

WetQual GUI

User Manual

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Section 1: Introduction

The process-based Wetland Water Quality Model, *WetQual* (Hantush et al. 2013; Kalin et al. 2013; Sharifi et al. 2013) can simulate the hydrology as well as water quality including nitrogen (N), phosphorous (P), carbon (C), and sediment (including total suspended sediment [TSS]) cycles in natural and constructed wetlands. *WetQual* can be used in continuously flooded environments or in wetlands going through wetting and drying cycles.

The model partitions a wetland into three basic compartments: (1) (free) water column, (2) wetland soil layer, which is further portioned into aerobic and anaerobic zones, and (3) plant biomass (Hantush et al., 2013). The model simulates oxygen dynamics and the impact of oxidizing and reducing conditions on nitrogen transformation and removal, and approximates phosphorus precipitation and releases into soluble forms under aerobic and anaerobic conditions, respectively. Processes in the surface water and the bottom-active soil layer are described by a system of coupled ordinary differential equations (Hantush et al., 2013). The model runs on daily time scale, while the model internally divides the one-day time interval into smaller intervals for numerical integration.¹

This document describes the graphical user interface (GUI) developed for the *WetQual* model. The *WetQual* GUI enables users with a basic knowledge of hydrology and water quality to easily apply the model to their wetland sites and related projects. This GUI has been developed to handle continuously flooded wetlands (i.e., with free water above soil bed). The GUI reads in forcings data (i.e., climate/weather, runoff and nutrient loading) and geometry table (i.e., depth-area-volume-outflow relationship) to calculate wetland outflow, reference depth of water in wetland, wetland surface area, and volume of wetland surface water. The GUI allows the *WetQual* model to be run either in a deterministic or stochastic mode. In the stochastic mode, users need to select the probability distributions (uniform, log-normal, or triangular) and relevant statistics for each model parameter. The GUI generates random parameter sets and performs Monte Carlo simulations (MCS) to generate an ensemble of outputs. It provides an opportunity to visualize both deterministic and stochastic model outputs through series of graphs. With the latter, users can visualize the time series of various *WetQual* outputs for a particular parameter set. Alternatively,

¹ See the Appendix for a short description of *WetQual* subroutines and a flowchart which explains the internal structures/steps and processes of the *WetQual* model.

the GUI can also summarize the ensemble of model runs through prediction intervals. If observed data are available, the GUI can also perform Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Freer, 2001) and Bayesian Monte Carlo simulation or maximum likelihood estimation (BMCML) analyses so users can perform uncertainty analyses (Hantush and Chaudhary, 2014; and Chaudhary and Hantush, 2017).

Section 2: Installing the GUI

2.1 Minimum System Requirements

2.1.1 Hardware Requirements

- Personal computer using a Pentium IV processor or higher, running at 2.0 GHz or faster.
- 4 GB RAM.
- 700 MB free space on the hard drive for installation (including example project folder).
- Additional hard drive if MCS are going to be performed. For instance, 4 GB of additional free space on the hard drive are required to store the outputs of a run with 10,000 simulations for a 2-year run, to visualize the outputs and have a successful post-processing analysis. This is the most extreme case where the user had observed data for all the constituents. This is just an example of the space required so that users are aware of the space requirements for a *WetQual* GUI run and analyses.

2.1.2 Software Requirements

- Windows operating system (Windows 7 or higher version).
- Microsoft .NET Framework 4.5.2 or higher version.
- MATLAB® Compiler Runtime R2017a (9.2) (see Section 2.2 for its installation). (Only needed for the stochastic model. If the user will not run any stochastic simulations, there is no need to install this software.)

2.2 MATLAB Runtime Installation

MATLAB Compiler Runtime R2017a (9.2) is freely available online (<https://www.mathworks.com/products/compiler/matlab-runtime.html>). If MATLAB 2017a or MATLAB Compiler Runtime R2017a (9.2) is already installed on the computer, skip these steps and proceed to GUI installation in Section 2.3.

1. Download the MATLAB Compiler Runtime R2017a (9.2) software. The downloaded file name needs to be MCR_R2017a_win64_installer.exe. Double click the file to start the installation. During the installation, if any warning or permission requests appear, select **Yes** or **Accept** to continue the installation. After MATLAB Runtime installer extracts the necessary files (Figure 2.1), click the **Next** button to continue installation (Figure 2.2).

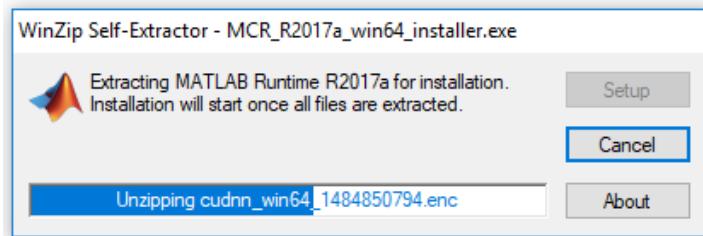


Figure 2.1

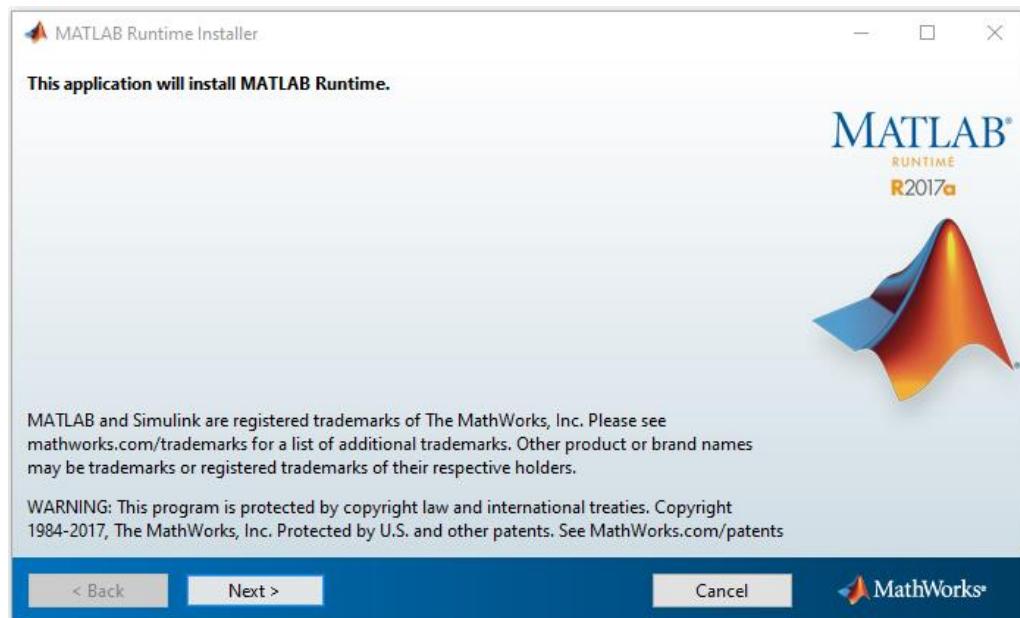


Figure 2.2

2. The next window asks for the MATLAB Runtime installation folder location. It is advised to keep the default folder (Figure 2.3). The license agreement on the next screen must be accepted to install MATLAB Compiler Runtime (Figure 2.4).

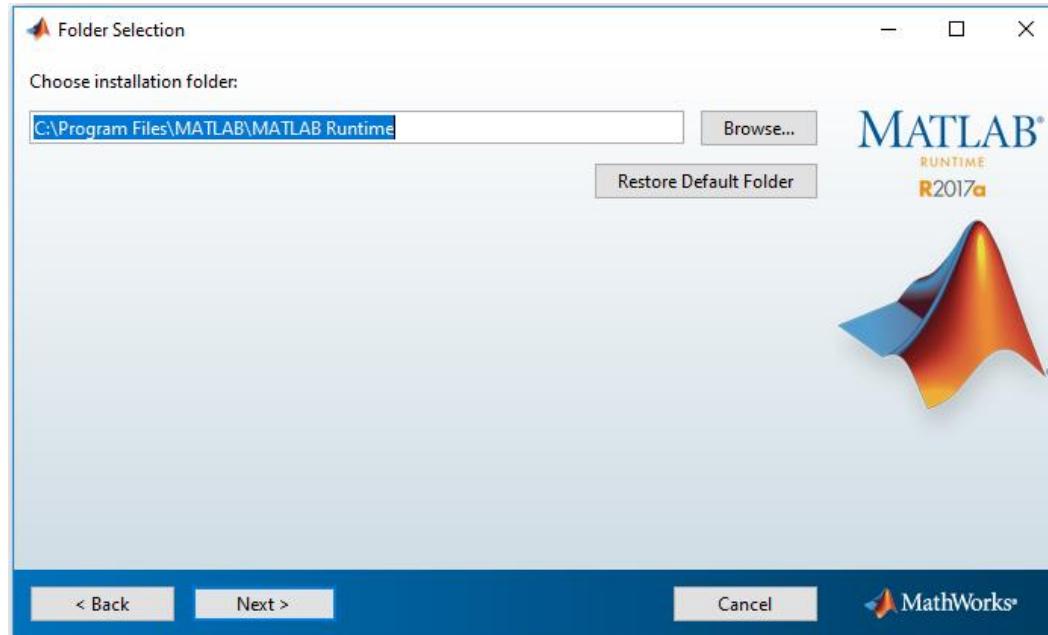


Figure 2.3

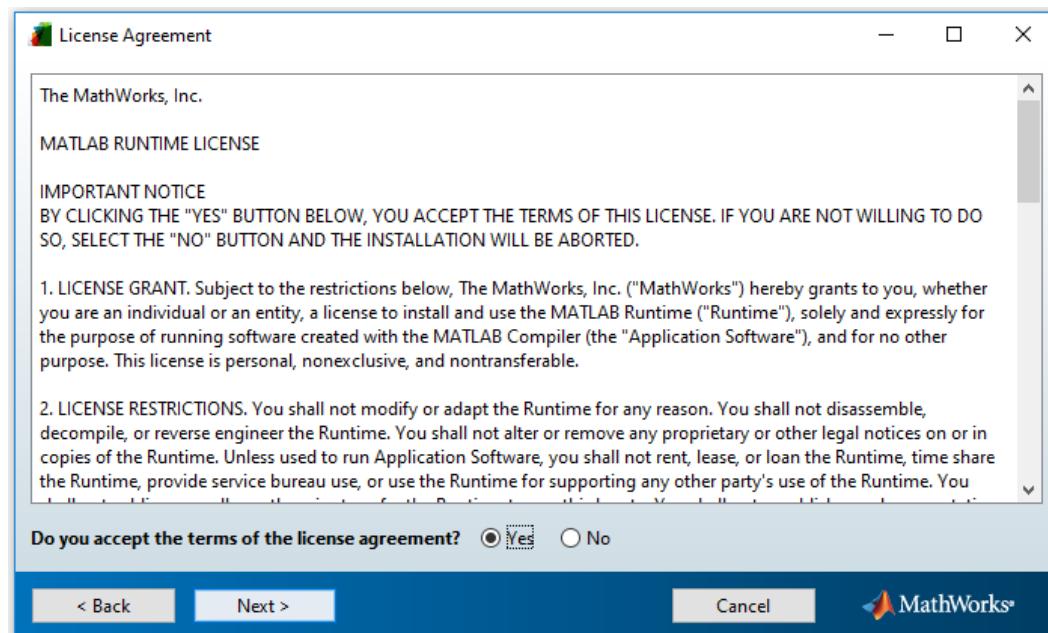


Figure 2.4

3. On the next window, click **Install** to start the MATLAB Runtime installation. The installation can take several minutes depending on the computer speed (Figure 2.5 and Figure 2.6).

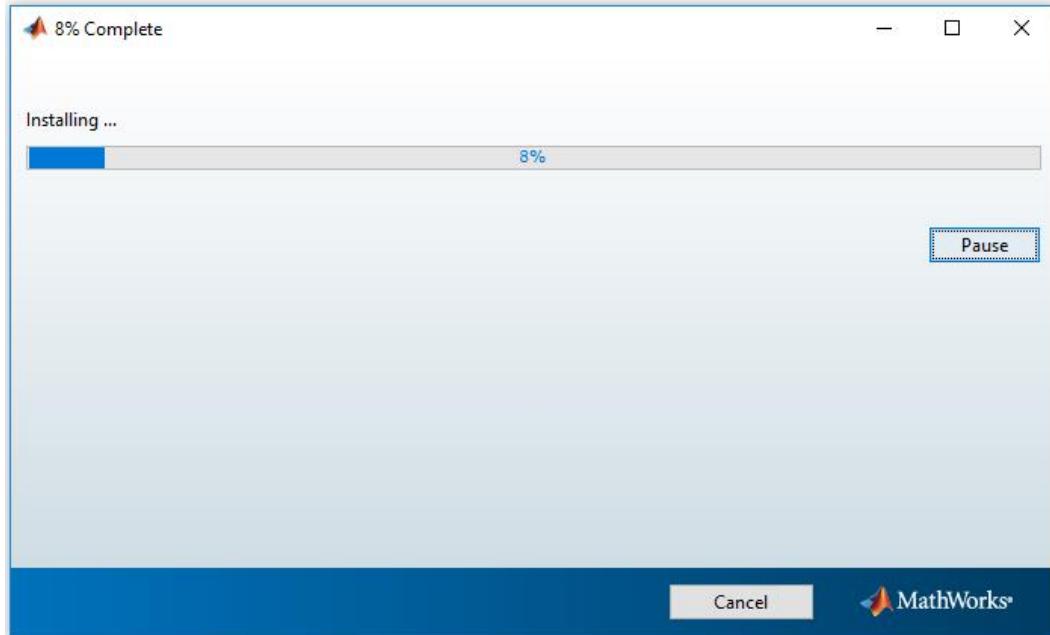


Figure 2.5

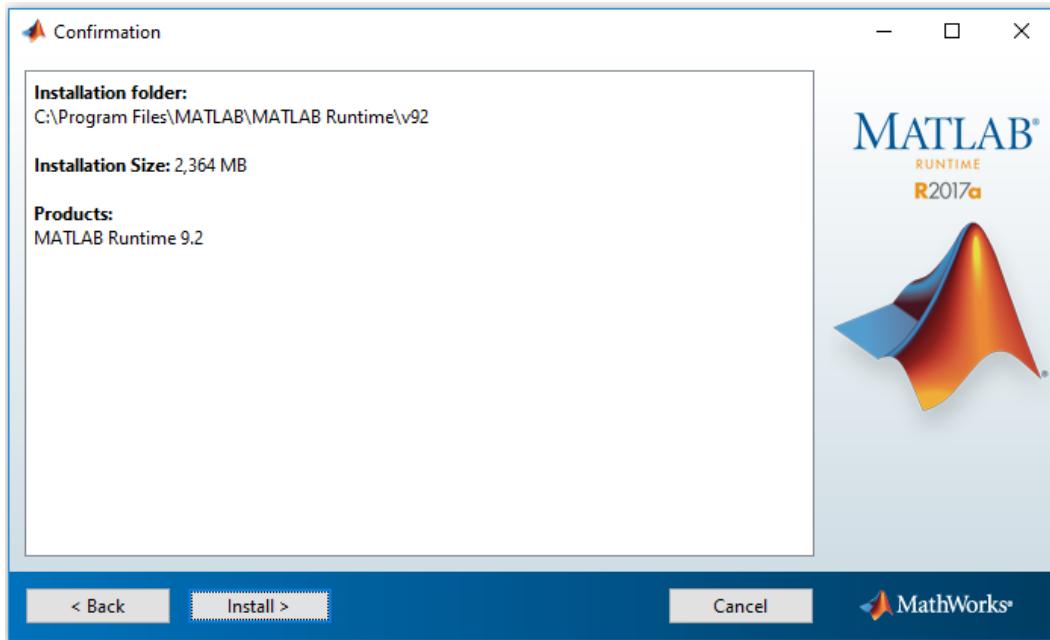


Figure 2.6

4. After the installation is complete, click **Finish** to close the installation window (Figure 2.7).

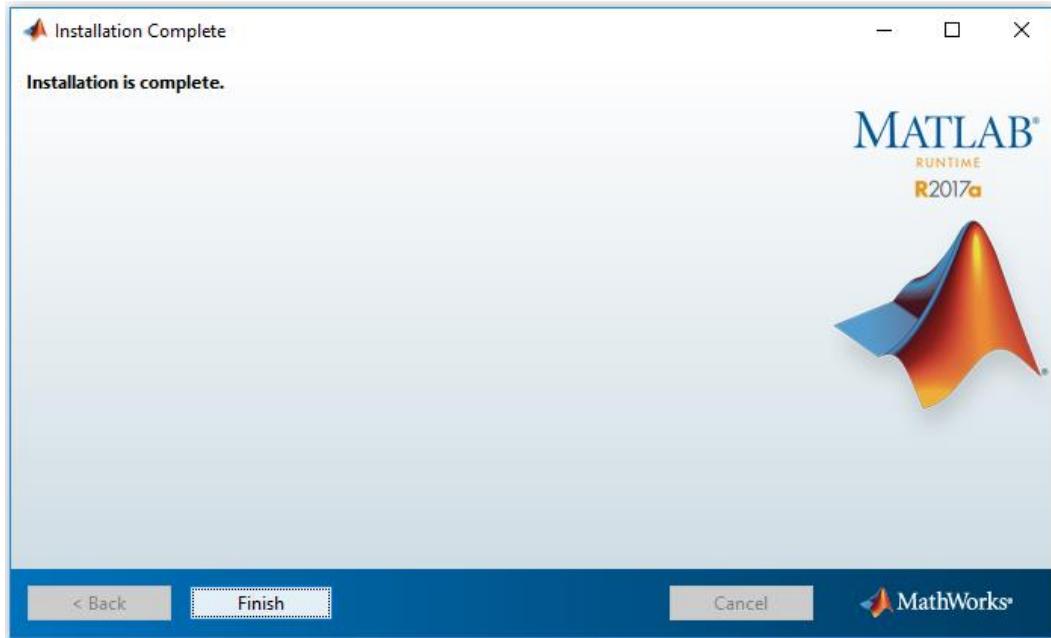


Figure 2.7

2.3 GUI Installation

1. All previous versions of the GUI must be uninstalled before installing the GUI (i.e., *WetQual_Install.msi*) using **Add/Remove Programs in Programs and Features** under Control Panel.
2. Double click the *WetQual_Install.msi* file and the following dialog window will appear (Figure 2.8).

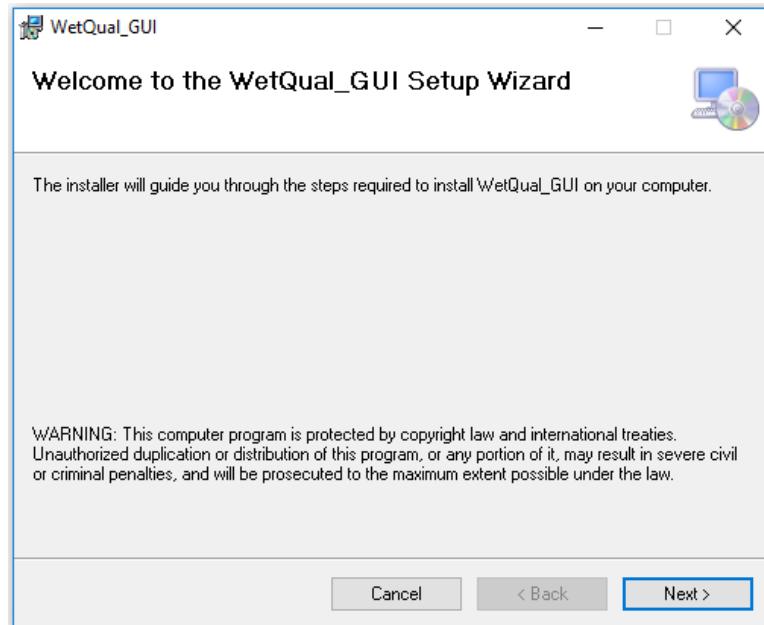


Figure 2.8

3. Click **Next** and then choose the installation folder. The default folder, *C:\WetQual*, is recommended (Figure 2.9).

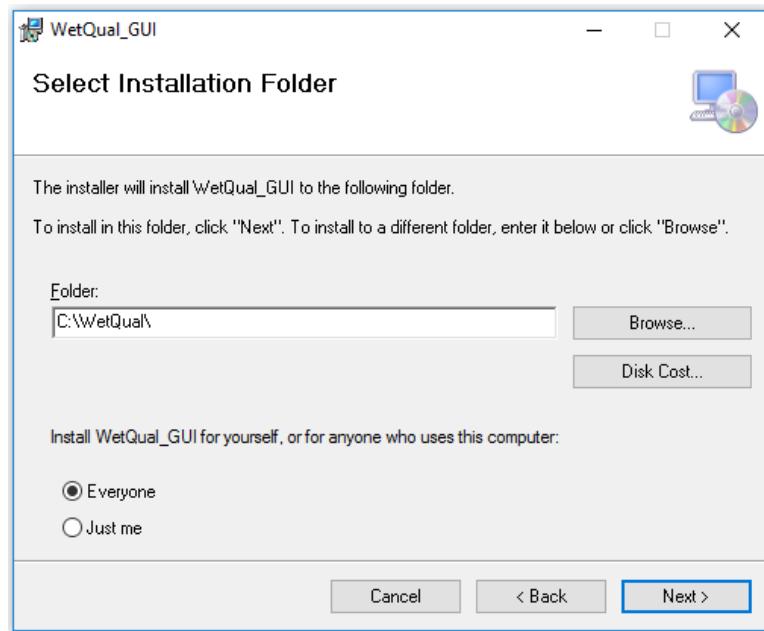


Figure 2.9

4. Click **Next** and confirm installation in the next dialog (Figure 2.10).

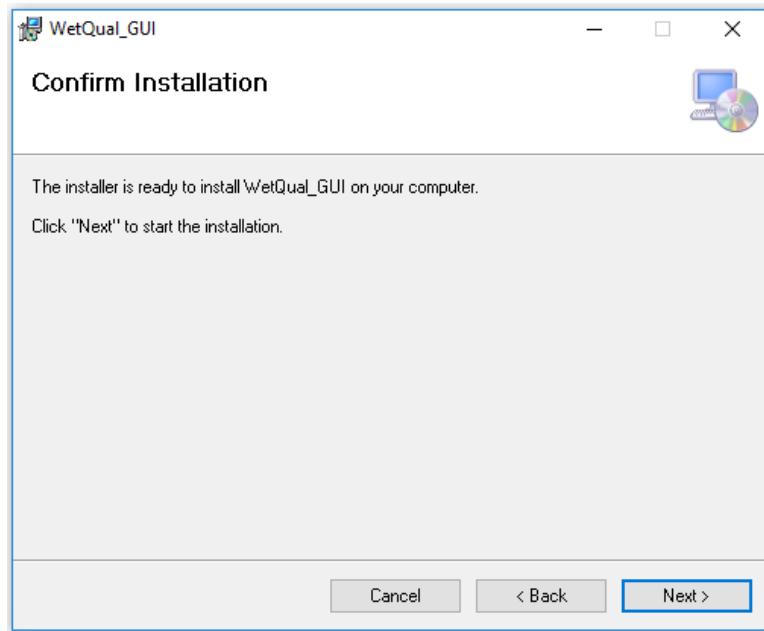


Figure 2.10

2.4 Structure of the Installation Folder

Under the *WetQual* installation folder, the process creates two folders: *InputOutput* and *Observations* (Figure 2.11).

Name	Date modified	Type
InputOutput	10/5/2017 9:36 AM	File folder
Observations	10/5/2017 9:36 AM	File folder

Figure 2.11

The *InputOutput* folder contains all the input files required for running *WetQual* (listed below). When a new project is created, the GUI program will initially copy those files from the installation source files. The user needs to update those with their own data. Only short descriptions of those files are given below. Detailed descriptions and formats of input/output files and all the model parameters are explained later in relevant sections. The GUI is interactive in reading necessary files and generating outputs.

- ***1_input_control.txt***: This file acts as a master (control) file for running *WetQual* where the names of the required input files need to be provided. The name of the file *1_input_control.txt* should not be changed. The GUI requires the six input files shown in Figure 2.12.

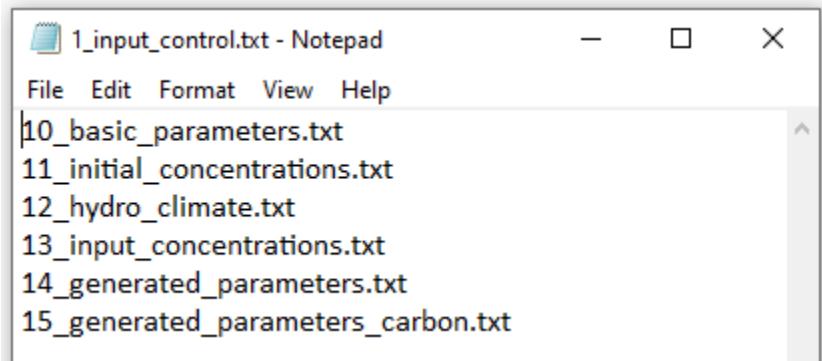
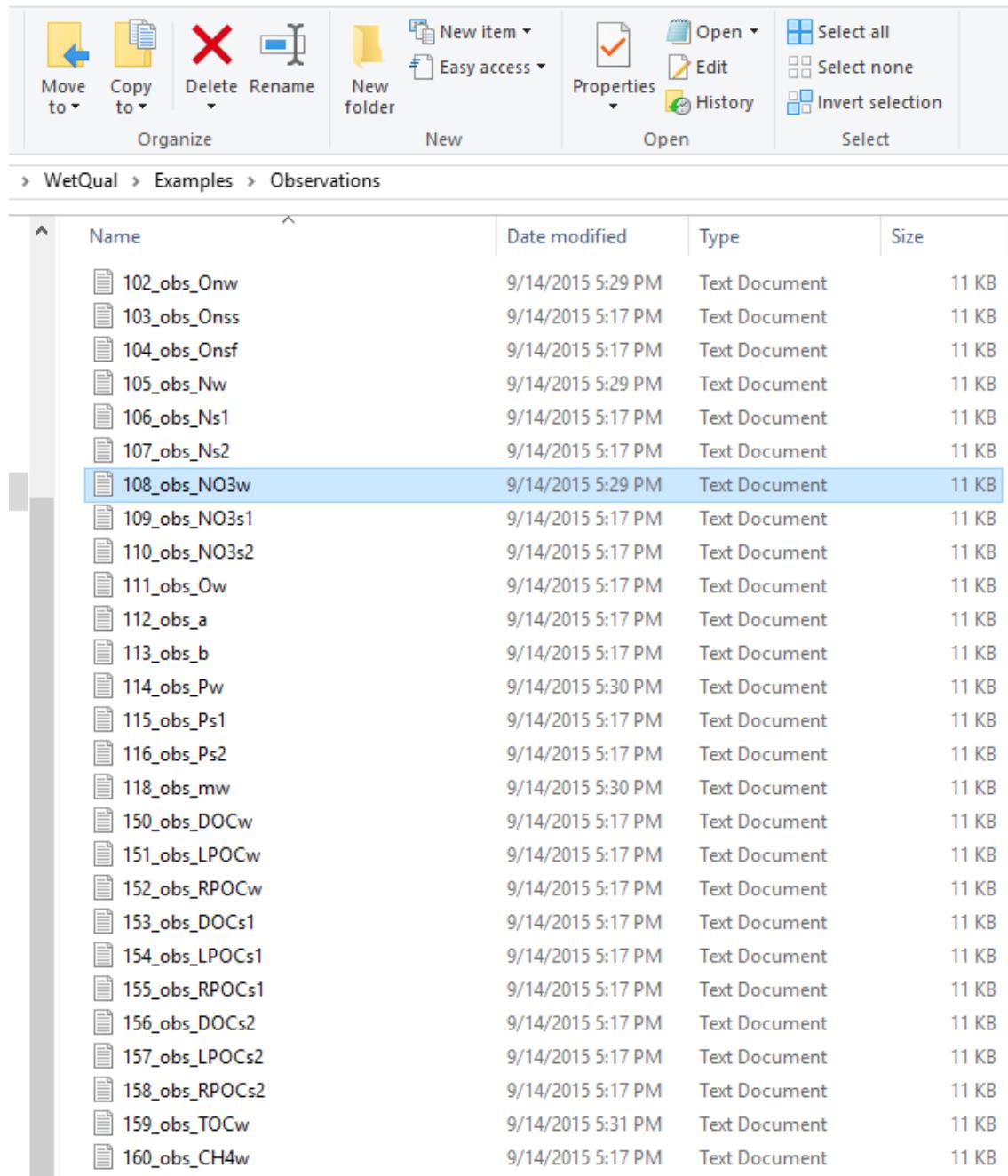


Figure 2.12

- ***10_basic_parameters.txt***: This input file provides basic parameters of *WetQual* (i.e., model parameters that are not calibrated or considered random during stochastic simulations).
- ***11_initial_concentration.txt***: Initial concentrations of nitrogen (N), phosphorus (P), total suspended sediment (TSS), and carbon (C) are provided to *WetQual* within this file.
- ***12_hydro_climate.txt***: The time series of hydro-climate input forcings are read and imported to *WetQual* with this file.
- ***13_input_concentrations.txt***: Time series of nutrient concentrations in incoming flow.
- ***14_generated_parameters.txt***: Some of the *WetQual* parameters related to N, P, and TSS processes, which are considered to be random in stochastic mode or need calibration in deterministic mode are provided in this file. Each row represents one parameter set. If a deterministic run is selected, there will be only one row of data. The user does not need to prepare this file externally. The GUI populates the parameter values from selected distributions. This is explained in more detail later.
- ***15_generated_parameters_carbon.txt***: This file is similar to *14_generated_parameters.txt* with parameters related to carbon.

If observed data exist for any of the model output variables (e.g., suspended sediment concentration in water column, nitrate concentration in aerobic sediment layer), then copy the files containing such data into the *Observations* folder. See Table A.6 in the appendix for a list of

WetQual output filenames. During post-processing, the GUI looks for the exact same filename as a particular output in the *Observations* folder. For example, to see NO_{3w} post-processing results, the file *108_obs_NO3w.txt* should be placed in the *Observations* folder (Figure 2.13). The formats of the observed files are explained in Section 3.6.2.



Name	Date modified	Type	Size
102_obs_Onw	9/14/2015 5:29 PM	Text Document	11 KB
103_obs_Onss	9/14/2015 5:17 PM	Text Document	11 KB
104_obs_Onsf	9/14/2015 5:17 PM	Text Document	11 KB
105_obs_Nw	9/14/2015 5:29 PM	Text Document	11 KB
106_obs_Ns1	9/14/2015 5:17 PM	Text Document	11 KB
107_obs_Ns2	9/14/2015 5:17 PM	Text Document	11 KB
108_obs_NO3w	9/14/2015 5:29 PM	Text Document	11 KB
109_obs_NO3s1	9/14/2015 5:17 PM	Text Document	11 KB
110_obs_NO3s2	9/14/2015 5:17 PM	Text Document	11 KB
111_obs_Ow	9/14/2015 5:17 PM	Text Document	11 KB
112_obs_a	9/14/2015 5:17 PM	Text Document	11 KB
113_obs_b	9/14/2015 5:17 PM	Text Document	11 KB
114_obs_Pw	9/14/2015 5:30 PM	Text Document	11 KB
115_obs_Ps1	9/14/2015 5:17 PM	Text Document	11 KB
116_obs_Ps2	9/14/2015 5:17 PM	Text Document	11 KB
118_obs_mw	9/14/2015 5:30 PM	Text Document	11 KB
150_obs_DOCw	9/14/2015 5:17 PM	Text Document	11 KB
151_obs_LPOCw	9/14/2015 5:17 PM	Text Document	11 KB
152_obs_RPOCw	9/14/2015 5:17 PM	Text Document	11 KB
153_obs_DOCs1	9/14/2015 5:17 PM	Text Document	11 KB
154_obs_LPOCs1	9/14/2015 5:17 PM	Text Document	11 KB
155_obs_RPOCs1	9/14/2015 5:17 PM	Text Document	11 KB
156_obs_DOCs2	9/14/2015 5:17 PM	Text Document	11 KB
157_obs_LPOCs2	9/14/2015 5:17 PM	Text Document	11 KB
158_obs_RPOCs2	9/14/2015 5:17 PM	Text Document	11 KB
159_obs_TOCw	9/14/2015 5:31 PM	Text Document	11 KB
160_obs_CH4w	9/14/2015 5:17 PM	Text Document	11 KB

Figure 2.13

The installation folder *WetQual_Install* includes some other files that are automatically generated as complementary files of the GUI (Figure 2.14).

A desktop icon is created to run *WetQual* once installation is complete.

