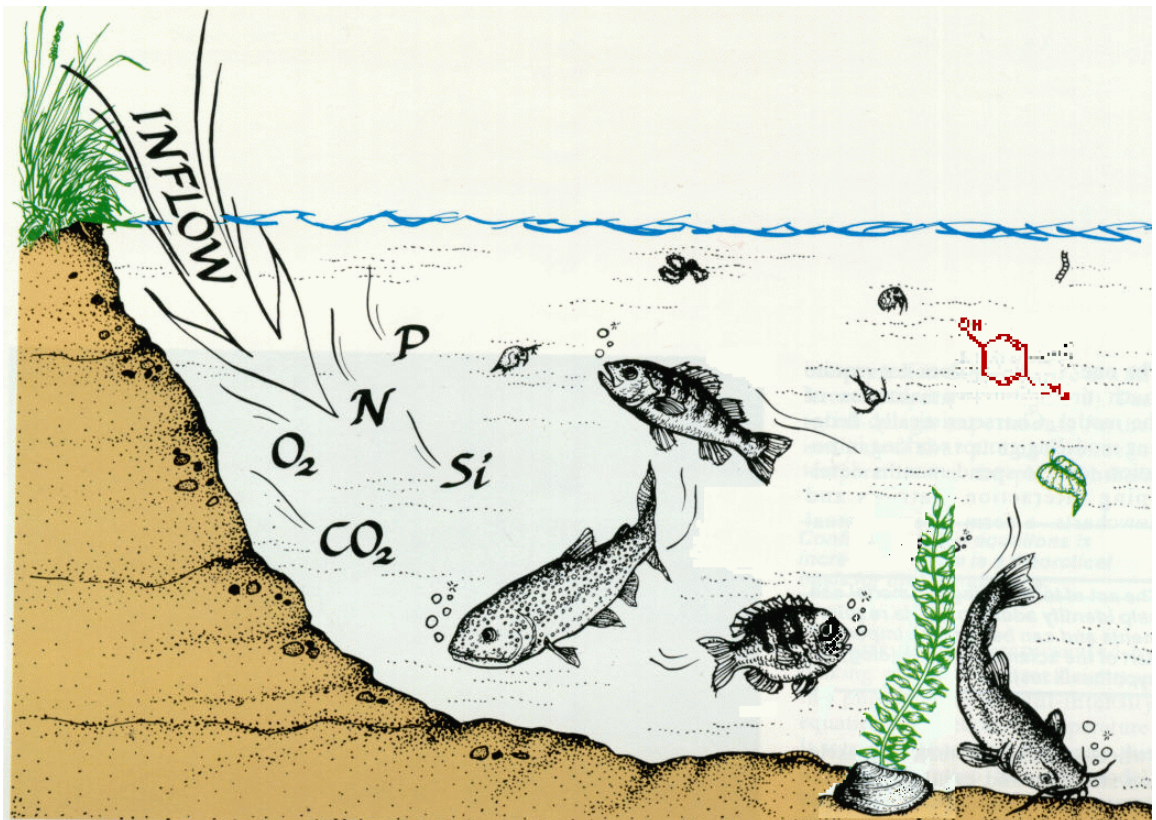




# AQUATOX (RELEASE 3.1 Beta)

## MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS

### VOLUME 1: USER'S MANUAL



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# **AQUATOX (RELEASE 3.1 Beta)**

## **MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS**

### **VOLUME 1: USER'S MANUAL**

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September 2011

**U.S. ENVIRONMENTAL PROTECTION AGENCY  
OFFICE OF WATER  
OFFICE OF SCIENCE AND TECHNOLOGY  
WASHINGTON DC 20460**

## **Disclaimer**

This document describes the interface of the aquatic ecosystem model AQUATOX, Release 3.1. Anticipated users of this document include persons who are interested in using the model, including but not limited to researchers and regulators. The model described in this document is not required, and the document does not change any legal requirements or impose legally binding requirements on EPA, states, tribes or the regulated community. This document has been approved for publication by the Office of Science and Technology, Office of Water, U.S. Environmental Protection Agency. Mention of trade names, commercial products or organizations does not imply endorsement or recommendation for use.

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# AQUATOX (RELEASE 3.1) VOLUME 1: USER'S MANUAL

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## Getting Started

### AQUATOX: A Brief Overview

AQUATOX is a simulation model for aquatic systems. AQUATOX predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including fish, invertebrates, and aquatic plants. AQUATOX is a valuable tool for ecologists, biologists, water quality modelers, and anyone involved in performing ecological risk assessments for aquatic ecosystems.

AQUATOX simulates the transfer of biomass, energy and chemicals from one compartment of the ecosystem to another. It does this by simultaneously computing each of the most important chemical or biological processes for each day of the simulation period; therefore it is known as a process-based or mechanistic model. AQUATOX can predict not only the environmental fate of chemicals in aquatic ecosystems, but also their direct and indirect effects on the resident organisms. Therefore it has the potential to establish causal links between chemical water quality and biological response and aquatic life uses.

AQUATOX is the only general ecological risk model that represents the combined environmental fate and effects of conventional pollutants, such as nutrients and sediments, and toxic chemicals in aquatic ecosystems. It considers several trophic levels, including attached and planktonic algae and submerged aquatic vegetation, invertebrates, and forage, bottom-feeding, and game fish; it also represents associated organic toxicants. It has been implemented for streams, ponds, lakes, estuaries, reservoirs, and experimental enclosures.

The fate portion of the model, which is applicable especially to organic toxicants, includes: partitioning among organisms, suspended and sedimented detritus, suspended and sedimented inorganic sediments, and water; volatilization; hydrolysis; photolysis; ionization; and microbial degradation. The effects portion of the model includes: acute toxicity to the various organisms modeled; and indirect effects such as release of grazing and predation pressure, increase in detritus and recycling of nutrients from killed organisms, dissolved oxygen sag due to increased decomposition, and loss of food base for animals.

AQUATOX is the latest in a long series of models, starting with the aquatic ecosystem model CLEAN (Park et al., 1974) and subsequently improved in consultation with numerous researchers at various European hydrobiological laboratories, resulting in the CLEANER series (Park et al., 1975, 1979, 1980; Park, 1978; Scavia and Park, 1976) and LAKETRACE (Collins and Park, 1989). The MACROPHYTE model, developed for the U.S. Army Corps of Engineers (Collins et al., 1985), provided additional capability for representing submersed aquatic vegetation. Another series started with the toxic fate model PEST, developed to complement CLEANER (Park et al., 1980, 1982), and continued with the TOXTRACE model (Park, 1984) and the spreadsheet equilibrium fugacity PART model. AQUATOX combined algorithms from these models with an ecotoxicological construct borrowed from the FGETS model (Suárez and Barber, 1992); and additional code was written as required for a truly integrative fate and effects model (Park, 1990, 1993). In the late 1990s, AQUATOX was restructured and linked to Microsoft Windows interfaces to provide even greater flexibility, capacity for additional compartments, and user friendliness.

- AQUATOX Release 1 was produced in 2002 and was the first EPA release to run under Windows.
- AQUATOX Release 2 was completed in 2003 and included more state variables and multi-age-class fish along with a refined user-interface.
- AQUATOX Release 2.1 was completed in 2005 and included additional chemical modeling options and variable stoichiometry among numerous other refinements.

- AQUATOX Release 2.2 was completed in 2006 and included updated simulations and parameter databases along with minor interface enhancements.
- AQUATOX Release 3 was completed in 2009 and includes linked segments, simulations of estuaries, dramatically improved output capabilities, and many other model improvements.
- AQUATOX Release 3.1 was completed in 2011 and includes a steady-state diagenesis model, updated ICE data (toxicity regressions), modified denitrification code, and many interface enhancements.

## Installation Considerations

To install the AQUATOX Model, an "InstallAware" installer is utilized.

Through its install program, AQUATOX will produce the following folder structure:

- **DATABASE:** holds libraries of parameters, chemical toxicity databases, and interspecies regression models for toxicity (see ICE ).
- **OUTPUT:** holds files produced by AQUATOX to produce tabular data and graphs. Also a default location for exporting results.
- **PROGRAM:** holds the executable itself and helper files
- **STUDIES:** holds the simulations included with the Installshield. New simulations may be saved in this location or anywhere else that is desirable. A "Tutorial" directory is also included here with files required for the tutorials in this document. This directory also includes some ancillary files such as a parameter import template, descriptions of files, etc.

Be sure that you have read-write access to each of these directories wherever you are installing AQUATOX.

If you install AQUATOX in the same location as a previous installation, you will no longer be able to access the previous version and any modifications you made to the databases or default study files (\*.APS) may be lost.

The Borland Database Engine is also installed as part of the installation of AQUATOX.

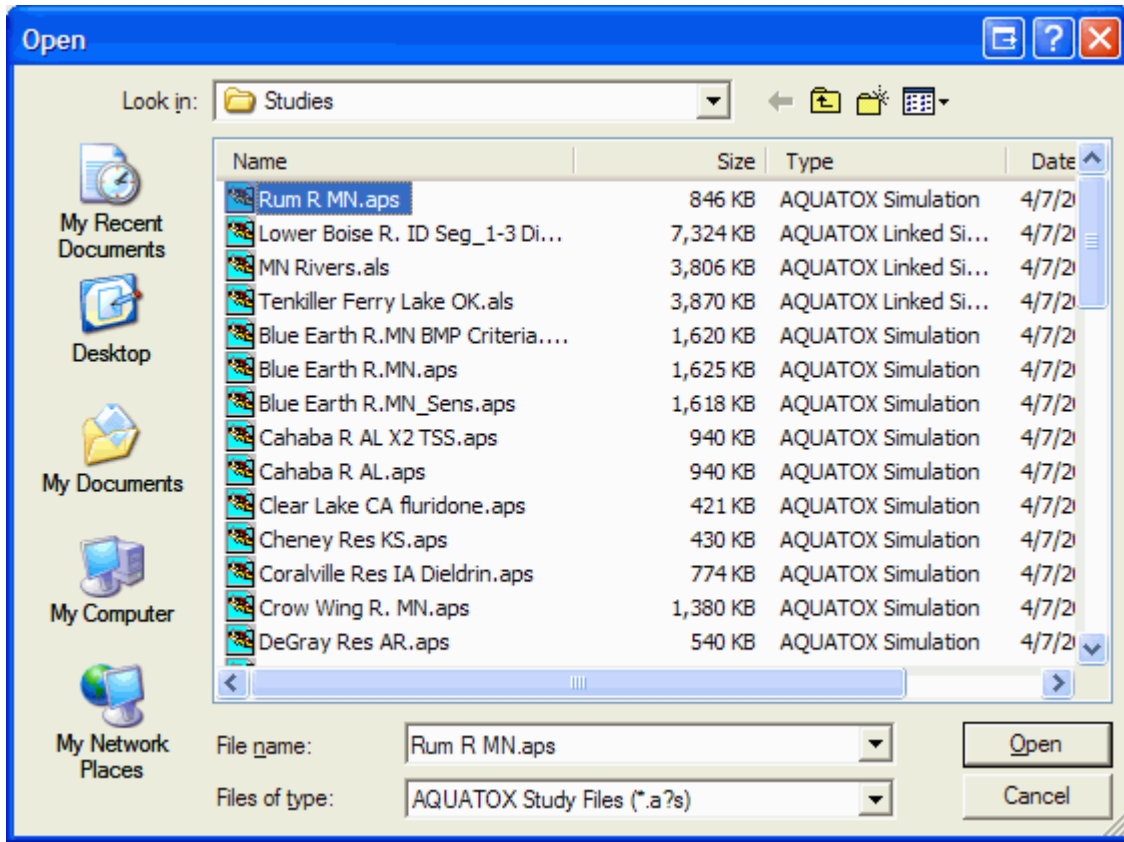
Some additional notes:

- AQUATOX must be initially installed by an Administrator.
- If AQUATOX will exclusively be run using an "administrator" account, no additional changes need to be made.
- If AQUATOX will be run by a user with a "standard" account, full read and write privileges must be given to that user for the directory in which AQUATOX has been installed.
- An alternative to adding read and write privileges: is to install AQUATOX in a directory where the user already has read and write privileges. This is the best choice for managed desktop systems.

For more information see the *AQUATOX Release 3.1 Installation Guide*.

## Loading a Study

The APS file is the basic unit in AQUATOX; it contains site data, loadings, and parameter values used in a simulation; and it may contain results from a prior simulation. Click on **File** in the menu bar to get the pull-down file menu, and click on **Open**. You will then be given a choice of AQUATOX study files to load.



When a study is opened, a new window is opened within the AQUATOX multi window interface. You may open many studies at the same time and switch back and forth between them by clicking or using the **Window** menu at the top of the screen.

A single segment AQUATOX simulation is designated as a **\*.APS** file while a multi-segment AQUATOX simulation is designated as **\*.ALS**.

### The Main Window

The main window includes the name of the study, the list of state variables used, and buttons from which to choose various operations. At the top of the screen is an editable **Toolbar**. Linger the mouse over each button to get a "hint" that describes the function of each toolbar button.

The **Study Name** can be edited; it is separate from the name of the file, which you loaded and which is displayed at the top of the screen. The study name is used as a title in graphical output, so is best capitalized.

The **Status** window tells when the perturbed and control runs were made, and warns if they are incomplete or outdated.

The **Initial Conditions** button brings up a screen with all the state variable values at the beginning of a simulation.

The **Chemical** button brings up the loadings screen for the organic toxicant, if modeled. Double clicking on the state variable named "**Dissolved org. toxicant**" that will appear at the top of the list of state and driving variables (if a chemical is included in the simulation) has the same effect.

The **Site** button loads the site characteristic screen .

**Setup** allows the user to set the dates of the simulation, and to specify various options such as the **control setup**, uncertainty analysis, and saving biologic rates.

**Notes** provides a window for writing comments on the study.

**Birds, Mink...** links to a model of chemical uptake for shorebirds or any other animals that feed exclusively on aquatic prey.

The **Sed Layers** button brings up parameters and initial conditions for the multi-layer sediment model or the sediment diagenesis model if they are included in the simulation.

**Perturbed** starts the simulation with changed conditions, such as with a toxicant.

**Control** starts a simulation without the stressor; the user can use **Control Setup** to specify what is changed and what is held constant, or parameters may be changed between running the control and perturbed simulations.

**Output** presents the results as a series of charts and graphs .

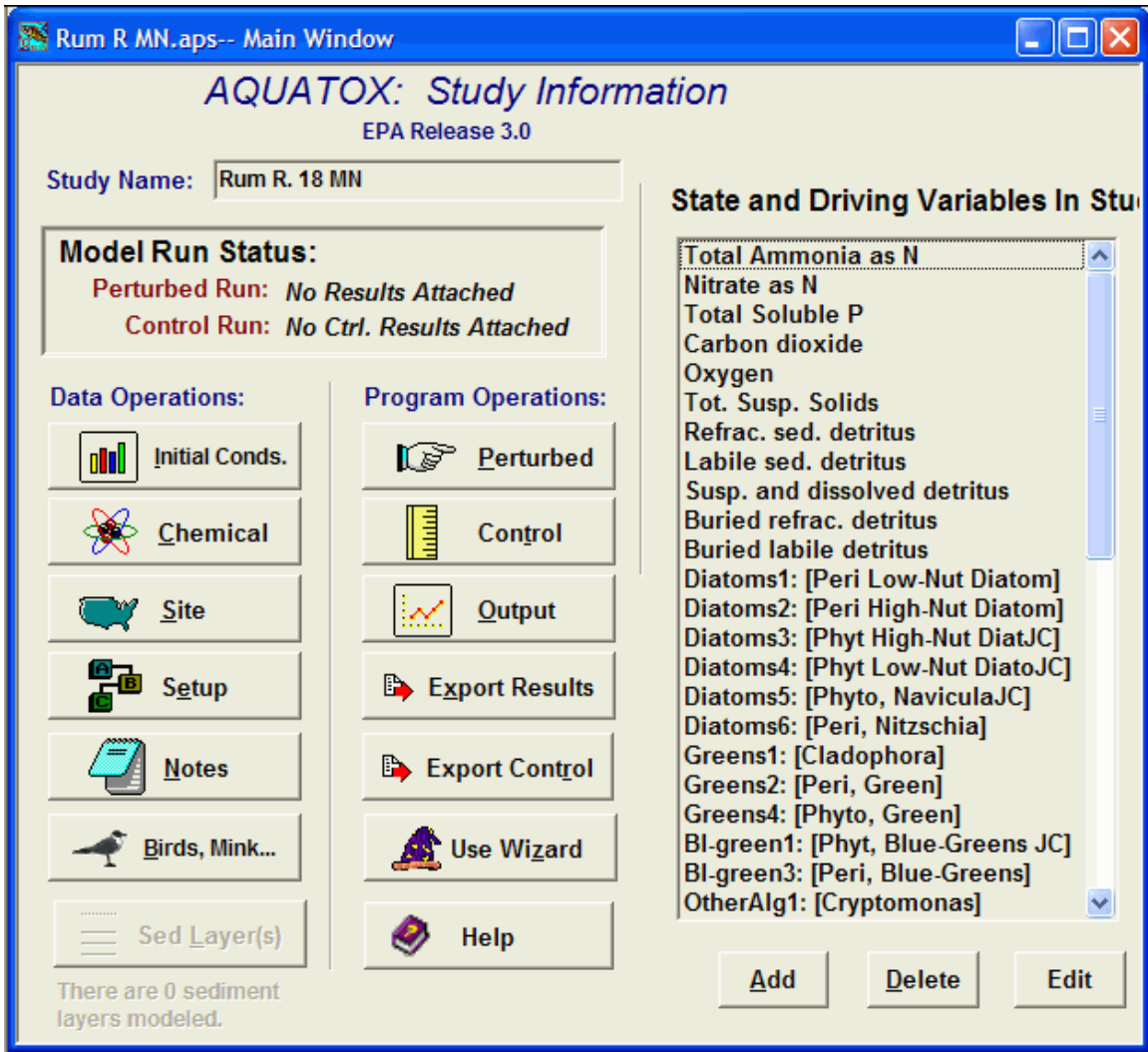
The output can be exported as database, spreadsheet, or text files by clicking on **Export Results** or **Export Control**

The **State and Driving Variables In Study** show the full list of state variables within the simulation. Variables can be added to or deleted from this list using the buttons at the bottom of the list. Animals, plants, and detritus within this list can have up to twenty organic chemicals associated with them.

The **Edit with Wizard** button allows you to edit the current simulation with the **AQUATOX Wizard**.

If you hit the **Help** button from the Main Screen, you will jump to this topic in the help screen.

When this screen is viewed in Linked Mode it represents a single linked segment. In this case, two additional buttons are available. **Stratification** affects the setup of vertically stratified segments in linked mode. **Morphometry** allows the user to specify a time series of cross section areas for each segment.



## Saving a Study

To save a file, click on **File** then **Save** or **Save As** on the menu bar; you will also be given an opportunity to save an altered file before exiting or loading another file. Study files range in size from 25 KB to well over 2 MB. If you wish to minimize the size of a study—for example, to transmit to someone else—you can strip out the results by clicking on **Study** and choosing **Clear Results** from the menu bar. The study files distributed with AQUATOX have been minimized in this way.

