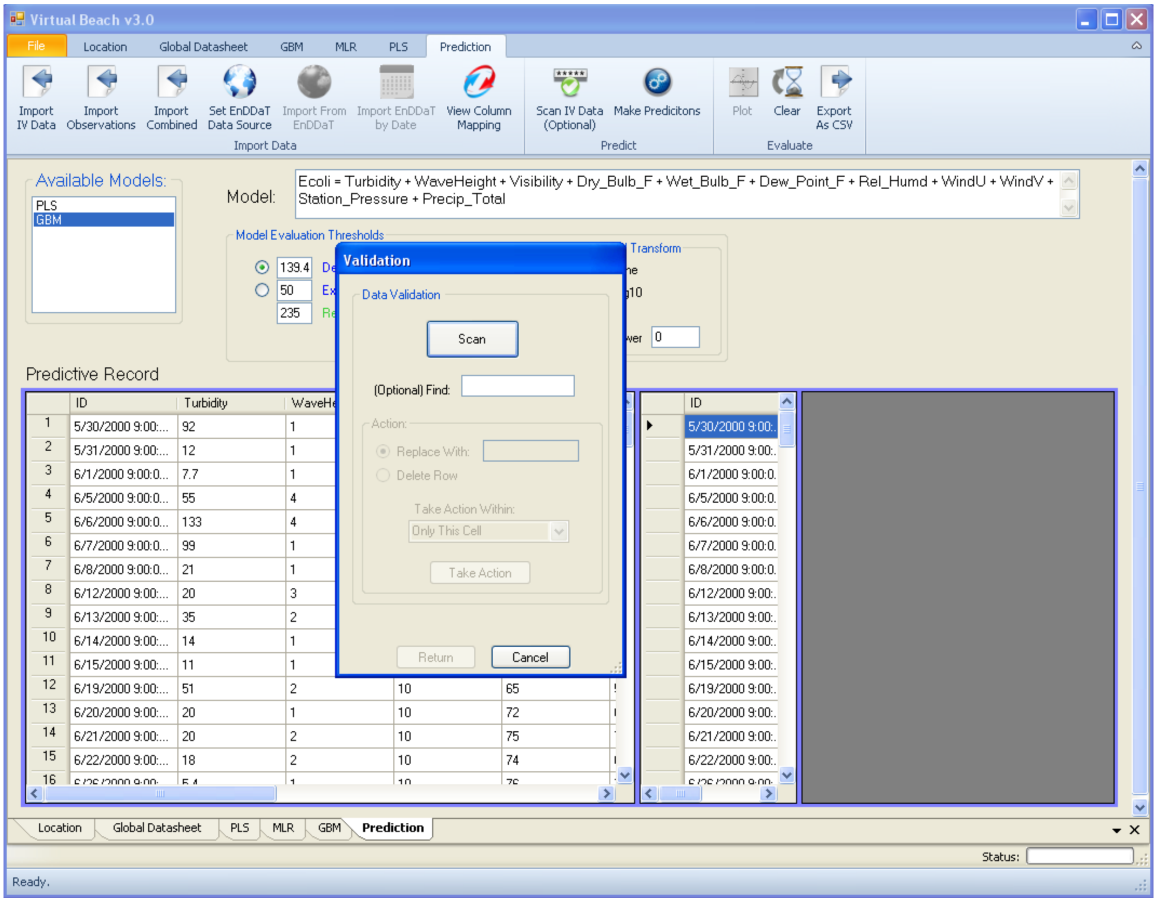


	Obs IDs	Obs
▶	ID	Tstamp
	LogCFU_Ecoli	LogCFU_Ecoli

Figure 60. Importation of observational data using the "Column Mapper" window.

After observations have been imported or manually entered, users specify the correct data transformation to ensure proper comparison to model predictions. This is done by right-clicking on the observation column header (the right column of the middle panel) and choosing an option from the "Define Transform" drop-down menu: none, log$_{10}$, log$_e$, or a power transformation; "none" is the default choice. For example, if Log$_{10}$ observations are imported, the user must change the "Define Transform" menu option to "Log10." If untransformed (raw) values of the observations are entered/imported, then the appropriate "Define Transform" menu choice would be "none."

The IV data are automatically scanned for errors (e.g., blank or non-numeric cells) when "Make Predictions" is clicked on the ribbon (however, this button is not enabled until data are entered into the IV data panel). If bad data cells are found, VB$_3$ will tell the user to run an IV data scan by clicking the "Scan IV Data" button on the ribbon (Figure 61). The IV scan pop-up window is very similar to the one seen on the Global Datasheet; however, "Delete Column" is not a choice. "Replace With" and "Delete Row" are the only options for dealing with problems in the IV data grid.