Name	Date modified	Type	Size
InputOutput	5/9/2018 12:14 PM	File folder	
Observations	5/9/2018 12:14 PM	File folder	
Accord.dll	12/10/2015 3:08 PM	Application extens...	64 KB
Accord.dll.config	12/10/2015 3:08 PM	XML Configuratio...	1 KB
Accord.Math.dll	12/10/2015 3:08 PM	Application extens...	588 KB
Accord.Math.xml	12/10/2015 3:08 PM	XML File	1,262 KB
Accord.Statistics.dll	12/10/2015 3:08 PM	Application extens...	624 KB
Accord.Statistics.xml	12/10/2015 3:08 PM	XML File	2,781 KB
Accord.xml	12/10/2015 3:08 PM	XML File	186 KB
AcroPDF.dll	7/31/2017 5:31 PM	Application extens...	469 KB
AxInterop.AcroPDFLib.dll	5/9/2018 12:13 PM	Application extens...	8 KB
Interop.AcroPDFLib.dll	5/9/2018 12:13 PM	Application extens...	12 KB
MathNet.Numerics.dll	11/17/2015 2:01 PM	Application extens...	1,128 KB
MathNet.Numerics.xml	11/17/2015 2:01 PM	XML File	3,078 KB
MWArray.dll	1/11/2016 4:58 PM	Application extens...	114 KB
OxyPlot.dll	11/1/2015 1:42 PM	Application extens...	472 KB
OxyPlot.pdb	11/1/2015 1:42 PM	Program Debug D...	1,024 KB
OxyPlot.Wpf.dll	2/10/2016 9:25 PM	Application extens...	157 KB
OxyPlot.Xps.dll	2/10/2016 9:25 PM	Application extens...	13 KB
System.Net.Http.dll	5/28/2014 5:35 AM	Application extens...	82 KB
User_Manual_WetQual_GUI_V.1.0.pdf	2/13/2017 4:32 PM	Adobe Acrobat D...	2,317 KB
WetQual.exe	5/9/2018 12:13 PM	Application	1,706 KB
WetQual.exe.config	12/10/2015 3:08 PM	XML Configuratio...	1 KB

Figure 2.14

2.5 Preparing Input Files for the GUI

It is strongly recommended that the input files are prepared before getting started with the GUI. Sample input files are provided in the *Project* folder. An Excel file named *Sample_InputFiles_for_WetQual.xls*, which includes all necessary input files, is also provided in

the *Project* folder. Each sample input file is available as a separate sheet named with the input file name.

Templates are provided for *10_basic_parameters.txt*, *11_initial_concentration.txt*, *12_hydro_climate.txt*, and *13_input_concentrations.txt* in the Excel file. The GUI can automatically generate the files *14_generated_parameters.txt* and *15_generated_parameters_carbon.txt*, so templates are not provided for these files.

In addition to the input files described above that are needed to run *WetQual*, other input files are required to perform a flow routing analysis for preparing hydrologic input files to *WetQual*. The hydrologic routing calculation in *WetQual* requires three input files: *1_basic_inputs.txt*, *2_input_time_series.txt*, and *3_bathymetry_inputs.txt*. Templates of these three files are also available in the Excel file. If evapotranspiration (ET) will be calculated by the GUI (user can provide ET data externally too), the *1_ET_inputs.txt* input file is also needed. A sample of this input file is also provided in the Excel file.

Note: The input files do not need to be in the project folder. However, placing the input files in the project folder will reduce the chance of any potential errors. Note that the format of all input files is space delimited.

Section 3: Using the GUI

3.1 GUI Toolbar Items

The following sections describe the functionality of the different menus available from the GUI Toolbar. As can be seen in Figure 3.1, the toolbar includes Home, Input Files, Model Parameters, Run, Post-processing, Forecasting, and Help menus, which are explained in the following sections.

The Input Files, Model Parameters, Run, Post-processing, and Forecasting menus are not active initially (Figure 3.1). They will be unlocked as the project setup progresses.

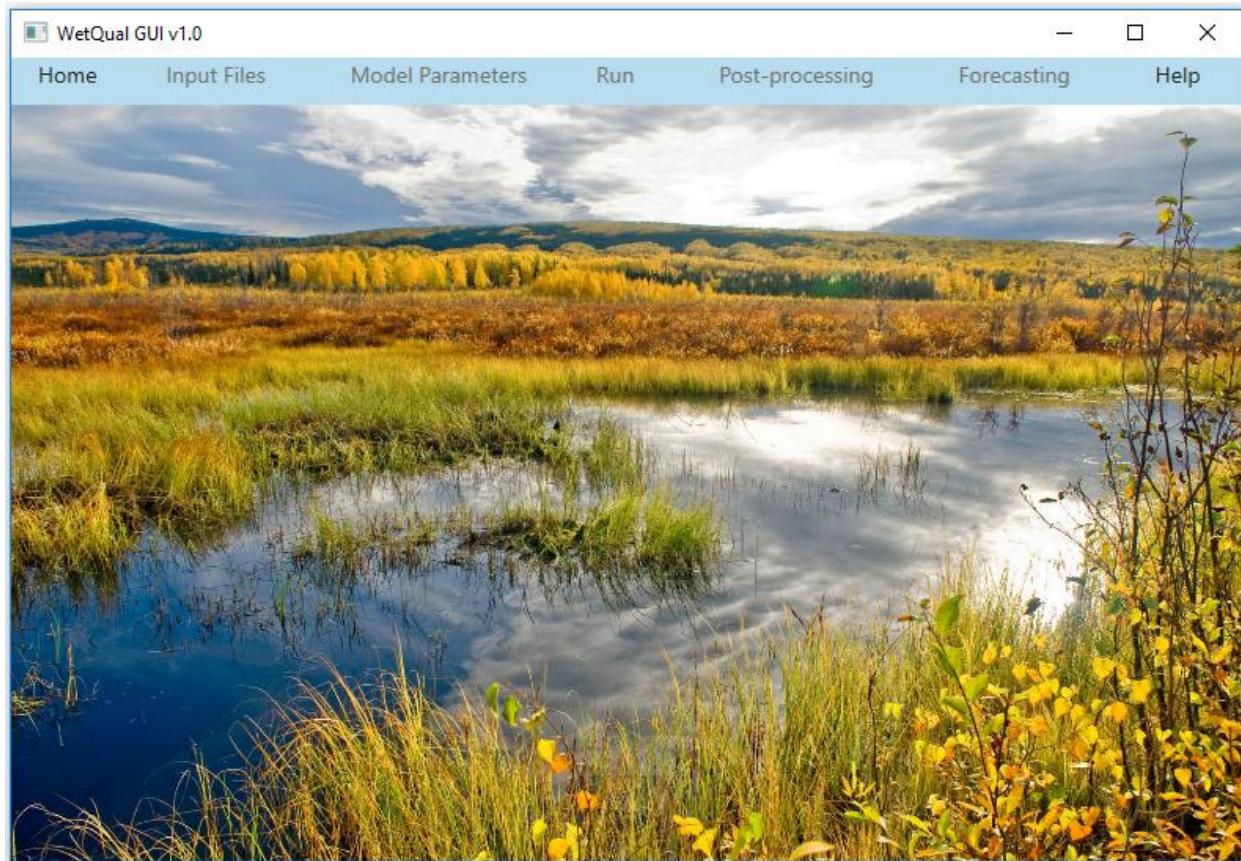


Figure 3.1

3.2 Home

The Home menu includes items that control the setup and management of projects. This menu includes the Open Project, New Project, Save As, and Exit options (Figure 3.2).



Figure 3.2

3.2.1 Open Project

Select **Open Project** under the **Home** menu to load a previously created project or one of the example projects provided with the GUI. Loading an existing project activates all the menus in the GUI, meaning that the user will have access to the **Post-processing** and **Forecasting** (only with the stochastic runs) menus.

On the navigation bar, clicking **Home>Open Project** will pop up the window shown in Figure 3.3. After selecting the folder where the project resides, press **OK** to open the selected project.

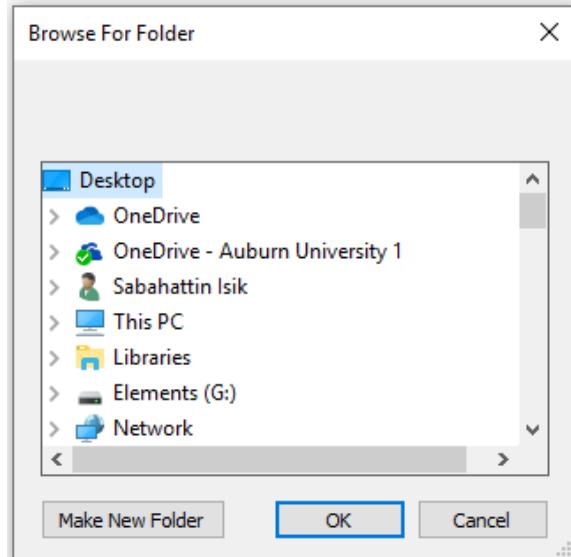


Figure 3.3

If the wrong folder is opened through **Open Project**, the error message shown in Figure 3.4 will appear. The selected folder needs to contain at least the *InputOutput* and *Observations* folders with the required input files inside them.

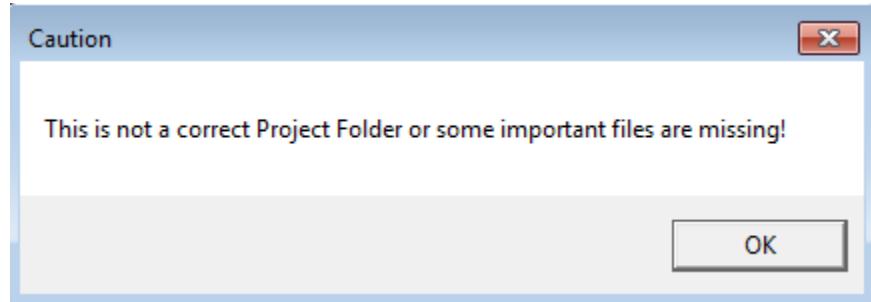


Figure 3.4

3.2.2 New Project

This option is for creating a new project. When a project is created, the **Input Files** menu will be activated. A starting date of simulation, hydro-climate data, basic parameters, initial concentration, and input concentrations must be provided for the project.

On the navigation bar, click on **Home>New Project** and it will pop up the *Browse For Folder* dialog box as shown in Figure 3.3. In this box, navigate to the folder where the new project will be stored. Use **Make New Folder** (Figure 3.3) or select an available folder (not necessarily an empty folder) and click **OK**.² The GUI copies the sample input/output files/folders under the selected or newly created folder. The GUI guides the user to update these files step by step.

3.2.3 Copying a Project

The **Save As** option copies the project the user is currently working on to a new folder. No separate Save option is available since clicking any button or requesting a process saves the results in each step.

3.3 Input Files

The **Input Files** menu contains **Select Start Date**, **Hydro-Climate Parameters**, **Basic Parameters**, and **Water Quality** sub-menus, which are needed to setup a new project. Figure 3.5 displays these sub-menus.

² User needs to have administrative rights to access and create new files inside the folder.

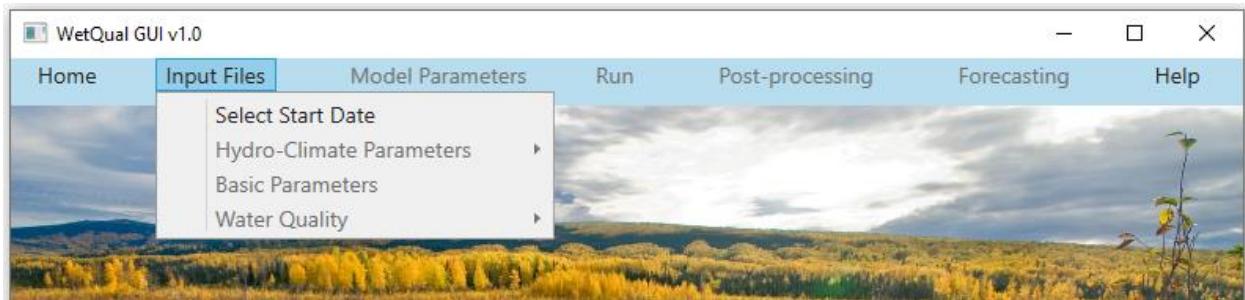


Figure 3.5

3.3.1 Select Start Date

This opens a window that asks for a start date for the simulations (Figure 3.6). The default start date is 5/9/1995 (month/day/year format), which is the start date of the example project. If the computer's date format is not month/day/year, this should be changed in the computer's region settings. *WetQual* needs the day number within a year (Julian days) for the equations governing rooted/benthic plant growth/death. Hence, having a starting day for the simulation helps keep track of the number of days for related calculations in the model. After choosing the date, click **Confirm**.

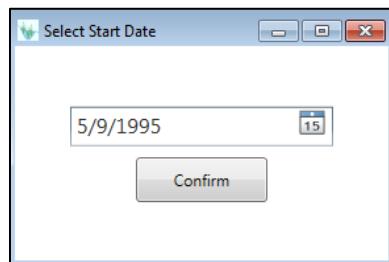


Figure 3.6

3.3.2 The Hydro-Climate Parameters

The **Hydro-Climate Parameters** menu can be used to upload pre-existing hydro-climatic data and perform flow routing to calculate time series of wetland area, volume, and outflow (Figure 3.7). If time series of wetland area, volume, and outflow values are available in advance, flow routing is not needed. If ET data are not available, the GUI can calculate ET as explained later (enter zero for all ET values initially). If *Twater*, *Qout*, *Area*, and *Vw* are also not available, they can be entered as zero or any other number. In this case, they should be replaced using the steps below. Selecting **Pre-existing Data** opens the *Select a File for Hydro-Climate Data* window (Figure 3.8) for

browsing and selecting the related file (here, hydro-climate input file). The name of the file does not need to be *12_hydro_climate.txt* as shown in the figure.

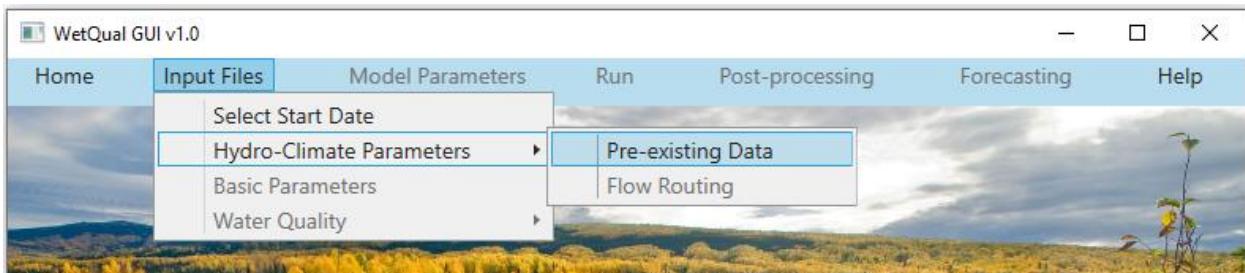


Figure 3.7

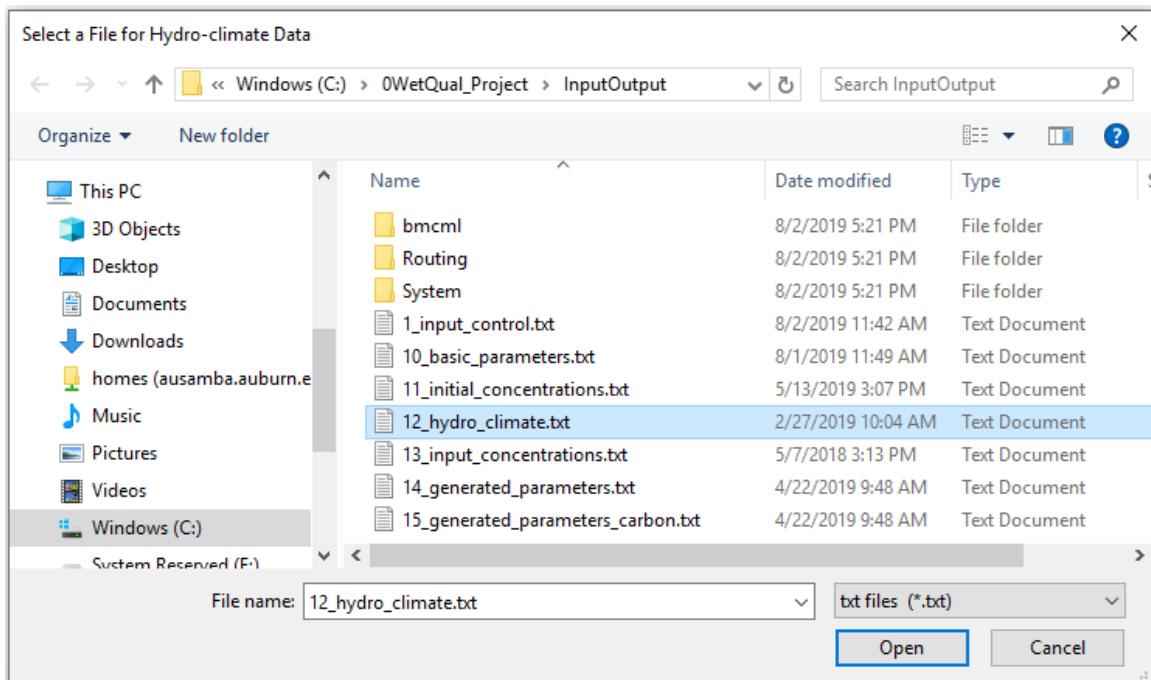


Figure 3.8

Figure 3.9 shows sample hydro-climate data. As with other input files, data in this file are space delimited. The first two rows are for parameter symbols and their units. Follow the same format when defining a new project. Once the file is selected, the GUI reads and checks the data and places it in the *12_hydro_climate.txt* file in the *InputOutput* folder.

The screenshot shows a Notepad window titled "12_hydro_climate.txt - Notepad". The data is presented in a tabular format with the following columns:

Date	Qin	Qout	Vw	Area	ET	ip	Qg	Uw	air temp	water temp
5/9/1995	0	0	2324.4	7922.2	0.22	0.01	0	3.3975	16.48	0
5/10/1995	126.59	0.82	2502.6	8259.1	0.24	2.34	0	4.1575	17.07	0
5/11/1995	75.35	22.34	2692.9	8598.1	0.29	0.7	0	2.414	18.56	0
5/12/1995	2.86	17.97	2676.4	8569.6	0.3	0.1	0	4.0234	18.88	0
5/13/1995	0	11.29	2643	8511.5	0.29	0	0	3.4869	18.55	0
5/14/1995	76.41	15.78	2658.6	8538.5	0.27	0.68	0	4.0234	17.84	0
5/15/1995	0	18.85	2679.2	8574.5	0.32	0.07	0	4.828	19.41	0
5/16/1995	0	7.74	2619.9	8470.9	0.29	0	0	2.6375	18.4	0
5/17/1995	22.37	3.68	2584.5	8408.2	0.34	0.36	0	3.1293	20.06	0
5/18/1995	542.73	122.14	2800.4	8772	0.4	1.3	0	2.5034	21.55	0
5/19/1995	92.52	281.55	3078	9220.1	0.34	1.33	0	4.6045	19.89	0
5/20/1995	0	124.95	2905.1	8950.5	0.31	0	0	4.381	19.09	0
5/21/1995	0	50.22	2773.6	8735	0.36	0	0	3.8445	20.36	0

Figure 3.9

Once the hydro-climate file is selected, the *Hydro-Climate Data* window opens (Figure 3.10), which shows the same hydro-climate data in table format. If data in the selected file are not in the correct format, or a wrong file is selected, the GUI will give an error (see Figure 3.11 and Figure 3.12). In such case, the GUI will not continue to the next step and will not allow further processing until valid data are provided. The user needs to close the window and try again after correcting the data format.

The screenshot shows the "Hydro-Climate Data" window. At the top, there are buttons for "View Graph" and "Tair to Twater". Below the buttons is a row of input fields for each column header: Date, Qin, QOut, Vw, Area, ET, ip, Qg, Uw, Tair, and Twater. A "Save" button is located to the right of the Twater field. The main area contains a table with the same data as Figure 3.9.

Date	Qin	QOut	Vw	Area	ET	ip	Qg	Uw	Tair	Twater
05/09/1995	0	0	2301.2800	7935.4487	0.22	0.01	0	3.3975	16.48	17.36
05/10/1995	126.59	11.99072	2613.5029	8515.8105	0.24	2.34	0	4.1575	17.07	17.8025
05/11/1995	75.35	115.34381	2877.94185	8918.61621	0.29	0.7	0	2.414	18.56	18.92
05/12/1995	2.86	65.64739	2787.2189	8776.69141	0.3	0.1	0	4.0234	18.88	19.16
05/13/1995	0	20.49546	2663.4943	8576.34961	0.29	0	0	3.4869	18.55	18.9125
05/14/1995	76.41	36.91365	2708.4834	8650.2363	0.27	0.68	0	4.0234	17.84	18.38
05/15/1995	0	36.93112	2708.5312	8650.3144	0.32	0.07	0	4.828	19.41	19.5575
05/16/1995	0	13.61504	2626.8378	8530.5761	0.29	0	0	2.6375	18.4	18.8
05/17/1995	22.37	11.39325	2608.5979	8510.3544	0.34	0.36	0	3.1293	20.06	20.045
05/18/1995	542.73	282.95932	3076.0605	9215.0771	0.4	1.3	0	2.5034	21.55	21.1625
05/19/1995	92.52	326.02722	3115.1245	9271.4345	0.34	1.33	0	4.6045	19.89	19.9175
05/20/1995	0	106.58932	2865.6418	8899.5712	0.31	0	0	4.381	19.09	19.3175

Figure 3.10

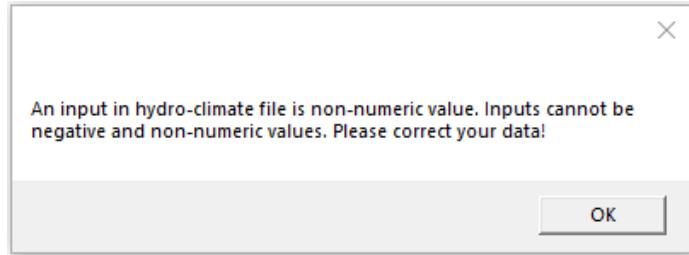


Figure 3.11

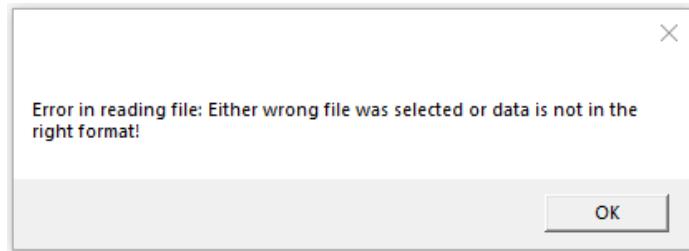


Figure 3.12

Hydro-climate data require time series data for inflow rate (Q_{in} , m³/day), outflow rate (Q_{out} , m³/day), volume of wetland (V_w , m³), wetland surface area (A , m²), evapotranspiration rate (ET , cm/day), precipitation rate (ip , cm/day), groundwater discharge (Q_g , m³/day; negative for infiltration/recharge), wind speed (U_w , m/s), daily average air temperature (T_{air} , °C), and daily water temperature (T_{water} , °C), respectively. More details about the definitions, symbols, and units are given in the Appendix. This order must be followed when preparing hydro-climate data for projects. If T_{water} data are not available, daily average air temperature (T_{air}) can be provided and daily water temperature (T_{water}) data can be entered as zeros. The *WetQual* GUI can use T_{air} to estimate T_{water} using the equation developed by Stefan and Preud'homme (1993) for a well-mixed stream:

$$T_{water} = 5.0 + 0.75 T_{air}$$

Clicking the **T_{air} to T_{water}** button on the *Hydro-Climate Data* window causes the T_{water} values to be computed in both the *Hydro-Climate Data* window and the hydro-climate input file (Figure 3.13). This step is not necessary if T_{water} data are in the hydro-climate input file.

Note: Do not add any blank rows at the end of input files.

Values can be edited by choosing the row where the data are located. In Figure 3.13, the third row is selected as an example. The GUI shows the selected row at the top that can be edited. After editing the value(s), click the **Save** button to save the changes. If the window is closed without saving, any changes made will be lost. Also, the parameters come with a tooltip that shows the definition and unit (if applicable) of a parameter when the cursor is held over the parameter's symbol. Click the **View Graph** button to open a new window where a parameter can be selected to see its time series graph. On the graphical report page (Figure 3.14), pick other parameters from pull down menus and the graph will automatically be updated. The graphs are dynamic and the view can be zoomed in or out.

The screenshot shows a software window titled "Hydro-Climate Data". At the top, there is a toolbar with buttons for "View Graph" and "Tair to Twater". Below the toolbar is a table with various parameters: Date, Qin, QOut, Vw, Area, ET, ip, Qg, Uw, Tair, and Twater. The third row of the table is highlighted in blue, indicating it is selected for editing. The "Qin" cell in this row contains the value "75.35". To the right of the table is a "Save" button. Below the table is a scrollable data grid showing historical data for the same parameters across several dates from 1995 to 1996.

Date	Qin	QOut	Vw	Area	ET	ip	Qg	Uw	Tair	Twater
	75.35	115.34381	2877.9418	8918.6162	0.29	0.7	0	2.414	18.56	18.92
05/09/1995	0	0	2301.2800	7935.4487	0.22	0.01	0	3.3975	16.48	17.36
05/10/1995	126.59	11.99072	2613.5029	8515.8105	0.24	2.34	0	4.1575	17.07	17.8025
05/11/1995	75.35	115.34381	2877.9418	8918.6162	0.29	0.7	0	2.414	18.56	18.92
05/12/1995	2.86	65.64739	2787.2189	8776.6914	0.3	0.1	0	4.0234	18.88	19.16

Figure 3.13

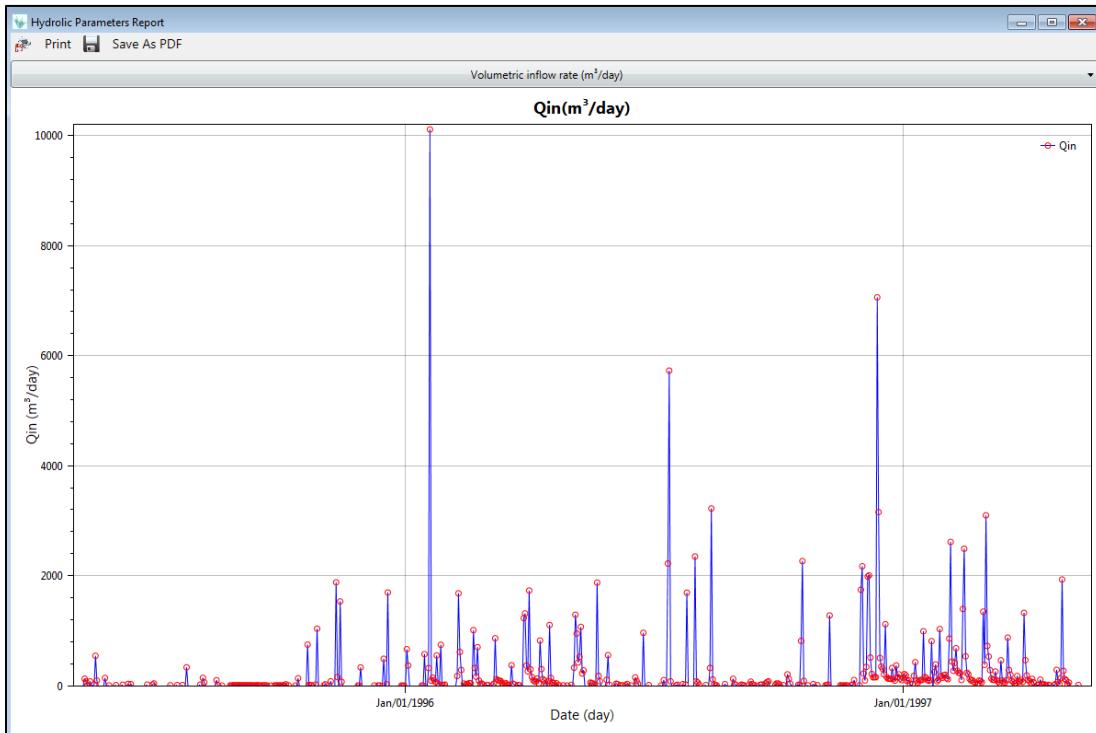


Figure 3.14

3.3.3 Flow Routing

If time series of wetland area, volume, and outflow data are unavailable, flow routing using the **Flow Routing** menu (Figure 3.15) is needed to generate the necessary hydrologic data. Flow routing in the *WetQual* GUI is based on solutions of the continuity equation using the third-order Runge-Kutta method. Navigate to the **Flow Routing** section by following: **Input Files>Hydro-Climate Parameters>Flow Routing**. Follow the pre-existing data importing procedure described above before performing flow routing and enter zero for Q_{out} , V_w , and $Area$ in the hydro-climate data file. Those values will be updated once flow routing is completed.

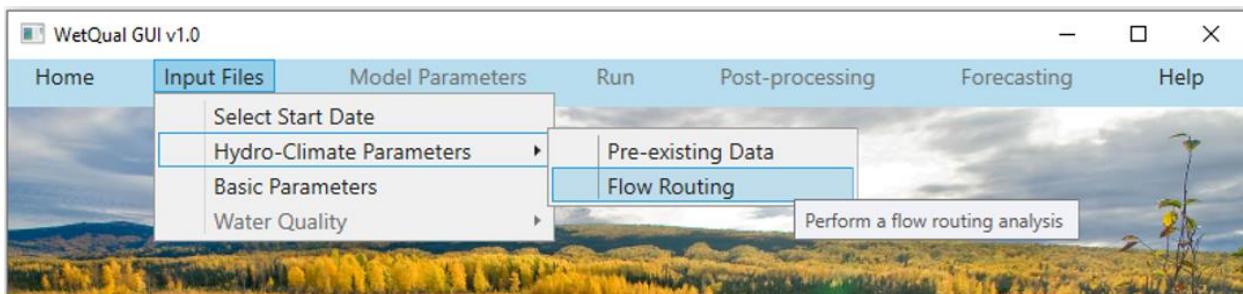


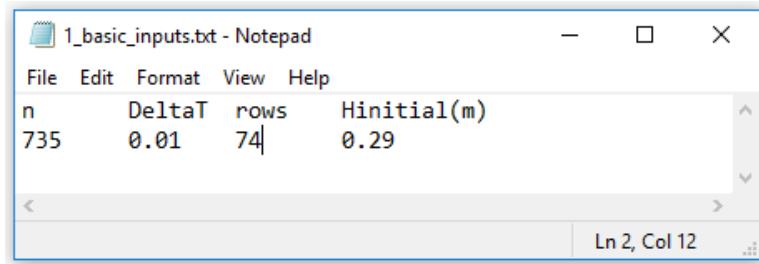
Figure 3.15

Clicking the **Flow Routing** menu opens up the *Flow Routing* window as shown in Figure 3.16. As can be seen, there are four tabs, which are explained below.



Figure 3.16

Basic Inputs: In this window (Figure 3.16) provide the time step (dt) of flow routing simulations and the antecedent water level in the wetland ($H_{initial}$). Once $H_{initial}$ and dt are provided and the **Save** button is clicked, the GUI will create the *1_basic_inputs.txt* control file that is needed for the flow routing module (Figure 3.17) and display the message in Figure 3.18.



The screenshot shows a Windows Notepad window titled "1_basic_inputs.txt - Notepad". The menu bar includes File, Edit, Format, View, and Help. The content of the file is as follows:

	DeltaT	rows	Hinitial(m)
n	0.01	74	0.29

Below the table, the status bar indicates "Ln 2, Col 12".

Figure 3.17

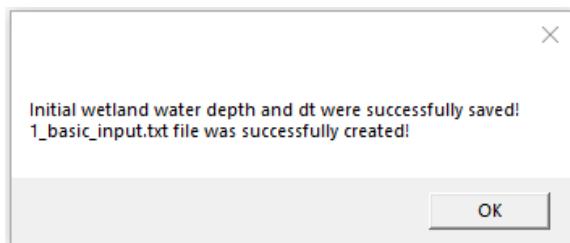


Figure 3.18

Time Series Inputs: After clicking **Save** in the *Basic Inputs* tab, the *Time Series Inputs* header will be activated. As can be seen in Figure 3.19, after clicking the *Time Series Inputs* header, a message appears stating “*2_time_series_inputs.txt* file was successfully created!” This file is automatically created by the GUI in the *InputOutput\Routing* folder using the hydro-climate data described earlier. If an error message appears, check and correct the data format. This file consists of the data shown in Figure 3.20: inflow to the wetland, Q_{in} (m^3/day), evapotranspiration rate, ET (cm/day), precipitation rate, ip (cm/day), and groundwater discharge into the wetland, Q_g (m^3/day).