## Working With Existing Simulations

### What is in an "APS" file?

An APS file is the basic unit in which AQUATOX simulations are loaded and saved. Each APS file contains the following items:

- List of state variables and driving variables utilized and their loadings, "underlying parameters," and initial conditions;
- Site specific and remineralization Parameters;
- Model setup information;
- Boundary condition loadings for a simulation;
- Results from any simulation that may have previously been run, including "rates";
- External data that has been imported into the simulation for plotting against results;
- The graph library that has been produced for that simulation;
- The uncertainty mode or sensitivity mode setup including distributions chosen and correlation information.

Not included in the APS file are uncertainty output, which is saved in a database format (\*.db or \*.dbf) and sensitivity output which is in Excel format (\*.xls). Libraries of parameters are not included in the APS file either, other than those parameters that have been "loaded" into a simulation and therefore have relevance to that simulation.

## **Libraries and Parameters in a Simulation**

There is a basic dichotomy in working with AQUATOX. You have a choice of editing database files in the general "library" or of opening and editing a particular study. Studies are self-contained files with all the information on a particular simulation, including initial conditions, loadings, parameter values, first and last dates for the simulation, and simulation results. Parameter values can be edited, but changes apply *only* to that study. The intent is to be able to archive a model application so that all assumptions and results are saved for future reference. This is especially important for regulatory applications that are subject to later review. (Of course, you also should archive the version of AQUATOX that was used.)

Parameter and site records that will be used repeatedly should be saved in the appropriate library. Each library is a database in Paradox format with records for each organism, chemical, or site. Generally, editing of parameters should be done in the library mode to maintain consistency among studies. In contrast, if a site record is only going to be used for a single study, it may be desirable to create it within the study. Study records can be copied into the library; so the choice of where to edit parameters is up to the user. It is the user's responsibility, though, to synchronize parameter values among studies. This can be done by saving a record to a library and then loading that record to each study.

To create or edit a record for general use, click on **Library** in the menu bar. You can then click on the specific library from the pull-down menu.

See Also: **Types of Libraries**

## **Exploring State Variables**

### **State Variables**

State variables are those ecosystem components that are being simulated. These include organic toxicants, nutrients and dissolved gasses, organism and detrital compartments and their associated toxicants, and other variables traditionally considered driving variables, such as water inflow, temperature, pH, light, and wind.

AQUATOX is a powerful model because you can add or delete state variables. It is even possible to remove all biotic components in order to model a tank or other sterile system. In general, the fewer state variables, the better. In particular, unnecessary state variables slow down the simulation and create additional requirements for verification. This is especially true for

streams, which tend to be more dynamic and therefore slower to simulate. Nevertheless, often it is desirable to model a food web rather than a food chain, for example to examine the possibility of less tolerant organisms being replaced by more tolerant organisms as environmental perturbations occur. The choice of which state variables to model depends to a large extent on the purpose of the modeling application and the availability of data pertaining to the state variables.

### **Modifying the State Variable List**

**To Delete** a state variable, select the variable you wish to delete from the state variables list by clicking on it. To select multiple state variables, hold down the control key while clicking more than one variable on the list. Then, click on the **delete** button and confirm the deletion. There are several state variables (such as nutrients) that are basic to an AQUATOX simulation, and that therefore cannot be deleted.

**To Add** a state variable, click on the **Add** button and choose the variable you wish to add from the dialog box that appears. Note that the names of the taxonomic groups and ecologic guilds on the main study screen are followed by the names of the specific groups in brackets. After clicking the **Add** button, you will first be prompted to choose the taxonomic group, ecologic guild, or chemical compartment you wish to add. Then, you will be prompted to load the chemical or species specific **parameters** from the appropriate library.

You may also modify the state variable list using the AQUATOX Wizard.

After animal or plant state variables have been added or removed one **critical step** is to view the **trophic interactions** for the simulation to ensure that the resulting food web is reasonable. AQUATOX *does* have default trophic interactions within each organism, but not knowing which organisms are going to be included in each simulation, it will usually require modification. The best way to access trophic interactions is by selecting "**Edit Trophic Interactions**" under the "**Study**" menu, or by clicking on "**Trophic Matrix**" which is a button found within Animal state variable loadings screens.

### **Initial Conditions and Loadings**

Initial values and loadings are needed for all the state variables or compartments simulated. These are input on the loadings screen. If one or more toxicants are modeled, then initial concentrations associated with the biota can also be specified. Constant loadings for plants and invertebrates can be considered as "seed" values, although care should be taken to use small values or the loadings can dominate the simulation. Even periphyton and zoobenthos may be maintained through drift from upstream, and a constant loading is appropriate. Likewise, macrophytes may die back in winter and sprout from rhizomes; because rhizomes are not explicitly modeled, a small loading is the mechanism for reestablishing the population in the simulation when environmental conditions become more favorable.

Of course, upstream loadings may be significant inputs to a reach or lake. These may be represented by constant or dynamic (time-varying) loadings. AQUATOX has a very flexible interpolation routine to obtain daily values from irregular data points and even time series occurring or extending outside the simulation period. Dynamic loadings can be entered directly on the loadings screen, or they can be entered or obtained offline and imported into the model. Imported data can be in a variety of formats, which are evident when the "**Change**" button is used. Loadings can be altered by means of a multiplier (the "**Multiply loading by**" button). This procedure is especially useful for analyzing various loading scenarios. It is also a way to correct or convert data series. However, ordinarily the multipliers are set to 1 for the Control simulation, so use for other than perturbations is discouraged.

Loadings in "inflow water" are closely related to the volume of inflow water specified (or calculated as a result of choices) in the water volume screen. In other words, loadings in unit per liter of water must have an associated inflow of water in order to be relevant to the simulation.

On the other hand, nonpoint-source (NPS), and point-source (PS) loadings are input in units of grams per day and are not affected by the quantity of inflow water. AQUATOX ignores the quantity of water that is associated with NPS and PS loadings as a model simplification; however, this water can be directly modeled in the multi-segment model with the use of Tributary Input Segments.

Direct precipitation loadings are a function of the site's surface area with units of grams per meter squared per day. This input field includes both wet and dry precipitation.

Any of the time-series loadings may be imported, exported, or cleared using the "**Change**" button found directly below their listing.

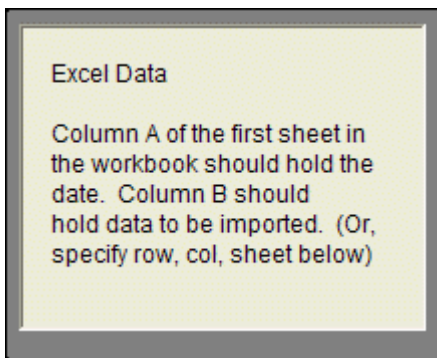
Also see this note about dynamic loadings.

For carbon dioxide loadings the **Import CO2 Equil.** button is also available. This enables a user to import a time series of equilibrium carbon dioxide values (if air to water exchange were perfect). This interface is designed for linkage with CO2SYS, CO2calc or other similar salt-water carbon chemistry models. More information about this interface may be found in section 5.6 of the *Technical Documentation*.

### **Importing and Exporting Loadings**

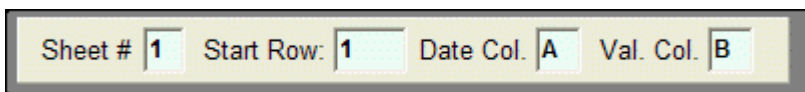
Loadings and other time series may be imported from Excel format, Tab delimited format, DBase format, Paradox Database Format, or Comma Separated Value (CSV) format.

To change the format, move to the List Files of Type menu and select a different format. The required input format will be specified in the box at the upper left. For example, an Excel data file should have the date in column A of the first worksheet and the data to be imported in Column B.



When you select a file, a preview will appear in the lower box. You can "update" this preview by pressing the button above it.

For Excel only, you may specify where the data you wish to import appears. This is helpful when working with very large spreadsheets with multiple sets of data on them. The worksheet number is specified first and then the start row, date column, and value columns may also be specified as shown below.



Sheet # 1 Start Row: 1 Date Col. A Val. Col. B

To import from Excel, Microsoft Excel 2000 or a later version of Microsoft Excel must be installed on the computer.

Some data, for which there are units conversions available, may be converted on the fly using the conversion check-box.



Convert Imported Data from uEin./m2 s to Ly/d

Loadings may also be exported from AQUATOX by selecting the "Export" tab at the top of the screen. Time series that are no longer relevant may be cleared from AQUATOX by selecting the "Clear Data" tab at the top of the screen.

### Important Note about Dynamic Loadings:

Dynamic loadings are loadings that are variable over the simulation's time-period. These loadings are entered using a list of dates and associated loadings.

During a simulation, if the date that is being simulated appears on the input list of dates, the loading is taken directly from the list. If the current date in a simulation occurs **between two dates**, interpolation is used to determine the correct loading value. Because of this interpolation, if the intent is to represent a spike such as from storm runoff on a particular day, the spike loading should be bracketed by zero ("0") loadings.

If the current date in a simulation occurs **before the first date or after the last date** of the loading time series, AQUATOX assumes that the loadings "wrap around" with an annual cycle. Specifically, the AQUATOX algorithm will step towards the input data in one-year increments until the derived date falls within the input time series. The model will then interpolate the results, if necessary, and assign the results to the date being modeled. In this manner, if you had two years of loadings but ran the model for eight years, the model would repeat the second year of loadings in an annual cycle for the last seven years of the simulation. (Note: if a different type of annual cycle or interpolation is desired this can be derived outside of the AQUATOX interface and then imported into the model.)

Exercise caution when modeling multiple years using loadings data from only one or a few years. Sporadic loadings, which would be expected in that one particular year may inappropriately be repeated in successive years. If you do not wish loadings to be repeated, enter values ("0" or otherwise) for the first and last days of the simulation.

If there is only one dynamic loading point present, this is interpreted in the same manner as a constant load.

### Dissolved Org. Tox Loadings

This initial conditions and loadings screen contains a few items that are unique to dissolved organic toxicants.

The **gas-phase concentration** input allows the user to enter a constant concentration of toxicant in the air (g/m<sup>3</sup>) that affects the degree of volatilization (potentially in either direction).

The **biotransformation** button may be used to access the biotransformation screen which is only relevant when multiple chemicals are modeled, and only then when parent compounds and daughter products are both included in the mix.

The **toxicity data** button allows the user to specify direct effects from the toxicant to biotic elements in the simulation in the chemical toxicity data screen.

### **Nutrient Loadings**

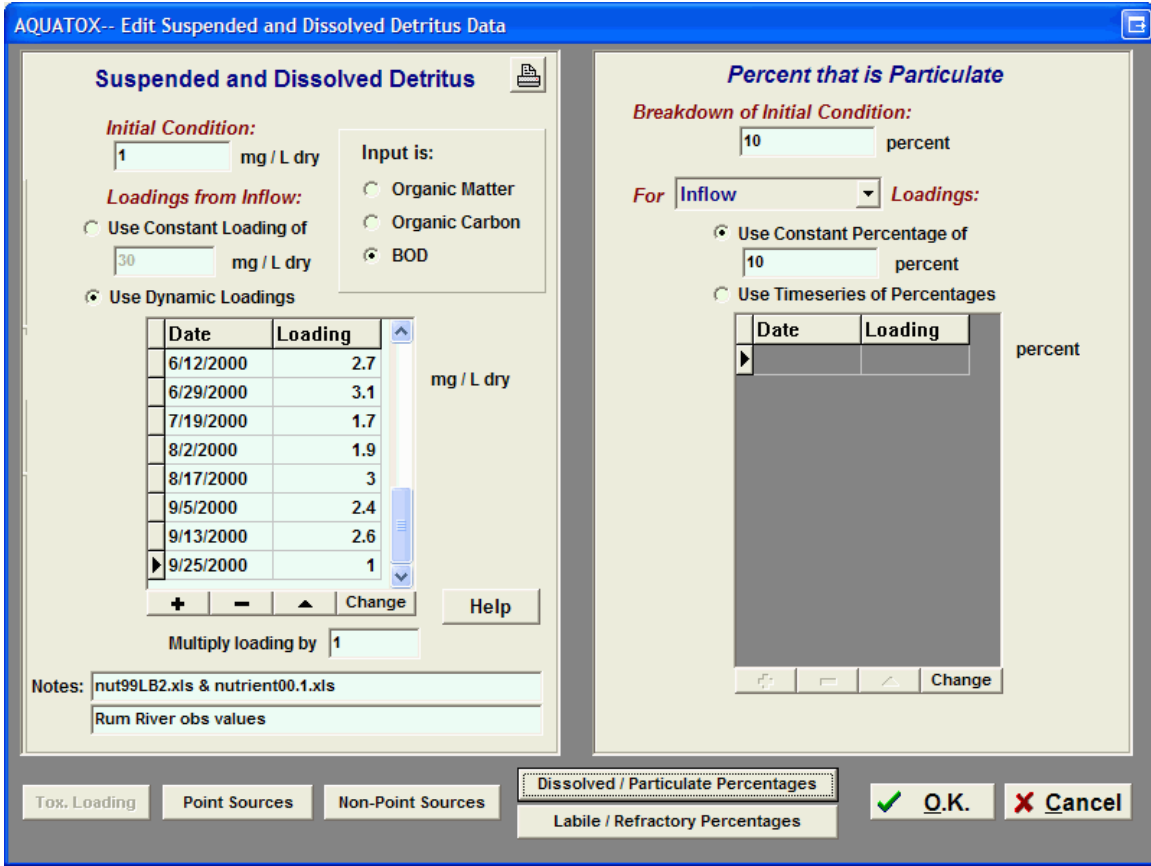
The nutrient initial conditions and loadings screens include the capability to model **Total N** and **Total P** along with all of the items contained on other loadings screens.

When initial conditions, inflows, or other loadings are entered as Total N, by selecting the appropriate check-box (e.g. "**Init. Cond. is Total N**"), model inputs are located in the "Nitrate" initial conditions and loadings screen and loadings on the ammonia screen are grayed out as they are not relevant. (Total N is assumed to be 12% ammonia for inflow and nonpoint-source loadings and 15% ammonia for point-source loadings.)

When Total N or Total P are used as model inputs, AQUATOX calculates the dissolved content by subtracting out loading inputs for suspended and dissolved detritus and suspended algae as discussed in section 5.4 of the technical documentation.

### **Detrital Initial Conditions and Loadings**

A complex loading screen is necessary for organic matter inputs in the water column. AQUATOX simulates **Organic Matter** (dry weight); however, the user can input data as **Organic Carbon** or **Biochemical Oxygen Demand (BOD)** and the model will make the necessary conversions. (See the technical documentation for more information about how the model converts organic carbon and BOD loadings into organic matter.)



Organic matter initial conditions and loadings are divided into four compartments:

- particulate refractory detritus;
- particulate labile detritus;
- dissolved refractory detritus; and
- dissolved labile organic matter.

Initial conditions and loadings are parsed by specifying % **Particulate** and % **Refractory** which can be entered as constant or time-varying percentages (0-100). Loadings of organic matter can be constant or dynamic (time series) for concentrations in inflowing water (mg/L), and for mass from point sources and non-point sources (g/d). Toxicants associated with detritus also can be specified (ug/kg).

Organic matter loadings in "inflow water" are closely related to the volume of inflow water specified (or calculated as a result of choices) in the water volume screen. In other words, loadings in unit per liter of water must have an associated inflow of water in order to be relevant to a simulation.

Separate state variable input screens are provided for refractory and labile organic matter within the sediment bed. The initial conditions are given as g/m<sup>2</sup>, and the loadings are given as mg/L. Associated toxicants are given as ug/kg (ppb).

See section 5.1 of the technical documentation for more information. Also see this note about dynamic loadings.

### Temperature Data Screen

The annual mean and range in temperature from the site underlying data screen can be used, or time series can be entered—in which case make sure that the complete time period being simulated is covered. If the system stratifies then temperatures must be given for both epilimnion and hypolimnion.

If a system may thermally stratify then hypolimnion temperature data may also be entered here. Under the model's default behavior, thermal stratification will be assumed when vertical temperature differences exceed three degrees; at all other times a well-mixed system is assumed and modeled. However, there is an additional button on this screen labeled "**Stratification Options**" that allows a user to modify this behavior by specifying dates of stratification, thermocline depth, and flow routing options.

For more information on temperature modeling, see section 3.5 of the technical documentation. If time series are entered you may wish to see the note about dynamic loadings.

### Wind Loadings Screen

(To access this screen double-click on "Wind Loading" on the state variables list in the main window.)

Within the wind loadings screen, you can either use a default time series for loadings, a constant wind loading, or enter **dynamic loadings**.

Wind is an important driving variable because it determines the stability of blue-green algal blooms, affects reaeration or oxygen exchange, and controls volatilization of some organic chemicals. Wind also can affect the degree of mixing in estuaries. Wind is usually measured at meteorological stations at a height of 10 m and is expressed as m/s. Wind is less important for rivers and streams.

For the default time series, wind is computed using a complex Fourier series of sines and cosines for a 365-day repeating period with a user-supplied **mean value**. The edit box for the **mean value** (in m/s) appears in the upper right hand of the wind loadings screen.

For more information on wind, see section 3.6 of the technical documentation.

### Light Loadings Screen

(To access this screen double-click on "Light" on the state variables list in the main window.)

When entering light data, the user has three options: Constant, time series, or annual mean and range may be given for light in Langley's/day. If annual mean and range are used, these parameters must be filled-in in the site underlying data screen.

Also, photoperiod can be auto-calculated from latitude or entered manually. The latter can be useful when modeling experimental facilities.

Conversions into Langley's per day (Ly/d) are provided using the "convert" button; imported time series may also be converted.

See section 3.6 of the technical documentation. Also see this note about dynamic loadings.

### pH Screen

(To access this screen double-click on pH on the state variables list in the main window.)

pH is important in AQUATOX for several reasons.

- Ionization of ammonia is sensitive to pH;
- Nitrification rates are sensitive;
- Hydrolysis of organic chemicals can be sensitive to pH;
- Calcite precipitation is predicted as a function of pH;
- Conversion of refractory detritus to labile detritus is affected by pH; and
- Decomposition of organic matter is affected;

A user may input a time series of pH values here or calculate pH values using a simple semi-empirical formulation that requires a Mean Total Alkalinity input on this screen (see section 5.7 of the technical documentation for more information.)

When a time series is utilized the rules for dynamic loadings apply.

The pH state variable cannot be deleted from an AQUATOX simulation.

### **Water Volume Data**

(To access this screen double-click on "Light" on the state variables list in the main window.)

Considerable flexibility exists to compute or specify water volume. Depending on the method chosen, inflow or discharge values may be required. The Manning's equation can be used to compute changing volumes in a stream. The simplest procedure is to hold volume constant at the initial condition. Volume can also be computed dynamically using both inflow and discharge, which are input on this screen. Evaporation can also affect water volumes, this can be input as an annual evaporation rate on the site underlying data screen or using a time-series import available on the site-type screen. There is an "**Evaporation**" button available on this screen to directly link to the time-series evaporation output. When available, a known time series can be entered or imported. Flow data can be imported in several formats, including USGS tab-delimited; however, recent changes in the USGS format, including variable header material, makes this prone to problems. If the data do not appear in the preview window then the flow data will have to be converted in a spreadsheet from cfs to m<sup>3</sup>/d, and the date column and flow column then exported as a tab-delimited or comma-separated file suitable for importing into AQUATOX.