Model: Ecoli = Turbidity + WaveHeight + Visibility + Dry_Bulb_F + Wet_Bulb_F + Dew_Point_F + Rel_Humd + WindU + WindV + Station_Pressure + Precip_Total

● 139.4 De
○ 50 Ex
235 Re

he
g10
wer 0

(Optional) Find:

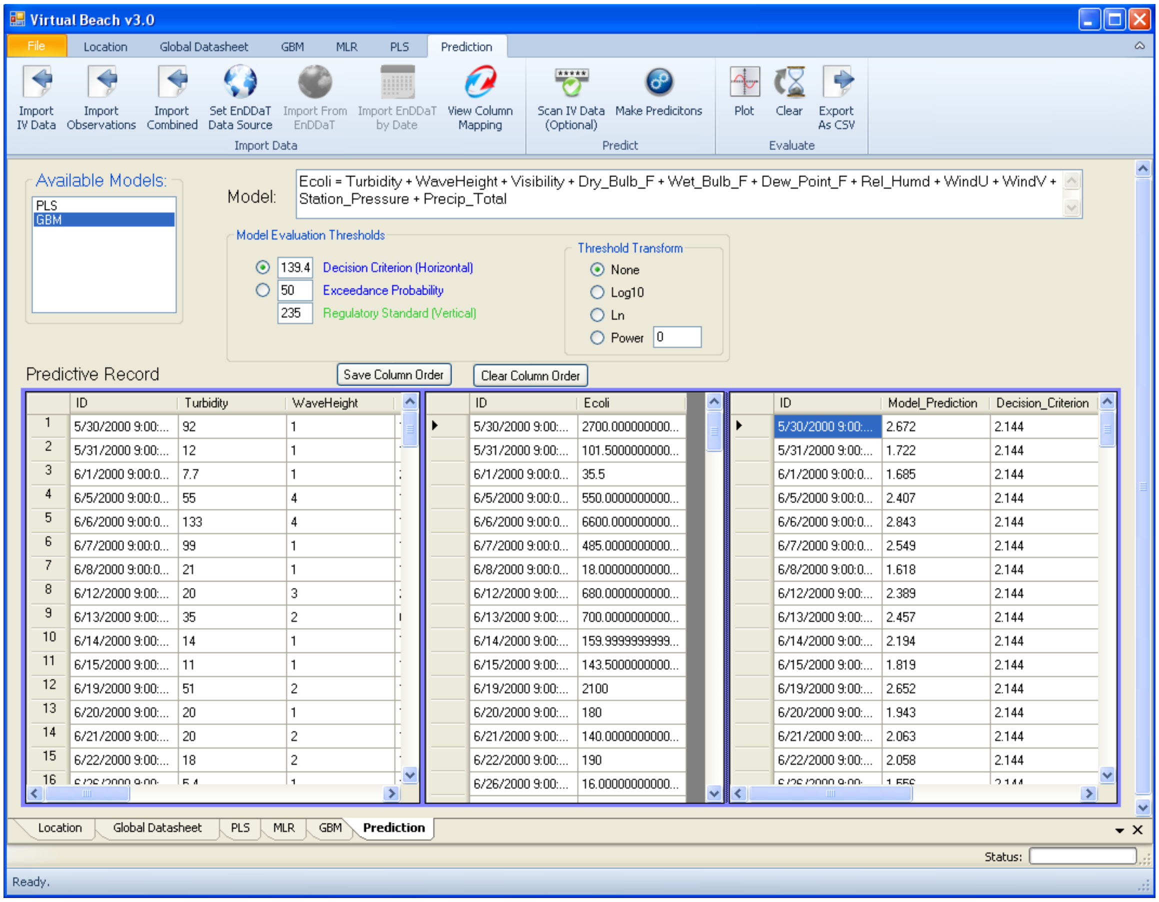
○ Replace With:
○ Delete Row
Take Action Within: Only This Cell

	ID	Turbidity	WaveHe			
1	5/30/2000 9:00:...	92	1			
2	5/31/2000 9:00:...	12	1			
3	6/1/2000 9:00:0...	7.7	1			
4	6/5/2000 9:00:0...	55	4			
5	6/6/2000 9:00:0...	133	4			
6	6/7/2000 9:00:0...	99	1			
7	6/8/2000 9:00:0...	21	1			
8	6/12/2000 9:00:...	20	3			
9	6/13/2000 9:00:...	35	2			
10	6/14/2000 9:00:...	14	1			
11	6/15/2000 9:00:...	11	1			
12	6/19/2000 9:00:...	51	2	10	65	
13	6/20/2000 9:00:...	20	1	10	72	
14	6/21/2000 9:00:...	20	2	10	75	
15	6/22/2000 9:00:...	18	2	10	74	