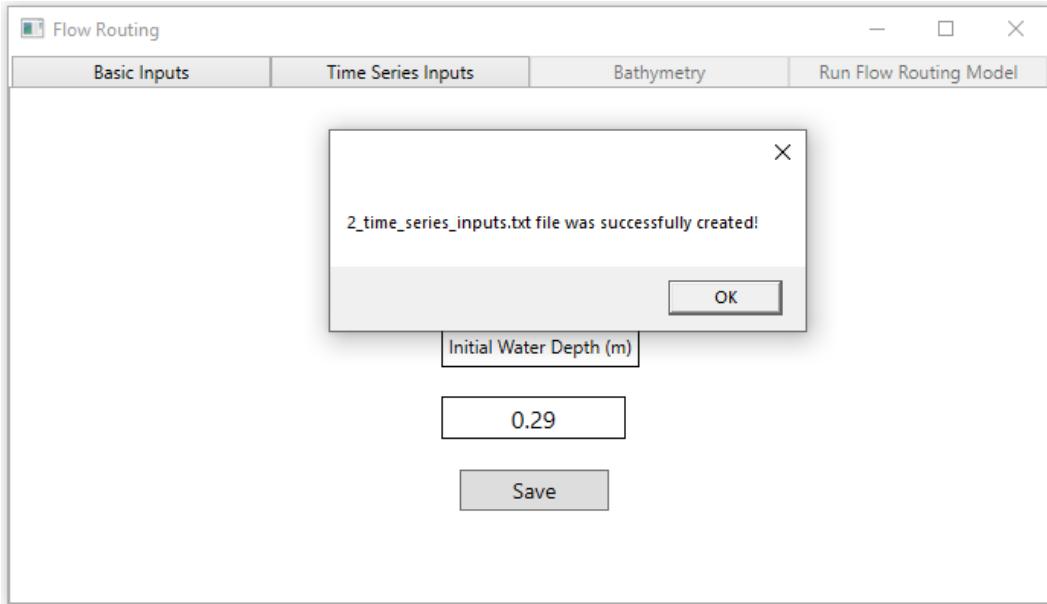


Figure 3.19

The screenshot shows the 'Flow Routing' software window with the 'Time Series Inputs' tab selected. The 'ET Calculation' sub-tab is active, showing a table of data. The table has columns: Date, Qin (m³/day), ET (cm/day), ip (cm/day), and Qg (m³/day). The data rows are:

Date	Qin (m ³ /day)	ET (cm/day)	ip (cm/day)	Qg (m ³ /day)
05/09/1995	0	0.22	0.01	0
05/10/1995	126.59	0.24	2.34	0
05/11/1995	75.35	0.29	0.7	0
05/12/1995	2.86	0.3	0.1	0
05/13/1995	0	0.29	0	0
05/14/1995	76.41	0.27	0.68	0
05/15/1995	0	0.32	0.07	0
05/16/1995	0	0.29	0	0
05/17/1995	22.37	0.34	0.36	0
05/18/1995	542.73	0.4	1.3	0
05/19/1995	92.52	0.34	1.33	0
05/20/1995	0	0.31	0	0
05/21/1995	0	0.36	0	0

Figure 3.20

If ET data are not available, the ET part of the Time Series Input file should have all zero values as mentioned earlier. In this case, calculate ET with the GUI using the Hamon method (Hamon, 1961). Clicking the **ET Calculation** button will prompt the GUI to ask for the latitude of the wetland (Figure 3.21). Click the **Save** button and the “1_ETinputs.txt file was successfully

created!” message will appear. This text file contains the data required for ET calculation. The GUI prepares this file using the data provided in the hydro-climate data and creates a copy of it under the name *1_ETinputs.txt* in the *InputOutput\Routing\ET Module* folder. Note that the *ET.txt* file in this folder is the output of the ET calculation.

As can be seen from Figure 3.22, the input file required for ET calculation requires the number of simulation days (*n*), latitude (decimal degree) of the study wetland, time series of Julian days, and daily average air temperature (°C).

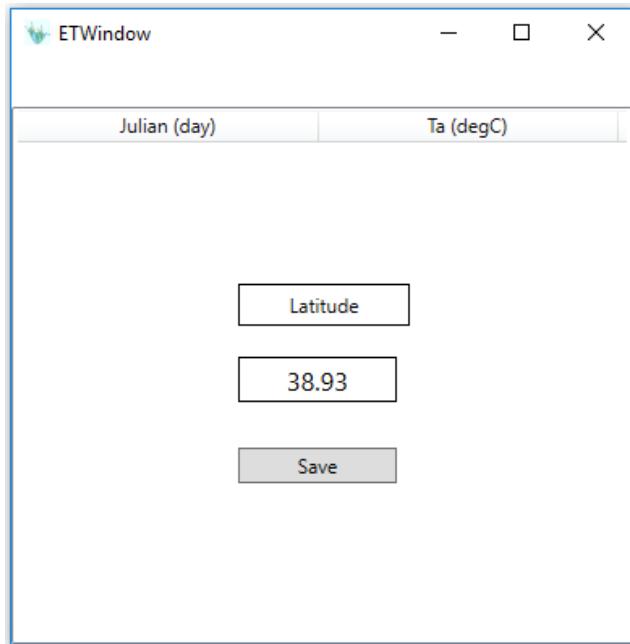


Figure 3.21

A screenshot of a Windows Notepad window titled "1_ETinputs - Notepad". The window shows a table of data with columns for Julian day and Ta (degC). The data is as follows:

	latitude
735	38.93
J (Julian day)	Ta(degC)
129	16.48
130	17.07
131	18.56
132	18.88
133	18.55
134	17.84
135	19.41

Figure 3.22

After required data are provided, click the **Calculate ET** button to perform the calculations and a confirmation message will appear once it is complete (Figure 3.23 and Figure 3.24). The ET column of the Input Time Series file, which was initially assigned zero values, will then be updated.

The screenshot shows a window titled "ETWindow" with a "Calculate ET" button at the top. Below the button is a table with two columns: "Julian (day)" and "Ta (degC)". The data rows are as follows:

Julian (day)	Ta (degC)
275	20.9
276	21.7
277	19.8
278	20.2
279	22.3
280	22.8
281	24.0
282	18.9
283	18.1
284	20.2
285	19.7
286	19.6
287	20.0
288	20.9

Figure 3.23

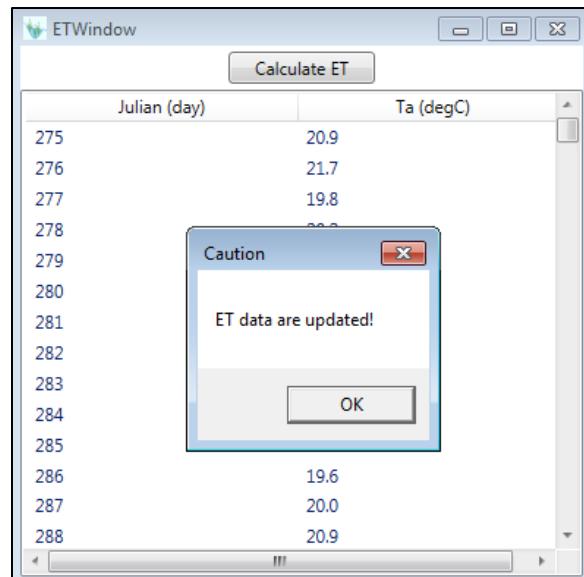


Figure 3.24

Bathymetry: After selecting the **Bathymetry** header, browse to the relevant folder and select the file that contains the wetland bathymetry data. The GUI reads, checks, and creates a copy of the input file, saving it with the name *3_bathymetry_inputs.txt* in the *InputOutput\Routing* folder (Figure 3.25). The *3_bathymetry_inputs.txt* file should contain reference depth of water in the wetland, *H* (m), wetland surface area, *Area* (m^2), water volume of wetland surface water, *Volume* (m^3) and outflow rate, *outflow* (m^3/day) (Figure 3.26). Figure 3.27 shows the bathymetry data in the table after the file is selected. This is essentially a depth-area-volume-outflow relationship table.

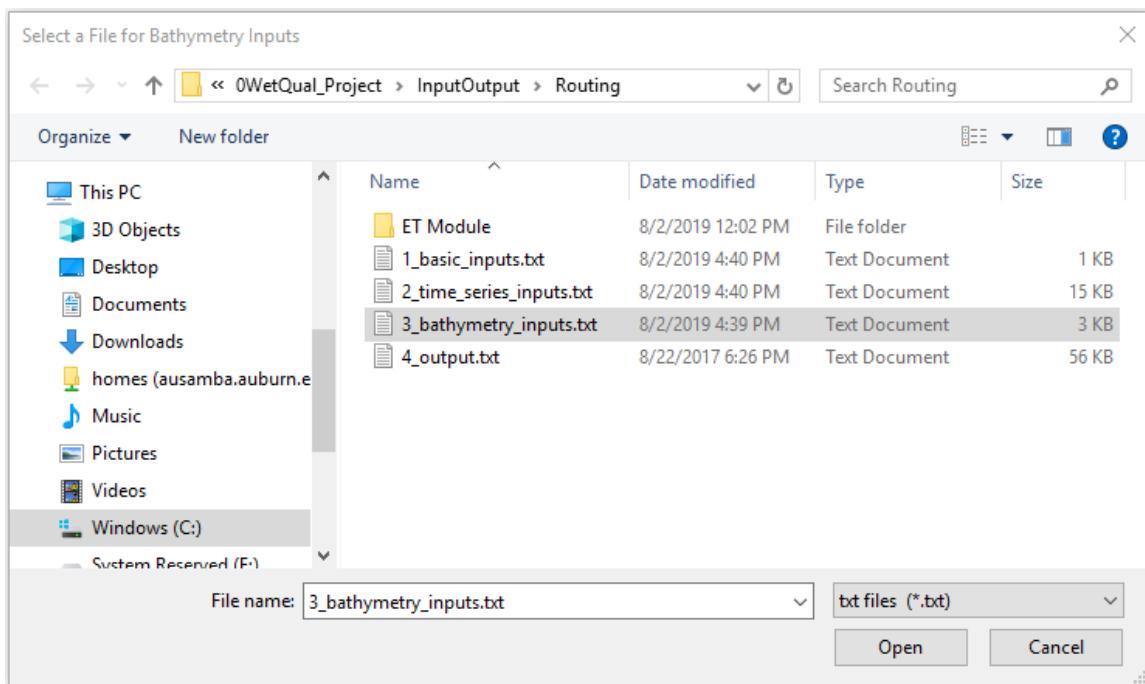


Figure 3.25

3_bathymetry_inputs - Notepad

H (m)	Area (m ²)	Volume (m ³)	Outflow (m ³ /day)
0	0	0	0
0.01	158.1528174	16.80905393	0
0.02	316.3056348	33.61810787	0
0.03	474.4584523	50.4271618	0
0.04	632.6112697	67.23621574	0
0.05	790.7640871	84.04526967	0
0.06	948.9169045	100.8543236	0
0.07	1107.069722	117.6633775	0

Figure 3.26

Flow Routing

Basic Inputs		Time Series Inputs		Bathymetry	Run Flow Routing Model
				View Graph	
H (m)	Area (m ²)	Volume (m ³)	Outflow (m ³ /day)		
0.00	0	0	0		
0.01	158.15	1.58	0		
0.02	316.31	6.33	0		
0.03	474.46	14.23	0		
0.04	632.61	25.30	0		
0.05	790.76	39.54	0		
0.06	948.92	56.94	0		
0.07	1107.07	77.49	0		
0.08	1265.22	101.22	0		
0.09	1423.38	128.10	0		
0.10	1581.53	158.15	0		
0.11	1767.37	194.43	0		
0.12	1960.60	224.02	0		

Figure 3.27

Clicking the **View Graph** button plots depth-area, depth-volume, and depth-outflow relationships of the wetland. Figure 3.28 shows the plot of volume vs. depth for the data shown in Figure 3.26.

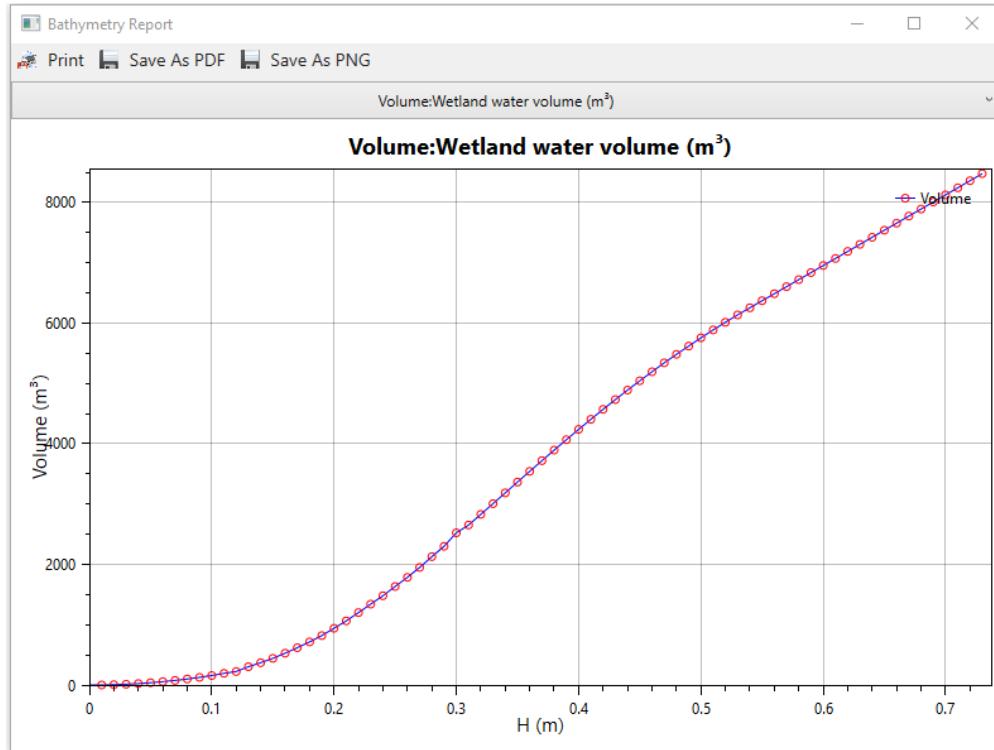


Figure 3.28

Output: After assigning the aforementioned input files, clicks the **Output** tab to run the flow routing process and see the results, which are time series of wetland water depth, outflow, area, and volume (Figure 3.29). The **Transfer Output** button transfers the calculated values to the pre-defined hydro-climate data file for the *WetQual* model run.

Flow Routing

Basic Inputs		Time Series Inputs		Bathymetry	Run Flow Routing Model
				View Graph	Transfer Output
Date	H (m)	Volume (m ³)	Calculated Outflow (m ³ /day)	Area (m ²)	
05/09/1995	0.29000	2301.28003	0.00000	7935.44873	
05/10/1995	0.30690	2613.50293	11.99072	8515.81055	
05/11/1995	0.32269	2877.94189	115.34381	8918.61621	
05/12/1995	0.31757	2787.21899	65.64739	8776.69141	
05/13/1995	0.31056	2663.49438	20.49546	8576.34961	
05/14/1995	0.31311	2708.48340	36.91365	8650.23633	
05/15/1995	0.31311	2708.53125	36.93112	8650.31445	
05/16/1995	0.30793	2626.83789	13.61504	8530.57617	
05/17/1995	0.30652	2608.59790	11.39325	8510.35449	
05/18/1995	0.33381	3076.06055	282.95932	9215.07715	
05/19/1995	0.33599	3115.12451	326.02722	9271.43457	
05/20/1995	0.32200	2865.64185	106.58932	8899.57129	
05/21/1995	0.31194	2687.79150	29.36241	8616.40332	

Figure 3.29

Clicking the **View Graph** button provides options to choose among the outputs to see the graph of the variable of interest. As an example, calculated H and Q_{out} are shown in Figure 3.30 and Figure 3.31.

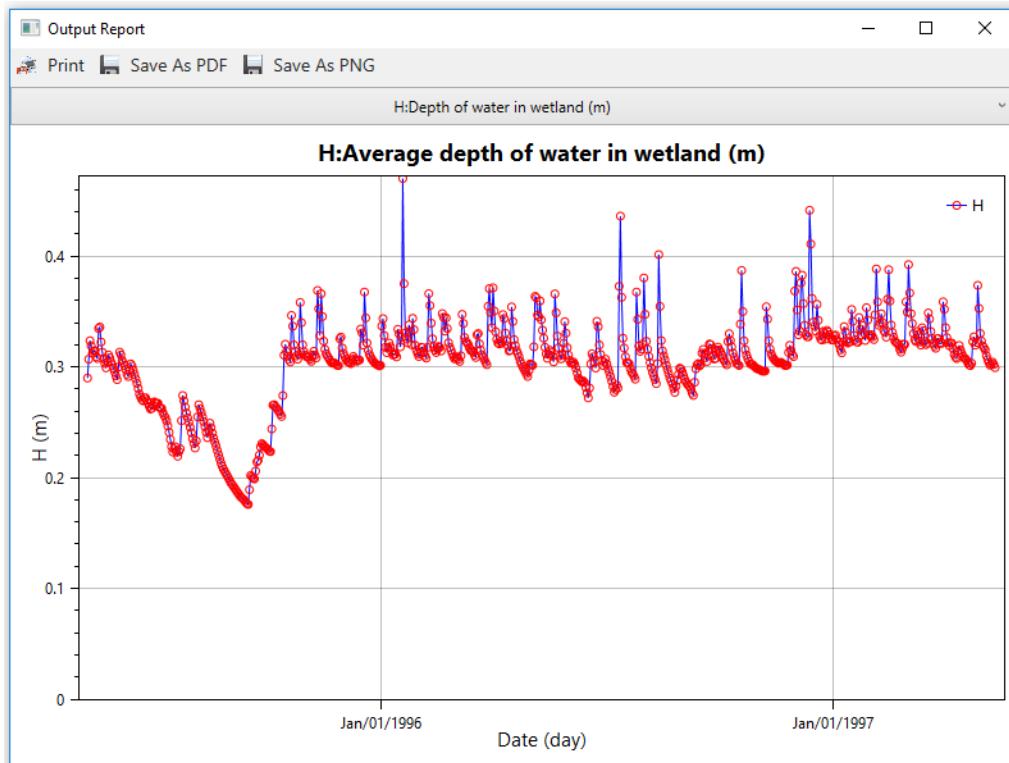


Figure 3.30

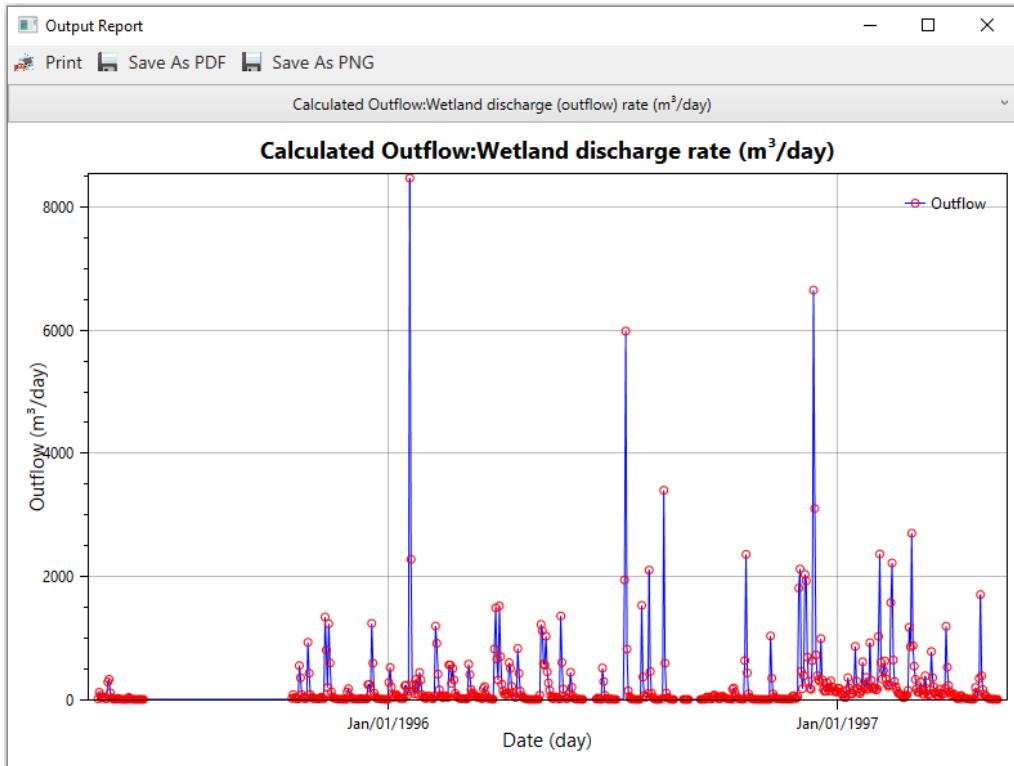


Figure 3.31

3.3.4 Basic Parameters

The **Basic Parameters** menu under **Input Files** (Figure 3.32) is used to assign the time-independent model parameters. Selecting **Basic Parameters** opens the window shown in Figure 3.33, which asks for the related input file. The basic parameters input file should include those parameters shown in Figure 3.34 (formatting should follow the same order; it is a space delimited file). The list of parameters in this menu is summarized in Table A.2 in the appendix. Selecting the basic parameters file opens the dialog window shown in Figure 3.35.

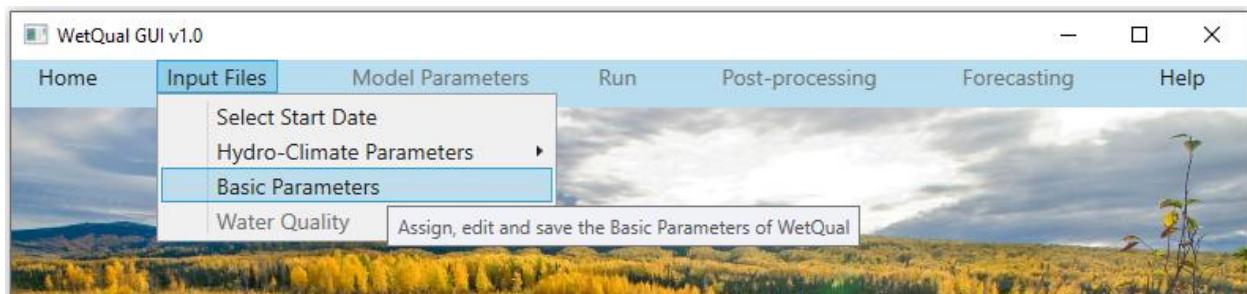


Figure 3.32

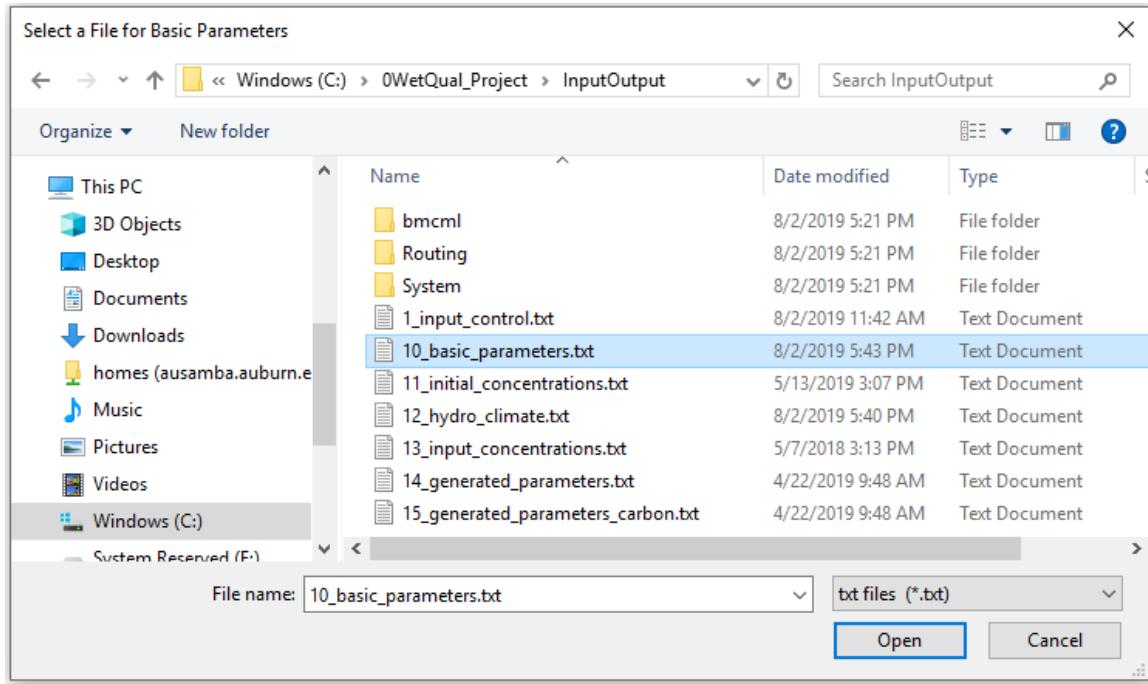


Figure 3.33

The screenshot shows a Notepad window titled "10_basic_parameters.txt - Notepad". The menu bar includes File, Edit, Format, View, and Help. The content of the file is as follows:

```
dt      n ronn(gO/gN)      rond(go/gN)      roc      sims
0.1    734     4.57      15.29      2.67      1000
fNw    fNs1    fNs2    fNO3w    fNO3s1    fNO3s2
0.5    0.5     0.5     0.5     0.5     0.5
apn    lat      amc(gr/gr)      lamdaR(m root m-3 soil)
0.139   0.68    0.267    0.0003
dn(day)
129
130
131
```

Figure 3.34

Basic Parameters

dt (day) [0.005; 0.1]	n (days) [1; 7305]	ronn (gO/gN) [4; 5]	rond (go/gN) [10; 20]	roc [2; 3]	
0.1	734	4.57	15.29	2.67	
fNw [0; 1]	fNs1 [0; 1]	fNs2 [0; 1]	fNO3w [0; 1]	fNO3s1 [0; 1]	fNO3s2 [0; 1]
0.5	0.5	0.5	0.5	0.5	0.5
apn [0; 1]	lat (radian) [-1.05; 1.05]	amc (gr/gr) [0.2; 0.3]	lamdaR (m root m-3 soil) [0.0001; 0.0005]	Save Values	
0.139	0.68	0.267	0.0003		

Figure 3.35

The recommended minimum and maximum values of all basic parameters are provided within brackets [] under each parameter. The parameter values can be edited and the **Save Values** saves the changes. There is a validation procedure that is carried out after clicking the **Save Values** button. The validation checks if the values of the parameters are within the defined ranges. Otherwise, an error message appears like the one seen at the bottom of Figure 3.36, “The value of the parameter is outside the range.” The box containing the relevant parameter will be highlighted in red. The recommended minimum and maximum values of basic parameters are provided in a text file named *MinMaxBasicParameters.txt* in the *InputOutput* folder (Figure 3.37). This file can be edited to change minimum and maximum values.

Basic Parameters

dt (day) [0.005; 0.1]	n (days) [1; 7305]	ronn (gO/gN) [4; 5]	rond (go/gN) [10; 20]	roc [2; 3]	
0	734	4.57	15.29	2.67	
fNw [0; 1]	fNs1 [0; 1]	fNs2 [0; 1]	fNO3w [0; 1]	fNO3s1 [0; 1]	fNO3s2 [0; 1]
0.5	0.5	0.5	0.5	0.5	0.5
apn [0; 1]	lat (radian) [-1.05; 1.05]	amc (gr/gr) [0.2; 0.3]	lamdaR (m root m-3 soil) [0.0001; 0.0005]		
0.139	0.68	0.267	0.0003	Save Values	

The value of the parameter is outside the range.

Figure 3.36

MinMaxBasicParameters.bat - Notepad

```

File Edit Format View Help
Min Max Parameters
0.005 0.1 //0-dt(day)
1 7305 //1-n(days)
4 5 //2-ronn(gO/gN)
10 20 //3-rond(go/gN)
2 3 //4-roc
0 1 //5-fNw
0 1 //6-fNs1
0 1 //7-fNs2
0 1 //8-fNO3w
0 1 //9-fNO3s1
0 1 //10-fNO3s2
0 1 //11-apn
-1.05 1.05 //12-lat(radian)
0.2 0.3 //13-amc(g/g)
0.0001 0.0005 //14-lamdaR(m-root_m-3_soil)

```

Figure 3.37

The message “Data saved successfully!” appears once the validation is successful (see Figure 3.38). Also, the parameters come with a tooltip that shows the definition and the unit (if any) of a parameter when the mouse cursor is held over the parameter’s symbol.

Basic Parameters

dt (day) [0.005; 0.1]	n (days) [1; 7305]	ronn (gO/gN) [4; 5]	rond (go/gN) [10; 20]	roc [2; 3]	
0.01	734	4.57	15.29	2.67	
fNw [0; 1]	fNs1 [0; 1]	fNs2 [0; 1]	fNO3w [0; 1]	fNO3s1 [0; 1]	fNO3s2 [0; 1]
0.5	0.5	0.5	0.5	0.5	0.5
apn [0; 1]	lat (radian) [-1.05; 1.05]	amc (gr/gr) [0.02; 0.3]	lamdaR (m root m-3 soil) [0.0001; 0.0005]		
0.139	0.68	0.267	0.0003		
<input type="button" value="Save Values"/> Data saved successfully!					

Figure 3.38

3.3.5 Water Quality Inputs

The Water Quality menu (Figure 3.39) is used to import initial concentrations and input concentrations of nitrogen (N), phosphorus (P), total suspended sediment (TSS), and carbon (C), and to view input concentrations. The related input files for these two menus are *11_initial_concentration.txt* and *13_input_concentrations.txt* files, respectively, located in the *InputOutput* folder of the project.

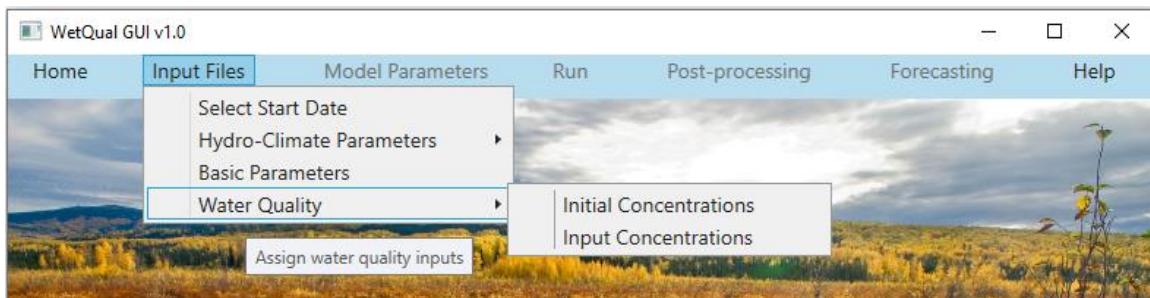


Figure 3.39

3.3.6 Initial Concentrations

Click Input Files>Water Quality>Initial Concentrations to navigate to the *Initial Concentrations* window. The window shown in Figure 3.40 will be displayed and the related input file should be selected (i.e., *11_initial_concentrations.txt*). The initial concentrations input file should include the parameters shown in Figure 3.41. The list of parameters in this file are

summarized in Table A.4 in the appendix. After selecting the file, the *Initial Concentrations* window shown in Figure 3.42 pops up. The values can be edited and click the **Save Values** button to save the changes. The parameters come with a tooltip that displays the definition and the unit (if applicable) of a parameter when the mouse cursor is held over the parameter's symbol.

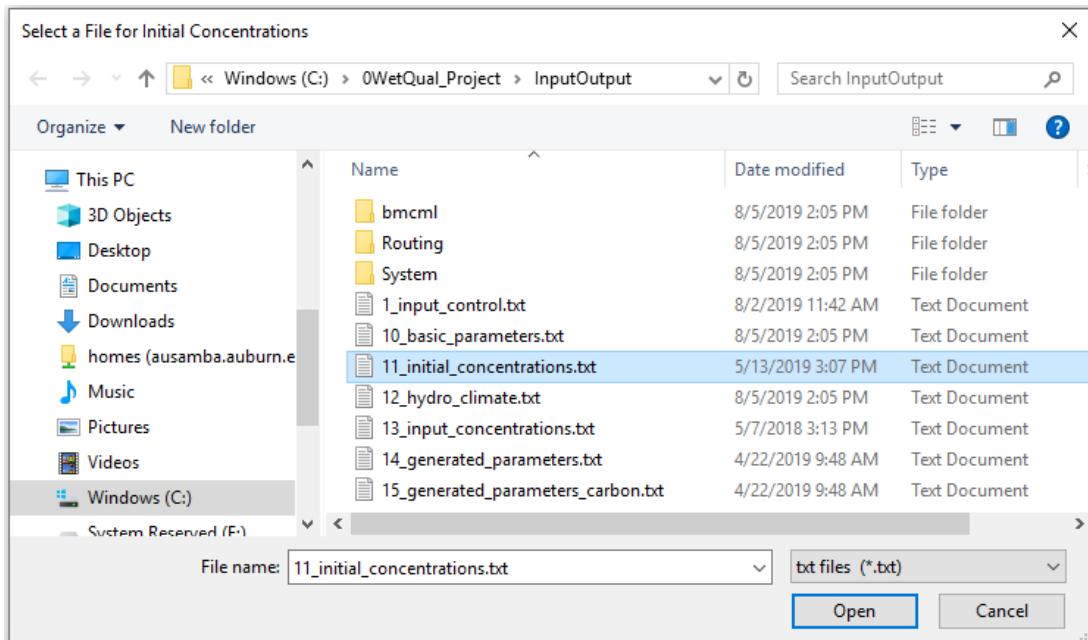


Figure 3.40

```

11_initial_concentration - Notepad
File Edit Format View Help
---- (mg/L) ----
ONw    ONsf    ONss    Nw      Ns1     Ns2     N03w      N03s1      N03s2
2.509   0.912   0.144   0.551   0.551   0.551   0.055   0.055   0.005
a(0)(g)  b(0)(g)
1        2000
mw(0)(mg/L)  ms(0)
110.5   0.3
Ow(0)(mg/l)  Pw(0)  Ps1(0)  Ps2(0)
5.967   0.621   0.621   0.621
---- (mg/l) ----
DOCw    LPOCw    RPOCw    DOCs1    LPOCs1    RPOCs1    DOCs2    LPOCs2    RPOCs2    Ch4w
4.00     9.50    13.10    4.00     9.50     13.10     0.68     1.00     1.41     2         2         2

```

Figure 3.41

As mentioned before, a validation procedure is completed after clicking the **Save Values** button. The validation checks for any empty fields or negative values and shows an error or success message (Figure 3.43 and Figure 3.44).