#### **Notes:**

The initial condition water volume is determined from the inputs on this screen and not from the site underlying data. However, a "**Get Initial Cond. from Site Data**" button exists to allow the initial condition to be copied from that screen.

The **Mannings Equation Method** (streams only) requires discharge data. Inflow data and site volume are calculated using Manning's Equation. Careful attention should be given to the "Channel Slope" and "Manning's Coefficient" parameters entered in the "Stream Data" screen (within the site underlying data screen.)

The **Keep Constant at Initial Condition Level** Method requires inflow data. Discharge is calculated based on inflow and evaporation.

If you choose to **Calculate Dynamically**, volume is calculated based on inflow, outflow and evaporation.

The **Utilize Known Values Method** requires a time series of known volumes and inflow data. Outflow is calculated taking evaporation into account.

The differential equation that calculates the water volume of the system is:

$$\delta \text{Volume} / \delta t = \text{Inflow} - \text{Outflow} - \text{Evaporation}$$

The "**Stratification Options**" button allows a user to modify default model behavior regarding stratification by specifying dates of stratification, thermocline depth, or flow routing options.

For more information on morphometry and volume, see section 3.1 of the technical documentation.

### **Initial Conditions Summary Screen**

Initial conditions can be displayed and printed for all state variables in this summary screen and any associated toxicants (reach this screen by clicking on the **Initial Conds.** button on the main screen.)

These initial conditions cannot be edited on this screen because of the complexities of the suspended and dissolved detritus screen.

### **Parameters**

Parameters provide values for coefficients in the process equations. Although default values are given, the user has great flexibility in specifying values to represent site-specific species or groups.

There are five **libraries** of parameter values that may be loaded into a simulation.

The **Chemical Library** contains parameters for organic chemicals that could be associated with a simulation. Within a simulation, chemical parameters may be found by double-clicking a **Dissolved org. toxicant** on the state-variable list and then choosing **Edit underlying data**. See also: **Chemical Data Screen**

The **Animal Library** contains parameters for fish and invertebrates that could be associated with a simulation. Within a simulation, animal parameters may be found by double-clicking an animal on the state-variable list and then choosing **Edit underlying data**. See also: **Animal Data Screen**

The **Plant Library** contains parameters for algae and macrophytes that could be added to a simulation. Within a simulation, plant parameters may be found by double-clicking a plant on the state-variable list and then choosing **Edit underlying data**. See also **Plant Data Screen**

The **Site Library** contains parameters for representative sites that could be modeled by AQUATOX. Within a simulation, the site parameters can be found by clicking the **Site** button and then by clicking on the **Edit Underlying Site Data** button that appears. See also **Site Data Screen**

The **Remineralization Library** contains parameters about the detritus and nutrients associated with a site. To find these parameters within a simulation click on the **Site** button and then by clicking on the **Remineralization** button that appears.

When editing libraries, a **GridMode** button may be pressed that toggles editing between a matrix of all parameters in the library or a close-up look at the parameters, units, and comments for one

specific entry in the library. When editing a particular simulation, this button allows the user to see a matrix of all of the animals, plants, or chemicals within that particular study. All parameters within the grid may be edited and the full set of parameters may be exported to Excel. All libraries may be searched using improved "Search Names" or "Search Scientific Names" interfaces. Searches are no longer case sensitive and a partial list of search results is shown for any entries that match the partial or complete search string entered.

To add a new library entry you may press the **New** button and a blank set of parameters is created for data entry. Alternatively, after modifying a parameter set in a simulation, those parameter values may be saved back into the library (either overwriting the original entry or the name may be changed to add additional information to the library.)

When you are editing the underlying data that applies to a simulation, you can either load from or save those parameters to the library file by clicking on the **Load from Library** or the **Save to Library** buttons at the top left of the screen.

### **Chemical Properties and Fate Data Screen**

Required chemical "underlying parameters" and units can be found on this screen. These parameters govern chemical fate and partitioning behavior.

Note that the organic-sediment/detritus and water partition coefficient can be calculated dynamically or entered manually by the user. Sorption to inorganic sediments is only relevant when the multi-layer sediment model is incorporated.

Parameters on this screen govern the chemical fate processes of

- ionization,
- volatilization,
- hydrolysis,
- photolysis,
- sorption, and
- microbial degradation.
- PFA Parameter Screen

You may also edit the toxicity data for the relevant chemical by selecting the Toxicity Data button at the top right of the screen.

To maximize comprehension, parameters on this user interface screen are described with several English words rather than symbolically. **Appendix B** of the **AQUATOX Technical documentation** contains a full description of each of the parameters shown here under "**Chemical Underlying Data**" as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this manner, a user can use this appendix as a reference to search the technical documentation and find all equations in which each parameter is utilized. Advanced users can also easily find the parameters within the AQUATOX source code as the "internal" variable names are also listed within Appendix B.

For more information on modeling organic chemicals, see chapter 8 of the technical documentation.

### **Chemical Toxicity Data Screen**

This screen is where all of the chemical toxicity parameters are located. To get to this screen go to Chemical **Underlying Data** and select the "**Toxicity Data**" button. Or use the button on the chemical's initial conditions and loadings screen

There are multiple options for entering uptake rate constant (k1), the elimination rate constant (k2) and the bioconcentration factor (BCF) or allowing the model to calculate these parameters (BCF=k1/k2)

Additionally, elimination rates may be estimated using the octanol water partition coefficient (Kow).

If the user only has toxicity data for a few species, an extensive library of regressions (Interspecies Correlation Estimation, or Web-ICE) is built into the model (Asfaw and Mayer, 2003). This may be accessed by using the button at the bottom of the screen ("**Interspecies Toxicity Correlation Models**").

By entering both LC50 and EC50 values for a species the application factor can be computed. The user has the option of applying that same ratio to the rest of the species in the animal or plant toxicity screen using the buttons **Estimate animal LC50s...** and **Estimate plant EC50s...** Animal and Plant toxicity require different parameters so they are given separate matrices on the screen. The animal toxicity data appears above the plant toxicity data.

The animal toxicity parameters are as follows:

**Animal Name**, must match the "toxicity data" record in the relevant Animal Data screen.  
**LC50**, ( $\mu\text{g/L}$ ), external concentration of toxicant at which 50% of population is killed  
**LC50 exp. time**, (h), exposure time in toxicity determination  
**Elim Rate Const. (K2)**, (1/d), elimination rate constant  
**K1 Uptake Const.** (L/kg) optional uptake rate constant (dry weight)  
**BCF**, (L/kg) optional Bioconcentration Factor (dry weight)  
**Biotransfm rate const**, (1/d), Daily rate of biotransformation of this toxicant  
**EC50 growth**, ( $\mu\text{g/L}$ ), external concentration of toxicant at which there is a 50% reduction in growth  
**Growth exp. time**, (h), exposure time in toxicity determination  
**EC50 repro.**, ( $\mu\text{g/L}$ ), external concentration of toxicant at which there is a 50% reduction in reproduction  
**Repro exp. time**, (h), exposure time in toxicity determination  
**Ave wet wt.**, (g), mean wet weight of organism  
**Lipid frac.**, (g lipid/g organism), fraction of lipid in organism (wet weight)  
**Drift Thresh**, ( $\mu\text{g/L}$ ), concentration at which invertebrate drift is initiated

The plant toxicity parameters are as follows

**Plant Name**, must match the "toxicity data" record in the relevant Plant Data screen.  
**EC50 photo**, ( $\mu\text{g/L}$ ), external concentration of toxicant at which there is 50% reduction in photosynthesis  
**EC50 exp. time**, (h), exposure time in toxicity determination  
**EC50 dislodge**, ( $\mu\text{g/L}$ ), external concentration of toxicant at which 50% of algae is dislodged (not applicable for phytoplankton)  
**Elim Rate Const. (K2)**, (1/d), elimination rate constant  
**K1 Uptake Const.** (L/kg) optional uptake rate constant (dry weight)  
**BCF**, (L/kg) optional Bioconcentration Factor (dry weight)  
**Biotransfm. rate const.**, (1/d), Biotransformation Rate  
**LC50**, ( $\mu\text{g/L}$ ), external concentration of toxicant at which 50% of population is killed  
**LC50 exp time**, (h), exposure time in toxicity determination  
**Lipid frac.**, (g lipid/g organism), fraction of lipid in organism (wet weight)

**Buttons at the bottom of the screen:**

**Estimate Animal or Plant K2s using Kow.** Elimination rate constants may be estimated using the chemical's KOW data. Animal estimates utilize the "wet weight" and "lipid frac." fields, whereas plant estimates utilize only the "fraction lipid" field within the plant's toxicity record. For a macrophyte-specific calculation to be performed, the plant name must include the substring "macroph."

In Release 3, an alternative K2 estimation is also available within the code, based on Barber (2003) that also requires the "wet weight" and "lipid frac." fields to be populated with data. For more information on this option, see the section on "Elimination" in section 8.7 of the *Technical Documentation*.

When the chemical being modeled is a PFA only animal K2 estimations are available as a function of the mean weight of the organism and the "chain length" of the chemical (equations 405 and 406 of the *Technical Documentation*). New to Release 3.1 the K2 values produced by this estimation procedure are now editable. However, all animals and plants must be linked to a chemical toxicity record with a populated K2 field for the model to work properly.

**LC50 / EC50 estimation:** Using the EC50 to LC50 ratio for one species, the EC50 or LC50 can be estimated for other species within the simulation.

**Interspecies Toxicity Correlation Models:** Utilize the integrated ICE regression databases.

Extensive information about the AQUATOX ecotoxicology model may be found in chapter 9 of the technical documentation.

Reference: Barber, M. C. 2003. A Review and Comparison of Models for Predicting Dynamic Chemical Bioconcentration in Fish. *Environmental Toxicology and Chemistry*, 22(9):1963-1992.

**Using ICE for Regressions**

This screen allows the user to utilize a database of regressions to populate all of the species in their simulation with toxicity data.

Often LC50 data will only be available for one or two of the many species that a user wishes to include in a simulation. To alleviate this problem, a substantial database of regressions is available (ICE) as developed by the US. EPA Office of Research and Development, the University of Missouri-Columbia, and the US Geological Survey (Raimondo 2010). The ICE database includes over 2000 models with over 100 aquatic species as "surrogates." Regressions may be made on the basis of species, families, or genera. The database also includes goodness of fit information for regressions so their suitability for a given application may be ascertained (see statistic definitions below).

The steps that a user can take to use ICE within AQUATOX are as follows:

- Invoke the ICE interface from the AQUATOX "Chemical Toxicity Parameter" screen;
- "Step 1:" Choose from the six available ICE databases (species, genus, and family by either scientific names or common names), by using the drop-down list provided;
- "Step 2 or 3:" Choose a "surrogate species" that matches a species for which there is observed LC50 data (drop-down list);

- "Step 2 or 3:" Choose a "predicted species" that matches a species that you wish to model (and for which *LC50* data is unavailable);
- "Step 4:" Examine the goodness of fit for your model and evaluate whether it is appropriate for your purposes. Where there are multiple surrogates for the desired predicted species, compare the statistics and choose the best surrogate/predicted pair.
- "Step 5:" Apply the model by assigning the surrogate and predicted species to species within the chemical's toxicity record. Use the drop-down menus shown to apply the correlation within your toxicity database. The changes will be made when you return to the toxicity screen from the ICE interface.

You may also visit the Web-ICE Website using the URL or the button displayed at the top of the screen in case an updated database is available.

Graphs may be displayed on a log-scale or arithmetic basis and the user may change the confidence interval plotted.

Statistics provided for goodness of fit are defined below (source: Raimondo et al., 2010)

- **Sample Size (n)** – The number of data points used to build the model. In general, the higher the number of samples, the more robust the model.
- **Intercept (a)** – The log<sub>10</sub> value of the predicted taxon toxicity when the log<sub>10</sub> of the surrogate species toxicity is 0.
- **Regression Coefficient (slope b)** – The regression coefficient, represents the change in log<sub>10</sub> value of the predicted taxon toxicity for every change in log<sub>10</sub> value of the surrogate species toxicity.
- **Average value of X (log *Ic50*)** – The average of toxicity values for the surrogate species used in the model, log-transformed.
- **Mean Square Error (MSE)** – An unbiased estimator of the variance of the regression line.
- **Standard Error of Slope (SEB)** – A measure of the variability of the derived slope.
- **Correlation Coefficient Sqr (R<sup>2</sup>)** – The proportion of the data variability that is explained by the model. The greater the R-squared value and the closer it is to one, the more robust the model is in describing the relationship between the predicted and surrogate taxa.
- **Probability (Pr) that slope <> 0, p-value** – The significance level of the linear association and the probability that the linear association was a result of random data. The lower the p-value, the stronger the association among the surrogate and predicted taxa. Model p-values of < 0.00001 are reported as 0.00000.

Raimondo, S., D.N. Vivian, and M.G. Barron. 2010. *Web-based Interspecies Correlation Estimation (Web-ICE) for Acute Toxicity: User Manual. Version 3.1.* EPA/600/R-10/004. Office of Research and Development, U. S. Environmental Protection Agency. Gulf Breeze, FL. FL.

## **Biotransformation Screen**

When **multiple chemicals are modeled**, the biotransformation screen indicates which chemicals can be converted to other chemicals within the simulation.

For the chemical indicated in the title of the screen, the columns of the matrix indicate the ecological compartments in which that chemical can break down and the rows of the matrix represent the other chemicals within the simulation into which the chemical could be transformed. Each cell indicates the percentage of the chemical that is biotransformed into the daughter product (chemical indicated in the row title). Each column must sum to 100 percent; the "other" row autocalculates to make this possible.

The rate of biotransformation in each species is governed by the biotransformation parameter found in the chemical toxicity record screen.

Categories in which biotransformation may be specified are:

- **Aerobic Microb.:** Aerobic microbial degradation within detritus;
- **Anaerobic:** Anaerobic microbial degradation within detritus;
- **In Algae:** Plant compartments;
- **Benthic Insect:** Invertebrates specified with an **animal type** of "Benthic Insect";
- **Other Invert:** Other invertebrates;
- **In Fish.**

In some cases, modeling a specific biotransformation pattern within a particular species will be desirable. In this case, using the "**Add Species Specific Data**" button will make this possible. You will be able to select a modeled species in the simulation and then specify the appropriate biotransformation rate within that species.

### **Plant Data Screen**

Several fields near the top of the screen require explanation. If you click on the arrow to the right of **Plant type**, you will be given a choice. The choice of **Plant type** is important because different types have different physical or biological processes that apply to them. For instance, phytoplankton are subject to sinking, but not periphyton, which are attached to a surface. Conversely periphyton are limited somewhat by very slow current velocity; but not phytoplankton, which are adapted to still water. If "macrophytes" are chosen the species must be distinguished as "benthic," "rooted floating," "or "free-floating." Table 5 in the Technical Documentation helps clarify some of the differences between plant types.

Although **Plant type** is important for determining which processes do or do not apply to the state variable, the **Taxonomic Type** field is included as an organizing tool and does not affect model output.

The **Toxicity Record** field within this screen links to the "plant name" within each chemical's toxicity data. In this manner, several plants could link to the same toxicity record if that is desired. You may select a record from the list or type a new name if the desired plant name does not appear in the pulldown list.

Phytoplankton and periphyton compartments may be linked together. When viewed in a simulation, a plant will have an "**Edit All Plant Linkages**" button available at the top of the screen. Periphyton also have a "**Periphyton Linkage**" button which allows you to edit the same information but only for the species shown. It is considerably more powerful and user-friendly to use the "Edit All" button.

A few notes regarding the some of the most important parameters:

- Photosynthesis and growth rates are quite sensitive to the saturating light and P half-saturation coefficients along with optimum temperature and the maximum photosynthetic rate;
- The sedimentation rate should be small for streams and much larger for lakes;
- The Critical Force (FCrit) for scour is quite important for periphyton;
- The phytoplankton mortality coefficient may be adjusted for a particular site;
- The exponential mortality coefficient (which increases the mortality for suboptimal conditions) may need to be adjusted if blooms crash too quickly or not quickly enough.

- Occasionally the extinction coefficient may need to be increased if algal growth is too strong--that is the principal means of negative feedback, and can vary among groups.
- Salinity effects are only relevant if "salinity" is included within the simulation in which case photosynthesis and mortality may be affected.

To maximize comprehension, parameters on this user interface screen are described with several English words rather than symbolically. **Appendix B** of the **AQUATOX Technical documentation** contains a full description of each of the parameters shown here under "**Plant Underlying Data**" as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this manner, a user can use this appendix as a reference to search the technical documentation and find all equations in which each parameter is utilized. Advanced users can also easily find the parameters within the AQUATOX source code as the "internal" variable names are also listed within Appendix B.

See section 4.1 and 4.2 of the technical documentation for extensive discussion of modeling algae and macrophytes.

### **Plant Linkages**

Individual periphyton to phytoplankton linkages may be edited using the "Periphyton Linkage button." Using the "**Edit All**" button allows you to edit these linkages for the entire simulation simultaneously. All periphyton in a simulation are listed here along with drop-down boxes that allow the user to link these to available phytoplankton compartments. For convenience sake, multiple periphyton compartments may be linked to the same phytoplankton compartment.

Periphyton may slough or be scoured, contributing to suspended algae; this may be reflected in the chlorophyll *a* observed in the water column. Using this screen, periphyton can be linked to a phytoplankton compartment so that chlorophyll *a* results reflect periphyton sloughing. One-third of periphyton is assumed to become the linked phytoplankton and two thirds are assumed to become suspended detritus in a sloughing event. When not linked, AQUATOX assumes that all sloughed periphyton becomes detritus.

Additionally, when phytoplankton undergoes sedimentation it will now be incorporated into the linked periphyton layer if such a linkage exists. If multiple periphyton species are linked to a single phytoplankton species, biomass is distributed to periphyton weighted by the mass of each periphyton compartment. If no linkage is present, settling phytoplankton are assumed to contribute to sedimented detritus.

### **Animal Data Screen**

This screen displays all of the relevant parameters for the animal that has been selected.

The **Toxicity Record** field within this screen links to the "animal name" within each chemical's toxicity data. In this manner, several animals could link to the same toxicity record if that is desired. You may select a record from the list or type a new name if the desired animal name does not appear in the pull-down list. To edit toxicity linkages for all plants and animals in a simulation simultaneously, click the "**Edit All**" button.

As was the case in the Plant Data Screen, the choice of **Animal type** is important because different types have different physical or biological processes that apply to them. For instance, benthic insects are subject to emergence but other animal types are not. Table 6 in the Technical Documentation describes the differences between animal types.

For "Benthic Invertebrates," a benthic designation box is available. This box does not affect model execution but has effects on the calculation of Biological Metrics (see section 4.6 of the technical documentation.)