ID
5/30/2000 9:00:.
5/31/2000 9:00:.
6/1/2000 9:00:0.
6/5/2000 9:00:0.
6/6/2000 9:00:0.
6/7/2000 9:00:0.
6/8/2000 9:00:0.
6/12/2000 9:00:.
6/13/2000 9:00:.
6/14/2000 9:00:.
6/15/2000 9:00:.
6/19/2000 9:00:.
6/20/2000 9:00:.
6/21/2000 9:00:.
6/22/2000 9:00:.

Figure 61. The scan IV window on the MLR Prediction tab.

Observational data need not be present to make predictions, but they are needed for model evaluation (sensitivity, specificity, false negatives, false positives, accuracy). After clicking "Make Predictions" on the ribbon, VB3 uses the model, IV data, and observational data to fill the right panel with these data columns: ID, Model Prediction, Decision Criterion, Exceedance Probability, Regulatory Standard, and Error Type (Figure 62).



Available Models:
PLS
GBM

Model: Ecoli = Turbidity + WaveHeight + Visibility + Dry_Bulb_F + Wet_Bulb_F + Dew_Point_F + Rel_Humd + WindU + WindV + Station_Pressure + Precip_Total

Model Evaluation Thresholds
● 139.4 Decision Criterion (Horizontal)
○ 50 Exceedance Probability
235 Regulatory Standard (Vertical)

Threshold Transform
● None
○ Log10
○ Ln
○ Power 0

Predictive Record

	ID	Turbidity	WaveHeight
1	5/30/2000 9:00:...	92	1
2	5/31/2000 9:00:...	12	1
3	6/1/2000 9:00:0...	7.7	1
4	6/5/2000 9:00:0...	55	4
5	6/6/2000 9:00:0...	133	4
6	6/7/2000 9:00:0...	99	1
7	6/8/2000 9:00:0...	21	1
8	6/12/2000 9:00:...	20	3
9	6/13/2000 9:00:...	35	2
10	6/14/2000 9:00:...	14	1
11	6/15/2000 9:00:...	11	1
12	6/19/2000 9:00:...	51	2
13	6/20/2000 9:00:...	20	1
14	6/21/2000 9:00:...	20	2
15	6/22/2000 9:00:...	18	2
16	6/26/2000 9:00:	5.4	1

ID	Ecoli
5/30/2000 9:00:...	2700.000000000...
5/31/2000 9:00:...	101.5000000000...
6/1/2000 9:00:0...	35.5
6/5/2000 9:00:0...	550.0000000000...
6/6/2000 9:00:0...	6600.000000000...
6/7/2000 9:00:0...	485.0000000000...
6/8/2000 9:00:0...	18.00000000000...
6/12/2000 9:00:...	680.0000000000...
6/13/2000 9:00:...	700.0000000000...
6/14/2000 9:00:...	159.9999999999...
6/15/2000 9:00:...	143.5000000000...
6/19/2000 9:00:...	2100
6/20/2000 9:00:...	180
6/21/2000 9:00:...	140.0000000000...
6/22/2000 9:00:...	190
6/26/2000 9:00:...	16.00000000000...

ID	Model_Prediction	Decision_Criterion
5/30/2000 9:00:...	2.672	2.144
5/31/2000 9:00:...	1.722	2.144
6/1/2000 9:00:0...	1.685	2.144
6/5/2000 9:00:0...	2.407	2.144
6/6/2000 9:00:0...	2.843	2.144
6/7/2000 9:00:0...	2.549	2.144
6/8/2000 9:00:0...	1.618	2.144
6/12/2000 9:00:...	2.389	2.144
6/13/2000 9:00:...	2.457	2.144
6/14/2000 9:00:...	2.194	2.144
6/15/2000 9:00:...	1.819	2.144
6/19/2000 9:00:...	2.652	2.144
6/20/2000 9:00:...	1.943	2.144
6/21/2000 9:00:...	2.063	2.144
6/22/2000 9:00:...	2.058	2.144
6/26/2000 9:00:	1.556	2.144

Figure 62. A prediction grid after IVs and observational data have been imported, and model predictions made.

The ID column of the model output panel is taken directly from the ID column of the IV panel, not IDs in the middle panel. VB3 will make one model prediction per row in the IV data panel, regardless of how many observations are entered in the middle panel.