The dialog box is titled "Initial Concentration". It contains two sections of input fields, each preceded by a "-----mg/L-----" label.

Top Section:

ONw	ONsf	ONss	Nw	Ns1	Ns2	N03w	N03s1	N03s2
2.509	0.912	0.144	0.551	0.551	0.551	0.055	0.055	0.005

Middle Section:

a(0)(g)	b(0)(g)
1	2000

mw(mg/L)	ms(0)s
110.5	0.3

Ow(0)(mg/L)
5.967

Pw(0)	Ps1(0)	Ps2(0)
0.621	0.621	0.621

Bottom Section:

DOCw	LPOCw	RPOCw	DOCs1	LPOCs1	RPOCs1	DOCs2	LPOCs2	RPOCs2
4.00	9.50	13.10	4.00	9.50	13.10	0.68	1.00	1.41

Ch4w	CH4s1	CH4s2
2	2	2

Buttons:

- A "Save Values" button located at the bottom right of the input area.

Figure 3.42

Initial Concentration

-----mg/L-----

ONw	ONsf	ONss	Nw	Ns1	Ns2	N03w	N03s1	N03s2
2.509	0.912	0.144	0.551	0.551	0.551	0.055	0.055	0.005

a(0)(g) b(0)(g)

1	2000
---	------

mw(mg/L) ms(0)s

110.5	0.3
-------	-----

Ow(0)(mg/L)

5.967

Pw(0) Ps1(0) Ps2(0)

0.621	0.621	0.621
-------	-------	-------

-----mg/L-----

DOCw	LPOCw	RPOCw	DOCs1	LPOCs1	RPOCs1	DOCs2	LPOCs2	RPOCs2
4.00	9.50	13.10	4.00		13.10	0.68	1.00	1.41

Ch4w CH4s1 CH4s2

2	2	2
---	---	---

This field cannot be empty or a negative number.

Save Values

Figure 3.43

Initial Concentration

-----mg/L-----

ONw	ONsf	ONss	Nw	Ns1	Ns2	N03w	N03s1	N03s2
2.509	0.912	0.144	0.551	0.551	0.551	0.055	0.055	0.005

a(0)(g) b(0)(g)

1	2000
---	------

mw(mg/L) ms(0)s

110.5	0.3
-------	-----

Ow(0)(mg/L)

5.967

Pw(0) Ps1(0) Ps2(0)

0.621	0.621	0.621
-------	-------	-------

-----mg/L-----

DOCw	LPOCw	RPOCw	DOCs1	LPOCs1	RPOCs1	DOCs2	LPOCs2	RPOCs2
4.00	9.50	13.10	4.00	9.50	13.10	0.68	1.00	1.41

Ch4w CH4s1 CH4s2

2	2	2
---	---	---

Data saved successfully!

Save Values

Figure 3.44

3.3.7 Input Concentrations

On the navigation bar, click **Files>Water Quality>Input Concentrations** to open the *Input Concentrations* window and provide the related input file (i.e., *13_input_concentrations.txt*) (Figure 3.45). The time series of the wetland water quality constituents in the example input concentration file is shown in Figure 3.46. The list and definitions of water quality constituents in this file are given in Table A.5 in the appendix. The GUI will read and check the data in the selected file. It will then copy it, name it *13_input_concentrations.txt*, and place it in the *InputOutput* folder. If the data are not in the required format, the GUI will give an error message and the data will need to be changed to the correct format. After selecting the file, the *Input Concentration* window shown in Figure 3.47 opens. The time series of the data in tables and graphs is viewable and the data can be edited and saved if necessary. By choosing a row, the related data can be edited and changes can be saved by clicking the **Save** button in the upper right side of the window (Figure 3.47).

As with other inputs, a validation procedure is also carried out after clicking the **Save** button that checks for any empty field or negative value.

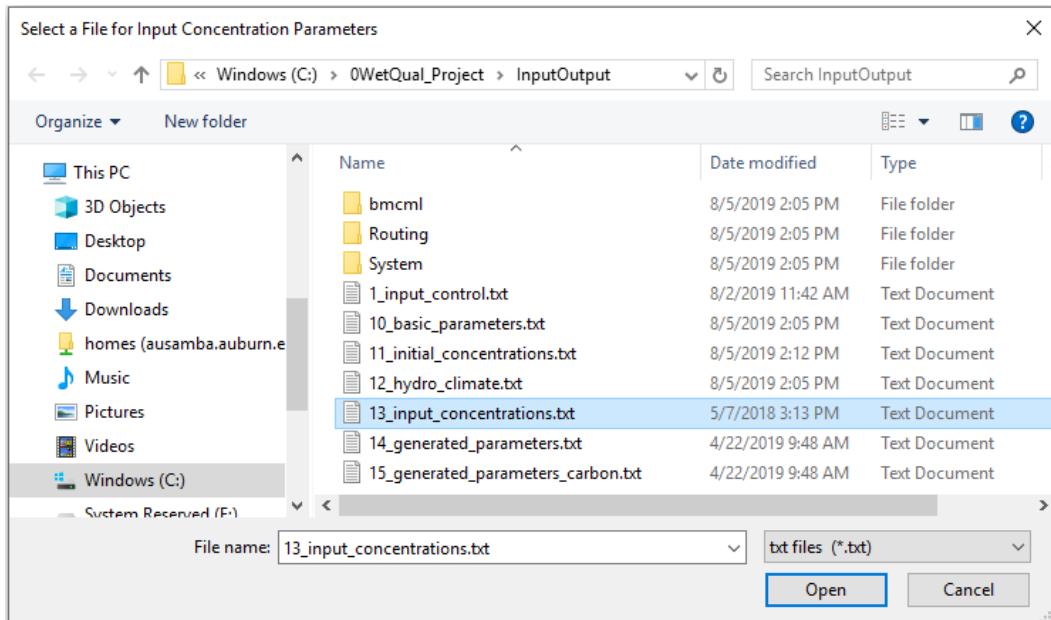


Figure 3.45

Date	ONin (mg/L)	NO3in (mg/L)	Nwin (mg/L)	NO3g (mg/L)	Ng	Owin (mg/L)	PO4in (mg/L)	Pg	mwini (mg/L)	NH4air (mg/L)	NO3air (mg/L)	Qa	Qn	LPOCin (mg/L)	RPOCin (mg/L)	DOCin (mg/L)	DOCatm (mg/L)
05/09/1995	2.509	0.055	0.551	0	0	5.9676	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82
05/10/1995	2.509	0.055	0.551	0	0	4.2982	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82
05/11/1995	2.509	0.055	0.551	0	0	5.3567	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82
05/12/1995	2.509	0.055	0.551	0	0	4.4224	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82
05/13/1995	2.509	0.055	0.551	0	0	7.6988	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82
05/14/1995	2.509	0.055	0.551	0	0	5.3347	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82
05/15/1995	2.509	0.055	0.551	0	0	6.1803	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82

Figure 3.46

Date	ONin	NO3in	NWin	NO3g	Ng	Owin	PO4in	Pg	mwin	NH4air	NO3air	Qa	Qn	LPOCin	RPOCin	DOCin	DOCatm	TOCgw
05/09	2.509	0.055	0.551	0	0	5.9676	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82	0
Date	ONin	NO3in	NWin	NO3g	Ng	Owin	PO4in	Pg	mwin	NH4air	NO3air	Qa	Qn	LPOCin	RPOCin	DOCin	DOCatm	TOCgw
05/09/1995	2.509	0.055	0.551	0	0	5.9676	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82	0
05/10/1995	2.509	0.055	0.551	0	0	4.2982	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82	0
05/11/1995	2.509	0.055	0.551	0	0	5.3567	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82	0
05/12/1995	2.509	0.055	0.551	0	0	4.4224	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82	0
05/13/1995	2.509	0.055	0.551	0	0	7.6988	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82	0
05/14/1995	2.509	0.055	0.551	0	0	5.3347	0.225	0	110.5	0.681	0.725	0	0	2.6285	2.6285	47.313	7.82	0

Figure 3.47

3.4 Model Parameters

In this step, some of the *WetQual* parameters that are considered to be random in the stochastic model (some biogeochemical parameters and reaction rates) are introduced. As can be seen from Figure 3.48, the GUI allows *WetQual* to be run in either deterministic or stochastic mode. To that end, after selecting the **Deterministic Model** or **Stochastic Model** option, the user can define the values of the model parameters or their statistical distributions. For stochastic model parameters, suggested ranges (Min, Max) and distributions for the listed parameters/coefficients were extracted from literature and expert knowledge (e.g., Schnoor, 1996; Chapra, 1997; Di Toro, 2001; Reddy and Delaune, 2008; Cerco and Cole, 1995, and Ji, 2008). See Hantush et al. (2013), Kalin et al. (2013), and Sharifi et al. (2013) to find details about *WetQual* parameters.

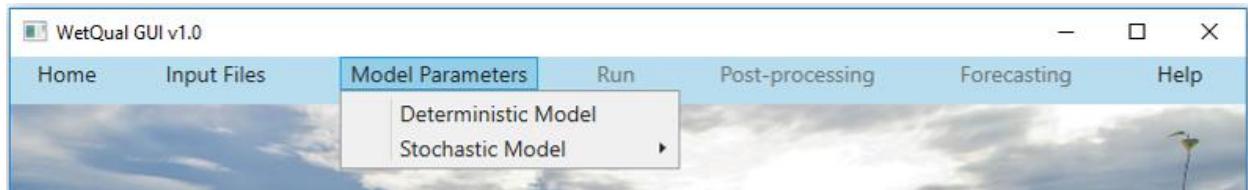


Figure 3.48

3.4.1 Deterministic Model

On the navigation bar, click **Model Parameters>Deterministic Model** to open the *Default values for model parameters* window. For a deterministic model, the median of the selected range for each model parameter was chosen as the default value. These can be seen in the related window (Figure 3.49). The GUI allows users to edit, save, and restore the values back to their defaults using the **Save Values** and **Default Values** buttons. A list of all parameters in this window is presented in the appendix. Clicking the **Save Values** button activates the **Run Simulations** option if there is no error. The parameters come with a tooltip that shows the definition and the unit (if any) of a parameter when the mouse cursor is held over the parameter's symbol. As with the previously described windows, a validation procedure starts after clicking the **Save Value** button that checks for any empty fields or negative values.

The screenshot shows the 'Deterministic Model Parameters' dialog box. The parameters are organized into two main sections: N,P,TSS and Carbon. The N,P,TSS section contains 18 parameters, and the Carbon section contains 12 parameters. Each parameter is represented by a text input field with its name and unit in parentheses above it. The 'Carbon' section includes buttons for 'Save Value' and 'Default Values' at the bottom.

N,P,TSS					
I2 (cm)	θ	ls (ly/day)	fN		
27.63	1.25	248.58	0.335		
kd (mL/g)	kep (1/m)	kga (1/day)	kgb (1/day)	kmr (1/day)	knw (1/day)
1.2	0.3	0.0014	0.0014	0.00003	0.0032
kmw (1/day)	kns (1/day)	kdn (1/day)	ρ_s	vso (cm/day)	vss (cm/day)
0.000032	0.32	1.29	2	0.8	299
vb (cm/day)	ana (cm/day)	rc,chl (gC/gChl)	Ss (g/L/day)	Sw (gr/cm ³ /day)	a
0.0034	10.56	60	0.0435	0	0.2155
fr	c1	c2	pH	S (mg-N/m ³ /hr)	Kw (cm ³ /g)
0.7514	0.09	2450	6.36	0.1266	31.54
apa (grP/grChl)	Dpw (cm ³ /day)	Ksa (cm ³ /g)	Ksb (cm ³ /g)	Ran1	fw
1.19	0.7452	31.73	317.46	0.5	0.75
fact	Cro	Crs	ϕ_w		
140	0.0318	0.0032	0.8005		

Carbon					
(gC/gChl)	faD	faL	faR	fbD	fbL
86.6	0.16	0.5	0.5	0.16	0.5
fbR	kL (1/day)	kR (1/day)	KO (mg/lit)	KinO (mg/lit)	KN (mg/lit)
0.5	0.00001	0.000001	0.6	0.25	0.038
KinN (mg/lit)	K1DOC (1/day)	K2DOC (1/day)	K3DOC (1/day)	K4DOC (1/day)	cp1
0.019	0.2	0.08	0.04	0.015	0.36
cp2	cp3	fbw (1/day)	k1CH4 (1/day)	k2CH4 (1/day)	Rv (cm/gr)
0.36	0.36	0.55	0.13	0.04	0.1

Figure 3.49

3.4.2 Stochastic Model

On the navigation bar, click **Model Parameters>Stochastic Model** (Figure 3.50) to activate the stochastic mode of the *WetQual* GUI and open the “N, P, TSS” (Figure 3.52) and “Carbon” windows (Figure 3.53). In these two windows, the user needs to select the distribution type and relevant statistics. Four options are available for probability distributions: uniform, normal, log-normal, or triangular (Figure 3.51).

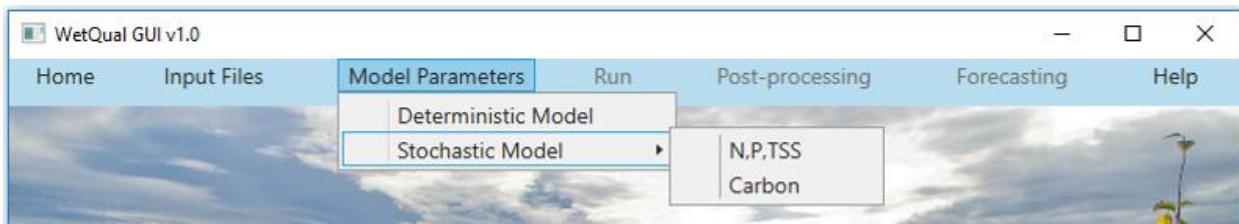


Figure 3.50

Minimum and maximum values are required for uniform and normal distributions. For log-normal distribution, provide either minimum and maximum values or mean (μ) and standard deviation (σ). Note, if minimum and maximum values are provided, they are assumed to correspond to probabilities of 0.1% and 99.9%. The GUI internally calculates μ and σ from those. For triangular distribution, the peak location (c) is required in addition to minimum and maximum values. Distribution types and parameter values can be changed for a specific project by clicking the **Save Values** button.

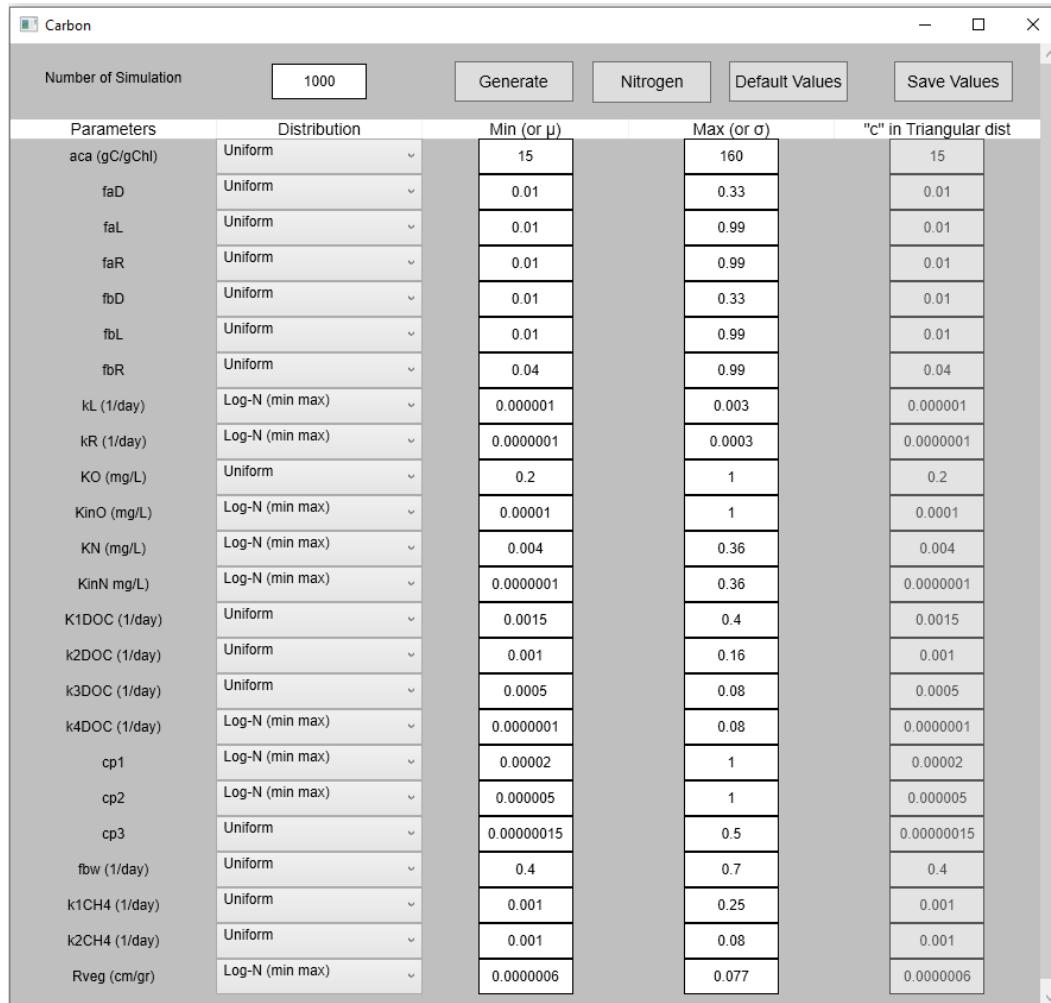
A screenshot of the "N, P, TSS" window. At the top, there is a "Number of Simulation" input field set to 1000, and several buttons: "Generate", "Carbon", "Default Values", and "Save Values". Below this is a table with columns for "Parameters", "Distribution", "Min (or μ)", "Max (or σ)", and "'c'" in Triangular dist. The table rows are: l2 (cm) - Uniform, Min: 5, Max: 50, c: 5; theta - Uniform, Min: 1.15, Max: 1.35, c: 1.15; ls (ly/day) - Uniform, Min: 100, Max: 400, c: 100; fNup - dropdown menu with options: Uniform, Normal (min max), Log-N (min max), Log-N (mu sigma), Tri; kd (mL/g) - Uniform, Min: 0.032, Max: 0.8, c: 0.032; kep (1/m) - Uniform, Min: 0.15, Max: 0.45, c: 0.15.

Figure 3.51

N, P, TSS

Number of Simulation		1000	Generate	Carbon	Default Values	Save Values
Parameters	Distribution	Min (or μ)	Max (or σ)	"c" in Triangular dist		
I2 (cm)	Uniform	5	50	5		
θ	Uniform	1.15	1.35	1.15		
Is (ly/day)	Uniform	100	400	100		
fNup	Uniform	0.29	0.38	0.29		
kd (mL/g)	Log-N (min max)	0.032	80	0.032		
kep (1/m)	Uniform	0.15	0.45	0.15		
kga0 (1/day)	Log-N (min max)	0.0009	0.002	0.0009		
kgb0 (1/day)	Log-N (min max)	0.0009	0.002	0.0009		
kmin1s (1/day)	Log-N (min max)	0.00001	0.0031	0.00001		
knw (1/day)	Log-N (min max)	0.0001	0.35	0.0001		
kminw (1/day)	Log-N (min max)	0.00001	0.001	0.00001		
kns (1/day)	Log-N (min max)	0.01	42	0.01		
kden (1/day)	Uniform	0.004	0.15	0.004		
rows (gr/cm ²)	Uniform	1.5	2.2	1.5		
vels_o (cm/day)	Log-N (min max)	0.025	138	0.025		
vels_s (cm/day)	Log-N (min max)	8	6750	8		
velb (cm/day)	Uniform	0.000274	0.006575	0.000274		
ana (gN/gChl)	Uniform	3.5	17.6	3.5		
rChl (gC/gChl)	Uniform	20	100	20		
Ss (g/L/day)	Uniform	0.022	0.065	0.022		
Sw (gr/cm ² /day)	Uniform	0	0	0		
c_uw	Uniform	0.0864	0.3456	0.0864		
frap	Uniform	0.5	1	0.5		
c1	Uniform	0.04	0.14	0.04		
c2	Uniform	1228	3686	1228		
PH	Uniform	4.5	8.2	4.5		
S (mg-N/m ² /hr)	Log-N (min max)	0.0004	3.5	0.0004		
Kw (cm ³ /g)	Log-N (min max)	1024	1193731	1024		
apa (grP/grChl)	Uniform	0.4	2	0.4		
Dpw (cm ² /day)	Uniform	0.66	0.83	0.66		
Ksa (cm ³ /g)	Log-N (min max)	1024	1193731	1024		
Ksb (cm ³ /g)	Log-N (min max)	8780	18549874	8780		
Ran1	Uniform	0	1	0		
fW	Uniform	0.5	1	0.5		
fact	Log-N (min max)	9.3	2021	9.3		
alfa_veir_o	Log-N (min max)	0.00001	61	0.00001		
alfa_veir_s	Log-N (min max)	0.00001	0.46121	0.00001		
porw	Uniform	0.65	0.95	0.65		

Figure 3.52



The screenshot shows the Carbon software window with the following configuration:

Number of Simulation	Distribution	Min (or μ)	Max (or σ)	"c" in Triangular dist
aca (gC/gChl)	Uniform	15	160	15
faD	Uniform	0.01	0.33	0.01
faL	Uniform	0.01	0.99	0.01
faR	Uniform	0.01	0.99	0.01
fbD	Uniform	0.01	0.33	0.01
fbL	Uniform	0.01	0.99	0.01
fbR	Uniform	0.04	0.99	0.04
kL (1/day)	Log-N (min max)	0.000001	0.003	0.000001
kR (1/day)	Log-N (min max)	0.0000001	0.0003	0.0000001
KO (mg/L)	Uniform	0.2	1	0.2
KinO (mg/L)	Log-N (min max)	0.00001	1	0.0001
KN (mg/L)	Log-N (min max)	0.004	0.36	0.004
KinN mg/L	Log-N (min max)	0.0000001	0.36	0.0000001
K1DOC (1/day)	Uniform	0.0015	0.4	0.0015
K2DOC (1/day)	Uniform	0.001	0.16	0.001
K3DOC (1/day)	Uniform	0.0005	0.08	0.0005
K4DOC (1/day)	Log-N (min max)	0.0000001	0.08	0.0000001
cp1	Log-N (min max)	0.00002	1	0.00002
cp2	Log-N (min max)	0.000005	1	0.000005
cp3	Uniform	0.00000015	0.5	0.00000015
fbw (1/day)	Uniform	0.4	0.7	0.4
k1CH4 (1/day)	Uniform	0.001	0.25	0.001
k2CH4 (1/day)	Uniform	0.001	0.08	0.001
Rreg (cm/gr)	Log-N (min max)	0.0000006	0.077	0.0000006

Figure 3.53

As shown in Figure 3.51**Error! Reference source not found.** and Figure 3.53, required options include the number of simulations for generation of parameter sets based on the assigned distribution types and the parameter ranges. By clicking the **Generate** button (Figure 3.52 and Figure 3.53), the GUI randomly generates parameter values and updates the files *14_generated_parameters.txt* and *15_generated_parameters_carbon.txt*. Click the **Carbon** button to move to that window. Hold the mouse cursor over the symbols of parameters in both the “N, P, TSS” and “Carbon” windows will show the definitions of parameters.

3.5 Run

After all parameters have been assigned (for the deterministic model) or randomly generated (for the stochastic model), click **Run>Run WetQual** (Figure 3.54). The GUI then runs the deterministic model or stochastic model depending on the previous step, respectively. Note that the models run are actually the same. The stochastic model performs Monte Carlos simulations with the same model. After executing **Run WetQual**, one of the following pop-up messages will display depending on the selection: “Deterministic model was successfully executed” or “Stochastic model was successfully executed” (Figure 3.55). As the deterministic model will perform only one simulation, it may take a couple seconds to finish. But, depending on the number of the simulations and the processor, it may take minutes to hours to complete a run under the stochastic scenario. Once the deterministic mode run is finished, the **Post-Processing** menu will be activated (see Figure 3.56). Running the *WetQual* GUI in stochastic mode will also activate the **GLUE** and **BMCML** sub-menus under the **Post-Processing** menu and the **Forecasting** menu.

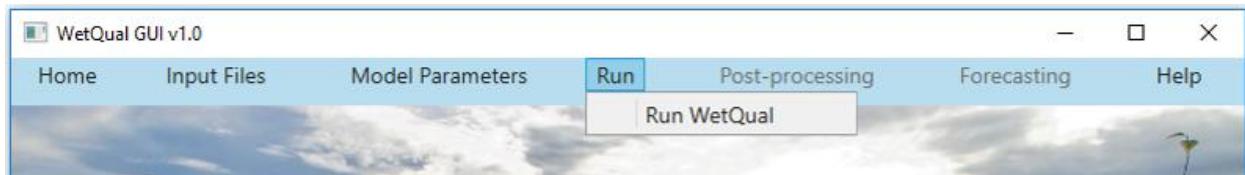


Figure 3.54

```
C:\Users\szi003\Desktop\00000NewTest1000\InputOutput\Wetlandmodel.exe
WetQual-Model

A numerical model for N, P and C cycling in ponded wetlands
Developed by:
    M.M. Hantush
    L. Kalin
    A. Sharifi
    S. Isik
USEPA and Auburn University (2014)
1
Deterministic model was successfully executed!
Fortran Pause - Enter command<CR> or <CR> to continue.
```

Figure 3.55

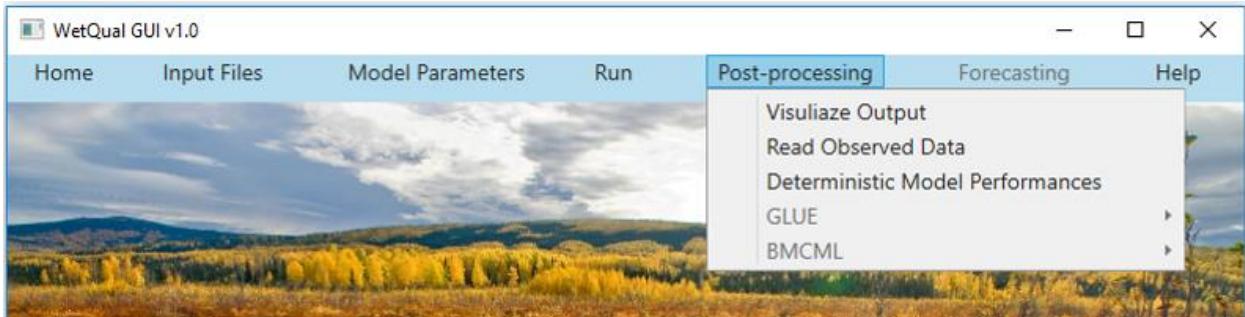


Figure 3.56

3.6 Post-processing

3.6.1 Visualize Output

Deterministic Model

Visualize Output provides an opportunity to visualize both deterministic and stochastic model outputs through a series of graphs. Figure 3.57 displays the windows that pops up after clicking Visualize Output for a deterministic model. Select the output of interest (out of 29 *WetQual* outputs for N, P, TSS, and C, see Table A.6 in the appendix) to see the time series graph for that output. As an example, the time series graph for particulate organic nitrogen concentration in free water (N_{ow}) is shown in Figure 3.58. In addition to the time series graph, by selecting the Time Series Table in this window, one can see the actual simulated values in time series (see Figure 3.59). Furthermore, the graphs can be printed or saved in pdf format. For the sake of simplicity and GUI performance efficiency, the *WetQual* output (text files) are saved in the *InputOutput* folder.

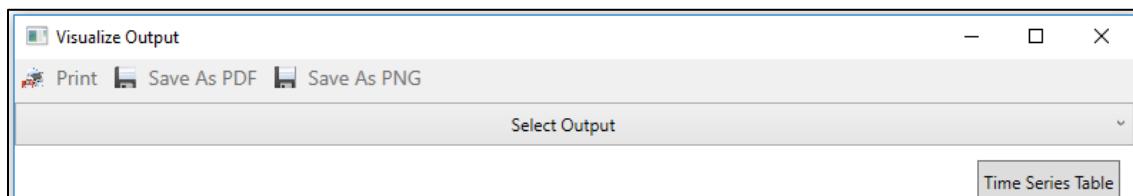


Figure 3.57

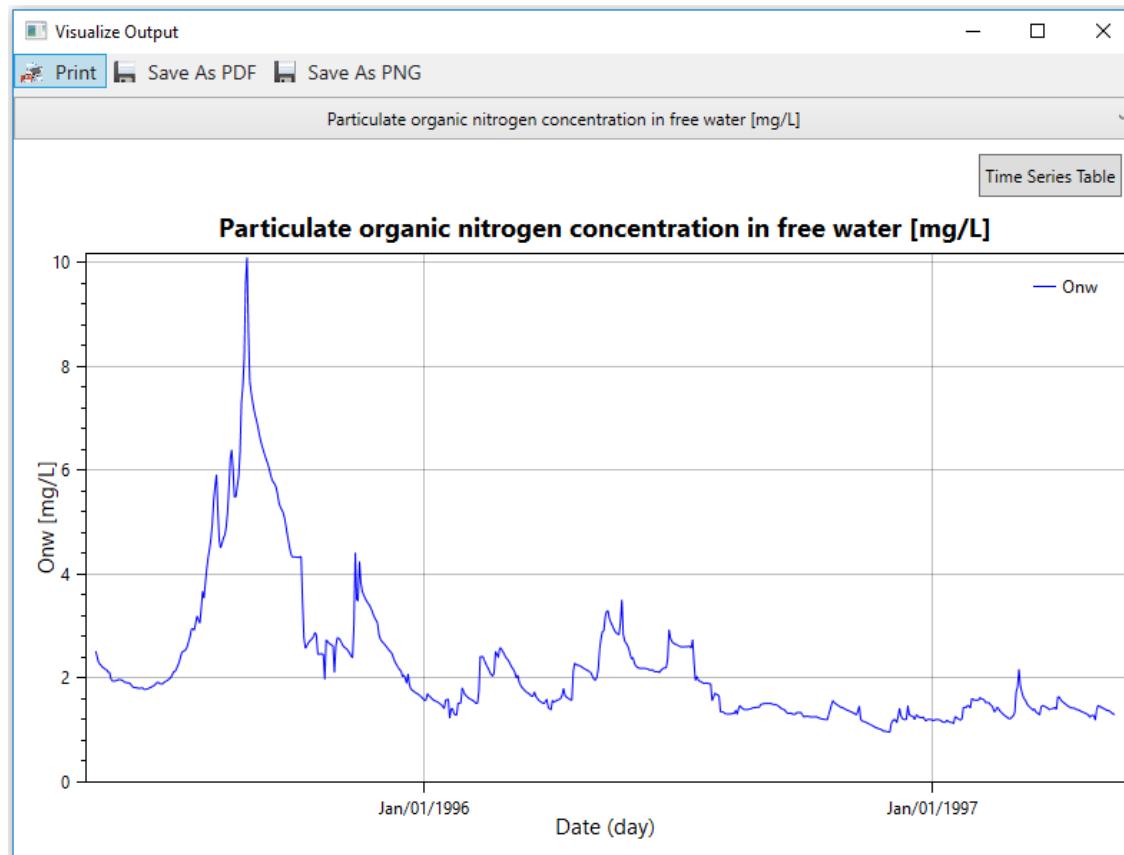


Figure 3.58

Date	Onw [mg/L]
05/09/1995	2.50900
05/10/1995	2.40680
05/11/1995	2.30236
05/12/1995	2.25715
05/13/1995	2.23309
05/14/1995	2.19691
05/15/1995	2.18335
05/16/1995	2.15833
05/17/1995	2.14878
05/18/1995	2.10193

Figure 3.59

Stochastic Model

The stochastic model results in an ensemble of outputs, so an option was added to allow the user to choose among the number of simulations in **Analyze Output Files**. Users can pick any simulation number and visualize its outputs. Figure 3.60 displays the **Analyze Output Files** window before a parameter of interest is selected.

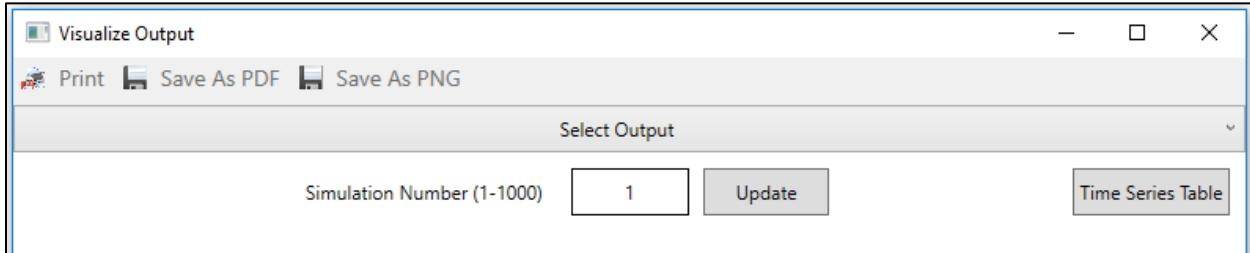


Figure 3.60

As an example, we ran *WetQual* with 1,000 simulations and simulation number 380 was selected to visualize the results (Figure 3.61). If a simulation number outside the range is picked, an error appears similar to Figure 3.62. There is also the option to visualize results of the previous or next simulations by clicking the **Previous** or **Next** buttons.