Although **Animal type** is important for determining which processes do or do not apply to the state variable, the **Taxonomic Type or Guild** field is included as an organizing tool and does not affect model output.

Sensitivity of animals to **sediments** comes into this parameter screen in several places. The feeding effects are found in the top of the screen with the feeding parameters. Lethal effects and percent-embeddedness effects are found towards the bottom of the screen with the other mortality parameters.

The **fraction in water column** field is only relevant to models running the multi-layer sediment model and determines how much of the organism is exposed to the water column as opposed to pore waters in the top layer of sediment.

**Bioaccumulation Data** includes the lifespan and fraction lipid. Uptake and maximum bioaccumulation of organic chemicals are sensitive to these parameters.

**Low Oxygen Effects** parameters are available for lethality and growth and reproduction effects. **Ammonia** toxicity parameters follow below that followed by **Salinity** effects.

AQUATOX can model two size classes for each fish species. Records for different size classes are linked by clicking on **Size-Class Links** and choosing the correct record from the list given.

Fish may spawn automatically using a formulation based on the **optimal temperature** parameter or specific spawning dates may be entered under **spawning parameters**.

For fish, consumption and respiration rates can be directly entered into the model (top of screen) or **allometric models** can be utilized (bottom of screen). Allometric models within AQUATOX can calculate consumption and respiration rates as functions of weight and temperature.

A few notes regarding the some of the more important parameters:

- Biomass predictions are sensitive to "Maximum Consumption" rate and "Endogenous Respiration" rates when not calculated based on weight (allometrics);
- Intrinsic mortality rate ("mortality coefficient") is often a site-specific response and is therefore subject to calibration;
- The optimum temperature can have a significant effect on biomass computations;
- The minimum prey for feeding affects the efficiency of foraging behavior;
- Allometric means the change in metabolic rate in relation to the size of the organism; allometric parameter values may be found in the Wisconsin Bioenergetics Model documentation (Hewett and Johnson, 1992; Hanson et al., 1997).

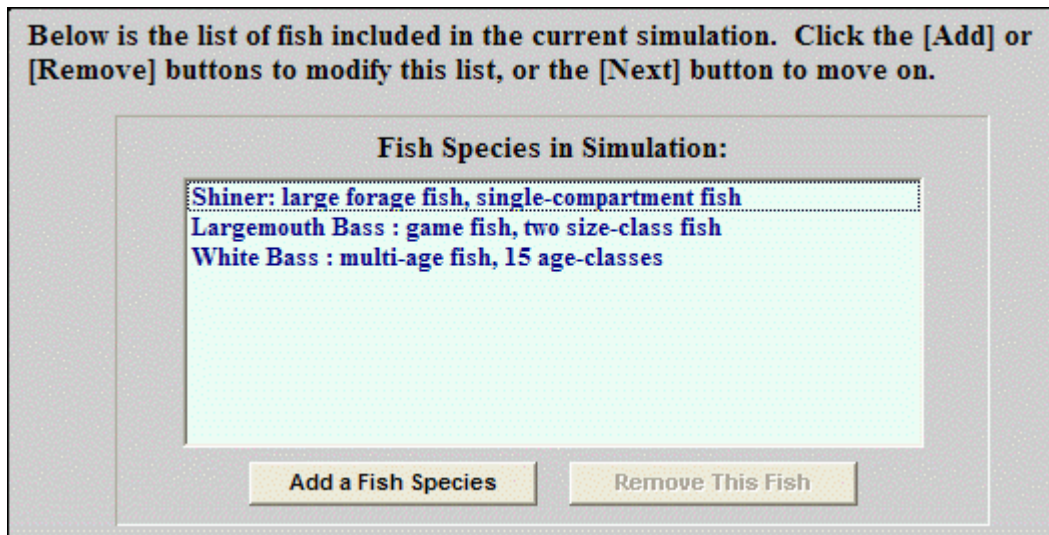
To maximize comprehension, parameters on this user interface screen are described with English words rather than symbolically. **Appendix B** of the **AQUATOX Technical documentation** contains a full description of each of the parameters shown here under **"Animal Underlying Data"** as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this manner, a user can use this appendix as a reference to search the technical documentation and find all equations in which each parameter is utilized. Advanced users can also easily find the parameters within the AQUATOX source code as the "internal" variable names are also listed within Appendix B.

See section 4.3 of the technical documentation for extensive discussion of modeling animals within AQUATOX.

### **Animal Linkages**

Fish may be modeled as a single "stand-alone" compartment, they may be linked by size-class, using the species data screen or an age-class fish may be modeled.

To get a good summary of the animal linkages currently utilized by the model, these can be viewed in Step-7 of the AQUATOX Wizard (example graphic below). This screen also provides a convenient interface to add size-class or age-class fish.



### **Trophic Interactions**

When you load an animal into an AQUATOX simulation, you are also loading a trophic interaction matrix for that particular animal. This trophic interaction table is important because it defines food-web relationships and assimilation efficiencies.

Within AQUATOX, there are two ways of viewing trophic interactions for a given simulation, on a species-by-species basis or to view the trophic interactions matrix for the whole simulation. The species-by-species manner of viewing trophic interactions is generally less useful but is maintained so that users can edit trophic interactions for libraries as well as for specific simulations.

**Species Specific Trophic Interactions:**

**Trophic Interactions of Single Species**

*Trophic Interactions of Tubifex tubifex:*

	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	0	
L detr sed	0.5	0.4	Leidy & Ploskey, 1980, p. C4
R detr part	0	0	
L detr part	0	0	
Peri Low-Nut D	0	0	

Trophic Interactions are not shown normalized, but will be normalized to 1.0 (100%) during a simulation.

View all data   
  View Organisms in Current Study Only   
    
    
    
    

This screen shows the preferences and egestion factors for a single species. To get to the single-species trophic interaction screen, within the Animal Library, click on the **Trophic Interactions** button that appears at the top right of the screen. To get to the trophic interaction matrix for an animal within a simulation, click on that same button within the animal's underlying data.

Within a simulation, you will generally only be interested in viewing an animal's trophic interactions with organisms within that simulation. To view preferences for all available organism compartments, clicking the **View All Data** button at the bottom of the screen.

The preference ratio indicates the animal's preference to consume a particular compartment on the list. Each preference is a fractional preference relative to the other food items on the list, and it need not add to one. Each time-step, AQUATOX will normalize these fractional preferences for the food sources that are available at that time.

The egestion fraction represents the portion of food that is not assimilated for a given animal and food compartment combination.

**Trophic Interaction Matrix Screen:**

AQUATOX-- Trophic Interaction Matrix

Preference percentages are initially normalized to 100% based on species in the simulation. Renormalize

Show Preferences  
  Show Egestion Coefficients  
  Show Comments

	Tubifex tubi	Daphnia	Rotifer, Bra	White Percl	Catfish	Largemouth	Largemouth
R detr sed	50.0				1.1		
L detr sed	50.0				4.6		
R detr part						2.9	
L detr part		30.0	40.0	1.0		2.9	
Cyclotella nan		40.0	5.0				
Greens		30.0	5.0				
Phyt, Blue-Gre							
Cryptomonad			50.0				
Tubifex tubife				42.3	45.7	55.9	0.8
Daphnia				41.1	2.9	38.2	0.8
Rotifer, Brach							
White Perch				15.6	45.7		38.5
Catfish							
Largemouth Bas							30.0
Largemouth Ba2							30.0

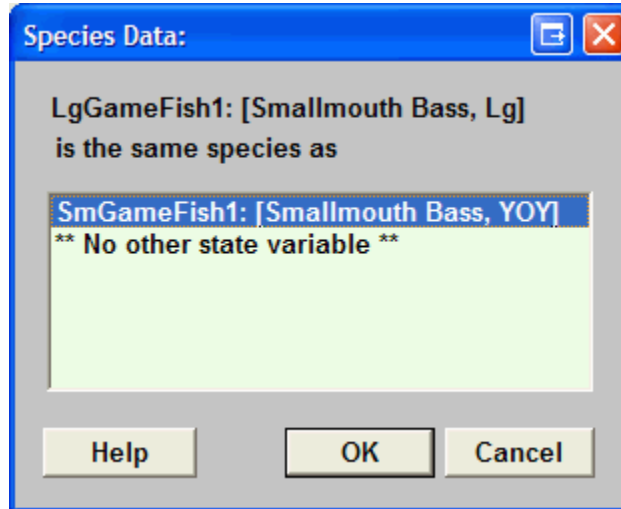
Export Preference Matrix to Excel  
 Help  
 OK  
 Cancel

This screen enables the user to see all trophic interactions for all animals in a particular species against all prey items. Generally, this is a more useful interface for examining and entering information about the food web. Preferences are normalized to 100% when the screen is first shown. After data are entered or modified, these preferences can be renormalized by clicking the "renormalize" button at the top of the screen.

By clicking on the radio buttons at the top of the screen, the user may toggle between preferences, egestion coefficients, and comments. The matrix may also be exported to Excel for printing or sharing.

**Species Data Screen**

The species data screen allows the user to represent a single species of fish with two state variables representing two size classes of that fish, generally young of the year (YOY) and adult. To access this screen select "Size Class Links" from the Animal's underlying data.



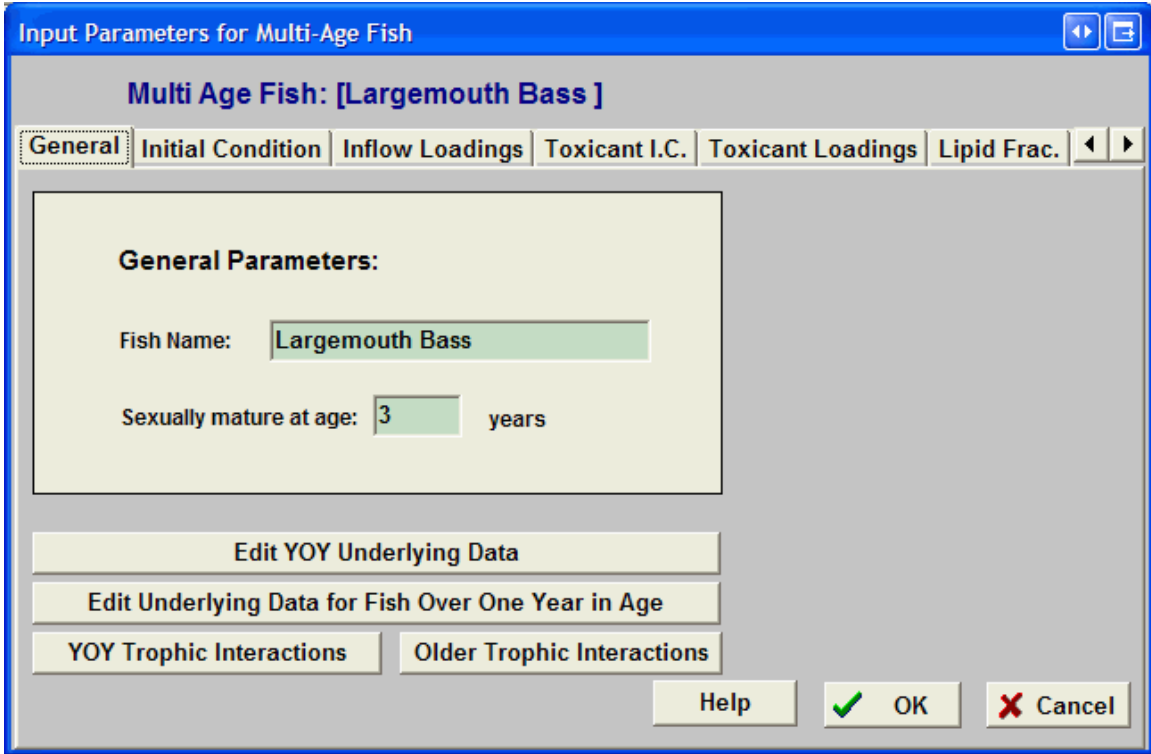
Large gamefish can only be paired with species loaded into a small gamefish compartment. Similarly, large bottom fish can only be paired with small bottom fish and large forage fish can only be paired with small forage fish compartments. Any species that can be matched within the simulation will appear on the list within this screen.

To get a good summary of the animal linkages currently utilized by the model, these can be viewed in Step-7 of the AQUATOX Wizard. This screen also provides a convenient interface to add size-class or age-class fish.

A similar dialog box may also be utilized to link periphyton to phytoplankton compartments, but the **Plant Linkages** screen (accessible by using the "Edit All" button in plant underlying data) is a preferable interface for this procedure as all plant linkages may be viewed simultaneously.

### Multi Age Fish Data Screen

AQUATOX can model one species of fish as having multiple age classes with input from this series of specialized screens. To access this screen one must first add a multi-age class fish to the simulation (see below) and then double-click on "**Multi.Age-Class Fish**" in the state variable list.



Tabs at the top enable the user to switch between the different screens, such as Initial Conditions, Inflow Loadings, Toxicant Initial Conditions and Loadings, Mean Weights, Lipid Fractions and Mortality Coefficients. Click on each tab name to move from one tab to the next. For each tab, the user can enter values for each age class or can choose one of several distributions, characterized by user-supplied statistics.

The values can be graphed as well to better display trends over the life of the fish.

Parameter screens and trophic interaction screens can be accessed for young-of-the-year (YOY) and older fish. When the "older fish" parameter screen and trophic interactions screens are entered, the parameters are relevant for all age classes one year old and older.

To add a multi-age class fish select to **Add** a state variable from the main study window and then select "**Multi.Age-Class Fish**" at the bottom of the available list of variables to add. A series of dialogs follows allowing you to designate the number of age-classes modeled (**Maximum Fish Age**) and to load parameters into the new fish. Alternatively, a multi-age fish may be added in Step 7 of the AQUATOX Wizard .

## Site Parameters

### The Site Type Screen

This screen allows a user to select which site type is being simulated. Six site types are available: pond, lake, stream (creek or river), reservoir, (experimental) enclosure, and estuary.

For standing water (ponds, lakes, and reservoirs) site type is not currently a sensitive parameter (these site-types can be used interchangeably).

Selecting to model a "stream" has the following effects:

- the sand-silt-clay model is enabled;
- Manning's coefficient may be used to model water volume;
- dynamic temperature stratification is disabled;
- periphyton scour and velocity limitation for plants is a function of water velocity;

Selecting "Estuary" produces a **salt-wedge model** and permanent stratification.

For a linked version, a seventh site type is available, that being a "**Tributary Input.**" State variables are not solved within this type of segment; rather, loadings of nutrients, organic matter, and biota to this type of segment are loaded directly into the directly modeled system.

Additionally, a user may edit a **site's underlying data, remineralization parameters, or stratification options** from this screen, or load default site or remineralization data from libraries.

Parameters that may be edited on this screen in a time series or constant manner are

- "Fraction of site that is shaded." See **modeling shade**.
- "Water Velocity." See **velocity**.
- "Mean Depth." See **mean depth**.
- **Evaporation of water** in cubic meters per day. If this time-series option is selected then the constant evaporation data in the "underlying site data" is not relevant.

### Site Data Screen

Each site can be characterized by a relatively small number of site constants. These can be seen and edited by clicking on **Edit Underlying Data** in the **Site Data** window, or they can be loaded from the **Library**. There is some redundancy in that **Volume, Area, and Mean Depth** all have to be specified. Based on mean and maximum depth, the bathymetry of the site is computed. Volume is a state variable and can be computed in a variety of ways (accessible through the **volume loading screen**); however, one option is to set it to remain constant using the value provided in the site screen.

The **Max. Length** is the distance, usually the long axis, across which wave buildup can occur; it determines the depth of mixing in stratified systems.

The epilimnetic and hypolimnetic temperature parameters are only used if the user has selected to "use annual mean and range loadings" on the **Temperature Screen**. If the user has selected to use this manner of calculating loadings, then both epilimnetic and hypolimnetic temperature parameters have to be specified on the site data screen, even for streams and ponds, where they can be set equal.

Likewise, if in the **Light Screen** a user has selected to "use annual mean and range loadings," that user must provide data about the **Average Light** and the **Average Light Range**, from which seasonal fluctuations are computed. These are not computed from the latitude because of local and regional differences in elevation, cloud cover, and maritime or continental climatic conditions.

**Latitude** is used to compute the seasonal variation in day length, though this can be overridden in the **Light Screen**. This override can be useful for laboratory simulations.

**Altitude** is used in the computation of oxygen saturation.

**Enclosure wall area** is used for experimental enclosures only and affects a site's morphometry. (Specifically, it increases the fraction of the site area within the euphotic zone.)

**Baseline Percent Embeddedness** is the initial condition percent embeddedness for a site. This value is used to calculate effects when organisms are sensitive to embeddedness, calculated as a function of TSS. See the "Interstitial Sediments" portion of section 4.3 of the Technical Documentation.

The **Minimum Volume Frac.** multiplied by the initial condition volume for a site represents the minimum volume that a water body can attain within the simulation. If the water volume drops below this level, numerical modeling of state variables stops and the simulation skips forward to the next period in time when the water volume is calculated to be above the minimum level.

Toward the bottom of the site screen are the parameters for the **phytoplankton retention function**. Phytoplankton and zooplankton will quickly wash out of a short reach, but may be able to grow over an extensive reach of a river, including its tributaries. To solve this problem, AQUATOX takes into account the "Total Length" of the river being simulated, as opposed to the length of the river reach, or "SiteLength" so that phytoplankton and zooplankton production upstream can be estimated. The assumption is that conditions upstream are similar to those in the reach being modeled.

For estuaries, a series of **tidal range parameters** is required (amplitudes and epochs). These are used to calculate the daily average tidal range for the site, which affects the average depth of the salt wedge on that day. These parameters are generally available for download from NOAA databases.

If a stream is being simulated (set in the **Site Type Screen**) the **Stream Data** button in the upper right is enabled. Clicking this button displays a series of important stream parameters regarding site morphometry, habitats represented, and parameters for the optional **sand-silt-clay sediment model**.

To maximize comprehension, parameters on this user interface screen are described with several English words rather than symbolically. **Appendix B** of the **AQUATOX Technical documentation** contains a full description of each of the parameters shown here under "**Site Underlying Data**" as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this manner, a user can use this appendix as a reference to search the technical documentation and find all equations in which each parameter is utilized. Advanced users can also easily find the parameters within the AQUATOX source code as the "internal" variable names are also listed within Appendix B.

## **Remineralization**

The parameters on the remineralization screen primarily govern the settling and degradation of organic matter and its nutrient stoichiometry.

Many of the parameters on the remineralization screen may be assumed to remain constant from one simulation to another. A few highlights that may be worth examination:

- Maximum degradation rates: If site-specific data are available.
- Detrital Sedimentation Rate (KSed): This governs the deposition of organic matter and phytoplankton from the water column to sediment (unless the sand-silt-clay model is utilized).

Because of these differences, there are three types of Remineralization records:

- Eutrophic -- should be used in highly nutrient-impacted high systems;
- Default – same as Eutrophic record;
- Mesotrophic -- should be used in moderately nutrient-impacted systems;
- Florida -- used for Florida lakes; this record is different because of the stoichiometry of labile detritus observed in Florida.