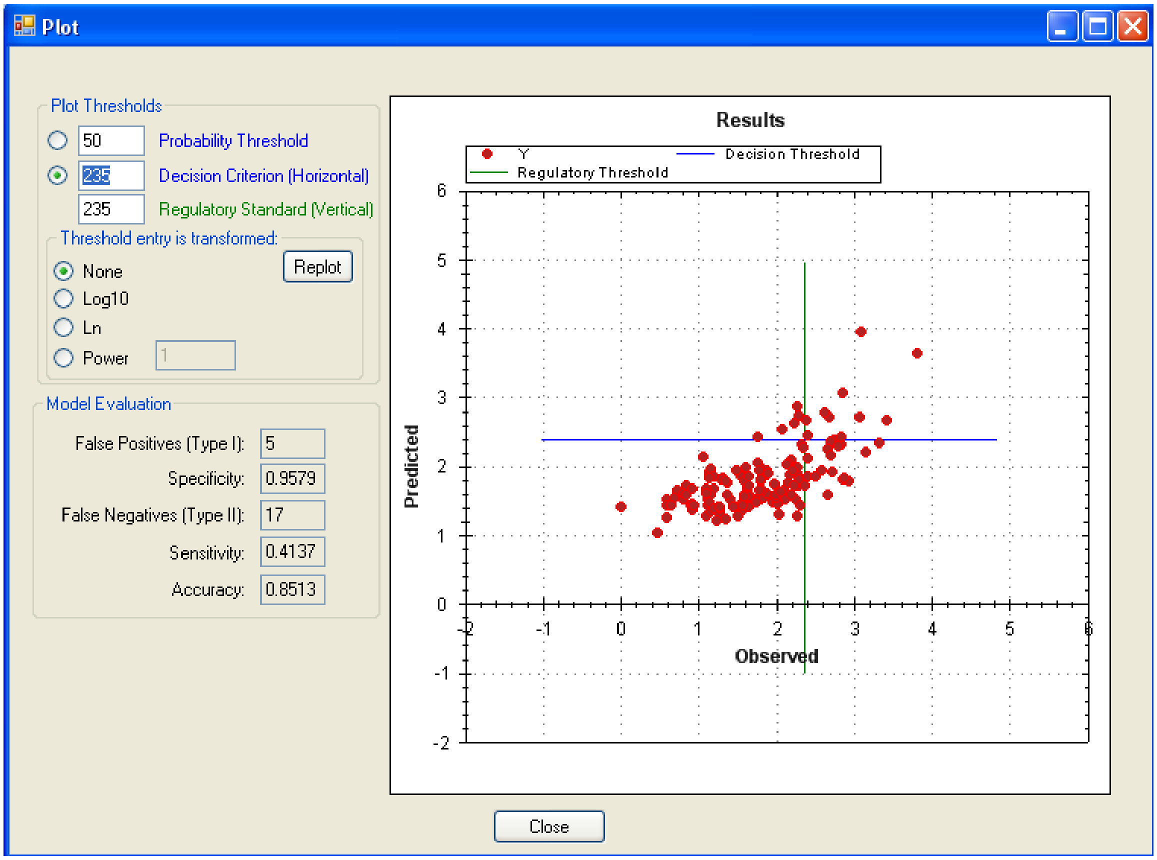
The Model Prediction column contains predicted values of the response variable, initially displayed in the same units as the model's response variable. Right-clicking on this column header changes how predictions are displayed in the table (raw, log, or power units). The Decision Criterion and Regulatory Standard are set by the user. They are displayed in the same units as the Model Predictions, and their column headers can be right-clicked to change the displayed units. The Exceedance Probability (displayed as a percentage, or 100 times the probability) is defined as the probability that the model's prediction will be larger than the Decision Criterion, based on uncertainty bounds (confidence intervals) of the model's predictions.

To compare model predictions to observations, VB3 looks at the prediction ID and attempts to find an observation in the middle panel with the same ID. It does not require unique IDs for each row in the observation panel, but a model prediction is compared to the first observation found with the same ID. When comparing model predictions to observations, an error ("False Negative" or "False Positive") will be reported in the "Error Type" column.

We again emphasize that assessing model output correctly depends on the synchronization of units of the Decision Criterion (DC), Regulatory Standard (RS), model predictions, and observations. VB3 will ensure this happens if the user correctly specifies the units for the observations (using the right-click column header menu of the right column of the middle panel) and for the DC and RS (using the radio buttons in the "Threshold Transform" box of the prediction window).