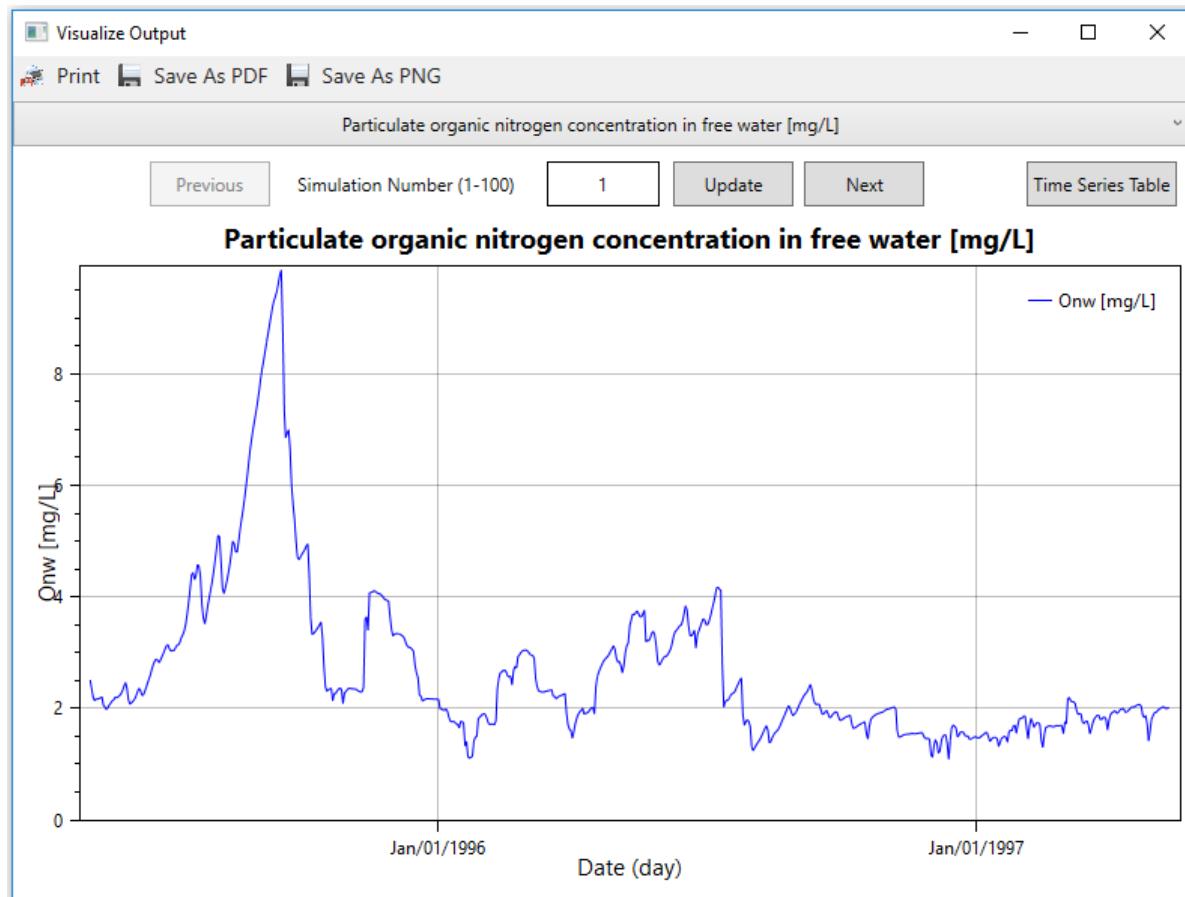


Figure 3.61

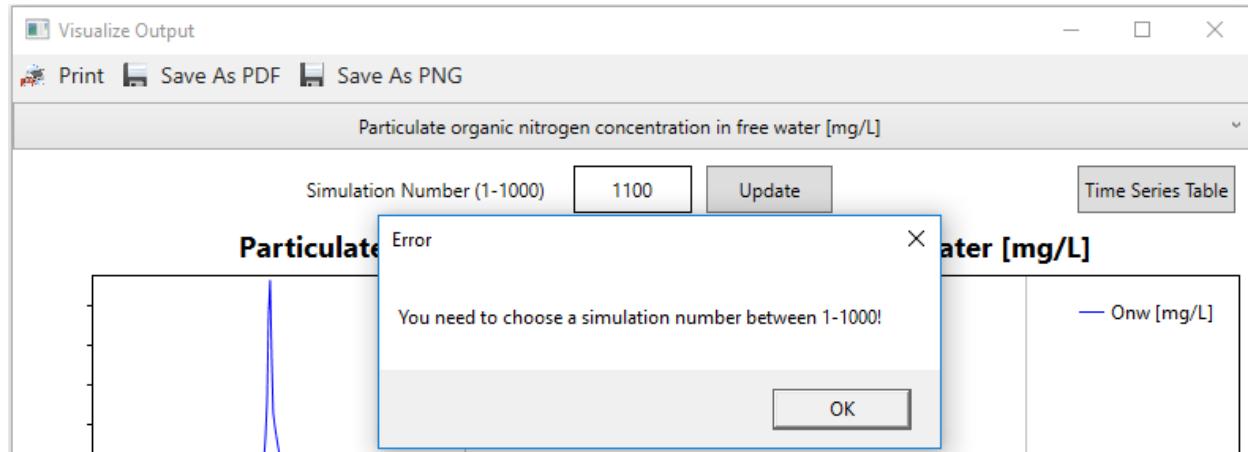


Figure 3.62

3.6.2 Read Observed Data

Observed values of model outputs are needed to assess model performance and complete uncertainty/sensitivity analysis. When **Read Observed Data** under the **Post-processing** menu (Figure 3.63) is chosen, the window in Figure 3.64 is displayed where the observed data file is selected. The observation data file format is shown on the top in Figure 3.65. Available constituent numbers, which are available in lines 3 through 6, should be given in the first line in the observation file. SD in the eighth line refers to the duration of the data collection period. If there are no data, SD should be “-999”. The user needs to provide data on the available dates.

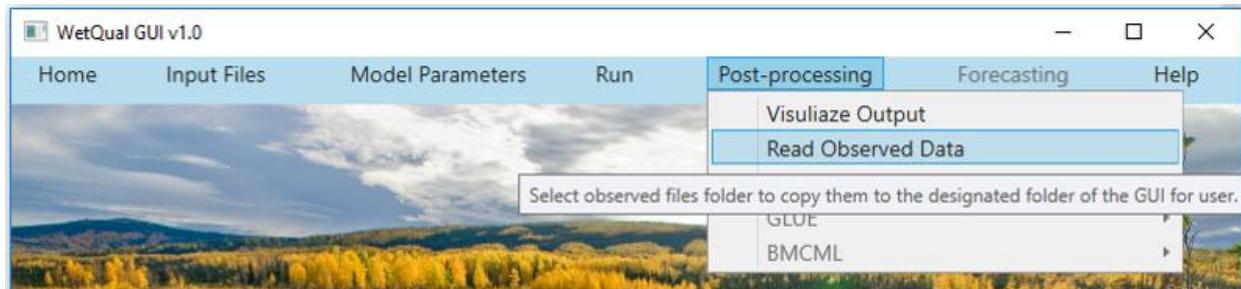


Figure 3.63

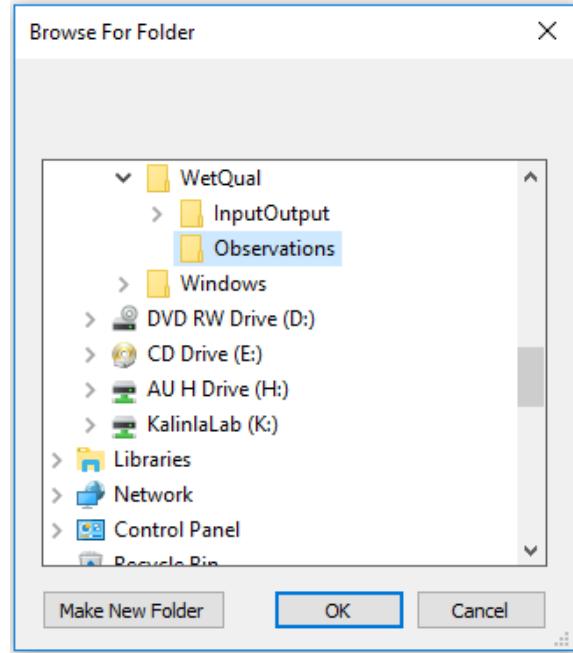


Figure 3.64

ObservedData.txt - Notepad

File Edit Format View Help

ObservedData	1	4	7	13	16	26	8:NO3s1					
1:Onw	2:Onss	3:Onsf	4:Nw	5:Ns1	6:Ns2	7:NO3w						
9:NO3s2	10:Ow	11:a	12:b	13:Pw	14:Ps1	15:Ps2	16:mw					
17:DOCw	18:LPOCw	19:RPOCw	20:DOCs1	21:LPOCs1	22:RPOCs1	23:DOCs2	24:LPOCs2					
25:RPOCs2	26:TOCw	27:CH4w	28:CH4s1	29:CH4s2								
Date	Onw(mg/L)	SD(d)	Nw(mg/L)	SD(d)	NO3w(mg/L)	SD(d)	Pw(mg/L)	SD(d)	mw(mg/L)	SD(d)	TOCw(mg/L)	SD(d)
05/15/1995	1.6350	6	0.2020	6	0.0140	6	0.0800	6	36.25	6	24.2798	6
05/22/1995	1.5920	7	0.1730	7	0.0310	7	0.0670	7	6.35	7	22.0165	7
05/30/1995	1.9110	8	0.1840	8	0.2810	8	0.1230	8	35.60	8	24.4856	8
10/31/1995	2.8890	5	0.8730	5	*	-999	0.2070	5	78.40	5	21.6049	5
11/07/1995	2.4340	7	*	-999	0.7980	7	0.1720	7	26.89	7	24.4856	7
11/15/1995	1.5090	8	0.1910	8	0.7590	8	0.2350	8	*	-999	14.7119	8
11/21/1995	2.7160	6	0.2280	6	*	-999	0.2800	6	234.80	6	16.7695	6
11/28/1995	3.7770	7	0.1480	7	0.7300	7	0.0370	7	*	-999	23.0453	7
12/06/1995	2.4990	8	0.1430	8	0.7990	8	0.1800	8	94.73	8	20.3704	8
12/18/1995	2.6150	7	0.1360	7	0.2620	7	0.1200	7	125.90	7	17.6955	7
12/27/1995	1.7030	7	0.1080	7	0.9770	7	0.0590	7	150.40	7	17.0782	7
01/03/1996	2.4500	7	0.1860	7	0.5820	7	0.0720	7	33.10	7	17.6955	7

< >

Ln 7, Col 122

105_obs_Nw - Notepad

File Edit Format View Help

Date	Nw(mg/L)	Sampling	Duration(day)
5/9/1995	*	-999	
5/10/1995	*	-999	
5/11/1995	*	-999	
5/12/1995	*	-999	
5/13/1995	*	-999	
5/14/1995	*	-999	
5/15/1995	0.0140	6	
5/16/1995	*	-999	
5/17/1995	*	-999	
5/18/1995	*	-999	
5/19/1995	*	-999	
5/20/1995	*	-999	
5/21/1995	*	-999	
5/22/1995	0.0310	7	
5/23/1995	*	-999	
5/24/1995	*	-999	
5/25/1995	*	-999	
5/26/1995	*	-999	
5/27/1995	*	-999	
5/28/1995	*	-999	
5/29/1995	*	-999	
5/30/1995	0.2810	8	
5/31/1995	*	-999	

< >

Ln 1, Col 9

Figure 3.65

The GUI will convert the observation data file to separate files for each constituent in the required daily format. On the bottom in Figure 3.65, the format and schematic of a typical

observation file is shown. The first column is for date and the second column is for the observations. The last column shows the duration of the data collection period for that entry in days (if data is flow-weighted average of certain number of days). If data are daily or instantaneous, “1” should be entered next to the observation in the last column. If data are flow-weighted averages, for example, of the previous 6 days, then “6” should be entered next to the observation value as seen in Figure 3.65. Days with no data need to have “*” in the second column and “-999” in the last column. Note that the format is space delimited. Users need to prepare their observation files in a folder and pick that folder from the **Read Observed Data** menu after selecting **Post-processing**. Note that users do not need to follow this procedure (of picking the *Observation* folder by using **Read Observed Data** menu) if the files with the observed data are already in the *Observations* folder for the project.

3.6.3 Deterministic Model Performance

If a deterministic model run was performed, then under the **Post-processing** menu only the **Deterministic Model Performances** sub-menu will be activated (Figure 3.66). When selected, a new window will open as illustrated in Figure 3.67. In this window, select the model outputs for which observations are available. The GUI provides time series graphs of observed data versus model outputs (Figure 3.68). On the upper right side of the window, the performance metrics Nash-Sutcliffe efficiency (E_{NS}), Mass Balance Error (MBE), and Normalized Root Mean Square Error (NRMSE which is RMSE divided by the average of observed values) are presented for the selected output variable. Performance metrics are calculated as

$$E_{NS} = 1 - \left[\frac{\sum_{i=1}^m (y_{obs,i} - y_{sim,i})^2}{\sum_{i=1}^m (y_{obs,i} - \bar{y}_{obs})^2} \right]$$

$$MBE (\%) = \left[\frac{\sum_{i=1}^m (y_{obs,i} - y_{sim,i})}{\sum_{i=1}^m (y_{obs,i})} \right] * 100$$

$$NRMSE = \frac{\sqrt{\frac{1}{m} \sum_{i=1}^m (y_{obs,i} - y_{sim,i})^2}}{\bar{y}_{obs}}$$

where, $y_{obs,i}$ and $y_{sim,i}$ denote observed and simulated values at the i^{th} observation, respectively, \bar{y}_{obs} refers to the average of observed values, and m represents the number of observations.

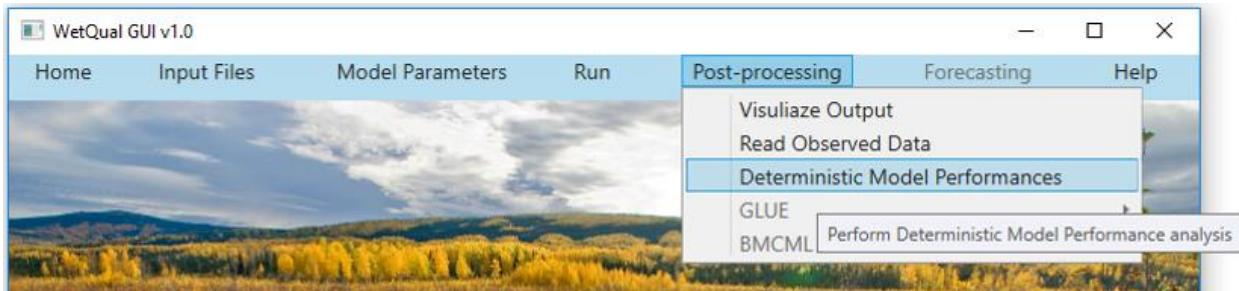


Figure 3.66

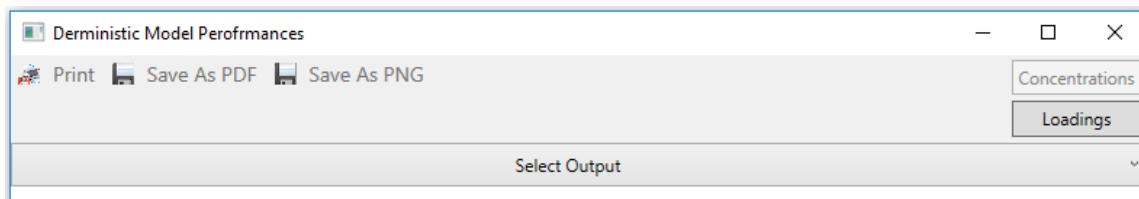


Figure 3.67

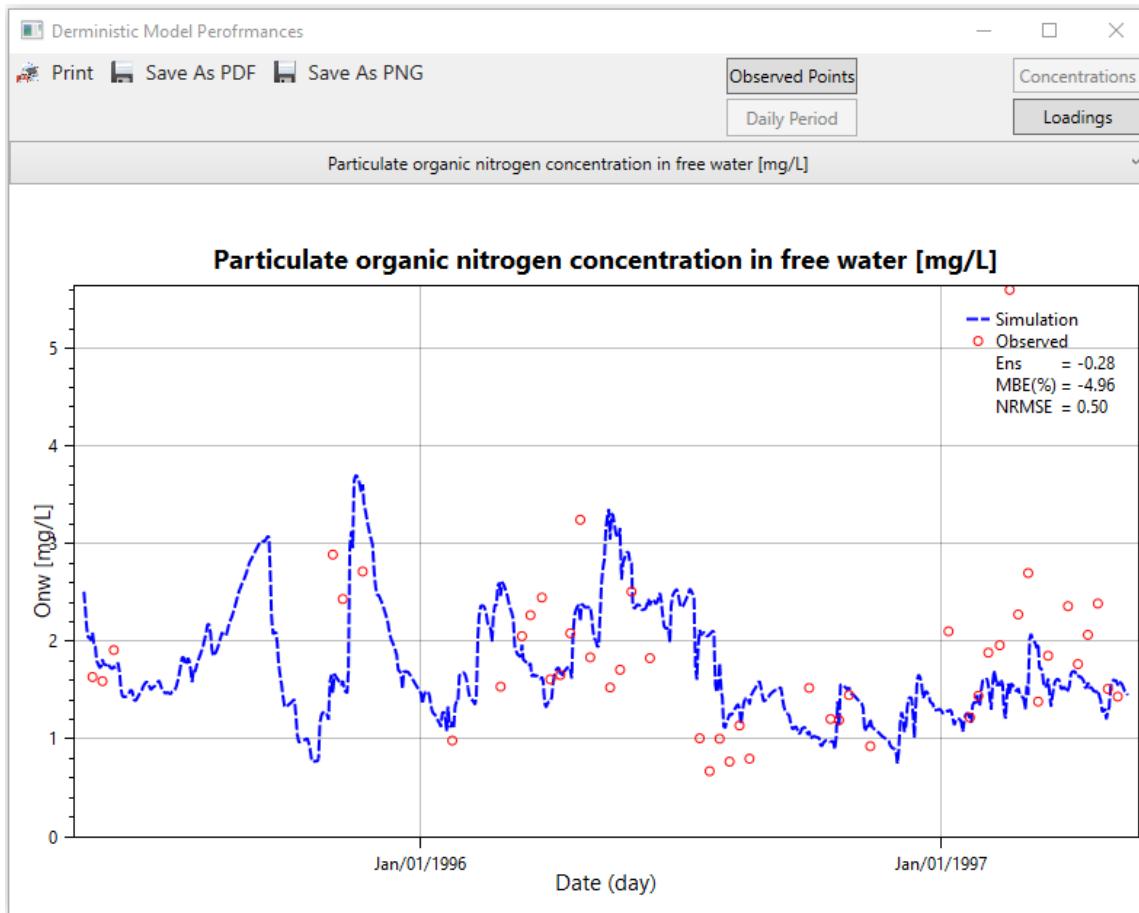


Figure 3.68

The GUI can plot the results only for the times where observed data are available or for the daily period. The **Observed Points** and **Daily Period** buttons can be used to switch between the two options. If observed data are flow-weighted averages of a certain number of days, the GUI will plot the results only for those periods with no time association as seen in Figure 3.69. The performance values are also calculated using the weighted values. The GUI can plot both concentration and loading results. The **Concentrations** and **Loadings** buttons can be used to select the desired option. More detailed information can be found for these buttons under Section 3.6.4.

If observed data for a selected constituent are not available or not provided in the *Observations* folder, the GUI will plot only the model output (Figure 3.70) and will not calculate or show any performance metrics.

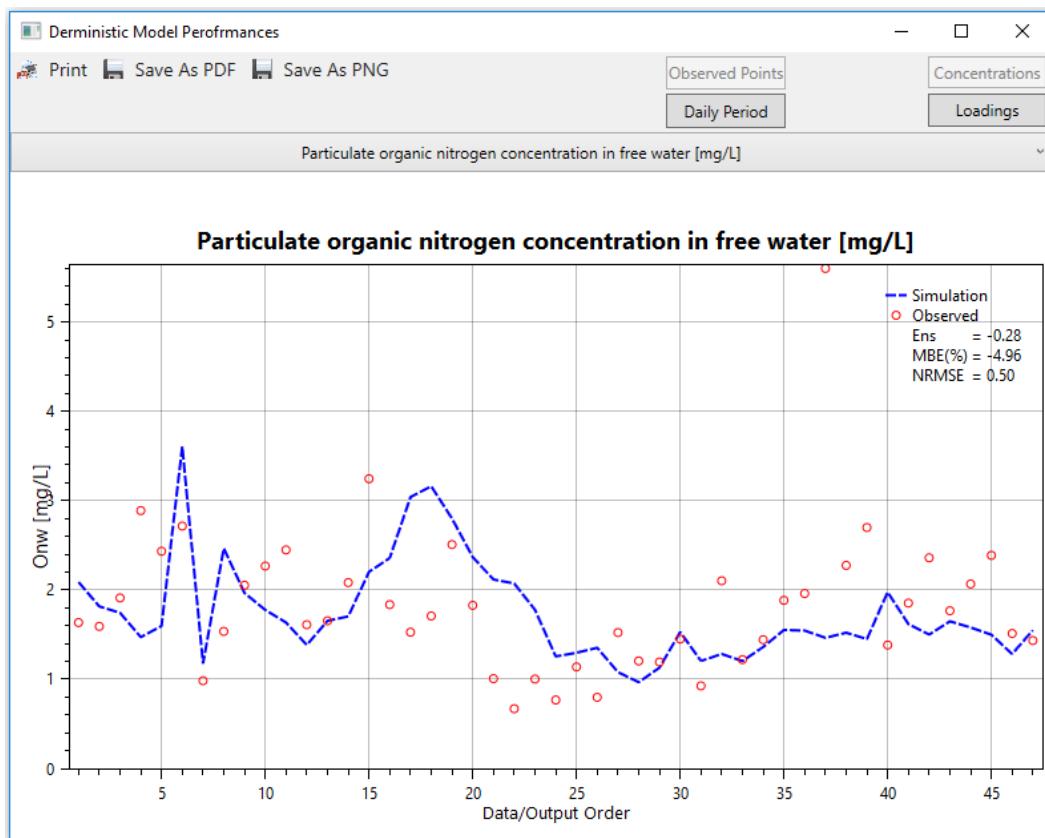


Figure 3.69

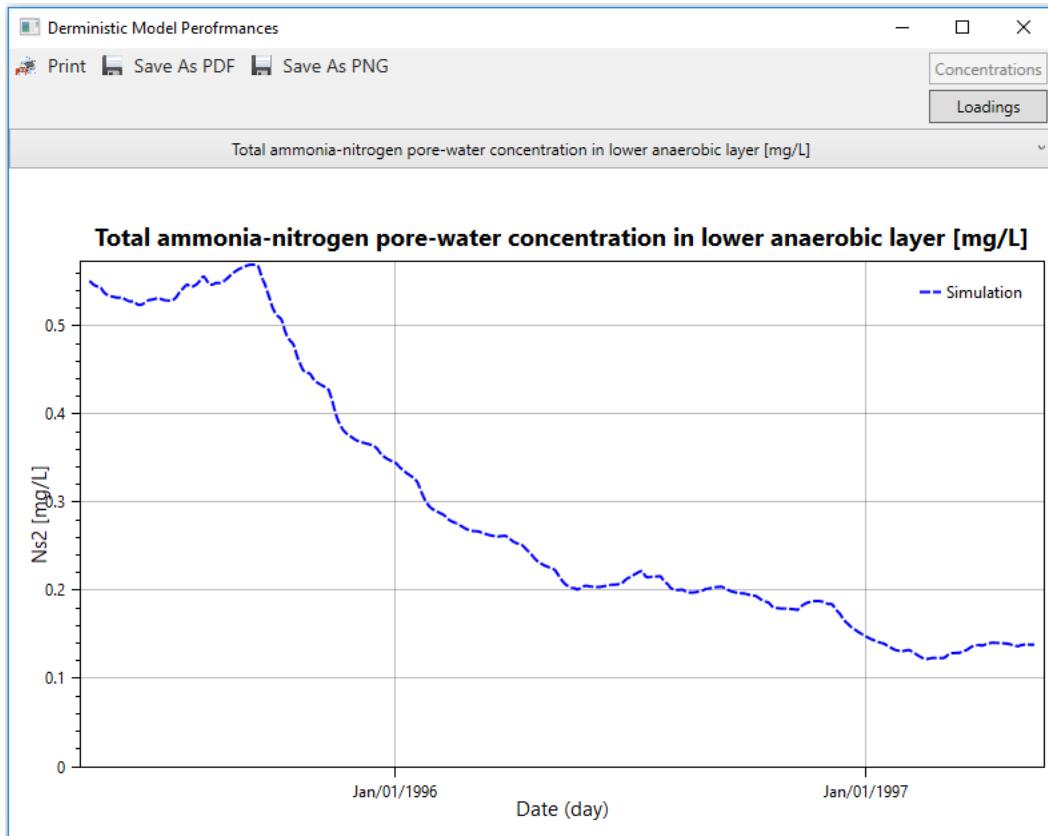


Figure 3.70

3.6.4 Uncertainty and Sensitivity Analysis

Figure 3.71 displays the Post-Processing menu for the stochastic model, which includes Read Observed Data, GLUE (Generalized Likelihood Uncertainty Estimation), and BMCML (Bayesian Monte Carlo simulation and maximum likelihood estimation) analyses. The Deterministic Model Performances sub-menu is deactivated during the stochastic model process.

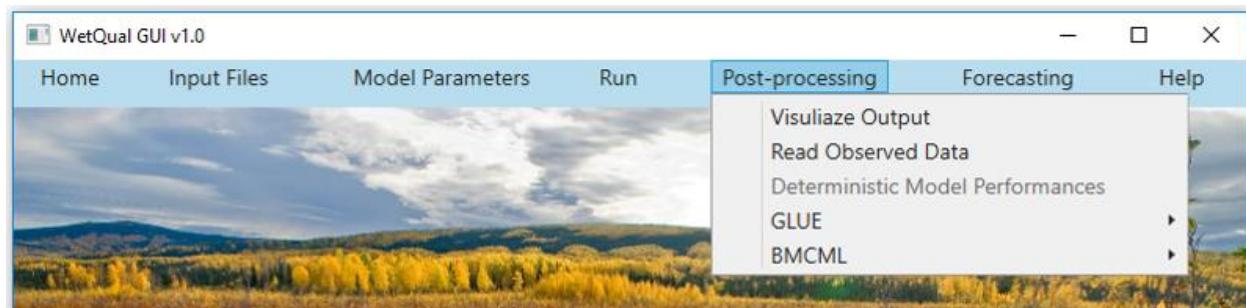


Figure 3.71

3.6.4.1 Uncertainty Analysis with GLUE

The **Uncertainty Analysis** and **Sensitivity Analysis** sub-menus are under the **GLUE** menu (Figure 3.72). Selecting **Uncertainty Analysis** displays Figure 3.73 before a model output of interest is selected. Here, select **Likelihood-1** or **Likelihood-2** (explained in the following paragraph) as the likelihood measure. These are used to separate the simulations and the related parameter sets into behavioral and non-behavioral sets. The default is “*Likelihood-1*” and there is an option to continue with the default or change it to *Likelihood-2* at the beginning. After prediction bands of selected parameters are displayed, the calculation method can be changed by clicking the **Likelihood-1** or **Likelihood-2** buttons, in which case the graph will be updated according to the selected method. A *WetQual* output can be selected under the “Select Output” list for GLUE analysis (Figure 3.74). These likelihoods can be calculated using either concentrations or loadings by clicking the **Concentrations** and **Loadings** buttons (Figure 3.74).

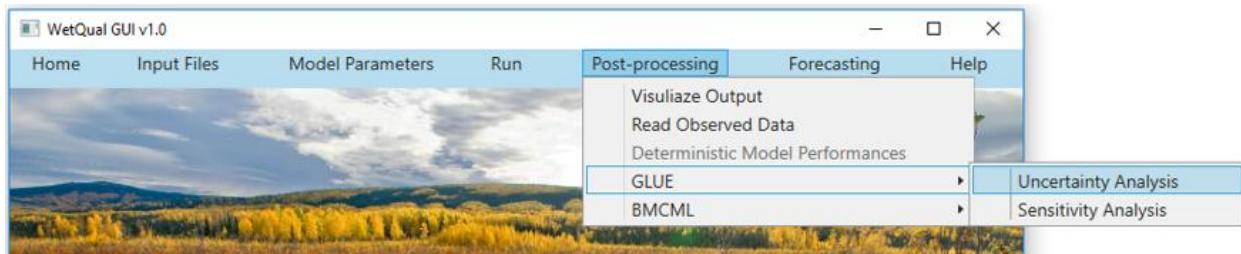


Figure 3.72

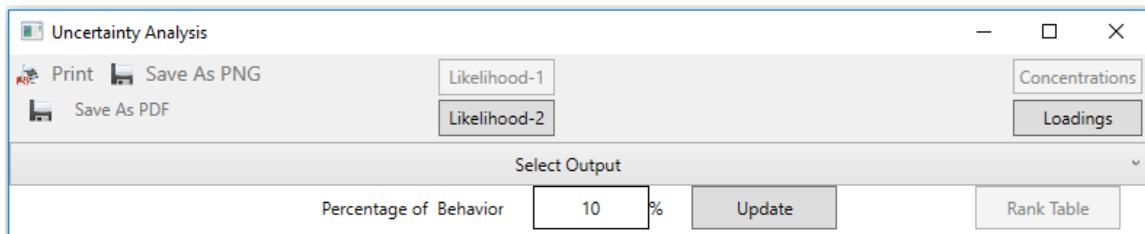


Figure 3.73

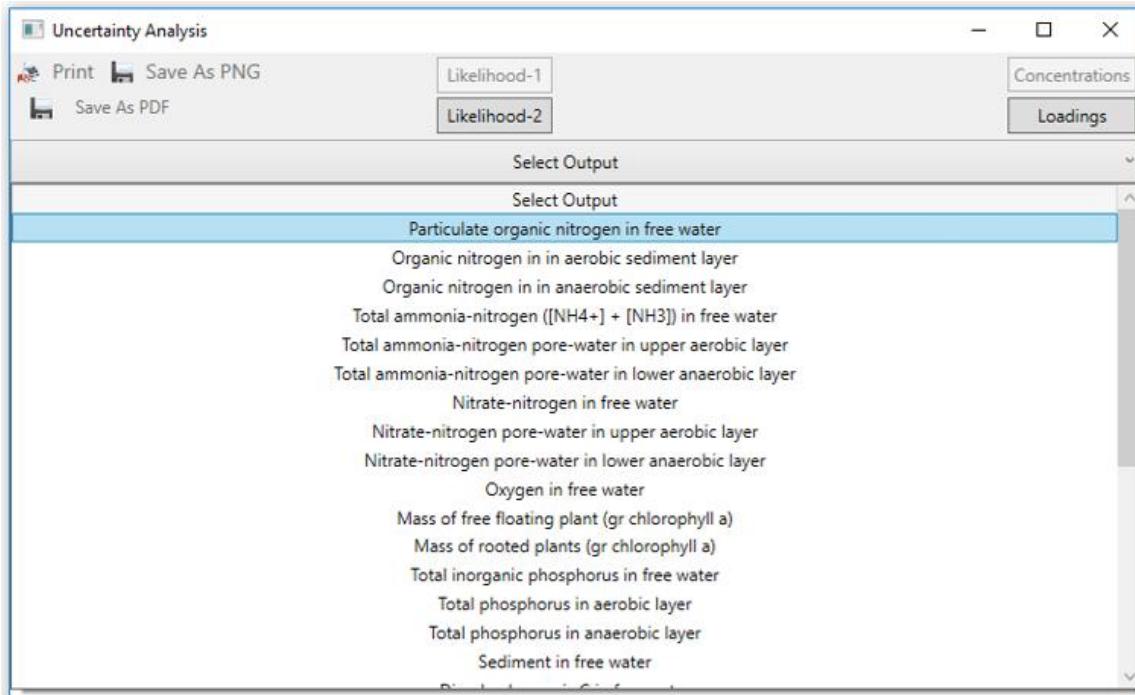


Figure 3.74

The *Likelihood-1* function utilized with GLUE in this GUI is a combination of Mass Balance Error (*MBE*) and *E_{NS}* such that

$$L_{k1} = \exp(E_{NS} - \frac{|MBE|}{100} - 1)$$

The *Likelihood-2* function utilizes the Nash-Sutcliffe efficiency (*E_{NS}*) and transforms it to a value is between 0 and 1 according to

$$L_{k2} = \exp(E_{NS} - 1)$$

The results of the likelihood calculations can be updated by changing the percentage of the behavioral simulations from 1 to 10. For instance, if 5% is selected, then the simulations that produced the highest 5% likelihoods are selected as behavioral (B), and the rest become non-behavioral (B'). The user needs to select the desired threshold. In the next step, behavioral (B) and non-behavioral (B') simulations are separated. Following this, a graph for each model output is depicted that includes observations, behavior set (B), the 95% prediction interval (P.I.) of all of the Monte Carlo generated simulations (BUB'), and the median of BUB'. Figure 3.75 shows an example graph of the *Uncertainty Analysis* window. The graph also shows the performance metrics *E_{NS}*, *MBE*, and *NRMSE* for the best simulation, which is the simulation having the highest *L_k* or *E_{NS}*.