### **Modeling Shade**

Shade can be an important limitation to light, especially in riparian systems. A user input “**fraction of site subject to shade from a canopy**” parameter can be entered either as a constant or as a time-series within the “Site” input screen. AQUATOX assumes that 2% of incident radiation penetrates the canopy so a site that has 100% canopy cover still receives 2% light transmission. See section 3.6 of the *Technical Documentation* for more information on this assumption, the equations utilized, and modeling light in general.

This "fraction shaded" parameter can be left as zero to simulate no shading effects on light.

### **Velocity**

Velocity in cm/s may be calculated by AQUATOX or entered as a time series. Otherwise, velocity is calculated as a simple function of flow and cross-sectional area.

Velocity has wide reaching effects including:

- deposition of phytoplankton and scour of periphyton;
- breakage of macrophytes;
- entrainment of zooplankton;
- deposition or scour of organic matter;
- scour and deposition in the sand-silt-clay model; and
- oxygen reaeration.

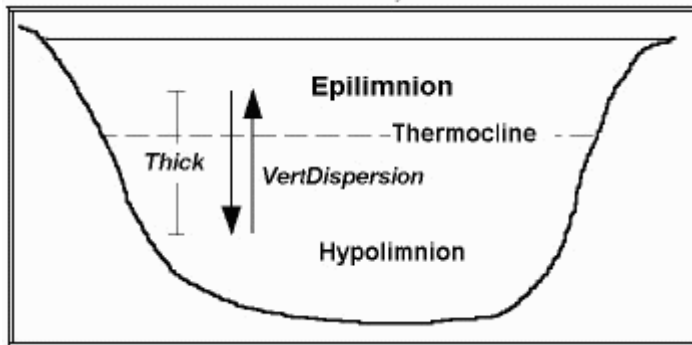
### **Mean Depth**

Mean depth may be kept constant or entered as a time series. Mean depth has significant effects on the average light climate that plants are exposed to (especially periphyton, which reside on the bottom of the water column.)

As noted on the entry screen, if "Use Bathymetry" is **not** selected, the mean depth calculation is irrelevant. In this case, mean depth is volume divided by surface area.

### **Stratification Options**

In the case of stratification, a site's thermocline depth may be calculated as a function of maximum depth and site-length. Alternatively, the depth of the thermocline may be entered as a constant or a time series. The model will interpolate between entered dates if necessary.



Inflow of water (and the loadings within that waterbody) can be routed to a specific vertical segment, as can the outflow of water.

AQUATOX calculates stratification based on the temperature difference between segments. When the temperature difference is less than three degrees, the system is assumed to be perfectly mixed, otherwise vertical stratification occurs. Alternatively, on this screen, users may enter the specific dates of stratification for their modeled systems. (A time-series may be entered. On each date where a "1" is entered, the system will stratify, if not already stratified. On each date where a "0" is entered, the system will undergo overturn and become completely mixed again.)

See section 3.4 of the technical documentation for more discussion of stratification and mixing.

## Exploring Model Setup

### Study Setup

The Setup Screen specifies important parameters about the simulation itself (as opposed to any of the components of the simulation.)

### Simulation Time and Relative Error

At the top of the setup screen you can modify the **first and last days of the simulation**. This defines the simulation period.

The **Relative Error** is the acceptable error in the simulation; if it is not achieved in a particular time step, the variable Runge-Kutta routine decreases the step size and tries again. If the relative error is too large, the results may be erroneous; if it is too small, the run time may be too long. Usually a value between 0.005 and 0.0005 is appropriate, but you may wish to experiment for a particular application.

**Daily and Hourly Simulations:** A user may set the native model time step to one day or one hour. If a daily simulation is utilized, average light conditions are utilized throughout the day. If an hourly simulation is selected, solar radiation is calculated as variable during the course of each day. Rather than calculating daily average oxygen concentrations, if an hourly simulation is selected, AQUATOX will simulate hourly average oxygen concentrations within the water column. These concentrations will be based on the hourly light climate (and optional hourly oxygen loadings). These hourly predictions will then be used to calculate lethal and non-lethal effects due to low oxygen. The user can output hourly values of DO or set a larger **Data Storage Step** and examine the minimum and maximum predictions over that time interval. Hourly inflow

loadings may be input for all nutrients, carbon dioxide, oxygen, inorganic suspended sediments, TSS, light, and organic matter.

### **Biota Modeling Options**

If the model is run in "**Spin-up Mode**" initial conditions for biota will be set based on the model results on the last time-step of the simulation. This can be useful in setting biotic initial conditions when there are insufficient available data. As initial conditions will be automatically overwritten it is best to first save a simulation before running in "spin-up mode."

If the model is set to "**Also spin up nutrients, suspended, and bed sediments**" then all nutrients suspended and bed sediment initial conditions are overwritten based on the spin up including initial conditions for diagenesis bedded sediments. Organic matter is also part of this enhanced spin up. The four modeled suspended and dissolved organic matter compartments (see section 5.1 in the *Technical Documentation*) are summed at the end of the simulation period and copied into the AQUATOX interface as the initial condition for "suspended and dissolved detritus." (Note: If inflow organic matter data are specified in BOD or TOC units, the spin-up procedure converts the AQUATOX final-step results from organic matter into the BOD or TOC units specified in the interface.)

With regards to nutrients, If TN or TP initial conditions were initially utilized, these are replaced with TSP, ammonia, and nitrate initial conditions at the end of the spin up. In this case, the "initial condition as TN" and "initial condition as TP" checkboxes become unchecked.

By default, nitrogen fixation in blue-green algae is assumed to occur when nitrogen concentrations are less than half of the *KN* value (the half-saturation constant for nitrogen). AQUATOX also provides an option to trigger nitrogen fixation as a function of an editable inorganic N to inorganic P ratio which may be selected and specified on this screen.

### **Toxicant Modeling Options** (collapsible with "show" or "hide" button)

If you wish to compute steady-state BAFs, you may wish to **keep the freely dissolved toxicant constant**; this was done in an application concerning PCBs in Lake Ontario (see Validation Studies document). Otherwise toxicant mass is balanced on the basis of loading, partitioning, washout, and other toxicant loss terms.

Toxic effects may be calculated based on **internal or external concentrations**. See Chapter 9 of the Technical Documentation for more information about the consequences of this choice.

When calculating effects based on external concentrations, internal concentrations may be less important. For this reason, a user may wish to **estimate toxicant uptake based on BCF** rather than using the default kinetic model of toxicant uptake. In many cases this will speed up simulation run time significantly.

The older literature often did not distinguish between freely dissolved contaminants and those complexed with dissolved organic matter. You may choose to **include the complexed contaminant in computing BAFs** so that the results are directly comparable with the older literature values.

### **Output Options**

The **Data Storage Step** represents the time period over which results are averaged. This obviously can have a significant effect on the amount of output that is produced by the model.

In plotting output for stratified systems it is usually more pleasing to plot continuous values for the hypolimnion, even when the system is not stratified. This is done by duplicating epilimnion values for the hypolimnion when the system is well mixed (by selecting the **Write Hypolimnion Data When System not Stratified** option); however, this option takes additional storage, so you may choose not to duplicate those data points, especially in systems that may not undergo stratification.

If you click on **Show Integration Info.** you will be able to see what time steps are used in solving the differential equations and which rates and associated relative errors are causing the integration to slow down while the model is running.

The default method of averaging results is by **Trapezoidal Integration**, which calculates the average value that has occurred since the last data storage step. A user may also bypass integration altogether and output "**instantaneous**" concentrations, that is to say, predictions that occur exactly at a given time-step.

For more information about the other buttons on the screen, please see the **Rate Output Screen, Uncertainty Setup Screen, Control Setup Screen, or Output Setup Screen** sections of the help file.

### **Rate Output Screen**

You may save state variable "rates" to be plotted in the output window.

In the Setup Screen, choose **Save Rates** and click on **Rate Specifications** to designate those state variables for which you want the additional output. Each element of a selected state variable's derivative will be integrated and saved along with the results for the simulation. They can then be graphed or viewed in tabular format.

Units for rates are "percent" which is short for "percent of state variable concentration per day." The only exception is for limitations to photosynthesis (variables ending with "\_LIM") which are expressed on a scale of 0.0 to 1.0 with 0.0 representing complete limitation of photosynthesis and 1.0 representing no limitation to photosynthesis.

For Release 3.1 two new light limitation variables are available to signal the occurrence of photoinhibition (too much light) as opposed to insufficient light. When low-light limitation causes light conditions to be sub-optimal then the LowLt\_LIM is equal to the overall light limitation and the "high-light limitation" is set to zero. When photoinhibition is occurring then the HighLtLIM is equal to the overall light limitation and "low light limitation" is set to zero.

### **Uncertainty Setup Screen**

AQUATOX can be run using point estimates for all available parameters (**deterministic mode**).

Alternatively, a Latin Hypercube **uncertainty analysis** can be utilized, or a nominal range **sensitivity analysis**.

#### **Deterministic Mode**

Deterministic mode is the default mode for the AQUATOX model. In this case, a single simulation is used, and all parameters are represented by point-estimates.

#### **Uncertainty Mode**

Another powerful feature of AQUATOX is that it can perform uncertainty or sensitivity analysis to provide probabilistic results. Latin hypercube sampling is performed, ensuring that all parts of the chosen distribution are sampled. Therefore, the number of iterations can be kept to a minimum, which is important because each iteration is a complete simulation. Twenty iterations is the default, meaning that the distribution is divided into 20 segments for purposes of sampling, and that twenty simulations will be run (besides the initial "deterministic" run). The number of iterations should be increased as the number of involved parameters increases.

The Uncertainty Setup screen enables you to view all of the parameters and loadings that can be chosen, either singly or in combination.

Nearly all AQUATOX parameters can be modified in an uncertainty analysis. Selecting the top branch of the tree interface (the "plus" next to **All Distributions** ") allows you to view all possible distributions that could be utilized (parameters that can be modeled as a distribution rather than a point estimate). Alternatively, distributions can be sorted by parameter type or by state variable. The bottom branch of the tree interface shows the distributions that are currently included in the model's uncertainty run. *(Click on the "+" or "-" symbols to expand or contract the various portions of the tree interface.)*

You may choose to **utilize a non-random seed** if you wish to be able to reproduce your simulation's results. A pseudo-random number generator requires a "seed" to start its sequence of "random" numbers. A random seed will be based on the exact clock time in which the simulation was started and this sequence will therefore not be reproduced in later simulations. A non-random seed will produce a repeatable sequence of random numbers.

When an uncertainty simulation is run, a log file (text file) listing the full set of parameter draws and the timing of model simulations is also produced. When **Save Each Iteration to CSV** is selected the full set of AQUATOX outputs for each iteration will be saved to a separate CSV (comma separated variable) file, that may later be examined using Excel or other software. This allows a user to see the full set of time-series results associated with each set of parameter draws.

A non-random set of draws may be utilized so that parameters are sampled at even intervals over their pre-defined range (also called a "statistical sensitivity analysis"). This also can assist in multivariate sensitivity analyses in which combined effects of parameter changes can be evaluated. If the **Sample Randomly within Intervals** option is not selected, the uncertainty analysis will sample the minimum probability for a distribution, the maximum probability, and will also sample at even intervals in between. *For example, a uniform distribution ranging from 0.0 to 1.0 when sampled non-randomly with 11 iterations will produce the following set of samples (though not sequentially ordered) [0.0, 0.1, 0.2, 0.3 ... 1.0].* For non-bounded distributions (normal and log-normal) the minimum and maximum probabilities are estimated as  $(1/num\_iterations)/2$  and  $1.0-(1/num\_iterations)/2$  respectively.

To turn off the uncertainty portion of AQUATOX, select the "**Deterministic Mode**" radio button, below the list of distributions.

By double-clicking on a variable one can access the **corresponding distribution information**.

**Correlations** between modeled distributions may also be modeled.

When you have left this screen and choose to run an uncertainty analysis, you will be prompted for a database file name in which to store the results. Based on all of the iterations, the minimum, maximum, mean, deterministic, and standard deviation result for each data-storage step will be saved in these database files. (Sometimes uncertainty results will not fit in one database file and

will need to be added to one or more additional successively numbered database files.) For more information on viewing these files, see **Viewing Uncertainty Output**.

Also see section 2.5 of the technical documentation for more discussion of the AQUATOX uncertainty analysis.

### **Distribution Information**

This screen shows whether a parametric distribution has been chosen for a given variable or whether a point estimate is used. The radio buttons at the bottom of the screen are used to toggle back and forth.

The default is a normal distribution with a mean of the point-estimate parameter value and a standard deviation of 60% that value. In most cases this will need to be overwritten with parameter-specific information.

A triangular, uniform, normal, or lognormal distribution may be chosen and the nature of the parameters changes based on the selected distribution. Graphs of the distribution will then be produced and can be used to ensure that the parameters chosen are producing the desired distribution. Please check these graphs (probability and cumulative distribution) carefully.

Often loadings are well represented by lognormal distributions. If less is known about the distribution, but minimum and maximum values and some central tendency can be defined, then a triangular distribution may be appropriate. If only minimum and maximum values are known, then a uniform distribution may be sufficient, and the number of iterations can be decreased.

Note for the lognormal distribution that the parameters are "mean" and "standard deviation" rather than geometric mean (GM) and geometric standard deviation (GSD). To convert a GM or GSD to the required parameters, take the natural logarithm of the GM or GSD.

### **Correlations**

This screen allows a user to specify correlations between two or more input distributions. All selected distributions for the uncertainty analysis are listed at the top of the screen. The user may then add a correlation, edit a correlation or remove a correlation from the list of correlated distributions.

Within AQUATOX, input distributions for uncertainty analyses are correlated using the method of Iman & Conover (1982). The Iman and Conover method induces a rank correlation between two randomly derived (stochastic) distributions such that the correlation of the two randomly derived distributions matches the correlation of the input data. Output distributions can be examined to verify that they closely match the correlation coefficient of the input distributions.

For the Iman Conover method to work, correlation matrices must be "Positive Definite." In the authors' experiments with input matrices, we have found this to mean three things in practice:

- No correlations greater than 0.8 or less than -0.8 may be used.
- When there are multiple correlations for the same variable, often correlations must be reduced to less than 0.75 (or greater than -0.75) due to interactions between variables.
- The method requires a minimum number of iterations to successfully impose correlations on input distributions. A specific error will be raised if insufficient iterations have been specified (asking the user to increase the specified number of uncertainty iterations).

To examine the input distribution correlation matrix and test for positive definite status, a user may use the "**summarize correlation matrix**" button. Unless an error is indicated, the output will summarize the user-specified correlation matrix followed by the rank correlation of draws produced by the correlation method.

For more information on this method, please see: Iman, R. L., and W. J. Conover. 1982. A distribution-free approach to inducing rank correlation among input variables. *Communications in Statistics* B11: 311-334.

## **Sensitivity**

"Sensitivity" refers to the variation in output of a mathematical model with respect to changes in the values of the model inputs (Saltelli 2001). It provides a ranking of the model input assumptions with respect to their relative contribution to model output variability or uncertainty (U.S. Environmental Protection Agency 1997).

AQUATOX can automate a nominal range sensitivity analysis (also known as a "one-at-a-time" sensitivity analysis). This analysis assumes independence among tested parameters.

As was the case for the uncertainty analysis, nearly all AQUATOX parameters can be tested for sensitivity. Selecting the top branch of the tree interface (the "plus" next to **All Distributions** ") allows you to view all possible parameters that can be tested for sensitivity. Alternatively, parameters can be sorted by parameter type or by associated state variable. The bottom branch of the tree interface shows the distributions that are currently included in the model's sensitivity analysis. (*Click on the "+" or "-" symbols to expand or contract the various portions of the tree interface.*) If you double-click on any of these parameters, or press <Enter> while the parameter is highlighted the parameter will be selected (or deselected) for the sensitivity analysis.

To run the model in sensitivity mode, the user must

- Select one or more parameters to test using the procedure given above;
- Select a set of output to track using the **Choose Output to Track** button; and
- Choose the percentage to vary by editing "Nominal Percent to Vary."

When the model is then executed, the user will be prompted for an Excel file-name in which to save model results. The model will run a deterministic run and then will run the model twice for each parameter selected (testing sensitivity to changes in each parameter in the positive and negative directions in the magnitude of "percent to vary.") In this manner, if a user selects **n** parameters, the model will run **(2n+1)** iterations. It should be noted that the number of output variables will not appreciably affect the simulation run time. However, the number of tested parameters obviously determines the number of iterations and therefore the total simulation time.

**One important note about sensitivity analyses:** Sensitivity analyses will calculate the percent difference between the results of the deterministic run and the modified simulation ***in the last averaged time-step of the simulation.*** In most cases the user will want to utilize a much longer averaging period within the model setup screen, for example, to calculate averaged sensitivities over the last year of the simulation or the entire simulation. If sensitivity at an intermediate date is desired, the simulation should be shortened so that the intermediate period is reflected in the last averaged time-step of the simulation.

Periphyton and phytoplankton may be linked within the AQUATOX model. If the "**Link Periphyton/Phytoplankton**" check-box is selected, whenever a linked periphyton or

phytoplankton parameter is varied, the same parameter will be varied within the linked algal state-variable by the same percentage.

After the run is complete, the output file can be viewed in Excel. Additionally, AQUATOX can automatically produce tornado diagrams of the results. See **Viewing Sensitivity Output** for more information. Also see section 2.4 in the technical documentation.

#### **References:**

Saltelli, A. 2001. Sensitivity Analysis for Importance Assessment. Paper read at Sensitivity Analysis Methods, June 11-12, 2001, at North Carolina State University, Raleigh NC

U.S. Environmental Protection Agency. 1997. Guiding Principles for Monte Carlo Analysis. Risk Assessment Forum. Washington, DC: U.S. Environmental Protection Agency

#### **Control Setup Screen**

There are two separate banks of memory for model results, one which is labeled "control" and one which is labeled "perturbed." The default is for the control simulation to have all organic toxicants zeroed out or omitted. However, there is considerable flexibility in setting up the control run. For example, toxicants can be kept and point-source nutrients can be omitted in the control run. In fact, it is possible with a few judicious choices to set up a factorial analysis to determine the effects of various combinations of pollution control scenarios.

If none of the check-boxes are selected, then the results of the control and perturbed simulations will be identical. A user could, however, first run a "control" simulation, then change parameters or loadings in the simulation as a "perturbation," and finally run a "perturbed" simulation. In this manner, the control and perturbed sets of results can be used with considerable flexibility, without even utilizing the "control-setup" screen.

Due to the multi-threaded nature of AQUATOX, it is often useful to run the control and perturbed simulations simultaneously, especially with multi-core computer processors.

#### **Output Setup Screen (Results Tracking)**

The Output Setup Screen, (available through a button on the setup screen) allows the user to select which output is saved by AQUATOX, and which output is not saved.

Because AQUATOX has the potential for modeling so many state variables, a user has the option of not saving given state variables, thus decreasing the memory requirements. This can be especially important when running simulations on a decadal scale or when outputting many data-points per day. However, given the RAM capacity of modern computers, this screen rarely needs to be utilized.

Use the "<" and ">" buttons to move results into the "Results to Track" or "Results NOT to Track" lists.