10.5 Viewing Plots

After predictions are made, a scatterplot of observations versus predictions, or observations versus the probability of exceedance, can be viewed by clicking "Plot" on the ribbon (Figures 62 and 63). If no observational data were entered, a message asking for observational data appears. The features of this plot are similar to those described in Section 7.6. Plotted points are based on comparing model predictions (right pane of the Prediction Form) with observations (middle pane) that share the same unique row ID. Note that the plotted exceedance probabilities are not automatically re-computed because the Decision Criterion is changed in this plotting window. To see updated exceedance probabilities for a new Decision Criterion, users must close this plotting window, change the DC in the "Model Evaluation Thresholds" box, re-click the "Make Predictions" button on the ribbon, and then click the "Plot" button again.



Plot

Plot Thresholds

○ 50 Probability Threshold

● 235 Decision Criterion (Horizontal)

235 Regulatory Standard (Vertical)

Threshold entry is transformed:

● None

○ Log10

○ Ln

○ Power 1

Model Evaluation

False Positives (Type I): 5

Specificity: 0.9579

False Negatives (Type II): 17

Sensitivity: 0.4137

Accuracy: 0.8513

Figure 63. Prediction interface plotting of the observations versus predictions, with model evaluation threshold controls.

10.6 Prediction Form Manipulation

Two other buttons found in the "Evaluate" section of the ribbon are "Clear" and "Export as CSV." To view the table in a spreadsheet or word processing program, "Export as CSV" saves the contents of the entire table (all three panels) in .csv format. "Clear" deletes all information in every panel of the table. As with most tabular information in VB3, data in individual panels can be selected with a left-click and drag. Control-c and Control-v are then used to copy and paste the data into another application such as Excel.

10.7 Importation of EnDDaT Data

The Environmental Data Discovery and Transformation (EnDDaT; http://cida.usgs.gov/enddat/) service accesses data from a variety of sources, compiles and processes it, and performs common transformations. The result is environmental data from multiple sources sorted into a single table. EnDDaT is a tool for compiling datasets prior to model development. Once models are developed, EnDDaT can create datasets for the VB3 Prediction tab. The "Set EnDDaT Data Source," "Import from EnDDaT" and "Import EnDDaT by Date" buttons on the ribbon (Figure 64) allow users to import data directly from the EnDDaT web service to the prediction tab of VB3, avoiding manual entry. See the EnDDaT user guide (available from the EnDDaT website link above) for step-by-step instructions on obtaining data, specifying transforms, processing data and developing a URL.

To import EnDDaT data to the IV panel of the prediction grid, click the "Set EnDDaT Data Source" button and insert an EnDDaT-generated URL that calls for the IVs needed to make predictions (Figure 65). Choose and activate the radio button for whether to collect data from a specific time (e.g., the time the beach was visited) or from the most recently available time. Users must also choose the desired time zone from the dropdown list. After clicking "OK," the "Import from EnDDaT" and "Import EnDDaT by Date" buttons are enabled on the ribbon. To import data for the current day, use the former button. Clicking the latter button opens a calendar for retrieval of data from a previous day (Figure 66). Whichever button is used, afterwards a pop-up window will indicate EnDDaT is being accessed (Figure 67). Once data have been retrieved, the "column mapper" window will open, allowing the user to specify which columns in the imported EnDDaT data should be matched to each IV in the selected model (see Section 10.4 for more details on column mapping).

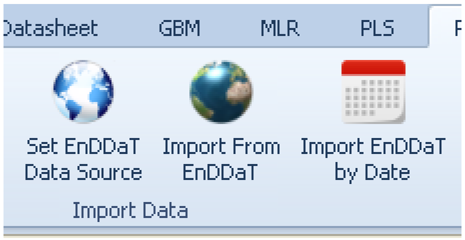
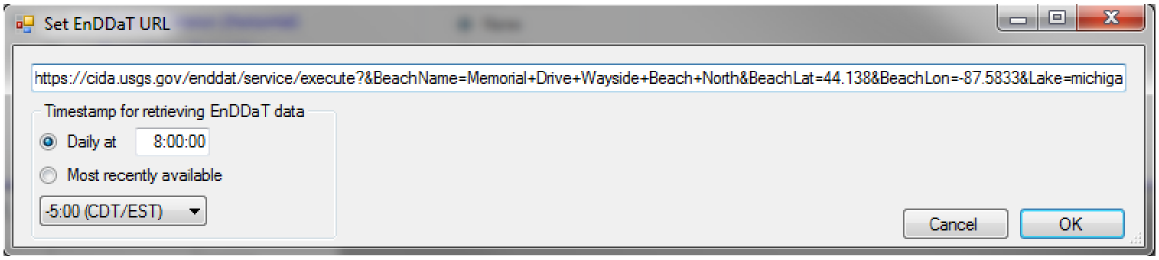