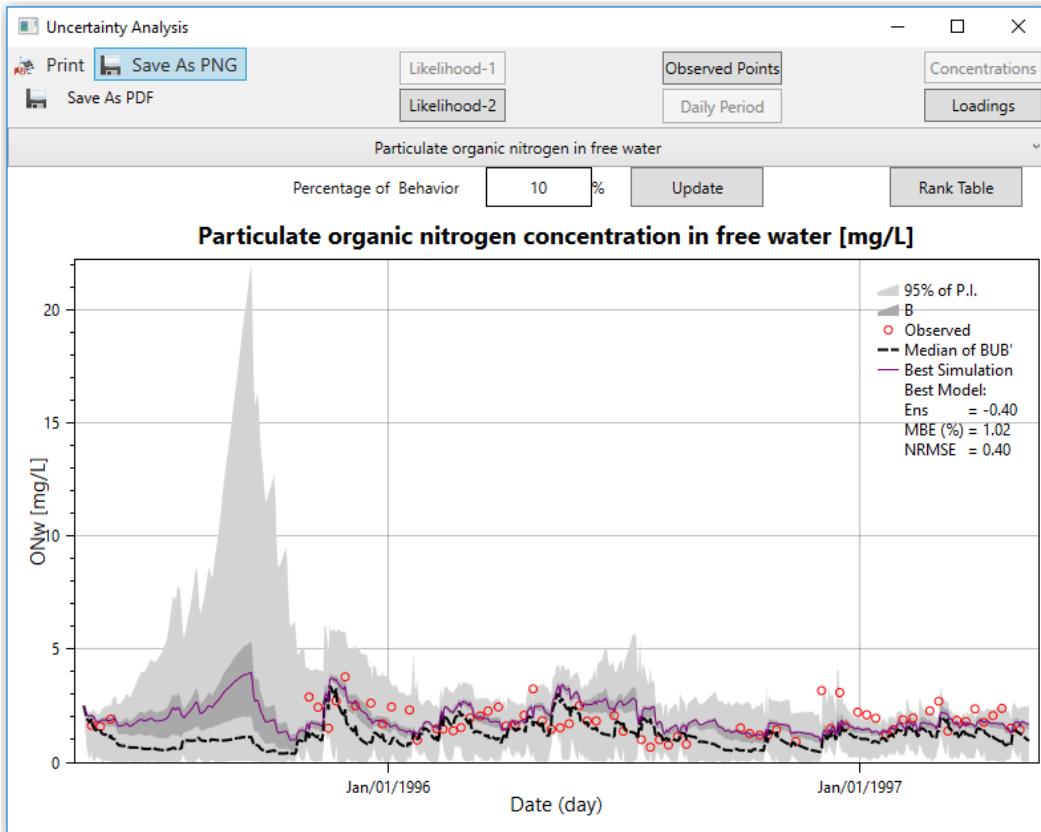


Figure 3.75

The GUI also writes these performance values to a text file and saves it as *Performances_GLUE_102_Onw.txt* (for *Onw* as selected model output) in the folder *ProjectName>InputOutput>glue*. When there are no observed data to calculate the likelihood values, the 95% P.I. for the whole simulation and the median of the whole simulation are displayed. If there are no observed data for a constituent but its immediate parent constituents have data, their joint likelihood values are used to determine the behavioral set. In this case, the GUI also plots behavior set (B). Figure 3.76 displays an example of the situation where there are no measured data but parent constituents have observed data.

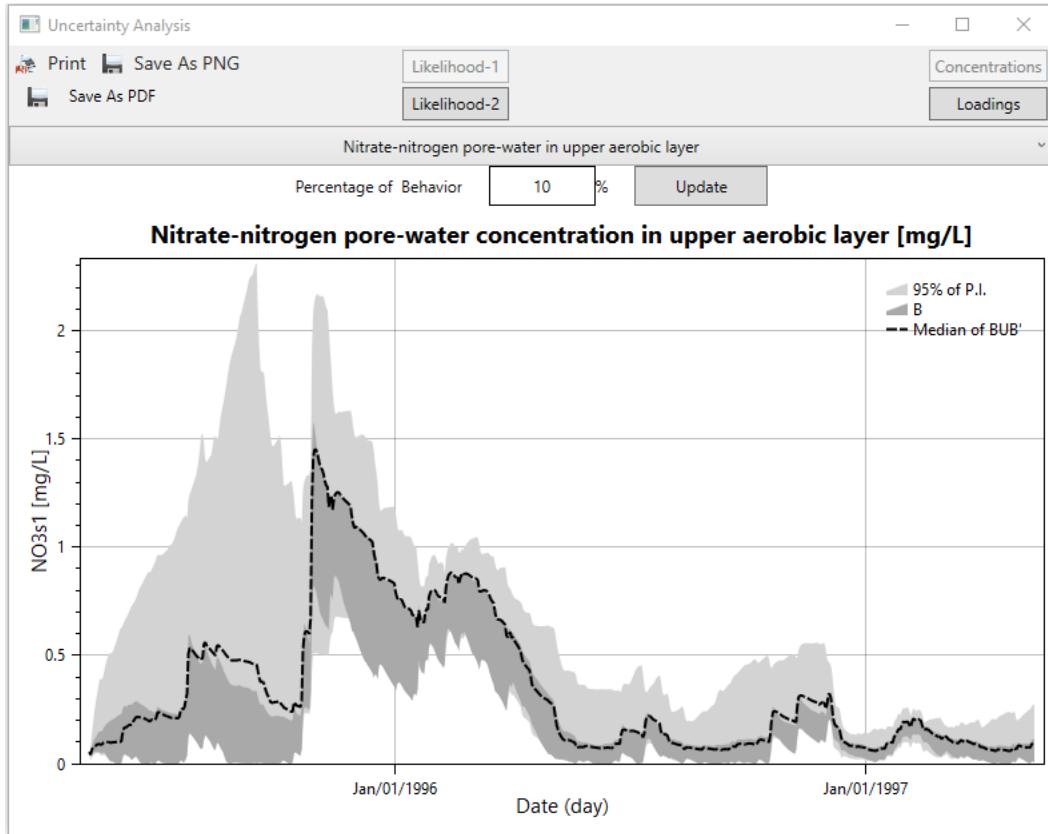


Figure 3.76

As can be seen in Figure 3.75, there is a **Rank Table** button on the upper right side of the window. Clicking this button generates a table similar to Figure 3.77, which provides a table summarizing all the calculated likelihoods and E_{NS} values in descending order. Whenever the *Rank Table* window is opened, the GUI saves it as a text file (e.g., *RankTables_102_Onw.txt*) in the *>InputOutput>glue* folder. The Rank Table file can be saved under a different file name and in any folder by clicking the **Save** button in the top right corner of the *Rank Table* window. As can be seen in Figure 3.76, the **Rank Table** button is invisible when there are no measured data.

Rank Table

Rank	Sim	Like1	Like2	ENash	Save
1	162	0.768769548628295	0.777229945833584	0.747980968187496	
2	745	0.665750544194042	0.775997088551986	0.746393489328046	
3	358	0.636114901482792	0.765502873075342	0.732777689309528	
4	638	0.631648597809414	0.759746540510539	0.725229599346733	
5	690	0.623287901525789	0.764101692604888	0.730945606830412	
6	926	0.594029337216825	0.755628350157066	0.719794376001	
7	647	0.562384848637025	0.731333009677017	0.687113630628336	
8	894	0.560045416757203	0.735674659417371	0.693032703183679	
9	114	0.552020756490404	0.736299433546481	0.693881596067888	
10	1	0.539502112286126	0.726478782709674	0.680453998797429	
11	717	0.538933049310035	0.724667962861417	0.677958288706517	
12	55	0.532054478320384	0.726073480837091	0.679895943995172	
13	580	0.530714100661875	0.719926497338818	0.671393840787309	
14	869	0.525707347612135	0.717034219980727	0.667368287090497	
15	147	0.524903950147632	0.70697238669357	0.653236329141182	

Figure 3.77

If observed data are daily or instantaneous values or not available, the GUI will plot GLUE results in a continuous time scale as shown in Figure 3.75 and Figure 3.76. If observed data are a flow-weighted average of a certain number of days, the GUI will plot the results only for those periods with no time association (Figure 3.78-top). The plot for the daily output can be seen by clicking the **Daily Period** (Figure 3.78-bottom). In this case, the observed data will be assigned to the last days of each sample collection on the graph. Clicking the **Likelihood-1** or **Likelihood-2** button reverts the plot to its previous state. The performance metrics will always be calculated using the flow-weighted values.

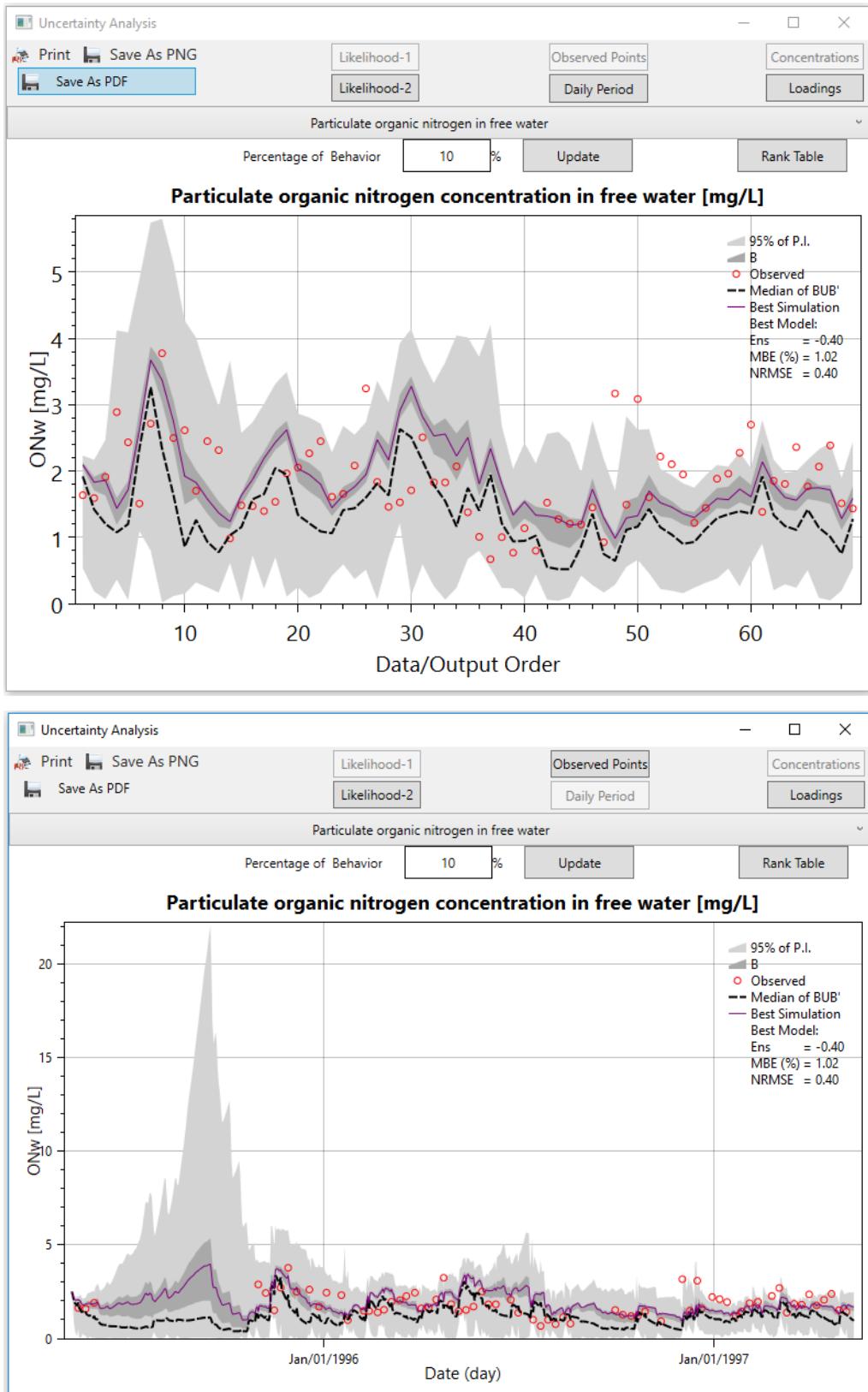


Figure 3.78

3.6.4.2 Sensitivity Analysis with GLUE

The Post-processing>GLUE>Sensitivity Analysis command opens the *Sensitivity Analysis* window (Figure 3.79). The user needs to select an output and then click the **Start Calculation** button to see the sensitivity analysis results. Examples of the graphs from the sensitivity analysis page (i.e., D_{\max} vs p -value) for organic nitrogen concentration in free water (mg/L) for a test run with 10,000 simulations are displayed in Figure 3.80. **We strongly suggest the users to have at least 1,000 simulations if they want to perform GLUE or BMCML analyses.**

In the **GLUE>Sensitivity Analysis** menu of the *WetQual* GUI, global sensitivity analysis (GSA) and dotty plots are considered in order to evaluate the sensitivity of the *WetQual* outputs to various parameters. The GUI performs the Kolmogorov-Smirnov (K-S) test in the *Sensitivity Analysis* window using the B and B' datasets. To that end, the cumulative distribution functions (CDFs) of the B and B' datasets are constructed for each parameter. Then, for each parameter, the maximum deviation (D_{\max}) between the two CDFs are determined (Kalin et al., 2013):

$$D_{\max} = \max |CDF_B(x) - CDF_{B'}(x)|$$

For a predetermined significance level of α , p -value less than α indicates a sensitive parameter. For the sake of space, the GUI displays the 20 most sensitive parameters by ranking the D_{\max} values from largest to smallest.

In addition to the K-S test, dotty plots were added to the *Sensitivity Analysis* window. Dotty plots provide information about sensitive parameters and most importantly depict the range in which the model is most sensitive to a given parameter. They also reveal the optimal ranges of the values of each parameter where the model performs best (Kalin et al., 2013).

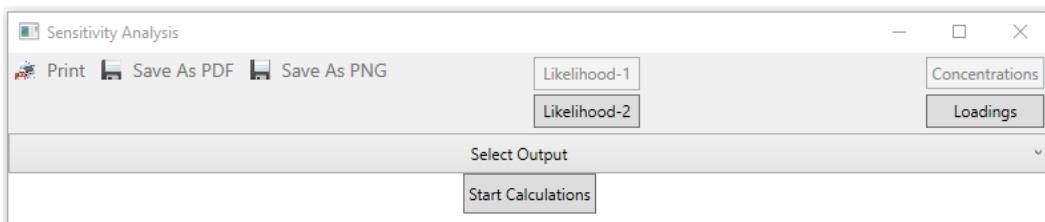


Figure 3.79

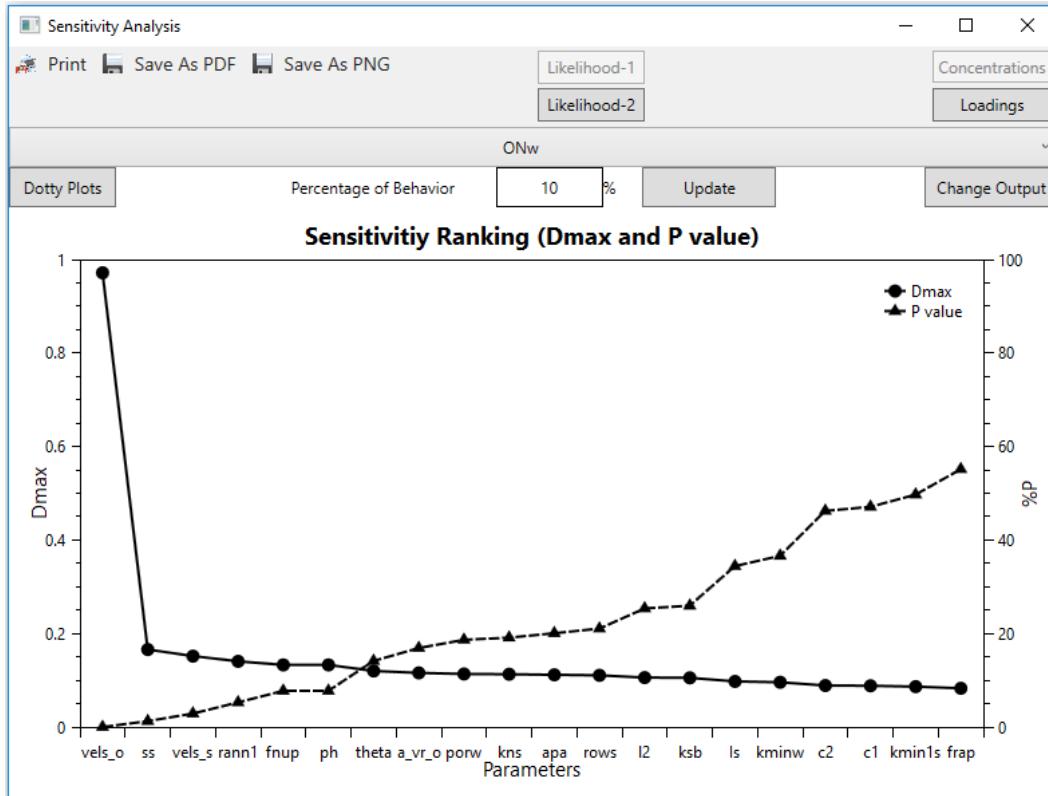


Figure 3.80

The **Change Output** button allows the user to select the desired output. The *Sensitivity Analysis* window of the GUI will display CDFs and dotty plots of the 20 most sensitive model parameters. By clicking **CDF** for a parameter of interest under the selected constituent bar (Figure 3.81), the GUI plots the CDFs of B and B' for the selected parameter (Figure 3.82). The graph can be saved using the **Save As PDF** or **Save As PNG** buttons for the appropriate format. The user can see the dotty plots of the 20 most sensitive parameters on the same window by clicking the **Dotty Plots** button on the upper left side of the *Sensitivity Analysis* window (Figure 3.83). These plots can also be saved using the **Save As PDF** or **Save As PNG** buttons. The GUI saves each dotty plot in the figure as separate files.

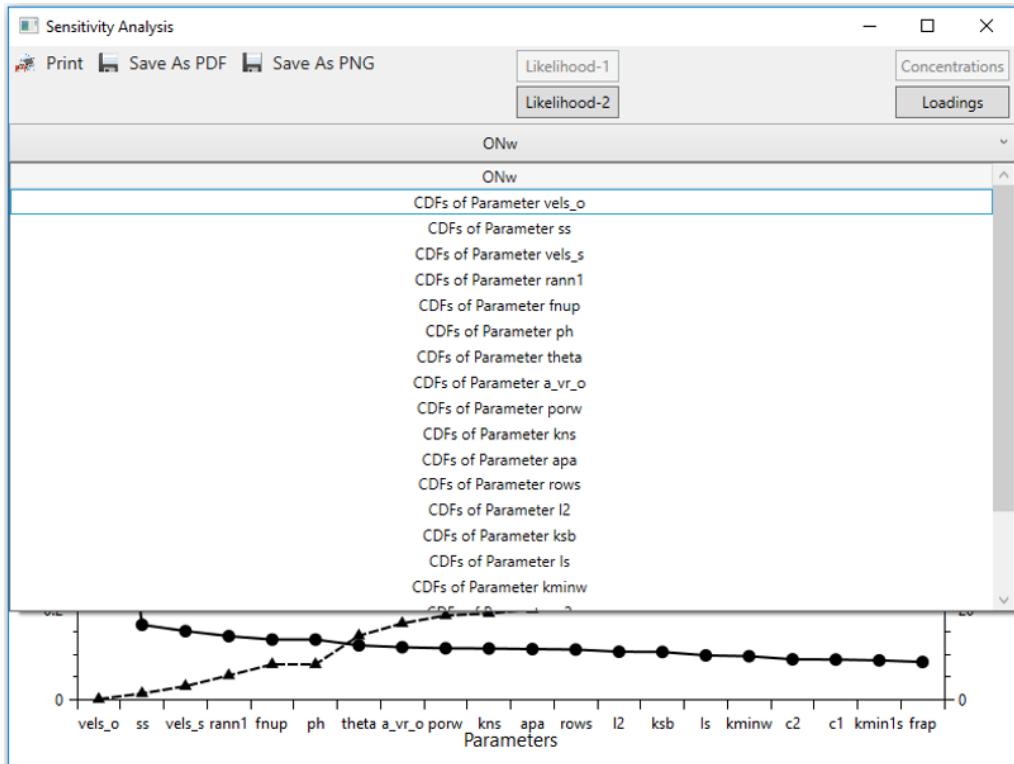


Figure 3.81

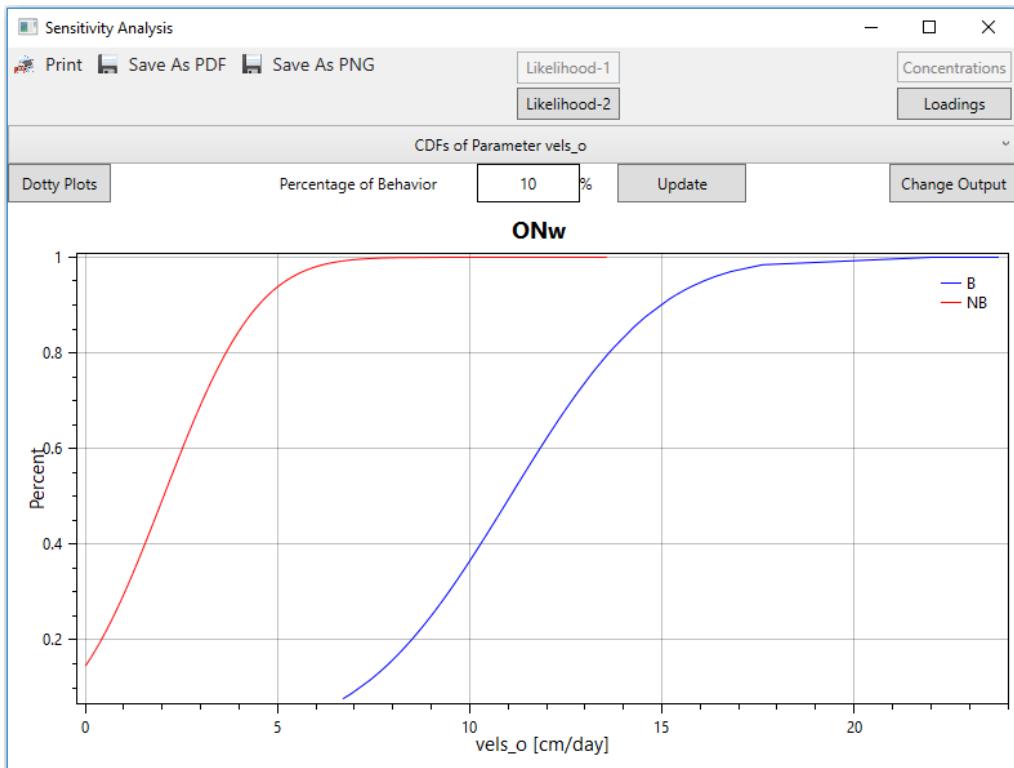


Figure 3.82

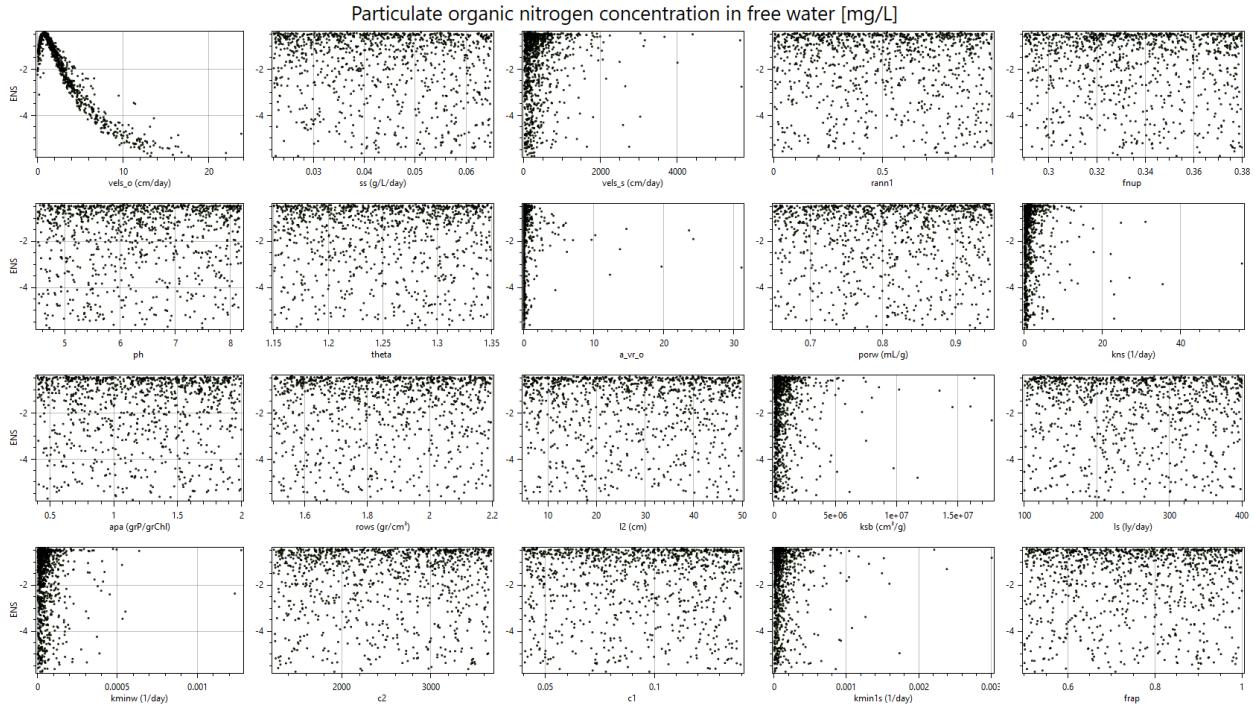


Figure 3.83

3.6.4.3 Uncertainty Analysis with BMCML

Post-processing for the stochastic model can also conduct a Bayesian Monte Carlo simulation and maximum likelihood estimation analysis (BMCML). This approach combines Bayesian Monte Carlo (BMC) simulation (e.g., Dilks et al., 1992) with the maximum likelihood estimation and borrows the concept of “equifinality” from the GLUE methodology (i.e., the emphasis is placed on the generated parameter sets).

In BMCML, the maximum likelihood value is obtained from $\hat{l}(\theta_i) = (2\pi e \hat{\sigma}_{\varepsilon i}^2)^{-\frac{m}{2}}$ where $\hat{\sigma}_{\varepsilon i}^2$ is the variance of model structural error (Hantush and Chaudhary, 2014).

The Bayesian estimate of each model output concentration Y at any point in time is the conditional mean of Y given the observation O , $E(Y|O)$, which in the discrete form can be approximated (assuming uniformly sampled parameter space) as (Hantush and Chaudhary, 2014):

$$E(Y|O) = \sum_{i=1}^n E(Y|\theta_i) P(\theta_i|O) = \sum_{i=1}^n C(\theta_i) P(\theta_i|O)$$

where $C(\theta_i)$ is the model-simulated output and $P(\theta_i|O)$ is the posterior probability mass of parameter set $\theta_i = (\theta_1^i, \theta_2^i, \dots, \theta_r^i)^T$.

The explicit expression for the posterior CDF of the model parameters and the expressions used to construct predictions (i.e., median and confidence limits) for future observed values of Y given the observed records, O , is (Hantush and Chaudhary, 2014):

$$E(Y|O) = \frac{1}{2} + \frac{1}{2} \sum_{i=1}^n \operatorname{erf} \left(\frac{y - C(\theta_i) - \hat{\mu}_i}{\sqrt{2}\hat{\sigma}_e} \right) P(\theta_i|O)$$

where $\hat{\mu}_i$ is the mean of residual errors. Refer to Hantush and Chaudhary (2014) and Chaudhary and Hantush (2017) for details about the BMCML method.

Similar to the uncertainty analysis with GLUE in Section 3.6.4.1, the joint likelihood of immediate parent constituents is used in BMCML analysis if there are no observed data for the constituent under study.

Under the Post-processing>BMCML menu, in order to plot priori/posterior the CDFs and the probability density functions (PDFs), the Prediction Bands and Posterior CDFs and PDFs sub-menus are available as shown in Figure 3.84. When the Post-processing>BMCML>Prediction Bands menu is selected, the *BMCML (Prediction Bands)* window will be displayed (Figure 3.85). The options are to select either the **Loadings** or **Concentrations** buttons. The results will be displayed based on the selection. The default is concentrations and the selected unit type is activated, and vice versa. By clicking the **Select Output** bar, the user can select the desired constituent under the bar as shown in Figure 3.86.

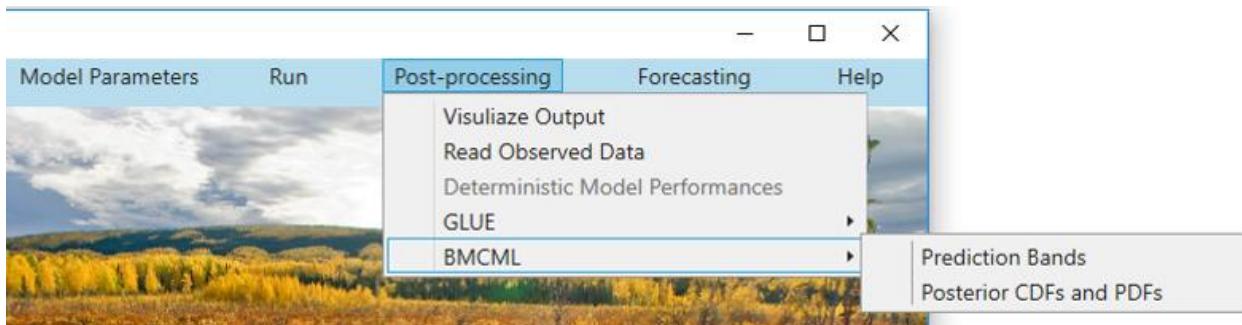


Figure 3.84

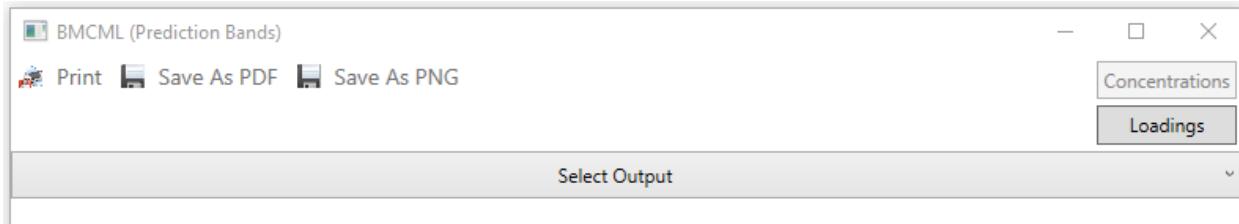


Figure 3.85

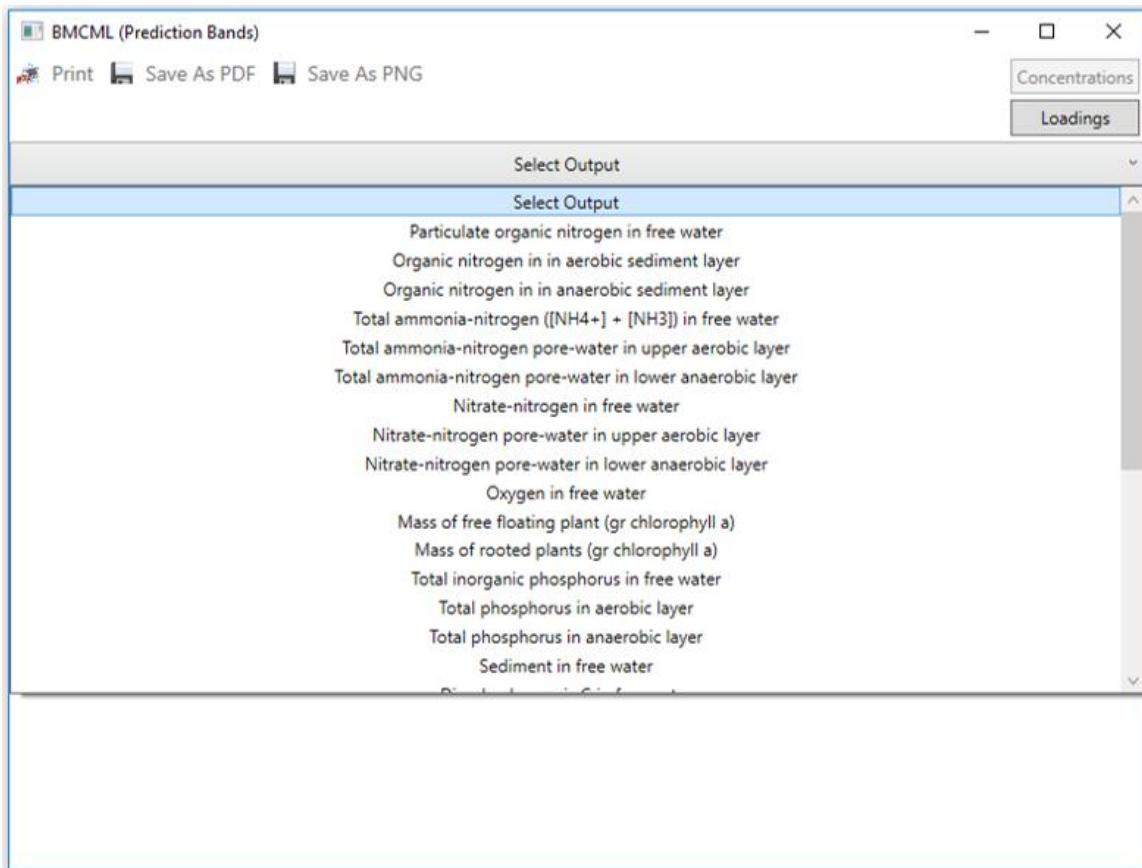


Figure 3.86

Figure 3.87 and Figure 3.88 display the prediction bands and performances for organic nitrogen (O_{nw}) based on loadings. Again, if observed data are a flow-weighted average of a certain number of days, the GUI will plot the results only for those periods with no time association. The user can also see the plot for the daily output by clicking **Daily Period**. See the GLUE section for more detail.