If "Save PPB Data" is unchecked, the model will not save concentrations of chemicals in biota with PPB units.

Note, when stratification is likely to occur, assume that RAM memory utilization will roughly double.

## Running the Simulation

To run an AQUATOX simulation, select the "Control" or "Perturbed" button in the main window.

The model will run for the amount of time specified in the setup screen. When the model has completed you may use the output button to view the model results.

You may work with the model while it is running and, for example, change parameters or open different models. If you change parameters though, AQUATOX will warn you when it is copying results back to the interface as your model results will no longer match the parameters or loadings associated with that study. In this case you will be able to optionally save the model results to a new file in which the model parameters will match the model output.

## Control vs. Perturbed Simulations

A powerful feature of AQUATOX is that it can run paired simulations for perturbed and control conditions. You can use the control setup screen to specify the differences between these two types of runs, or you can change parameters or loadings in between running the two different types of simulations.

The graphical output screen allows users to compare control and perturbed graphs and also to display difference graphs in which percentage differences are displayed.

## Viewing Graphical Output

AQUATOX has extensive capabilities for graphical and tabular output. By clicking on **Output** on the main screen one can create a new **Output Window**. There are four tabs available at the top of this window, each representing a different form of output. Click on the tabs at the top of the output screen to move from one type of output to the next.

The default window is the "Graph Library" window. Graphical output is often the most useful manner to quickly view and interpret model output. The AQUATOX graphing capabilities are quite powerful as described in the following sections.

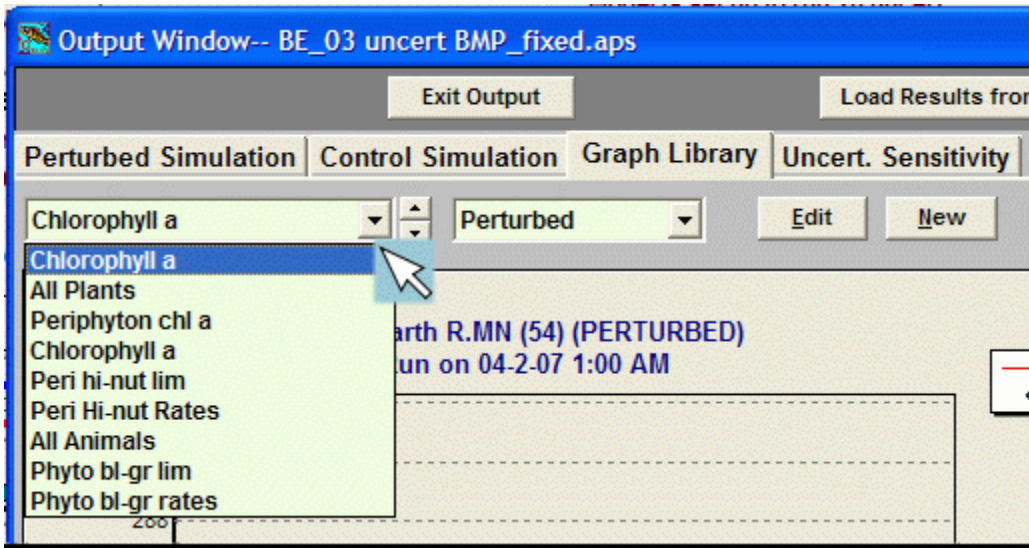
The first two tabs "**Perturbed Simulation**" and "**Control Simulation**" provide tables of output for the control and perturbed results.

The tab on the right leads to a window in which uncertainty and sensitivity results may be examined.

Within the output window you may also save the current bank of results and the "graph library" along with the current set of parameters using the "Save These Results" button. This is no different from exiting the output window and saving the existing "APS" file. Results may also be loaded using the "Load Results from File" button.

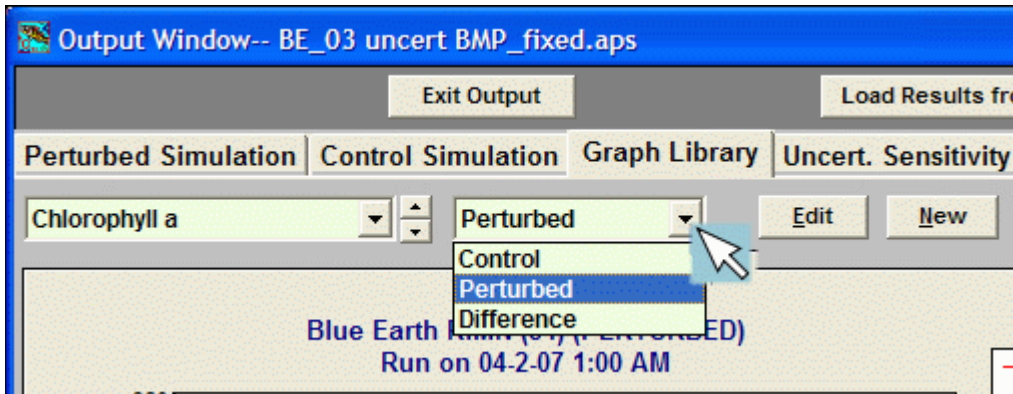
## Viewing Existing Graphs

To determine which graphs have been produced for the given simulation, click on the triangle at the top left of the graph. If there is more than one graph included, a drop-down list of graphs will be shown. The user may select a graph within this list or use the up and down arrows to the right of the list to scroll through the graph library.



## Control, Perturbed, and Difference Graphs

Each graph may be displayed in perturbed mode, control mode, or difference mode. By selecting from the drop-down menu next to the graph list, the user may toggle between these three modes.



The control graph will show a graph of the results saved as the "control" run and the perturbed graph will show the "perturbed" simulation's results.

One of the most useful forms of output is the **Difference Graph**, which plots the results of the perturbed simulation minus the control simulation as percent differences. The default minimum and maximum percentages are 400% and -100% (complete loss). However, these can be changed by using the "Edit" button.

If you click on any of the series shown on the graph, a pop-up box will appear that will tell you the value, the date, and the units for the point on which you clicked. For the difference graph it will describe the effect of the perturbation on that variable.

To add a new graph to the list of graphs in the graph library select the "New" button. To edit the existing graph select the "Edit" button.

Many additional options for graphing are found in the **Graph Menu**.

### **Setting Up a New Graph**

When the "New" button is pressed, a user has a choice of creating a custom graph or creating from a list of pre-produced graphs, for example:

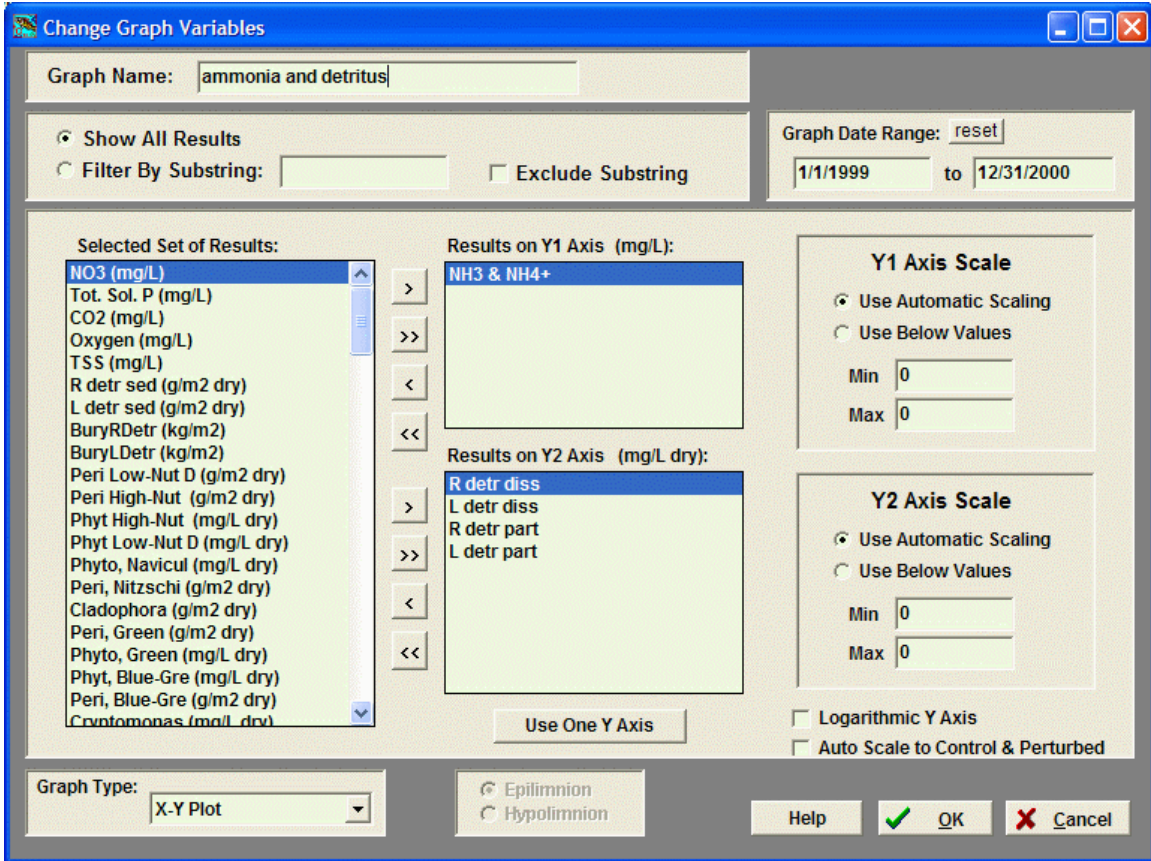
- **All Animals** will plot the biomasses of all animals in the simulation, those with units of "g/m<sup>2</sup>" on the Y1 axis and those with units of "mg/L" dry on the Y2 axis;
- similarly **All Plants** shows plant biomasses separated by units-type;
- **Nutrients** shows ammonia, nitrate, and phosphate
- **Chemical PPBs in animals and plants**,
- **Detritus** shows organic matter concentrations in the water column and sediment beds (located in the "other" pull-down menu).

The custom graph will create a new blank graph that the user can modify using the **Edit Graph** interface.

### **Editing an Existing Graph**

#### **Modifying a Graph**

By clicking on the "edit" button above a graph, one can get to this **Change Graph Variables** screen.



At the top of this window is the capability to edit the graph's name. This affects how the graph appears in the drop-down list.

Next, choose the output to place on each axis. There are potentially hundreds of output variables associated with each simulation. The filter tools help the user pick out relevant variables from this considerable list (see **Selecting from a List of Output.**)

State variables are organized in order of trophic level, starting with organic matter and working upward through plants, invertebrates, and fish.

**The Many Types of AQUATOX Output** (in order of output list)

- Concentrations of State Variables
  - toxicants in water
  - nutrients and gasses
  - organic matter, plants, invertebrates, fish
- Physical Characteristic State Variables
  - water volume, temperature, wind, light, pH
- Mass of Toxicants within State Variables (normalized to water volume)
  - T1-T20 in organic matter, plants, invertebrates, and fish
- Additional Model Calculations
  - Secchi depth, chlorophyll a, velocity, TN, TP, BOD
- Biological metrics
  - % EPT, Chironomids, Amphipods, % Blue-Greens, Diatoms, Greens, Gross Primary Production, Turnover, Trophic State Indices
- Sediment diagenesis state variables
- Toxicant PPB

- T1-T20 (PPB) in organic matter, plants, invertebrates, and fish
- Nitrogen and Phosphorus Mass Tracking Variables
- Bioaccumulation Factors for all organisms
- Uptake Rates (K1), Depuration Rates (K2), and Bioconcentration Factors (BCFs), for each animal in the simulation
- Uptake, Depuration, and Bioconcentration Factors
- State Variable Rates
  - These include limitations to photosynthesis
- Observed data imported by user

These output variables facilitate detailed analyses of simulated responses. Mass loadings and losses and mass balances are output for nutrients. K1, K2, and BCFs are output for toxicants. The ability to output in tabular and graphical form all the state-variable rates along with the limitations to photosynthesis is especially powerful.

You may graph variables on either one or two Y axes. Use the button under the results list to toggle between one or two Y axes. Use the "<" and ">" buttons to move results into and out of a particular axes' results. The ">>" button moves all variables into the selected axis. **Note:** all variables on the same axis must have the same units.

The **Graph Date Range** (x axis range) may be set to a smaller or larger range of dates than the AQUATOX simulation by typing dates in the edit boxes. Selecting "reset" above the date range will set the graph date range to the dates of available model results.

Scaling for each axis (Y1 and Y2) may be entered manually or automatically calculated by AQUATOX. Under the axis scale entry is the option to model a **Logarithmic Y Axis**.

The check-box to **Auto Scale to Control & Perturbed** will scale the Y axes to the minimum and maximum of **both** the control and perturbed simulations (if they both have been run). This enables the user to switch back and forth between control and perturbed graphs while looking at axis-scales that remain constant between the two graphs, enabling easier comparison.

By using the **Graph Type** pull-down menu, you can choose between the four types of plots:

- The **X-Y plot** is the standard, this plots observed results against dates.
- **Percent exceedance** graphs plot percent exceedance on the X axis against model results on the Y axes.
- **Duration graphs** plot duration of exceedance on the X axis against model results on the Y axes.
- **Scatter plots** allow you to examine correlations between model outputs by plotting one model output on the X axis against one or more different model outputs on the Y axis.

If the system has stratified results, you can choose the vertical layer that you wish to display results for using the **Epilimnion** and **Hypolimnion** radio buttons. This may also be toggled in the graph menu.

One additional note: if a duration or exceedance graphs is displayed, a **"Draw Threshold"** button is displayed on the lower right of the graph. When pressed, a dialog box comes up that both displays duration of exceedance above a threshold and draws a line on the graph.

### Selecting from a List of Output

There are potentially hundreds of output variables associated with each simulation. To help the user pick out relevant variables to be graphed, the **"Filter By Substring"** option is available at the

top of the screen. Typing a string in the box provided limits the list of variables to those with names that include the string. For example:

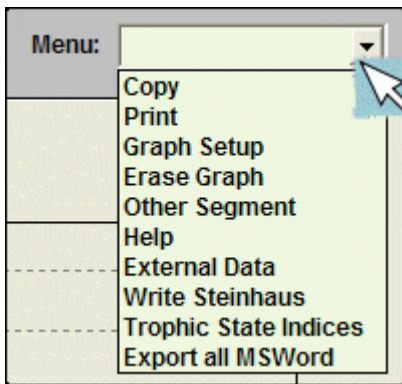
- Type "peri" to find all periphyton variables
- Type "mg/L" to find all variables with units of mg/L.
- Type "ppb" to find all parts per billion output.
- Type "detr" to find all results that pertain to detritus.
- Type "T1" to find all results that pertain to the first organic toxicant.

You may also exclude any results containing the substring by checking the "**Exclude Substring**" box.

Use the "<" and ">" buttons to move results into and out of the "Available Results" and "Results to Display" columns. Using "<<" and ">>" moves all results into or out of the relevant column.

### Graph Menu

At the top right of the graph is a menu that may be accessed as a pull-down menu. After the menu has been used, users may repeat their last action by clicking the "**(repeat)**" button that appears. Note: this menu may also be accessed by right-clicking on any AQUATOX graph.



#### Copy

The copy option allows a user to copy the current graph as a bitmap or a windows meta-file to be copied into presentations, documents, logs, or reports. Bitmaps are generally smaller files, but meta-files give better resolution.

#### Print

The print option allows the user to print the current graph. A "preview" window will first appear allowing the user to select printer, orientation, margins, etc.

#### Graph-Setup

The graph-setup menu allows the user to change the colors, symbols, default text, and fonts used on a graph through a dialog box. (See **Graph Setup Screen**).

#### Erase Graph

Erase graph will permanently remove the current graph from the graph library (after prompting).

#### Other Segment

If there are results for both the epilimnion and hypolimnion segments, this menu option toggles between the two segments. Currently, in linked mode, to view another segment, the user must first go into that segment and then open the output window for that segment.

### **External Data**

Allows the user to import observed data. (See **Importing Observed Data**)

### **Write Steinhaus**

This option enables a user to write a set of Steinhaus similarity indices in Microsoft Excel format. The Steinhaus index (Legendre and Legendre 1998) measures the concordance in values between two samples for each species. A Steinhaus index of 1.0 indicates that all species have identical biomass in both simulations (i.e., the perturbed and control simulations); an index of 0.0 indicates a complete dissimilarity between the two simulations.

A time series of indices is written for each day of the simulation representing the overall species similarity on that date. Separate indices are written out for all plants, all animals, invertebrates only, and fish only. Completed control and perturbed simulations (of the same length) must have been completed for this option to work.

### **Trophic State Indices**

AQUATOX will calculate and display trophic state indices (TSIs) for lakes using the methods identified in the EPA Nutrient Criteria Technical Guidance Manual (<http://www.epa.gov/waterscience/criteria/nutrient/guidance/lakes/lakes.pdf>). Separate TSIs are calculated based on average concentrations of **Total N**, **Total P**, and **Chlorophyll a**, as well as average **Secchi Depths**. The date range over which values are averaged may be specified in the TSI calculation screen as well as the AQUATOX scenario (control or perturbed) and the vertical segment (epilimnion or hypolimnion, if relevant).

### **Export All MSWord**

All graphs will be exported into a new Microsoft Word document in "Windows Metafile" format. When this option is selected, Microsoft Word will start up and each of the graphs will be pasted into a new document. Microsoft Word 2000 or later must be installed on the user's system for this option to work properly. Note, Windows Metafile does not always work properly when computer monitors are in "portrait mode," due to what is apparently a minor glitch in Microsoft Windows (fonts become distorted).

### **Arrange Graphs**

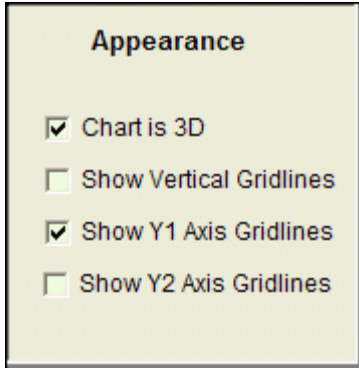
When dealing with a large number of graphs, it can be very useful to arrange them in a particular order. This also affects the order of the graphs when they are exported to Microsoft Word. When the "Arrange Graphs" menu item is selected, a dialog box appears showing all available graphs for the simulation. The user may drag and drop the graph names in the list to reorganize them or use "up" and "down" arrows next to the list to reorder them. Graphs may also be deleted using a "delete this graph" button or by pressing the <delete> key when a graph is selected. All changes made in this window may be undone using the "cancel" button.