Figure 64. The three EnDDaT-related buttons on the prediction tab.



https://cida.usgs.gov/enddat/service/execute?&BeachName=Memorial+Drive+Wayside+Beach+North&BeachLat=44.138&BeachLon=-87.5833&Lake=michiga

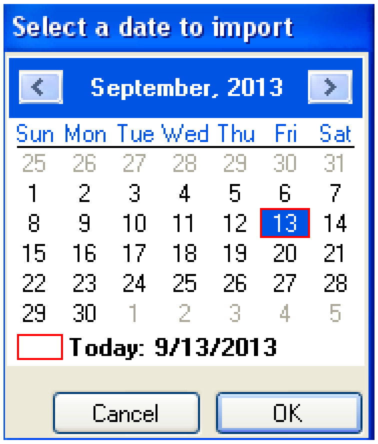
Timestamp for retrieving EnDDaT data

● Daily at 8:00:00

○ Most recently available

-5:00 (CDT/EST)

Figure 65. Setting URL options for retrieval of data from EnDDaT.

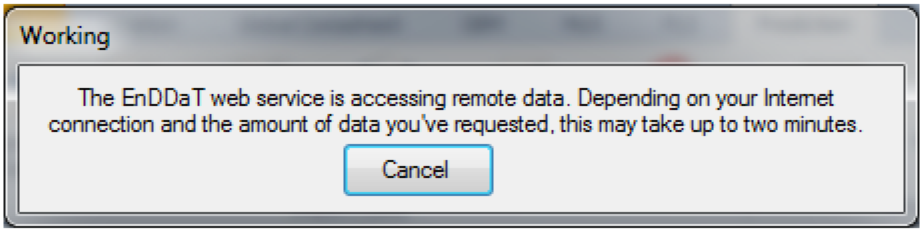


September, 2013

Sun	Mon	Tue	Wed	Thu	Fri	Sat
25	26	27	28	29	30	31
1	2	3	4	5	6	7
8	9	10	11	12	13	14
15	16	17	18	19	20	21
22	23	24	25	26	27	28
29	30	1	2	3	4	5

Today: 9/13/2013

Figure 66. Choosing a previous day for EnDDaT data retrieval.



The EnDDaT web service is accessing remote data. Depending on your Internet connection and the amount of data you've requested, this may take up to two minutes.

Figure 67. Pop-up window indicating that data have been requested from EnDDaT.

11. USER FEEDBACK

The USEPA and USGS provide no warranty, expressed or implied, as to the correctness of the furnished software or the suitability for any purpose. The software has been tested, but as with any complex software, there could be undetected errors. Suggestions and experiences from the user community are welcomed by the Virtual Beach design/development team, and users are encouraged to report problems, issues and likes/dislikes to:

Mike Cyterski, USEPA: 706.355.8142 (cyterski.mike@epa.gov)

The USEPA has limited resources to assist users; however, we make an attempt to fix reported problems and help whenever possible.

12. REFERENCES

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Ecosystems Research Division
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Ecosystems Research Division
Athens, GA

Any use of trade, product, or firm names is for descriptive purposes only and does not imply endorsement by the U.S. Government.

APPENDICES

A.1 Transformations

VB3 provides the following transformations, where X_t is the transformed IV and X is the original IV:

- Log_{10}: $X_t = \log_{10}(X)$
- Log_e: $X_t = \log_e(X)$
- Inverse: $X_t = 1/X$
- Square: $X_t = X^2$
- Square Root: $X_t = X^{0.5}$
- Quad Root: $X_t = X^{0.25}$
- Polynomial: $X_t = a + bX + cX^2$
- General Exponent: $X_t = X^z$ where the user specifies the value of z

For the polynomial transformation, the Pearson coefficient is calculated as the square root of the adjusted R^2 value derived from the regression of the response on X_t. Because this adjusted R^2 value can be negative, an empirically-derived formula is applied when adjusted R^2 values fall below 0.1:

$$\text{Polynomial Pearson Coefficient} = (-6.67*RE_1{}^2 + 13.9*RE_1 - 6.24)*(R^2)^{0.5}$$

where

$$RE_1 = 1.015 - 1.856*R^2 + 1.862*adjR^2 - 0.000153*N.$$

R^2 and $adjR^2$ are defined by the regression of the response on X_t, and N = number of observations.