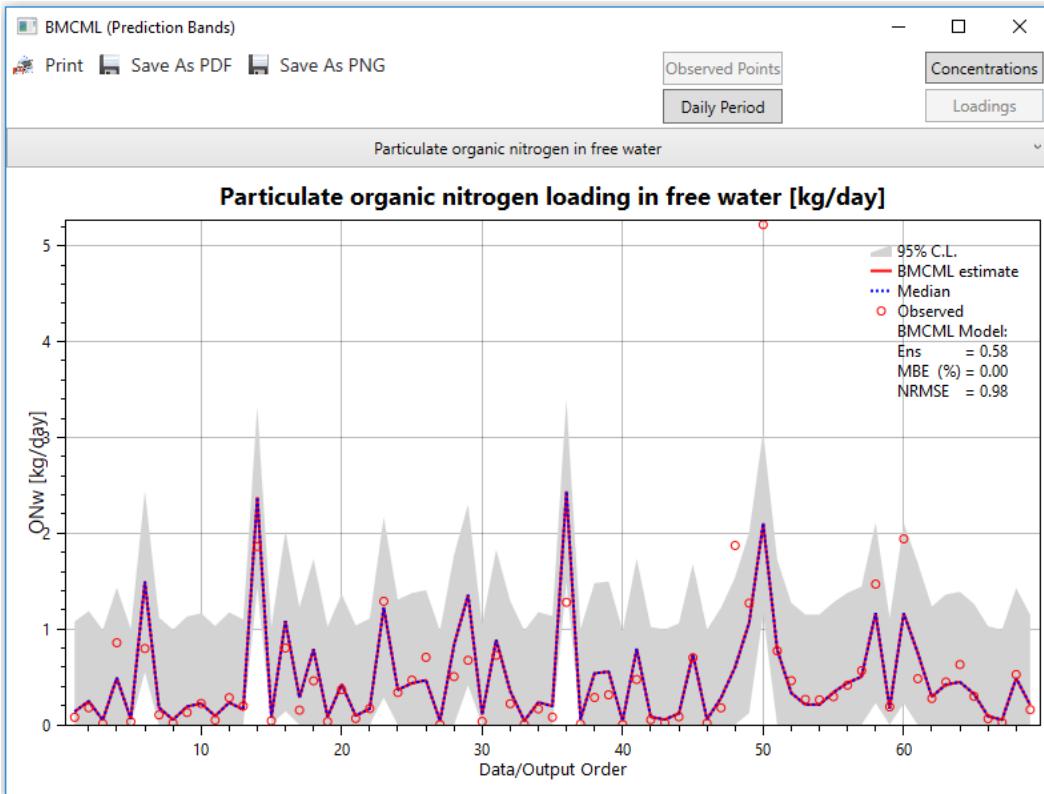


Figure 3.87

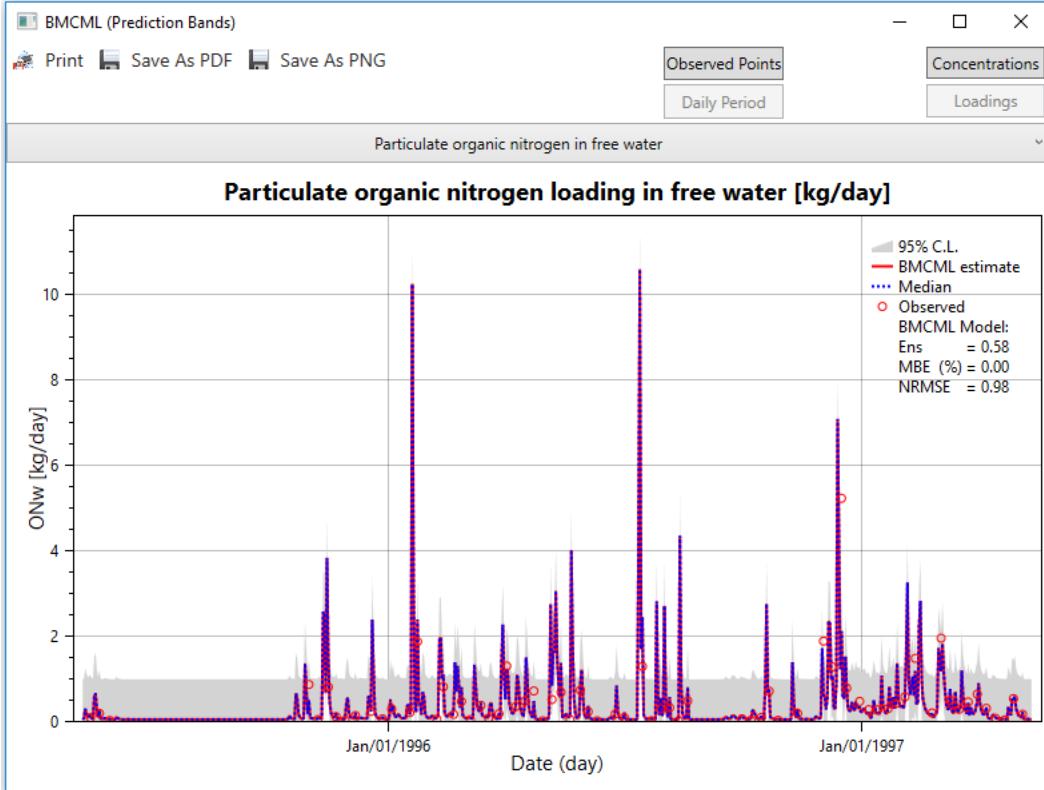


Figure 3.88

Both loadings (Figure 3.87 and Figure 3.88) and concentrations (Figure 3.89 and Figure 3.90) of observed and simulated values can be used in the BMCML calculations. The loading or concentration results can be viewed by clicking the **Loadings** or **Concentrations** buttons, respectively.

As explained in Section 3.6.4.1, if observed data are daily or instantaneous values, the GUI will plot BMCML results on a continuous time scale as shown in Figure 3.88 and Figure 3.90. If observed data are the flow-weighted average of a certain number of days, the GUI will plot BMCML results for those periods only, with no time association (Figure 3.87 and Figure 3.89).

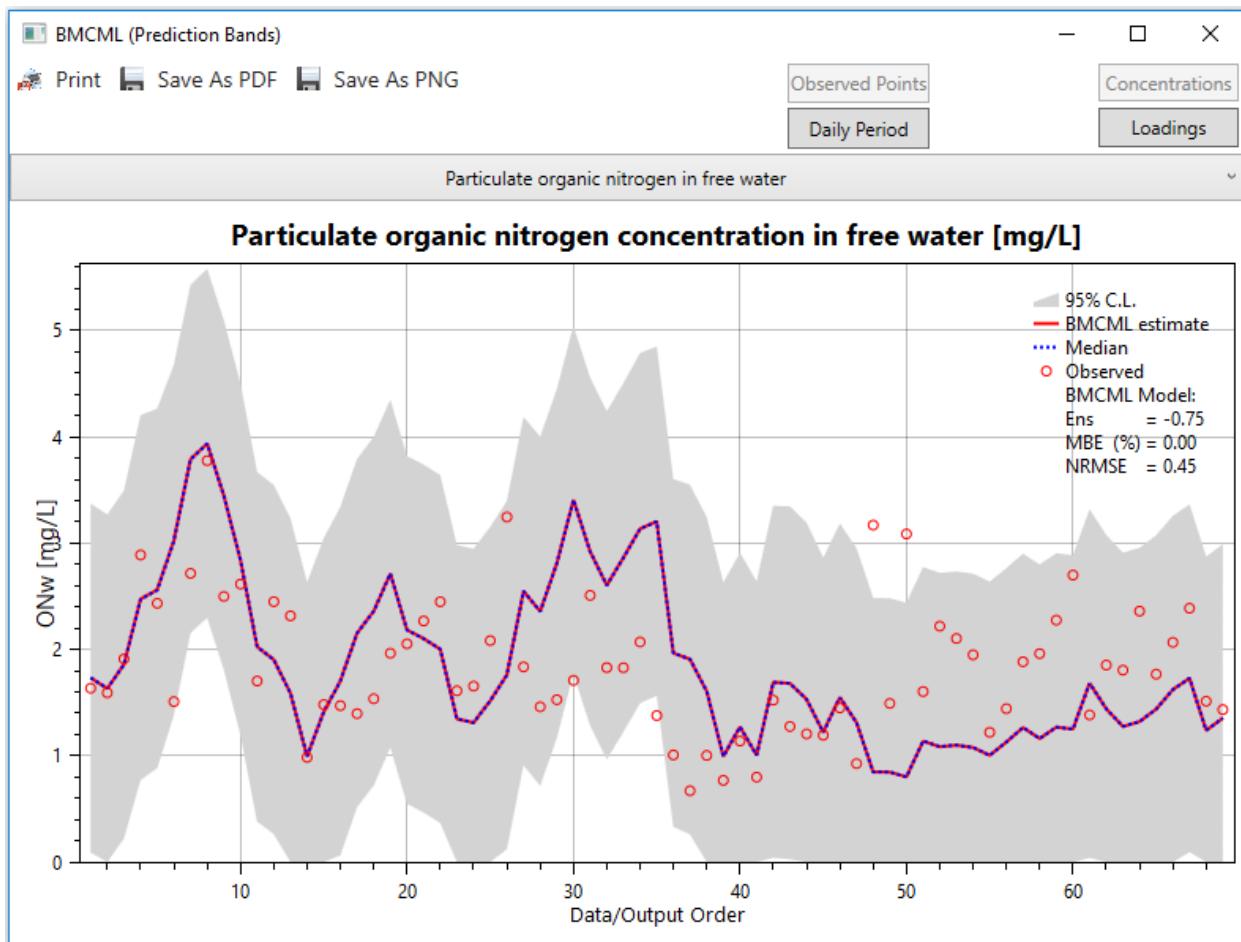


Figure 3.89

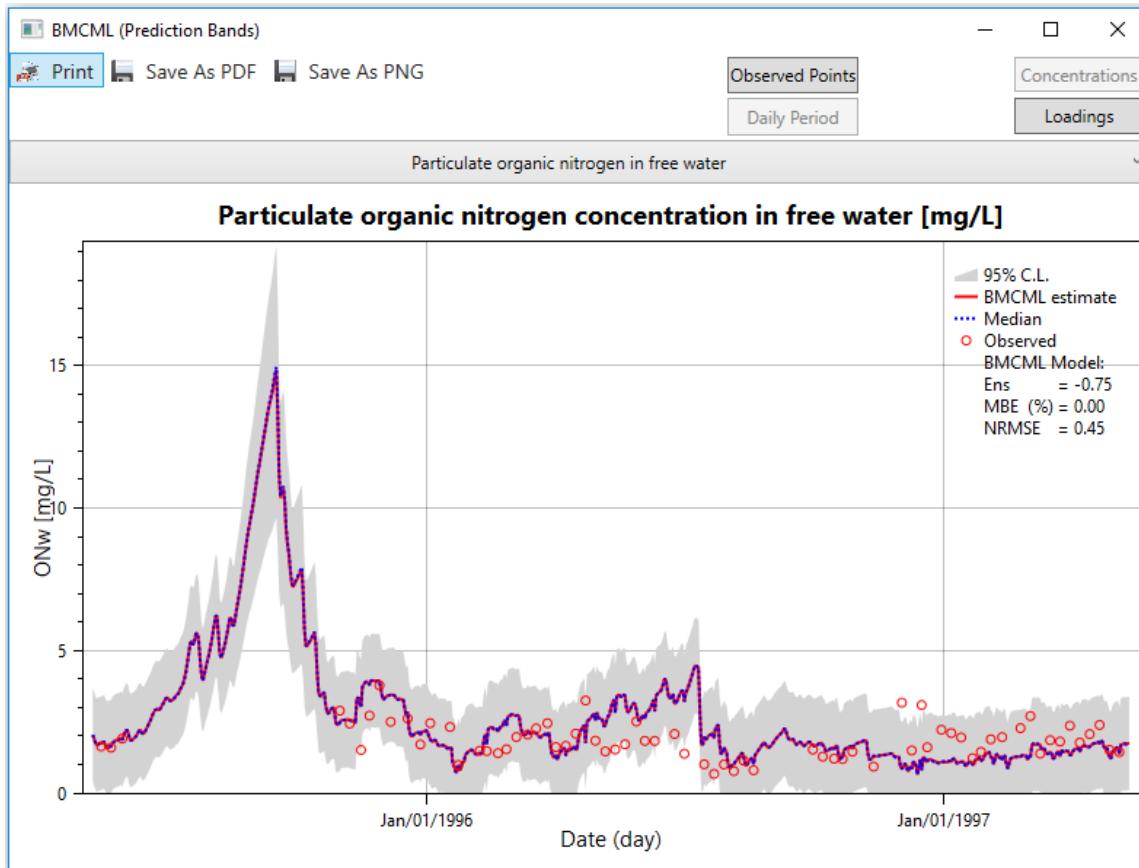


Figure 3.90

3.6.4.4 Posterior CDFs and PDFs

Under the Post-processing>BMCML menu, when the Posterior CDFs and PDFs sub-menu is clicked, the *Posterior Analysis* window is displayed as shown in Figure 3.91. Select a constituent under the “Select Output” bar and click **Start Calculation** to calculate posterior CDFs and PDFs (Figure 3.92) (refer to Hantush and Chaudhary, 2014 and Chaudhary and Hantush, 2017). It may take several minutes to a couple of hours depending on the number of simulations and the length of the period. After the calculations are completed, the CDF and PDF graphs of the 20 most effective parameters can be visualized by selecting a parameter under the selected constituent bar. The default percentage rate is displayed in the window. This rate can be changed to any value between 1% and 10%. Click the **Update** button to repeat the calculations based on the selected new percentage rate. If another constituent is needed, click the **Change Output** button. Figure

3.93 and Figure 3.94 display priori and posterior CDFs and PDFs for O_{nw} . Click the **CDF** or **PDF** buttons on the right upper side to see the CDF and PDF graphs sequentially.

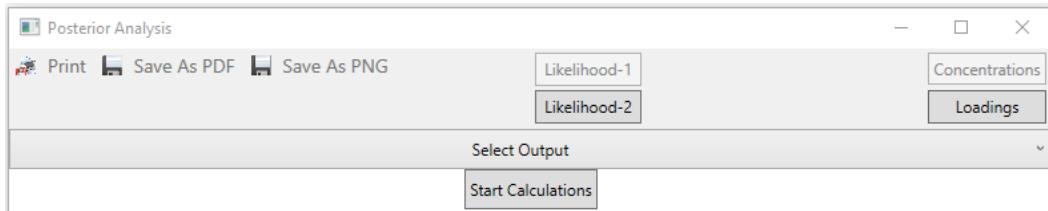


Figure 3.91

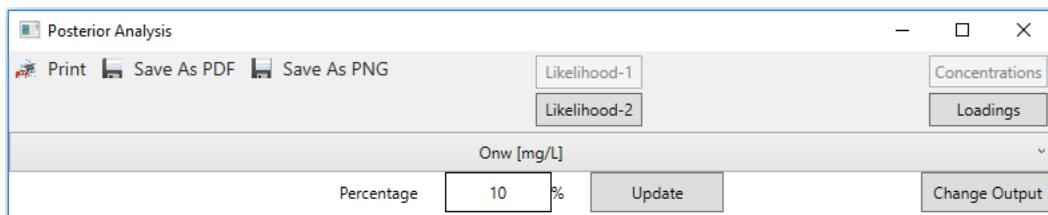


Figure 3.92

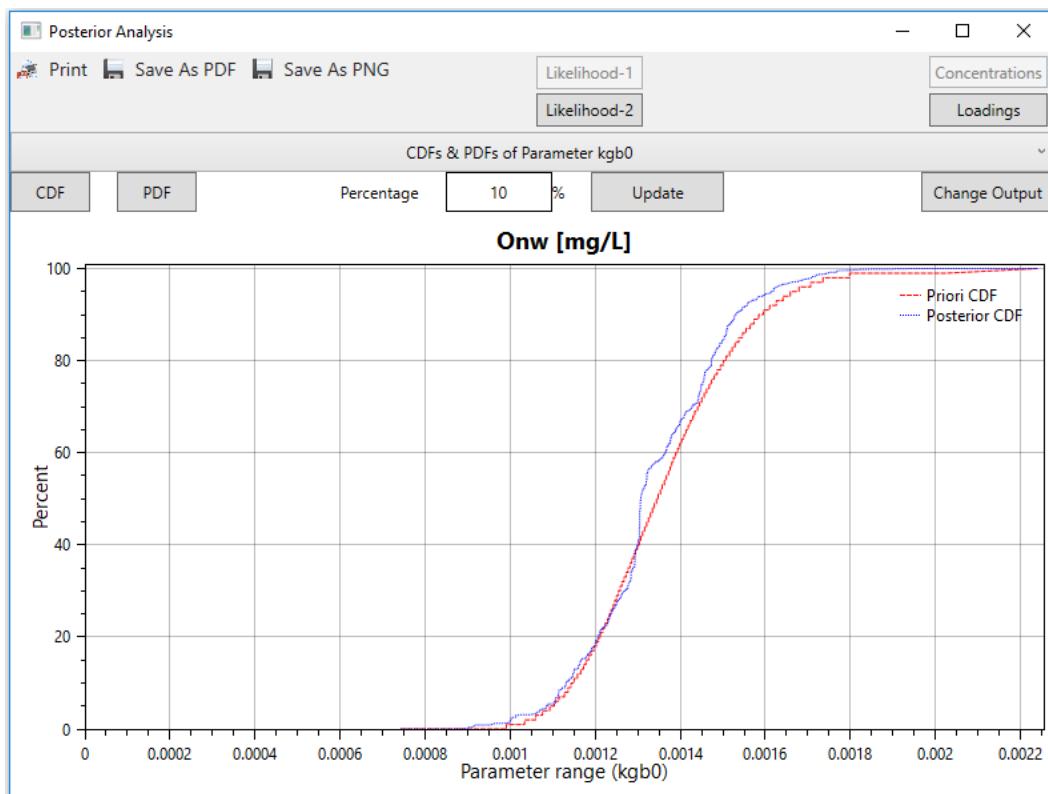


Figure 3.93

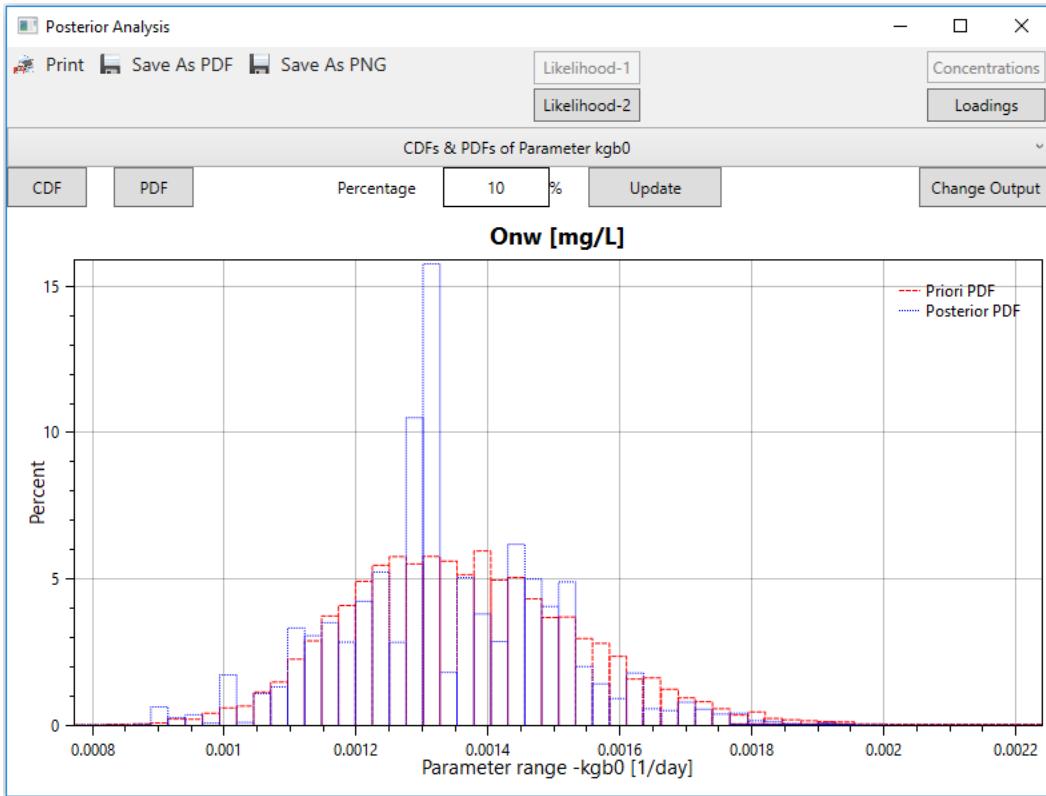


Figure 3.94

The **Print** and **Save As** (in PDF and PNG format) buttons near the top offer these options for all graph windows.

3.7 Forecasting/Validation

After analyzing the results of simulation(s) for a given period, the GUI activates the forecasting option. With this, the model can be run for a future period or any time span to forecast or validate data using the generated model parameter values and associated likelihood values of the main project. Forecasting/Validation window is displayed under **Forecasting>Start Forecasting/Validation** menu (Figure 3.95 and Figure 3.96). After clicking this menu, the GUI will copy all input files with sub-directories to the *Forecast* folder under the main project folder.

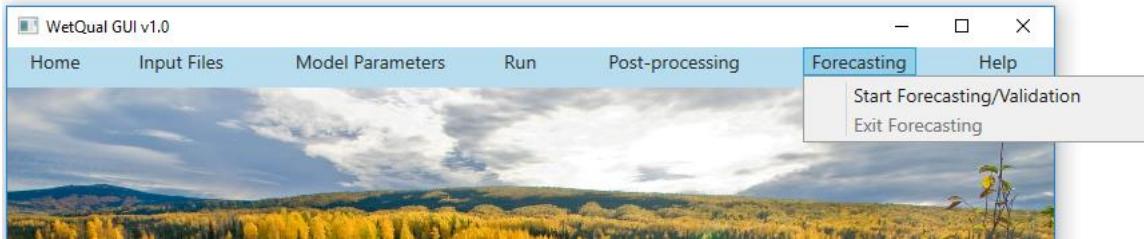


Figure 3.95

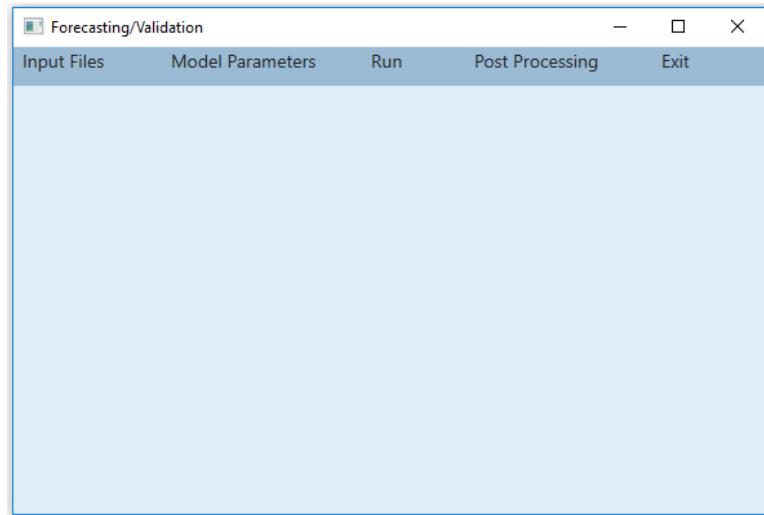


Figure 3.96

The procedures in Section 3.3 should be repeated for the forecasting period to prepare input files (Figure 3.97). The input files used in the main project simulation are copied under the *>Forecast>InputOutput* folder, so the related files under this folder can be selected and changed. As the GUI will use the likelihood values of the generated nitrogen and carbon parameters from the main project, the stochastic model parameters cannot be changed. The **Model Parameters>Stochastic Model** command (Figure 3.98) loads the parameters of the main project. On the other hand, *WetQual* can be run in a deterministic model by selecting one of the parameter sets. The **Model Parameters>Deterministic Model** menu (Figure 3.98) lets the user set the model parameter values as described in Section 3.4. If *WetQual* should be run with a particular parameter set from the generated set of parameters (for example, the one that had the highest likelihood value), do the following:

- Open the file *14_generated_parameters.txt* under the main project *InputOutput* folder and copy the row that has the desired parameter set (Figure 3.99).
- Open the file *14_generated_parameters.txt* under the *Forecast\InputOutput* folder and paste the copied parameter values (Figure 3.100).
- Repeat the same procedure for the carbon parameters.

After completing the input files, select the **Run >Run WetQual** menu to run *WetQual* for the forecasting period (Figure 3.101).

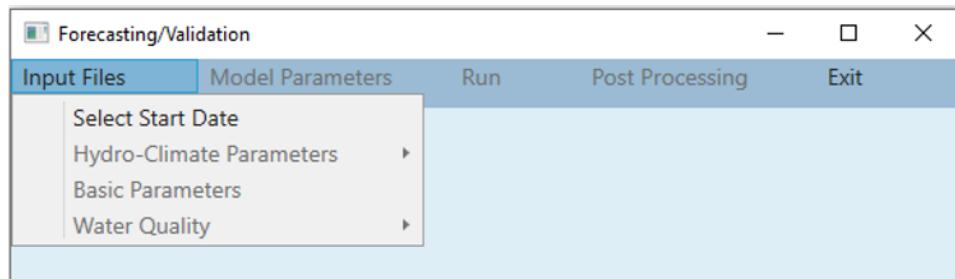


Figure 3.97

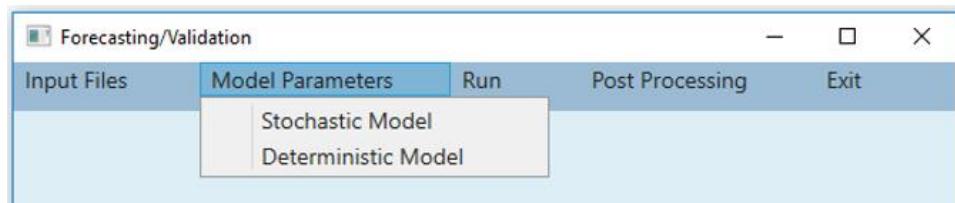


Figure 3.98

L2	theta	Is	fNup	kd	kep	kga0	kgb0	kmin1s	knw	kminw	kns	kden	rowp	vels_o	vels_s	v
26.66559909	1.24629155	195.35124111	0.31860537	0.87832615	0.35299275	0.00106241	0.00155355	0.000213!								
7.91917906	1.16297413	239.84497289	0.33195349	1.43686065	0.19825434	0.00153866	0.00123307	0.0004822!								
5.57840086	1.15257067	249.30196286	0.33479059	1.58822997	0.35444432	0.00154741	0.00127653	0.0006220!								
43.69842354	1.32199299	118.48267793	0.29554480	0.22733925	0.29300874	0.00157395	0.00113129	0.0005724!								
22.46881638	1.22763918	148.14460480	0.30444338	0.45547853	0.26527616	0.00139002	0.00128986	0.000784!								
10.19375502	1.17308336	167.16516356	0.31014955	0.61200306	0.21187464	0.00119699	0.00125239	0.000260!								
40.01634101	1.30562818	249.69741253	0.33490922	1.59488724	0.35036956	0.00152301	0.00136702	0.0001219!								
15.70002663	1.19755567	328.91332350	0.35867400	3.96131125	0.38699846	0.00150781	0.00127301	0.000360!								

Figure 3.99

L2	theta	Is	fNup	kd	kep	kga0	kgb0	kmin1s	knw	kminw	kns	kden	rowp	vels_o	vels_s	v
22.46881638	1.22763918	148.14460480	0.30444338	0.45547853	0.26527616	0.00139002	0.00128986	0.000784!								

Figure 3.100

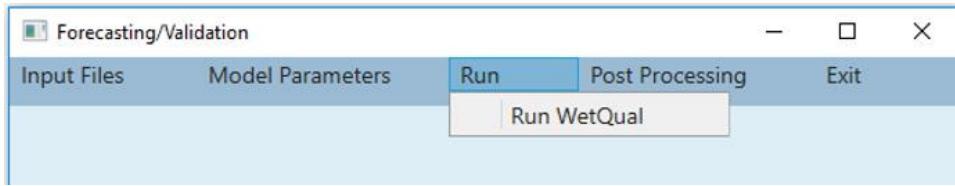


Figure 3.101

The results can be visualized as described in Section 3.6.1 using the **Visualize Output** menu. If the observed data are available for the forecasting period (validation period can be run under forecasting option), the results can be used for validation purposes. In this case, select the observed files using the **Read Observed Data** sub-menu as described in Section 3.6.2 (Figure 3.102). If the forecasting model is run with the whole parameter set (Stochastic mode), under the **Post-processing** menu, the **Deterministic Model Performances** menu is deactivated and the **GLUE** and **BMCML** menus are activated or vice versa (Figure 3.102). The function of the **GLUE** and **BMCML** menus in the *Forecasting* window are similar to the functions of the **GLUE>Sensitivity Analysis** and **BMCML>Prediction Bands** menus as described in Sections 3.6.4.1 and 3.6.4.3. The **GLUE** menu displays the *GLUE* window as shown in Figure 3.103. The Prediction band is displayed after a constituent is selected (Figure 3.104 and Figure 3.105). Prediction bands can be displayed for different likelihood functions based on concentrations and loadings by clicking the **Likelihood-1** or **Likelihood-2** and **Concentrations** or **Loadings** buttons, respectively.