### **Statistics from Graph**

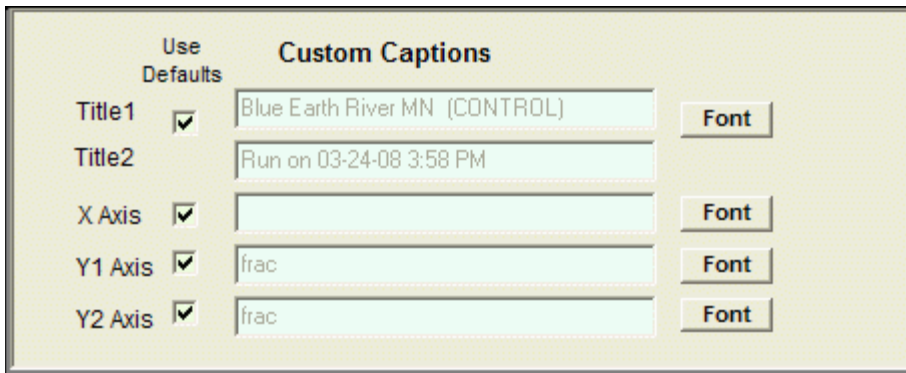
The statistics dialog allows the user to examine and export statistics based on the current graph. (See **Output Statistics**).

## The Graph Setup Screen

This screen allows a user to change the appearance of the current graph. The graph can be shown in 3D, and various grid-line options can be selected. The 3D option is somewhat flashy but not particularly flexible and of limited utility.



Additionally, captions, text, and font can be edited to personalize the graph. Un-check the relevant "Use Defaults" check-box and edit the text under "Custom Captions." Fonts may be modified using the **font** buttons.



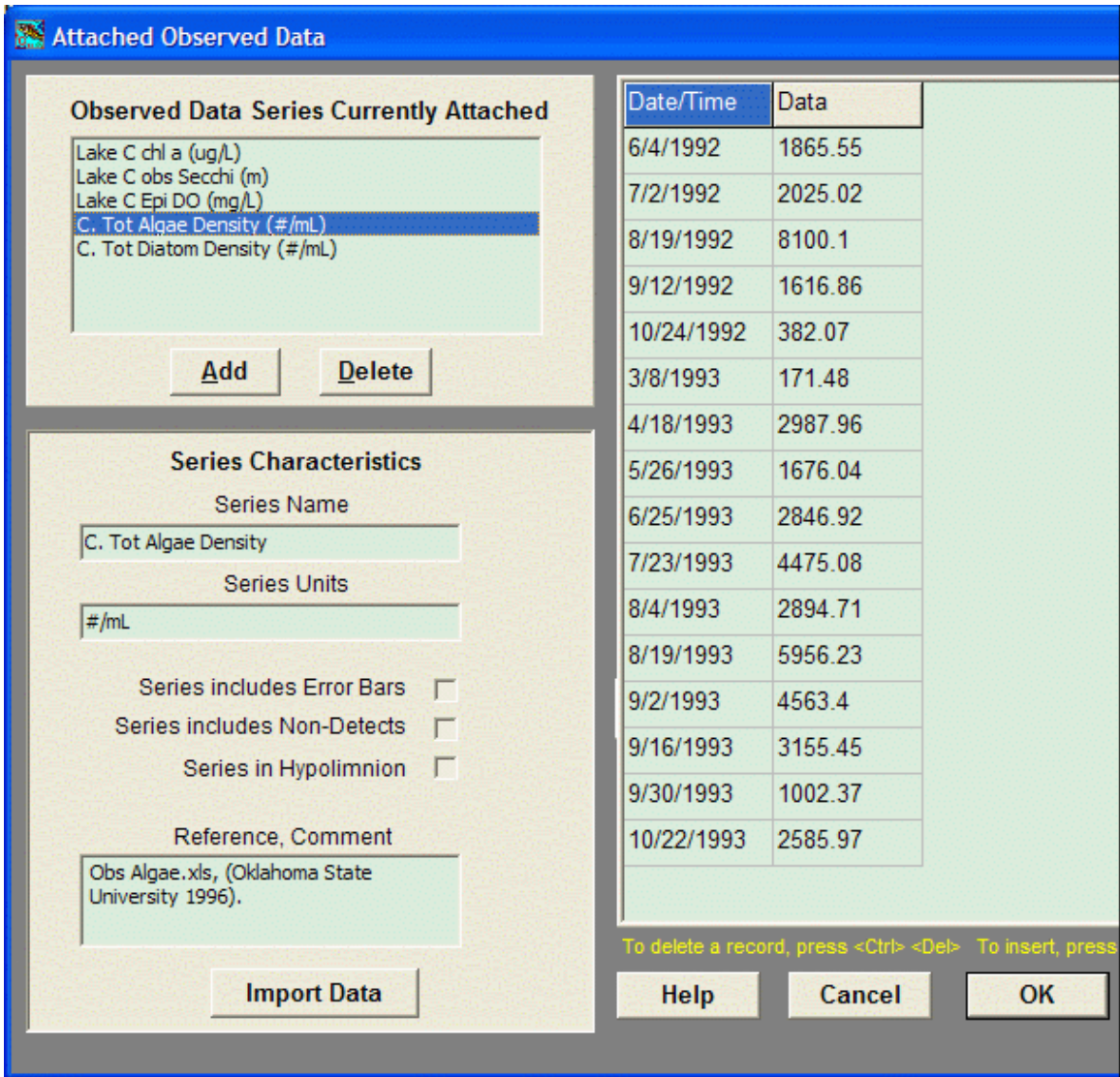
Finally, by selecting a data-series from the "Series Specific Characteristics" list, a user can select which color, line-thickness, symbol size, and symbol represents the selected series. The "SmallDot" symbol renders like a thin line, and is the AQUATOX default. Sometimes it is useful to change the symbol or line-thickness when it is desirable to emphasize one of several series on the graph.

All of the Graph Setup changes will be saved along with the graph when the study (APS) file is saved.

## Importing Observed Data

External "observed" data may be imported into AQUATOX for graphing against model results. After a data series has been imported, it will be displayed at the bottom of the list of data available for graphing in the edit graph dialog. You may also use the text filter within that dialog to find your observed data.

To access the "Attached Observed Data" window select "**External Data**" from the **Graph Menu**.



To add a series, use the **Add** button; the **Delete** button deletes the selected series.

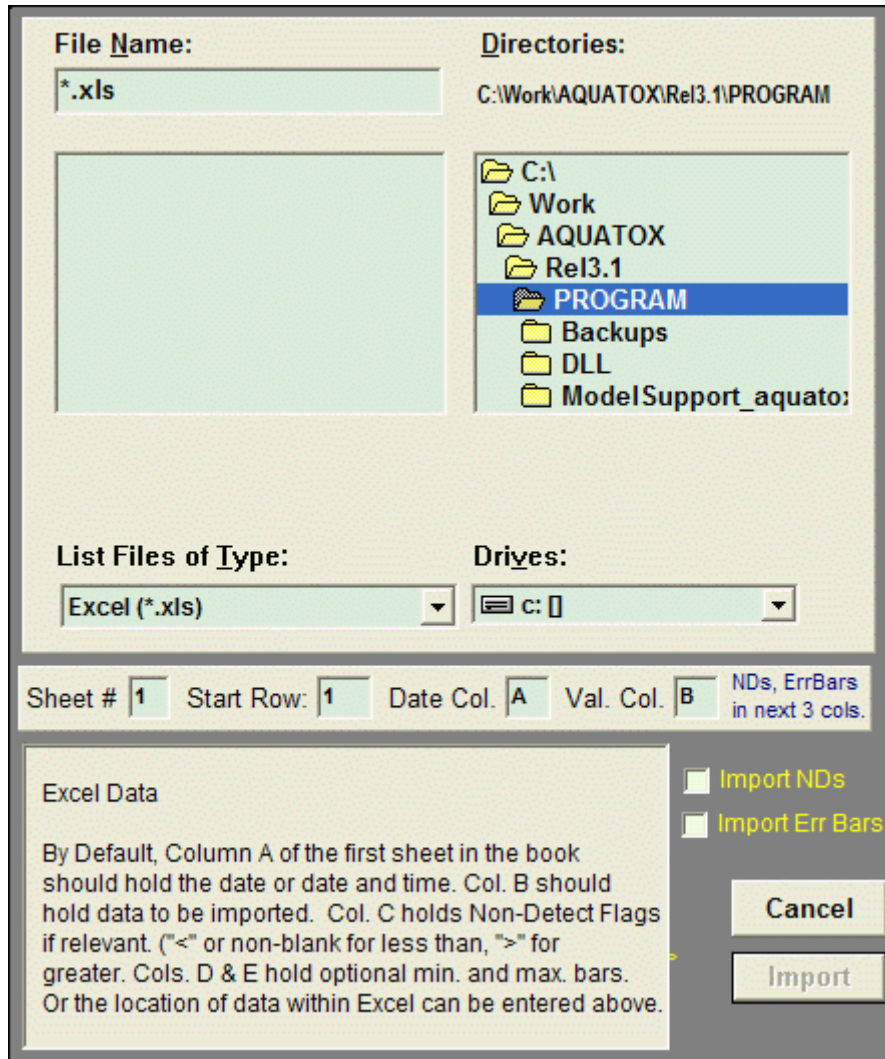
When a new series has been added, you may edit the **series name** and the **series units**. The series units are important as you may only put items with precisely the same units on a single Y axis. So copy the text format of any units that you wish to plot against your imported data precisely. A **reference or comment** may be added below in which the source of the external data is identified.

Imported series may contain **error bars**, in which case vertical bars will be plotted against every point in which error bars are included. Imported series may also contain **non-detects** in which case red arrows will be plotted at the location of the value (which is assumed to represent the detection limit). You may also flag whether the series belongs within the **Hypolimnion** segment.

After setting these flags, click the **Import Data** button.

The interface to import external data is almost identical to the one used to **import loadings**. The significant differences come because non-detects and Error bars may be imported. To change

the file type to import, click on the pulldown menu under "**List Files of Type.**" Directions about the precise file-format required will be found in the rectangle at the bottom of the screen.



Generally, the date appears in the first column of the file, with the values to be imported in the second column; however when importing from Excel you can change the column designations. If you are importing Non Detects check the yellow "**Import NDs**" box. Non-detects appear in the third column. If a value is not detected in the greater-than direction, use the ">" identifier, otherwise any non-blank value will be interpreted as a "lesser-than" non-detect which is much more common.

If you wish to import error bars, check the "**Import Err Bars**" box. Minimum bar values will be imported from the fourth column with maximum bars imported from the fifth column.

After data have been imported, they will be displayed along with their dates in a table. This table may be edited by double-clicking on a cell and editing it. Additional rows may be added or rows may be deleted from the table using the directions that appear below it. (<Ctrl><Del> and <Ctrl><Ins>)

When you have finished importing and editing your observed data series, select the OK button and it will appear in the list of output available to graph. The external data, and any plots created with it, will be saved and loaded along with your AQUATOX simulation.

### Output Statistics Screen

This dialog box enables the user to examine the following statistics that pertain to AQUATOX Output:

- **n:** number of data points evaluated;
- **Mean:** (Sum / n);
- **Median:** The 50th percentile. If there is an even number of data points, the average of the two middle values;
- **Minimum:** Minimum value given the time-period chosen;
- **Maximum:** Maximum value given the time-period chosen;
- **Variance:** A measure of statistical dispersion. Calculated using the robust two-pass algorithm;
- **Standard Deviation:** Square root of the variance;
- **5th Percentile:** 95% of values are greater than this value. The 5th percentile rank is calculated of the ordered data and, if the rank is non-integer, linear interpolation is used between the two nearest ranks;
- **95th Percentile:** 5% of values are greater than this value. Calculated using linear interpolation as above.

The date ranges, scenarios to export statistics for (i.e. "control" vs. "perturbed,") and the vertical segment (if relevant) may all be edited and the statistics will automatically update to reflect the changes from the various inputs and pull-down menus.

The "**Repeat Averaging Period for all years in the simulation**" checkbox allows you to export results on a seasonal basis. If this is selected, a user may put in a date range for a single year (e.g. "5-1-2011" to "9-1-2011") and the model will extract results between those calendar dates regardless of the year selected. (The year chosen when inputting the seasonal date range is not important.)

AQUATOX displays these statistics in a fixed-width basis and they may be copied and pasted to any spreadsheet or database software. The width of numbers and the width of the output names may also be varied using the entry boxes at the bottom of the screen. Statistics may also be exported to Excel using a button at the bottom of the screen.

The derivation of statistics from external "observed" datasets is not enabled at this time.

### Viewing Table Output

Tables can be obtained for both perturbed and control runs. Click on the tabs at the top of the output screen to move from one type of tabular output to the next.

Using the **Change Variables** button, the user can specify what variables are to be tabulated.

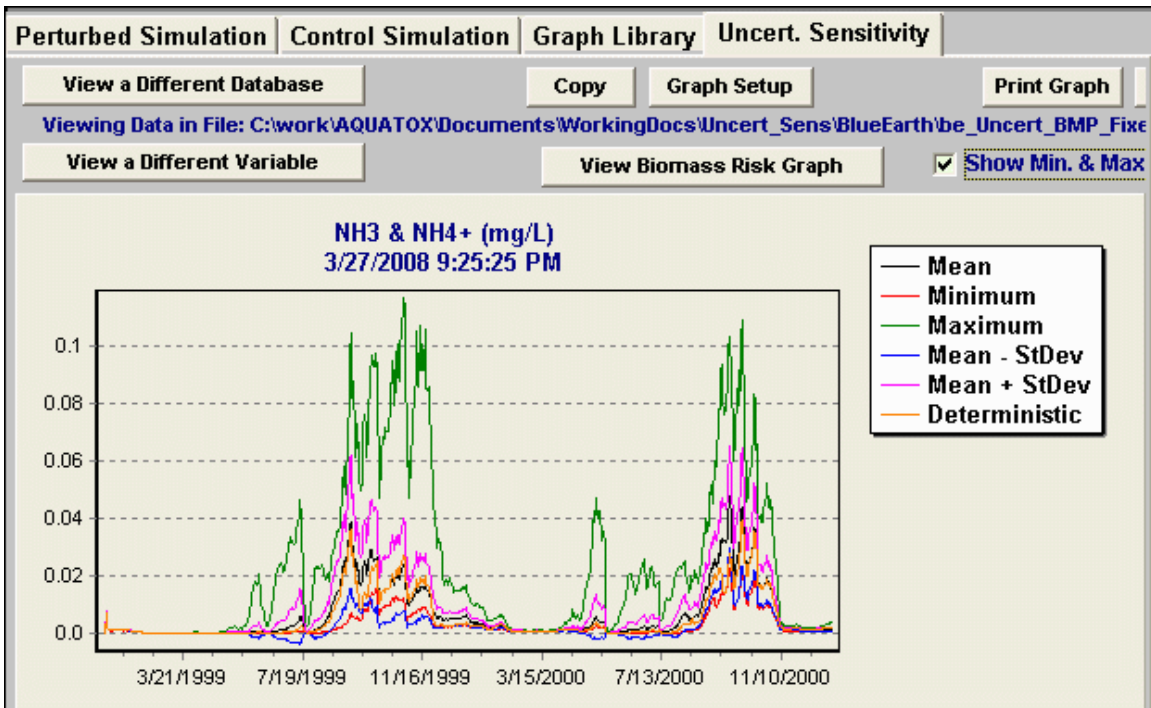
### Exporting Tabular Output

Using the **Save Table to Excel** button, the results can be saved to an Excel file. This button requires Microsoft EXCEL to be installed on the user's machine to work properly. After the export

is completed the user is prompted as to whether they wish to view the Excel file immediately or just leave it saved to disk in the specified location.

## Viewing Uncertainty Output

An additional form of graphical output is the **Uncertainty Graph**. If an uncertainty analysis has been performed, the results can be potted as a series of lines representing the mean, minimum, maximum, mean - 1 standard deviation, mean + 1 standard deviation, and deterministic results as tracked through the simulation time. Only one output variable can be viewed at a time, so click on **View a Different Variable** to view another. The multi-purpose uncertainty window may also used to view the results of a sensitivity analysis .

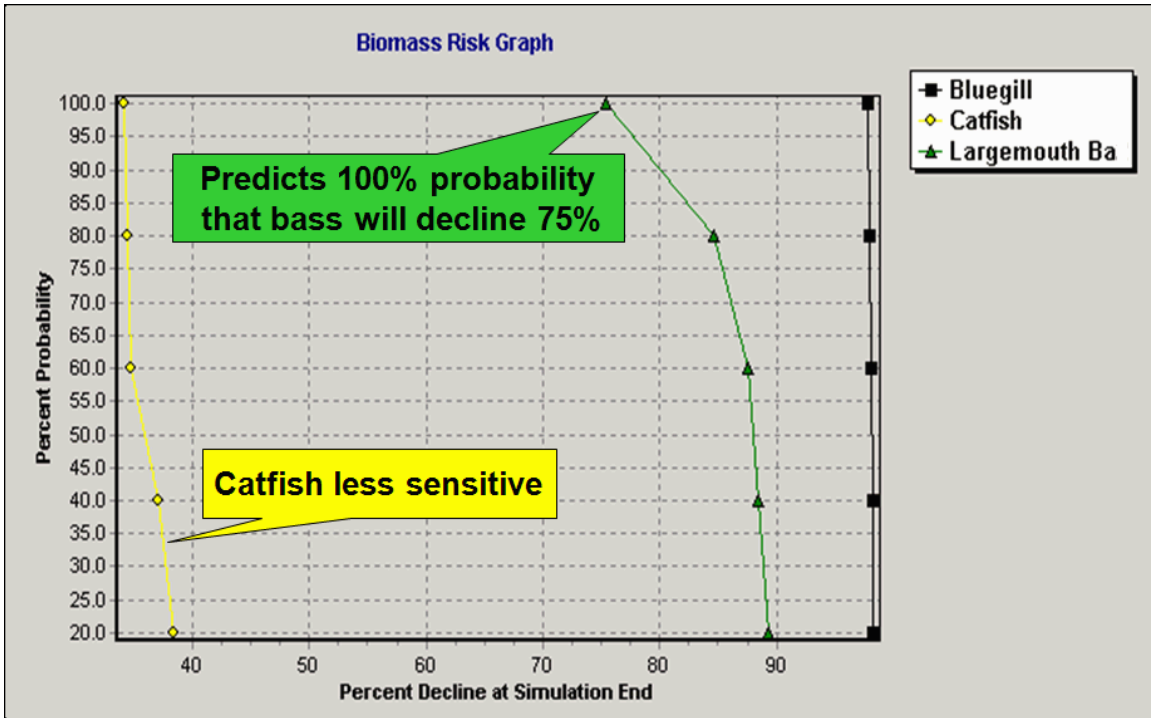


Uncertainty output is not saved as part of an APS file but is instead saved in Paradox databases (\*.db). Sometimes uncertainty results will not fit in one database file (which are limited to 255 columns); the results are then added to one or more successively-numbered database files. Immediately after running an uncertainty analysis, the uncertainty window will bring up the primary database file that is associated with the uncertainty run. However, if the study is closed and opened again, the pertinent database file will need to be re-opened using the **View a Different Database** button. This will also be required if the output variable you wish to graph is in one of the successively numbered database files.

When many iterations have been run, the minimum and maximum output become less relevant (existing far out on the tail of the output distribution, with very little probability of occurrence.) For this reason, the minimum and maximum scenarios can be toggled on or off again using the **Show Min & Max** checkbox.