VB3 transformations (primarily converting x into x^b) have specific processing for certain data values and are not pure mathematical transformations -- they were designed to maintain data order while helping to linearize the response-IV relationship. For the SQUARE (b = 2), SQUAREROOT (b = 0.5), QUADROOT (b = 0.25), INVERSE (b = -1) and GENERAL EXPONENT (user-defined b) transformations, VB3 uses the signed equivalent of the mathematical function:

$$x^b == \text{sign}(x)*(\text{abs}(x))^b$$

For example: $(-2)^2 = -4$ $\quad$ $(-9)^{0.5} = -3$ $\quad$ $(-4)^{-0.5} = -0.5$ $\quad$ $(-2)^{-2} = -0.25$

To avoid potentially undefined values (e.g., 1/x when x = 0), the INVERSE and GENERAL EXPONENT (if the user sets b < 0) transformations have special processing:

If x = 0, VB3 will find the minimum value of abs(z) where z is the set of all non-zero values for the IV in question. To compute the transformation after z is defined, VB3 substitutes z/2 for x. From this definition, note that z can be a positive or negative number.

LOG_{10} and LOG_e transforms are also the signed equivalent of their mathematical functions:

$$\log_e(x) == \log_e(x)$$
$$\log_e(-x) == -\log_e(x)$$
$$\log_{10}(x) == \log_{10}(x)$$
$$\log_{10}(-x) == -\log_{10}(x)$$

In addition, if $(-1 \leq x \leq 1)$, then $\log_e(x) = 0$ and $\log_{10}(x) = 0$

VB_3 will not compute the INVERSE, GENERAL EXPONENT (with a negative b), LOG_{10} and LOG_e transformations for data columns if more than 10% of the IV values are zero. Programmatically, zero is defined as any number whose absolute value is less than 1.0e-21.

POLYNOMIAL transformations are the result of a linear regression of the response variable on the IV and the square of the IV:

$$Poly(x) = a + b*x + c*x^2$$

where a, b, and c are determined by a multiple linear regression of x and x^2 on the response variable.

In general, the name of the transformed column of data that VB_3 creates is simply the type of transformation, with the original data column name in parentheses. For example, the $\log_{10}$ of WaterTemp becomes LOG(WaterTemp); however, there are some exceptions:

INVERSE(x,y) : x is the original data column name and y is the z/2 value discussed in the last paragraph on page 80.

POWER(x,y) : when y is positive, x is the original data column name and y is the exponent specified by the user.

POWER(x,y,z) : when y is negative, x is the original data column name, y is the exponent specified by the user, and z is the z/2 value discussed earlier in this section.

POLY(x, a,b,c) : x is the original data column name and a, b, and c are the values of the polynomial regression coefficients.

A.2 Singular Matrices and Nominal Variables

The solution to least squares regression (MLR modeling is discussed in Section 7) involves computing the inverse of the X'X matrix (the X matrix contains the IV values for the model). When one IV is a linear combination of other IVs, the X'X matrix is *singular*, and trying to invert it produces a mathematical quandary (i.e., division by zero). Examples of variables that are linear combinations of other IVs:

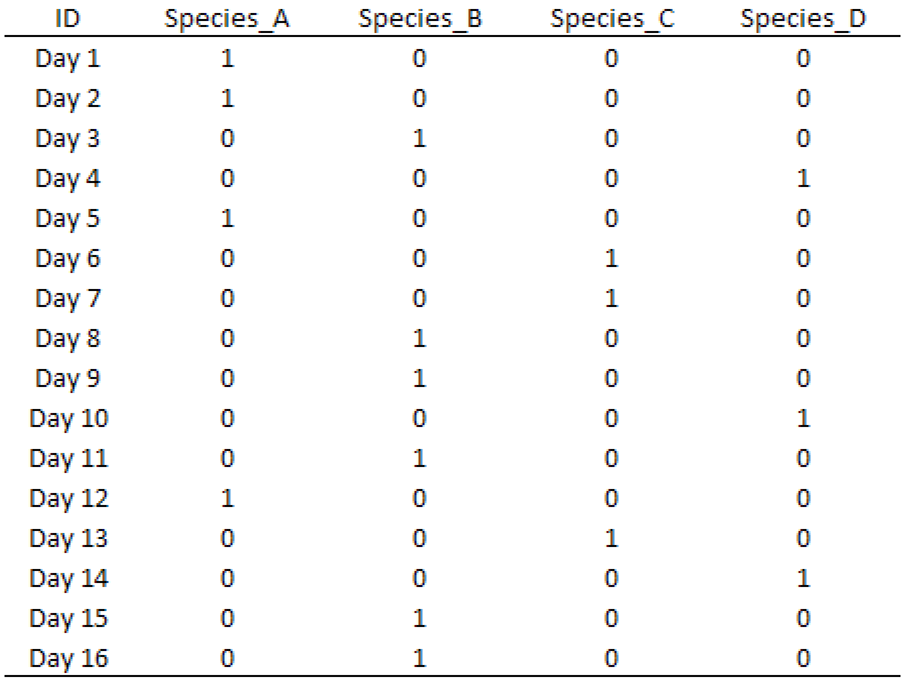
$$X_1 = 3.5 + 4.2*X_2$$
$$X_1 = 1 - X_2 - X_3 - X_4$$
$$X_3 = X_1 + X_2$$