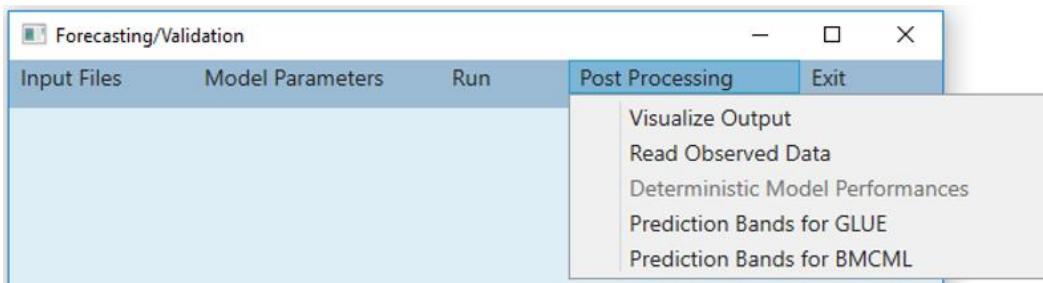


Figure 3.102

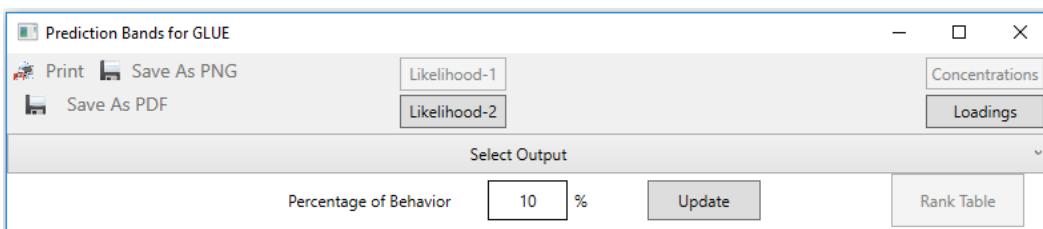


Figure 3.103

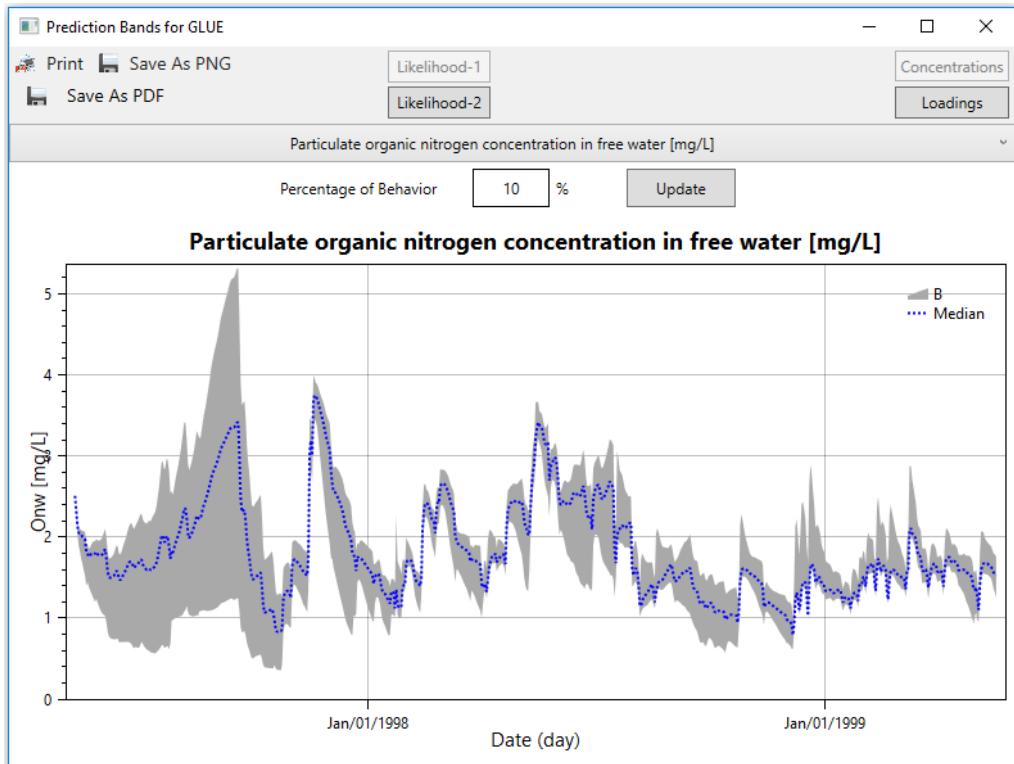


Figure 3.104

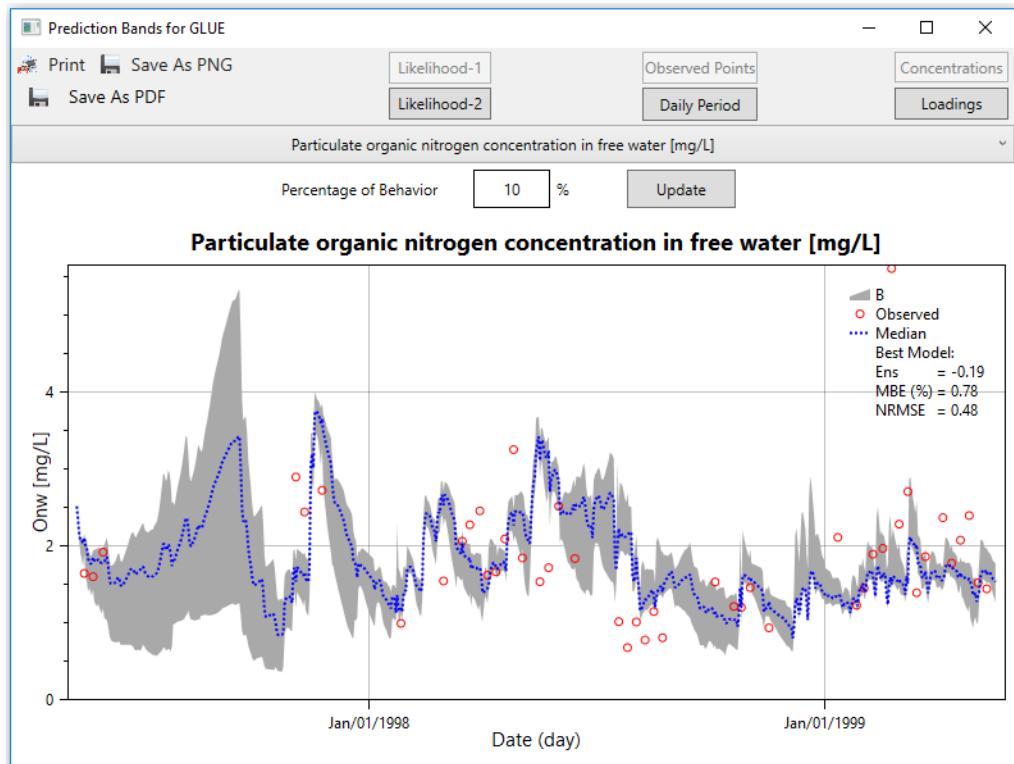


Figure 3.105

The **BMCML** menu opens the *BMCML* window as shown in Figure 3.106. The BMCML prediction band is displayed after selecting a constituent (Figure 3.107). The options are either **Loadings** or **Concentrations**. The calculations are based on the BMCML likelihood values of the main project. If the observed data are available for the projected period, the performance values are also displayed beside the band on the window as shown in Figure 3.108.

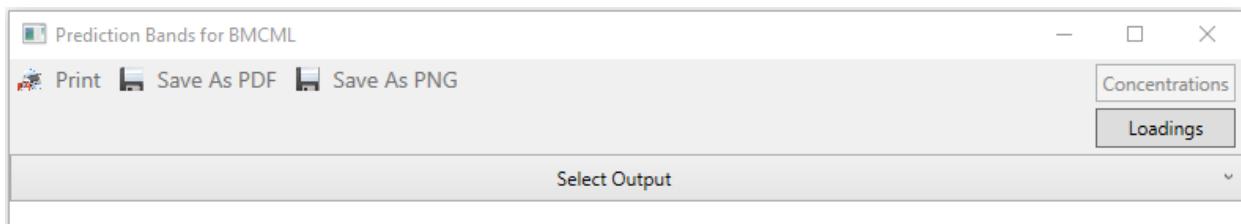


Figure 3.106

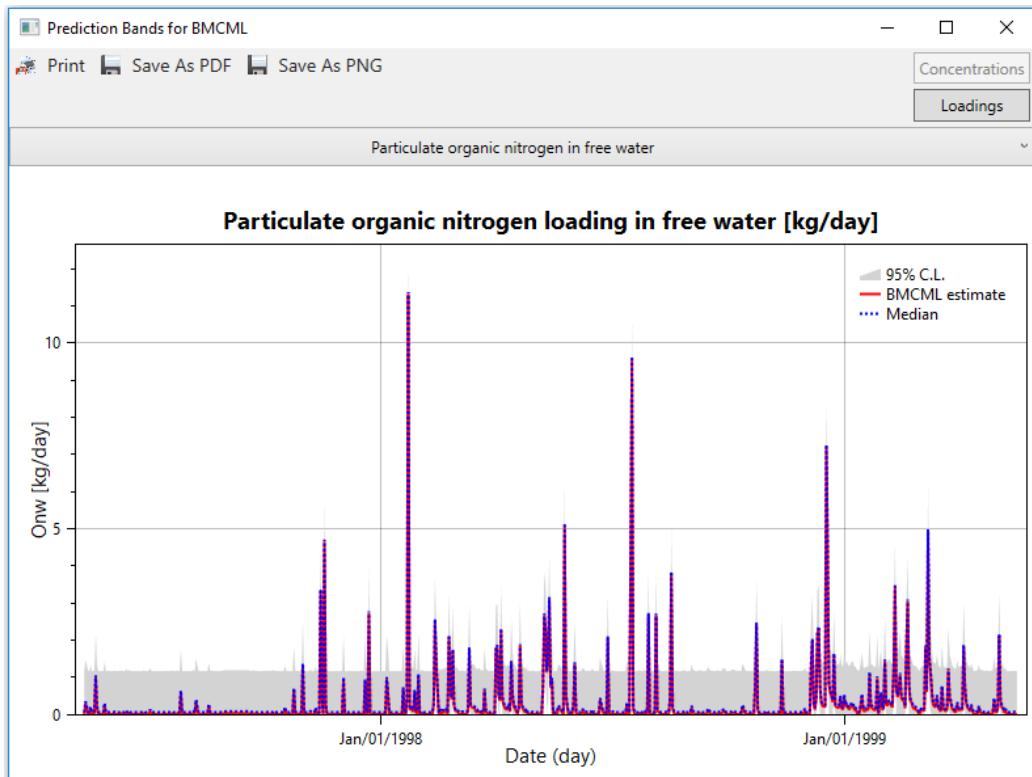


Figure 3.107

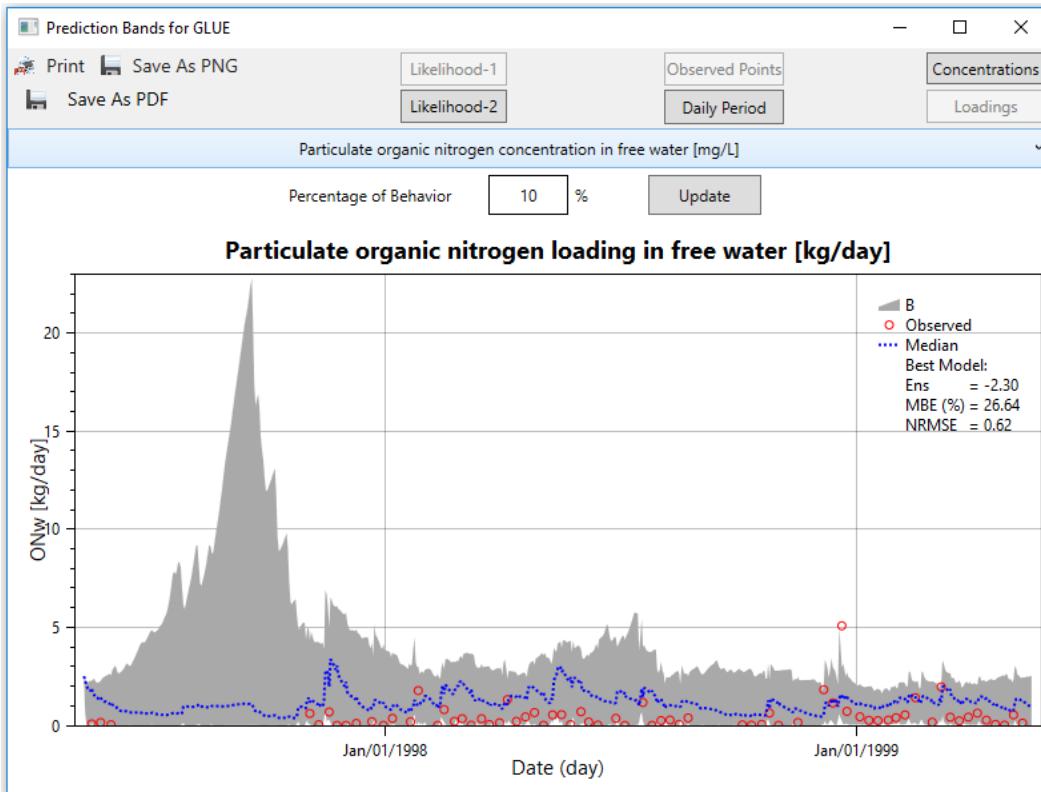


Figure 3.108

3.8 Help

The **Help** menu provides quick access to the *User Manual* of the *WetQual* GUI. It also provides some information about those who developed the *WetQual* GUI on the **About** page. Some key papers for the *WetQual* model (Hantush et al., 2013; Kalin et al., 2013, and Sharifi et al., 2013), GLUE methodology (Beven and Binley, 1992 and Beven and Freer, 2001), and BMCML methodology (Hantush and Chaudhary, 2014 and Chaudhary and Hantush, 2017) are available under the **Help>Publications** menu (Figure 3.109).



Figure 3.109

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Appendix: Definitions for Input Files, Parameters and Output Files of *WetQual*

Table A.1 A short description of *WetQual* subroutines

Subroutine name	Fortran file	Short definition
InOutTXT	2.1-InOutTXT.f90	To read master file and to create the text files to output the results.
FixedInitial	2.2-FIXEDINITIAL.f90	To read the basic model parameters, initial concentrations of nutrients, hydro-climate and input concentration time series.
ReadParms	2.3-Parms-Calc.f90	To read some of the <i>WetQual</i> parameters which are considered to be random.
Equal0	2.4-Neg-EqZero.f90	To check the calculated outputs for non-negativity.
OxyPlant	3.0-Plant-Oxygen.f90	To calculate sediment oxygen demand (SOD) and oxygen in water column as well as mass of floating plant.
Nitrogen	3.1-Nitrogen.f90	To simulate nitrogen transformation and removal in three layers including water column, aerobic and anaerobic soil layers.
PhosphorSed	3.2-Phos-sed.f90	To simulate phosphorus and sediment processes in wetlands.
Carbon	3.3-Carbon.f90	To simulate carbon cycle and removal in wetlands.
Printresults	5-PrintResults.f90	To print the <i>WetQual</i> outputs.

Table A.2 Hydro-Climate Parameters (“12_hydro_climate.txt” file)

Symbol	Definition, Units
Q_{in}	Volumetric inflow rate (m^3/day)
Q_{out}	Wetland discharge (outflow) rate (m^3/day)
V_w	Water volume of wetland surface water (m^3)
A	wetland surface area (m^2)
E_T	Evapotranspiration rate (cm/day)
i_p	Precipitation rate (cm/day)
Q_g	Groundwater discharge (negative for infiltration) (m^3/day)
U_w	Wind speed (m/s)
T_{water}	Daily water temperature ($^\circ\text{C}$) (note that the users have an option to calculate T_{water} if they have daily air temperature (T_{air}) available)

Table A.3 Basic Parameters (“10_basic_parameters.txt” file)

Symbol	Definition, Units
<i>dt</i>	Time step of simulation (day)
<i>n</i>	Number of days of simulation
<i>ronn</i>	Gram of oxygen consumed per gram of total ammonium nitrogen nitrified (gO/gN)
<i>rond</i>	Gram of oxygen consumed per gram of organic nitrogen mineralized(gO/gN)
<i>roc</i>	Gram of oxygen produced per gram of organic carbon synthesized
<i>sims</i>	Number of Monte Carlo (MC) simulations
<i>fNw</i>	Fraction of mineral nitrogen plant uptake as nitrate-N in free water
<i>fNs1</i>	Fraction of mineral nitrogen plant uptake as nitrate-N in the aerobic layer
<i>fNs2</i>	Fraction of mineral nitrogen plant uptake as nitrate-N in the anaerobic layer
<i>fNO3w</i>	Fraction of mineral nitrogen plant uptake as nitrate-N in free water
<i>fNO3s1</i>	Fraction of mineral nitrogen plant uptake as nitrate-N in the aerobic layer
<i>fNO3s2</i>	Fraction of mineral nitrogen plant uptake as nitrate-N in the anaerobic layer
<i>w</i>	Angular velocity of earth ($15^\circ/\text{h}$, or $\pi/12 \text{ rad/h}$)
<i>apn</i>	Phosphorus to nitrogen mass ratio produced by mineralization of particulate organic matter (POM)
<i>lat</i>	latitude in radians
<i>d_bound</i>	the thickness of a laminar (diffusive) boundary layer situated on top of the soil-water interface (cm)
<i>amc</i>	Stoichiometric yield of Methane from the anaerobic decomposition of gram of organic carbon during methanogenesis (gr/gr)
<i>lamdaR</i>	Specific conductivity of root system (m root m-3 soil)
<i>dn</i>	Day number of the year (day), Julian day

Note that “*n*” and “*dn*” parameters are updated automatically when the user picks and views the “Hydro-Climate Parameters”. Also, the “*sims*” parameter will be automatically updated when the user chooses between Deterministic and Stochastic modes. So, the access to these three parameters from “Basic Parameters” window has been limited. User can access them in “10_fixed_parameters.txt” file from “InputOutput” folder but it is recommended not to change values of parameter values from that file. Users can control all the required parameters directly from “Basic Parameter” window.

Table A.4 Initial Concentration (“11_initial_concentration.txt” file)

Symbol	Definition, Units
O_{nw}	Particulate organic nitrogen concentration in free water (mg/L)
O_{nss}	Concentration of refractory organic nitrogen in wetland soil (mg/L)
O_{nsf}	Concentration of labile organic nitrogen in wetland soil (mg/L)
N_w	Total ammonia-nitrogen ($[NH_4^+] + [NH_3]$) concentration in free water (mg/L)
N_{s1}	Total ammonia-nitrogen pore-water concentration in upper aerobic layer (mg/L)
N_{s2}	Total ammonia-nitrogen pore-water concentration in lower anaerobic layer (mg/L)
NO_3w	Nitrate-nitrogen concentration in free water (mg/L)
NO_3s_1	Nitrate-nitrogen pore-water concentration in upper aerobic layer (mg/L)
NO_3s_2	Nitrate-nitrogen pore-water concentration in lower anaerobic layer (mg/L)
a	Mass of free floating plant (gr chlorophyll a)
b	Mass of rooted plants (gr chlorophyll a)
m_w	Sediment concentration in free water (mg/L)
m_s	Wetland soil bulk density (mg/L)
O_w	Oxygen concentration in free water (mg/L)
P_w	Total inorganic phosphorus concentration in free water (mg/L)
P_{s1}	Total phosphorus concentration in aerobic layer (mg/L)
P_{s2}	Total phosphorus concentration in anaerobic layer (mg/L)
DOC_w	Concentrations of dissolved organic C in free water (mg/L)
$LPOC_w$	Concentrations of labile (fast reacting) particulate organic C in free water (mg/L)
$RPOC_w$	Concentrations of refractory (slow reacting) particulate organic C in free water (mg/L)
DOC_{s1}	Pore water concentrations of DOC in aerobic sediment layer (mg/L)
$LPOC_{s1}$	Pore water concentrations of $LPOC$ in aerobic sediment layer (mg/L)
$RPOC_{s1}$	Pore water concentrations of $RPOC$ in aerobic sediment layer (mg/L)
DOC_{s2}	Pore water concentrations of DOC in lower anaerobic sediment layer (mg/L)
$LPOC_{s2}$	Pore water concentrations of $LPOC$ in lower anaerobic sediment layer (mg/L)
$RPOC_{s2}$	Pore water concentrations of $RPOC$ in lower anaerobic sediment layer (mg/L)
$CH4w$	Methane concentration in free water (mg/L)
$CH4s_1$	Methane concentration in aerobic sediment layer (mg/L)
$CH4s_2$	Methane concentration in anaerobic sediment layer (mg/L)

Table A.5 Input Concentrations (“13_input_concentrations.txt” file)

Symbol	Definition, Units
<i>ONin</i>	Organic nitrogen concentration in incoming flow (mg/L)
<i>NO3in</i>	Nitrate-nitrogen concentration in incoming flow (mg/L)
<i>NWin</i>	Total ammonia-nitrogen ($[NH_4^+] + [NH_3]$) concentration in incoming flow (mg/L)
<i>NO3g</i>	Nitrate-nitrogen concentration in groundwater discharge (mg/L)
<i>Ng</i>	Total ammonia-nitrogen concentration in groundwater discharge (mg/L)
<i>Owin</i>	Oxygen concentration in incoming flow (mg/L)
<i>PO4in</i>	Phosphate concentration in incoming flow (mg/L)
<i>Pg</i>	Total phosphorus concentration in groundwater discharge (mg/L)
<i>mwin</i>	Sediment concentration in incoming flow (mg/L)
<i>NH4air</i>	Ammonium concentration in precipitation (mg/L)
<i>NO3air</i>	Nitrate-nitrogen concentrations in precipitation (mg/L)
<i>Qa</i>	Dry depositional rates of total ammonia nitrogen (mg/m ² /day)
<i>Qn</i>	Dry depositional rates of total nitrate-nitrogen (mg/m ² /day)
<i>LPOCin</i>	Labile particulate organic carbon concentration in incoming flow (mg/L)
<i>RPOCin</i>	Refractory particulate organic carbon concentration in incoming flow (mg/L)
<i>DOCin</i>	Dissolved organic carbon concentration in incoming flow (mg/L)
<i>DOCatm</i>	Atmospheric deposition for total organic carbon (mg/m ² /day)
<i>TOCgw</i>	Total organic carbon concentration in groundwater discharge (mg/L)

Table A.6 Definition of WetQual Outputs:

Output File Name	Observed File Name	Symbol	Definition, Units
102_Onw.txt	102_obs_Onw.txt	Onw	Particulate organic nitrogen concentration in free water (mg/L)
103_Onss.txt	103_obs_Onss.txt	Onss	Concentration of refractory organic nitrogen in wetland soil (mg/L)
104_Onsf.txt	104_obs_Onsf.txt	Onsf	Concentration of labile organic nitrogen in wetland soil (mg/L)
105_Nw.txt	105_obs_Nw.txt	Nw	Total ammonia-nitrogen ($[NH_4^+] + [NH_3]$) concentration in free water (mg/L)
106_NsI.txt	106_obs_NsI.txt	NsI	Total ammonia-nitrogen pore-water concentration in upper aerobic layer (mg/L)
107_Ns2.txt	107_obs_Ns2.txt	Ns2	Total ammonia-nitrogen pore-water concentration in lower anaerobic layer (mg/L)
108_NO3w.txt	108_obs_NO3w.txt	NO3w	Nitrate-nitrogen concentration in free water (mg/L)
109_NO3sI.txt	109_obs_NO3sI.txt	NO3sI	Nitrate-nitrogen pore-water concentration in upper aerobic layer (mg/L)
110_NO3s2.txt	110_obs_NO3s2.txt	NO3s2	Nitrate-nitrogen pore-water concentration in lower anaerobic layer (mg/L)
111_Ow.txt	111_obs_Ow.txt	Ow	Oxygen concentration in free water (mg/L)
112_a.txt	112_obs_a.txt	a	Mass of free floating plant (gr chlorophyll a)
113_b.txt	113_obs_b.txt	b	Mass of rooted plants (gr chlorophyll a)
114_Pw.txt	114_obs_Pw.txt	Pw	Total inorganic phosphorus concentration in free water (mg/L)
115_PsI.txt	115_obs_PsI.txt	PsI	Total phosphorus concentration in aerobic layer (mg/L)
116_Ps2.txt	116_obs_Ps2.txt	Ps2	Total phosphorus concentration in anaerobic layer (mg/L)
118_mw.txt	118_obs_mw.txt	mw	Sediment concentration in free water (mg/L)
150_DOCw.txt	150_obs_DOCw.txt	DOCw	Concentrations of dissolved organic C in free water (mg/L)
151_LPOCw.txt	151_obs_LPOCw.txt	LPOCw	Concentrations of labile (fast reacting) particulate organic C in free water (mg/L)
152_RPOCw.txt	152_obs_RPOCw.txt	RPOCw	Concentrations of refractory (slow reacting) particulate organic C in free water (mg/L)
153_DOCsI.txt	153_obs_DOCsI.txt	DOCsI	Pore water concentrations of DOC in aerobic sediment layer (mg/L)
154_LPOCsI.txt	154_obs_LPOCsI.txt	LPOCsI	Pore water concentrations of LPOC in aerobic sediment layer (mg/L)
155_RPOCsI.txt	155_obs_RPOCsI.txt	RPOCsI	Pore water concentrations of RPOC in aerobic sediment layer (mg/L)
156_DOCs2.txt	156_obs_DOCs2.txt	DOCs2	Pore water concentrations of DOC in lower anaerobic sediment layer (mg/L)
157_LPOCs2.txt	157_obs_LPOCs2.txt	LPOCs2	Pore water concentrations of LPOC in lower anaerobic sediment layer (mg/L)
158_RPOCs2.txt	158_obs_RPOCs2.txt	RPOCs2	Pore water concentrations of RPOC in lower anaerobic sediment layer (mg/L)
159_TOCw.txt	159_obs_TOCw.txt	TOCw	Concentrations of total organic C in free water (mg/L)
160_CH4w.txt	160_obs_CH4w.txt	CH4w	Methane concentration in free water (mg/L)
161_CH4sI.txt	161_obs_CH4sI.txt	CH4sI	Methane concentration in aerobic sediment layer (mg/L)
162_CH4s2.txt	162_obs_CH4s2.txt	CH4s2	Methane concentration in anaerobic sediment layer (mg/L)

Table A.7 N, P, TSS parameters (“14_generated_parameters.txt” file)

Symbol in publications	Symbols in the model files	Definition, Units
l_2	$L2$	Thickness of anaerobic soil layer (cm)
θ	$theta$	Temperature coefficient in Arhenius equation
I_s	I_s	Optimal light level (ly/day), range from about 100 to 400 ly/d (Chapra, 1997, p. 611)
f_N	$fNup$	Fraction of total ammonia nitrogen in ionized form
k_d	Kd	Ammonium ion distribution coefficient (mL/g)
k_{ep}	kep	Parameter required as input but not used in the model (1/m)
k_{ga}	$kga0$	Growth rate of free-floating plant (1/day)
k_{gb}	$kgb0$	Growth rate of benthic and rooted plant (1/day)
k_{mr}	$kminI_s$	First-order rapid mineralization rate in wetland soil (1/day)
k_{nw}	knw	First-order nitrification rate in wetland free water (1/day)
k_{mw}	$kminw$	First-order mineralization rate in wetland free water (1/day)
k_{ns}	kns	First-order nitrification rate in aerobic soil layer (1/day)
k_{dn}	$kden$	Denitrification rate in anaerobic soil layer (1/day)
ρ_s	$rows$	Wetland soil particle density (g/cm ³)
v_{so}	$vels_o$	Effective settling velocity (cm/day) for organic material
v_{ss}	$vels_s$	Effective settling velocity (cm/day) for sediment
v_b	$velb$	Effective burial velocity (cm/day)
a_{na}	ana	Gram of nitrogen per gram of chlorophyll-a in plant/algae (gN/gChl)
$r_{c,chl}$	$rChl$	Ratio of carbon mass to chlorophyll a mass in algae (gC/gChl)
S_s	Ss	Oxygen removal rate per unit volume of aerobic layer by other processes (g/L/day)
S_w	Sw	Volumetric oxygen consumption rate in water by other processes (gr/cm ³ /day)
α	c_uw	Empirical parameter used for calculating volatilization mass transfer velocity kv
fr	$frap$	Fraction of rapidly mineralizing particulate organic matter
$c1$	$c1$	Used for calculating pK (Keq, equilibrium coefficient)
$c2$	$c2$	Used for calculating pK (Keq, equilibrium coefficient)
pH	pH	pH
S	S	Rate of nitrogen fixation by microorganisms (mg-N/m ³ /hr)
K_w	Kw	Phosphorus sorption coefficient in water (cm ³ /g)
a_{pa}	apa	Ratio of phosphorus to chlorophyll-a in algae (grP/grChl)
D_{pw}	Dpw	Inorganic phosphorus free-water diffusion coefficient (cm ² /day)
K_{sa}	Ksa	Accounts for partitioning to phosphorus sorption site (cm ³ /g)
K_{sb}	Ksb	Accounts for association with iron hydroxide precipitate (cm ³ /g)
$Ran1$	$RanI$	Random number used for calculating soil porosity (ϕ) and free-water oxygen diffusion coefficient
f_w	fW	Fraction of nitrogen fixation in water
f_{act}	$fact$	Vertical diffusion magnification factor
C_{ro}	$alfa_velr_o$	Coefficient for resuspension/recycling of organic material
C_{rs}	$alfa_velr_s$	Coefficient for resuspension/recycling of sediment
φ_w	$porw$	Effective porosity of wetland surface water

Table A.8 Carbon parameters (“15_generated_parameters_carbon.txt” file)

Symbol in publications	Symbols in the model files	Definition, Units
a_{ca}	aca	ratio of carbon to chlorophyll-a in algae (gC/gChl)
f_{aD}	$FaDOC$	Fraction of dissolved organic C produced by death/loss of free floating plants and attached algae ($f_{aL} + f_{aR} + f_{aD} = 1$) (Dimensionless)
f_{aL}	$FaLPOC$	Fraction of labile particulate C produced by death/loss of free floating plants and attached algae ($f_{aL} + f_{aR} + f_{aD} = 1$) (Dimensionless)
f_{aR}	$FaRPOC$	Fraction of refractory particulate C produced by death/loss of free floating plants and attached algae ($f_{aL} + f_{aR} + f_{aD} = 1$) (Dimensionless)
f_{bD}	$FbDOC$	Fraction of dissolved organic C produced by death/loss of rooted and benthic plants ($f_{bL} + f_{bR} + f_{bD} = 1$)
f_{bL}	$FbLPOC$	Fraction of labile particulate C produced by death/loss of rooted and benthic plants ($f_{bL} + f_{bR} + f_{bD} = 1$)
f_{bR}	$FbRPOC$	Fraction of refractory particulate C produced by death/loss of rooted and benthic plants ($f_{bL} + f_{bR} + f_{bD} = 1$)
k_L	$kLPOC$	first order hydrolysis rate of labile particulate organic carbon (1/day)
k_R	$kRPOC$	First order hydrolysis rate of refractory particulate organic carbon (1/day)
K_O	$KsatO$	Michaelis–Menten half saturation concentration of dissolved oxygen required for oxic respiration (mg/L)
K_O^{in}	$KinO$	Michaelis–Menten oxygen inhabitation coefficient (mg/L)
K_N	KN	Michaelis–Menten nitrate N half saturation concentration required for denitrification (mg/L)
K_N^{in}	$KinN$	Michaelis–Menten nitrate-N inhibition coefficient (mg/L)
k_D^1	$K1DOC$	maximum dissolved organic C utilization rate for aerobic respiration (1/day)
k_D^2	$k2DOC$	maximum dissolved organic C utilization rate for denitrification (1/day)
k_D^3	$k3DOC$	maximum dissolved organic C utilization rate for methanogenesis in anaerobic water (1/day)
k_D^4	$k4DOC$	maximum dissolved organic C utilization rate for methanogenesis in anaerobic sediment (1/day)
cp_1	$cp1$	fraction of inflowing organic carbon (TOC_{in}) in form of dissolved organic carbon (DOC)
Cp_2	$cp2$	fraction of inflowing organic carbon in form of labile particulate organic carbon ($LPOC$)
Cp_3	$cp3$	fraction of inflowing organic carbon in form of refractory particulate organic carbon ($RPOC$)
f_{bw}	fbw	fraction of rooted plant biomass above soil-water interface (1/day)
k_M^1	$k1CH_4$	maximum methane utilization rate for aerobic respiration (1/day)
k_M^2	$k2CH_4$	maximum methane utilization rate for denitrification (1/day)
Rv	$Rveg$	root length density in soil (cm/gr) [L root/M chla]

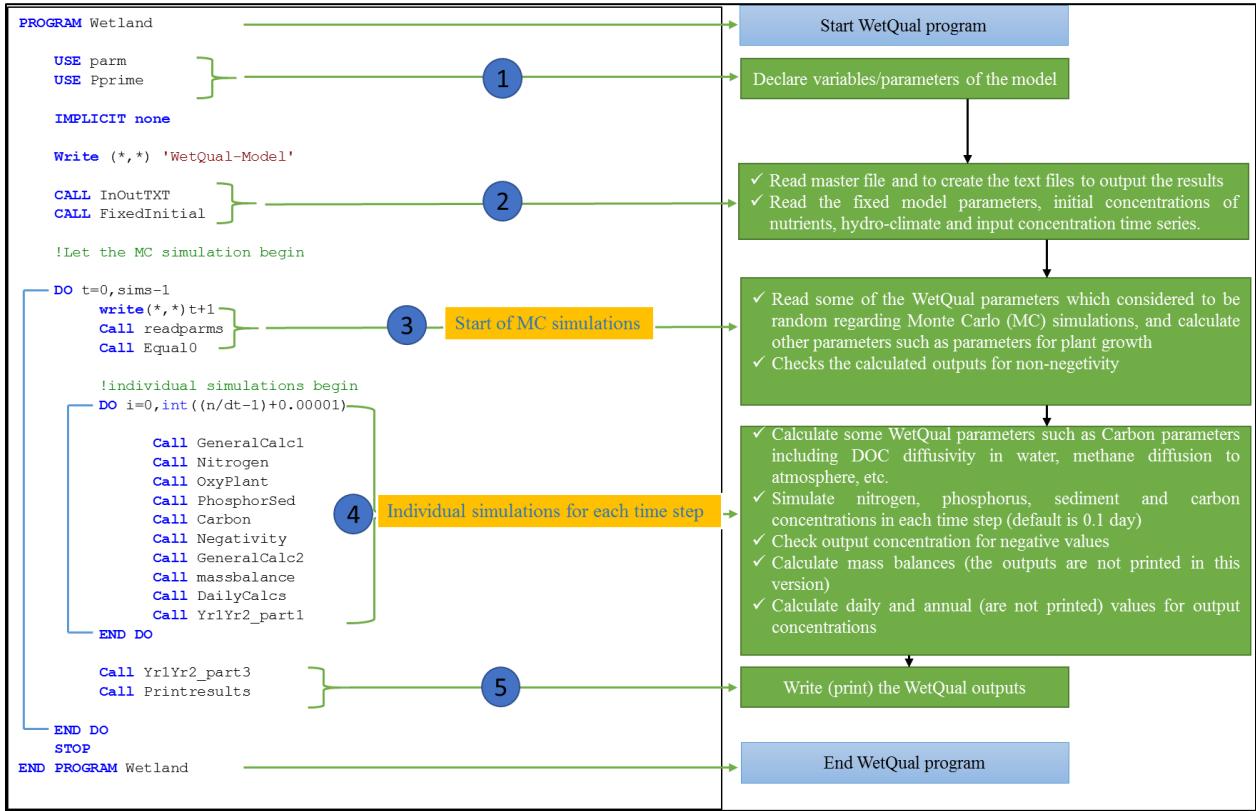


Figure A.1 A flowchart representing the internal structure and processes of *WetQual*