In these examples, it doesn't matter if the IVs are continuous (real numbers) or categorical (0/1 values). In fact, VB_3 allows the user to produce, using the "manipulate" button described in section 6.6, IVs that are linear combinations of others (like example c above). When VB_3 evaluates MLR models, it checks each model for highly correlated IVs because perfectly correlated IVs lead to a matrix singularity and throws out any model with this condition (as measured by the Variance Inflation Factor, explained in Section 7.2). Using example equation c: attempting to compute a regression model involving X_1, X_2, and X_3, VB_3 will issue an error message.

Singularities are often produced if an IV with several categories is being defined using multiple indicator variables. Let's say there is an IV for cloud cover. One could make this categorical measure a continuous variable by using a single column with values ranging from 1 (no clouds) to 5 (completely overcast). This is acceptable because this IV is "ordinal" -- there is a natural order to its values. As values increase from 1 to 5, it implies more clouds.

There may be other categorical IVs that are "nominal," meaning there is no real order to their values. An example is the species of bird most abundant at the beach on a given day. If there are four possible species (A, B, C, D), it would be incorrect to code this IV in a single column with values 1, 2, 3, and 4. A value of 2 doesn't imply any larger mathematical quantity than a value of 1 or a smaller quantity than a value of 4. So the bird species should be coded as a series of indicator variables, using 0's and 1's (Table A.1):

Table A.1. Example of using 0/1 indicator variables for a multi-category IV



ID	Species_A	Species_B	Species_C	Species_D
Day 1	1	0	0	0
Day 2	1	0	0	0
Day 3	0	1	0	0
Day 4	0	0	0	1
Day 5	1	0	0	0
Day 6	0	0	1	0
Day 7	0	0	1	0
Day 8	0	1	0	0
Day 9	0	1	0	0
Day 10	0	0	0	1
Day 11	0	1	0	0
Day 12	1	0	0	0
Day 13	0	0	1	0
Day 14	0	0	0	1
Day 15	0	1	0	0
Day 16	0	1	0	0

A "1" denotes when a species is dominant and "0" when it isn't. Looking closely, we see that the four columns form a linear combination:

Species_D = 1 – Species_A - Species_B - Species_C

Given this relationship, VB$_3$ cannot evaluate a MLR model that includes all four columns (mathematically impossible due to a matrix singularity), but a model that contains three or fewer of the columns is acceptable, as is including all four columns in the dataset (but they will never occur together in a model). An advantage of PLS (Section 8) and GBM (Section 9) modeling is that they are not constrained by the collinearity of IVs and can compute solutions for models that include all four columns.

A.3 MLR Model Evaluation Criteria

If *p* is defined as the number of parameters in a model, *n* as the number of observations in the dataset, RSS as the residual sum of squares for a model, and TSS as the total sum of squares for a model, then the evaluation criteria for any model can be defined as:

- Akaike Information Criterion (AIC): $2p + n*\ln(RSS)$

- Corrected Akaike Information Criterion (AICC): $\ln(RSS/n) + (n+p)/(n-p-2)$

- R^2: $1 - RSS/TSS$

- Adjusted R^2: $1 - (1-R^2)(n-1)/(n-p-1)$

- Bayesian (Schwarz) Information Criterion (BIC): $= n*\ln(RSS/n) + p*\ln(n)$

- Root Mean Squared Error (RMSE): $(RSS/n)^{1/2}$

- Predicted Error Sum of Squares (PRESS): $1 - \Sigma(y_i - \hat{y}_{-i})^2 / \Sigma(y_i - y_m)^2$

where y_i is the i_{th} observation, $\hat{y}_{-i}$ is the model estimate of the i_{th} observation when the model coefficients are fitted with the i_{th} observation removed from the dataset, and y_m is the mean value of y in the dataset

- Accuracy: (true positives + true negatives) / number of total observations

- Specificity: true negatives / (true negatives + false positives)

- Sensitivity: true positives / (true positives + false negatives)