Of particular interest to risk assessors is the **Biomass Risk Graph**, which plots the probabilistic results as "percent probabilities" against "percent declines" by the end of the simulation. Any number of organisms can be plotted simultaneously on the Risk Graph, so that the responses of both tolerant and intolerant organisms can be analyzed. If an organism increases in biomass, for example because of release of herbivory (for plants) or predation (for animals), then the percent

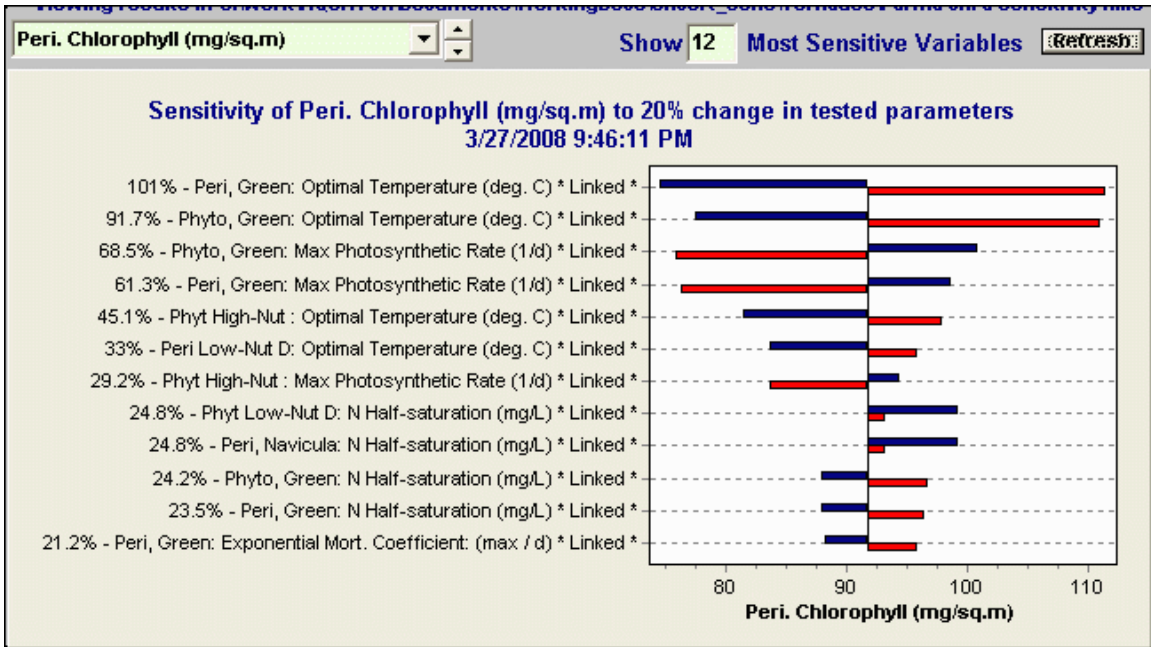
declines are shown as negative values. Data to support the biomass risk graph are stored in CSV files with the suffix "\_decline" added to the end of the file-name. A different CSV file may be loaded using the **View a different CSV file** button, though the CSV file that is relevant to the simulation will be initially displayed.



Uncertainty graphs may be copied to the clipboard using the "Copy" button, or printed using the "Print Graph" button. The "Graph Setup" button brings up the **graph setup window** allowing the appearance of the graph to be edited.

### Viewing Sensitivity Output

The same screen that is used to view uncertainty output can automatically produce tornado diagrams which is a visual manner of interpreting the results of a sensitivity analysis .



For a particular model output, a tornado diagram displays the parameters that cause the most sensitivity, sorted in decreasing order of sensitivity. Red bars plot results in which the parameter has been reduced by the given percent and blue bars plot results in which the parameter has been increased. The black vertical line in the middle of the blue and red bars represents the baseline model result (in which no sensitivity test was performed.) Clicking on any of the bars will give the user information about which parameter was tested and the result as compared to the baseline result.

The statistic shown in front of the parameter names is the "sensitivity" statistic which is a normalized average sensitivity for that parameter. If a given parameter was varied by 20% in each direction and the output result also varied by 20% (on average) the "sensitivity" for that parameter/output pairing would be calculated as 100%.

Sensitivity analysis results are stored in Excel files. Immediately after running a sensitivity analysis, the proper Excel file will be loaded. Otherwise, the user will need to select "**View a Different Database**" change the file-type to "**Sensitivity Results, (\*.xls)**" and load the file in which sensitivity results have been saved. If there are many results in the given Excel file loading the data from Excel could take several minutes.

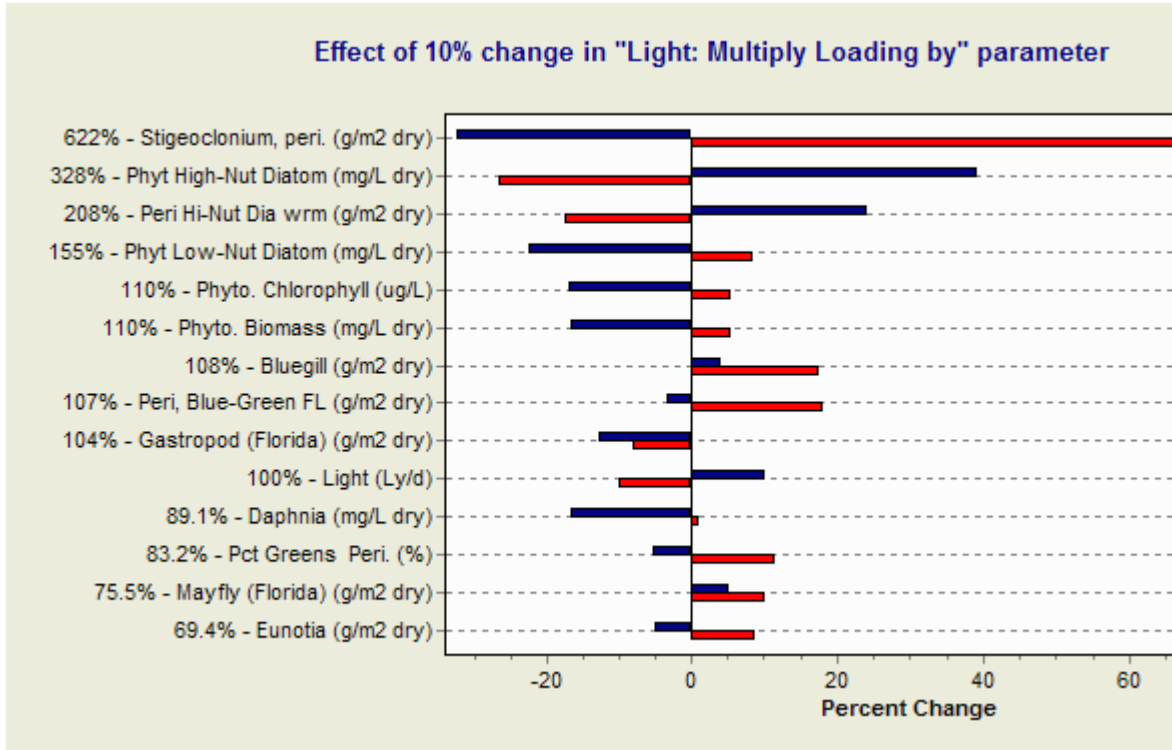
All the model outputs that were tested for sensitivity may be scrolled through, using the drop-down menu at the top left of the tornado diagram. The user may also scroll through these tornado diagrams using the up and down arrows immediately to the right of the drop-down menu.



The number of rungs on the tornado diagram can be changed by changing the "**Show \_\_\_ Most Sensitive Variables**" edit box. For a full accounting of all parameters tested for this particular endpoint and their ordered sensitivity statistics press the "List Sensitivities" button

**New to Release 3.1 -- "Effects Diagrams"**

A user can also set up an alternative tornado diagram in which the effects of a single parameter change on all tracked outputs can be examined. To convert the diagrams, the user should click the "Show Effects" button. A diagram such as the one shown below will be produced. The drop-down menu can now be used to select from all of the tested parameters. Because output variables have many different units, this metric is tracked in terms of "percent change."



Clicking on an individual rung of the diagram will show precisely the percentage change predicted by a given perturbation. As was the case with the sensitivity tornado diagram, the number of effects may be edited and the individual effects may be listed in text format by clicking on the (renamed) "List Effects" button.

## Exporting Results

Control and perturbed results may be exported to a variety of formats by clicking the **Export Results** or **Export Control** buttons on the main study window.

Providing there are available results for export, a dialog box will appear allowing you to choose the output variables you wish to export. After output variables are chosen, the user is prompted for a file-name in which to save the results. Results may be saved in Excel format (\*.xls), Paradox database format (\*.db), DBase IV format (\*.dbf), or Comma Separated Value format (\*.csv). To change the format of the export, choose a different format from the "Save as type" pull-down menu.

An alternative means of exporting data is to save tabular output (viewed in the output window) to Excel.

As part of the BASINS linkage, when exporting results, if GenScn is installed on your machine, the "Export all Results to GenScn" button is available. This automatically starts the GenScn

program with all available AQUATOX output attached. However, most of the GenScn functions are now available within the AQUATOX interface.

## Clearing Results

AQUATOX study files include results of any control or perturbed simulations that have been run. When a long simulation has been executed, with a small data storage step, these results can take up a lot of disk space. To clear these results from memory, select **Study** and choose **Clear Results** from the menu bar. The results will be disposed of so that your study file will be smaller but you will not be able to view output using the output window until the simulation is re-executed.

## Export to Release 2.2/3.0 Databases

When a simulation is open, in the Study menu, there are two options to "**Export to 2.2 Databases**" and "**Export to Rel3 Databases.**" This option will export all animal and plant parameters from the simulation into databases with the chosen file-format. The user will be prompted as to which databases the data should be written to. Any available database entries with the same plant or animal names will be overwritten as part of this procedure, so it may be wise to back-up the original databases before exporting.

## "Taking Parameters" from Another Study

When a simulation is open, in the Study menu there is an option to "**Take Parameters from Another Study.**" This will copy all "non-site-specific" parameters from another study (which is required to have exactly the same state variable list). This procedure allows a user to test a single set of parameters at multiple sites.

Parameters that are copied include:

- Animal "underlying data" and trophic interactions
- Plant "underlying data" and linkages
- Chemical and Diagenesis parameters, if relevant
- Settings in the Control Setup Window

The user also will be prompted as to whether initial conditions should be copied into the given simulation.

## Other Interface Components

### Using the Toolbar

Virtually every function in AQUATOX can be accessed by clicking on the applicable icon on the toolbar. For the experienced user this provides a quick way to bring up a particular screen or to perform a function, such as saving a simulation, without going through several layers of options in the menu bar or the "big buttons." (The big buttons can be suppressed entirely through the **View** menu option.)

To determine the purpose of a given button, hover the mouse cursor over the button for a moment and a "hint" which describes the purpose of the button will become visible.

Toolbar icons can be added, deleted, or moved by clicking on **Edit Toolbar** under the **View** menu option. This is also a good way to learn the functions of the icons. There are 32 icons that are

listed and can be used, compared to the 24 icons shown on the default toolbar. One can also use dividers to visually group icons representing similar functions.

## Editing the Toolbar

When you have entered this screen, you may edit the toolbar by dragging and dropping buttons onto the toolbar from the available list. Alternatively, you can drop buttons from the toolbar into the large trash-can icon and they will no longer appear on the toolbar.

Your custom toolbar will be saved when you exit AQUATOX and reloaded when you start the program the next time.

Dividers appear at the bottom of the button list and they can be used to group tool-button functionality. You cannot drag dividers from the toolbar into the trash, instead, the **Remove all Dividers** button (at the bottom of the tool-button list) must be selected and new dividers can then be dragged onto the toolbar.

## The AQUATOX Wizard

### Wizard Overview

The AQUATOX Setup Wizard is intended to guide the user through the 19 steps necessary to set up a new simulation. Even experienced users may find it to be a convenient checklist, providing a measure of quality assurance not usually found in models. Most steps consist of several parts, and one can move systematically through these by making choices or entering values, then clicking on **Next**.

Wizard Components:

- Progress Screen
- Summary Screen
- Step 1: Simulation Type
- Step 2: Simulation Period
- Step 3: Nutrients
- Step 4: Detritus
- Step 5: Plants
- Step 6: Invertebrates
- Step 7: Fish
- Step 8: Site Characteristics
- Step 9: Water Volume
- Step 10: Water Temperature
- Step 11: Wind Loading
- Step 12: Light Loading
- Step 13: Water pH
- Step 14: Inorganic Solids
- Step 15: Chemicals
- Step 16: Inflow Loadings
- Step 17: Direct Precipitation
- Step 18: Point-Source Loadings
- Step 19: Non Point-Source Loads

### Wizard: Progress Screen

The **Progress Screen** lists all the Wizard's steps and shows which step is currently active.

It also provides a means of skipping from one step to another by double-clicking on any step in order to move there.

If a user decides to create a new AQUATOX study from scratch, the wizard's progress screen also displays the status of each step (whether the user has completed entering data for that step or if data gaps still exist for the step).

The progress screen can be hidden by selecting the **Hide Progress** button. It can be shown again at any time by selecting the **Show Progress** button that is always available on the main wizard window.

### **Wizard: Summary Screen**

The **Summary Screen** provides a list of the state and loading variables as they are changed while going through the Wizard. This is for informational purposes only, to give the user a sense of how their actions are changing the state variable list they will see when the wizard is complete. The list is not editable through the summary screen.

The summary screen can be hidden by selecting the **Hide Summary** button. It can be shown again at any time by selecting the **Show Summary** button always available on the main wizard window.

### **Wizard: Step 1- Simulation Type**

In order to create a simulation from scratch, you must access the Wizard from the File menu ("New Simulation Wizard"). If you have an existing study open, selecting the Wizard "big button" means that you wish to edit that particular study with the wizard.

When creating a new simulation with the AQUATOX setup wizard, you have the choice to start a simulation from scratch, or work with a default study. When starting a study from scratch, every parameter within the simulation will be specified by you or loaded from the data libraries. Otherwise, a simulation will be based on an existing simulation and you will have the opportunity to make modifications to the default parameters.

The name for the simulation will appear on the main screen and will be used as a heading in the output. Six site types are available: pond, lake, stream (creek or river), reservoir, experimental enclosure, and estuary.

### **Wizard: Step 2- Simulation Period**

This screen allows you to specify the time period for the simulation.

The time period for the simulation may be a few days, corresponding to an experiment, or a year, or even several decades. The time period does not have to correspond to the loadings, because the loadings can be interpolated automatically. However, it is advisable to consider the correspondence between the start date and the initial conditions; if the initial conditions are poorly known then a start date in the middle of winter may allow the simulation to "spin up" before going into the growing season. (This is different than "spin-up mode" from the model-setup window which sets biotic initial conditions to the value at the end of the simulation)

### **Wizard: Step 3- Nutrients**

Initial conditions for dissolved nutrients must be entered. Phosphate can be considered as soluble reactive phosphate; by going into the phosphate loading screen phosphate can be adjusted for availability. Because of interchange with the atmosphere, the model is not very sensitive to the initial conditions for carbon dioxide and dissolved oxygen.

#### **Wizard: Step 4- Detritus**

This set of screens allows you to specify initial conditions of detritus in the sediment bed and in the water column.

Labile detritus is readily decomposed and assimilated, refractory is resistant to decomposition.

Initial conditions and loadings of detritus in the water column can be input as Organic Matter (dry weight), Organic Carbon, or Biochemical Oxygen Demand (BOD) and the model will make the necessary conversions. Suspended and dissolved detritus initial conditions and loadings are divided into four compartments: particulate refractory and labile detritus and dissolved refractory and labile organic matter. Initial conditions and loadings are parsed by specifying % particulate and % refractory.

#### **Wizard: Step 5- Plants**

The user is provided with a list of plants within each taxonomic group from which to choose. These taxonomic groups can be scrolled through using the "**next >>**" and "**<< back**" buttons. Drag the plant name from the list provided into the simulation list to include it in the simulation.

After the plants have been specified, an initial conditions entry screen is reached. Initial conditions should be entered for each plant group; as with any biotic group, a value of "0" will keep the group from being simulated. Note that the units are sensitive to whether the plant is planktonic or benthic.

The list of available plants corresponds to those species that have entries in the **Plant Library**. As the library continues to expand with additional applications, the set of plants available within the wizard also expands.

#### **Wizard: Step 6- Invertebrates**

The user is presented with a list of invertebrates for each ecological guild from which to choose. Some are general taxonomic groups and some are genera and species. These groups can be scrolled through using the "**next >>**" and "**<< back**" buttons. Drag the invertebrate name from the list provided into the simulation list to include it in the simulation.

After the invertebrates have been specified, an initial-conditions entry screen is reached. The initial conditions are either mg/L or g/m<sup>2</sup>, depending on the mode of life (pelagic or benthic).

The list of available invertebrates corresponds to those species that have entries in the **Animal Library**. As the library continues to expand with additional applications, the set of invertebrates available within the wizard also expands.

#### **Wizard: Step 7- Fish**

Fish are classified as forage fish, bottom fish, and game fish. At least two species can be modeled for each general class. Furthermore, two size classes can be modeled for each species, and one species can be modeled as multiple year classes.

For each trophic guild (forage fish, bottom fish, and gamefish) the user can choose from a list of appropriate species in the database.

After fish species are specified, an initial conditions screen can be reached by selecting "**next >>**." Initial conditions are given as  $g/m^2$  because it is easiest to express biomass on an areal basis.

The list of available fish corresponds to those species that have entries in the **Animal Library**. As the library continues to expand with additional applications, the set of fish available within the wizard will also expand.

More information on Fish Type and Fish Class follow.

### **Wizard: Select Type of Fish Compartment(s)**

You can choose to model a fish species either as a single state variable, as two state variables representing size classes, or as up to fifteen state variables representing age classes.

### **Wizard: Select Class of Fish**

Each fish species that is modeled within AQUATOX must be classified as a forage fish, bottom fish, or game fish.

If you are modeling this species as a single state variable you must also choose whether it is of large or small size. When modeling a species as a single state variable this has little effect on the model's results but food preferences for any predators of the species must be set accordingly.

### **Wizard: Step 8- Site Characteristics**

The most important morphometric characteristic is mean depth because that controls light penetration, volatilization, and attached plant distribution. Mean annual evaporation is used for computing the water balance. Latitude is used to compute photoperiod for photosynthesis.

The data entered here is used to parameterize the site underlying data.

The wall area is important for an experimental enclosure because it represents additional area for attachment of periphyton. This is only visible if your site type is an experimental enclosure.

### **Wizard: Step 9- Water Volume**

This screen presents the options for modeling water flow in an AQUATOX simulation. Depending on the method chosen, inflow or discharge values may be required. The Manning's equation can be used to compute changing volumes in a stream. The simplest procedure is to hold volume constant at the initial condition. Volume can be computed dynamically, given the inflow and outflow (and factoring in evaporation). Finally, time series of known values can be entered.

For more information about modeling water volume in AQUATOX see **Water Volume Data**.

### **Wizard: Step 10- Water Temperature**

A constant temperature, annual mean and range in temperature or time series can be entered. Depending on your selection, you will be required to enter additional information about temperature patterns in the next screens.

For more information about modeling temperature in AQUATOX see **Temperature Data Screen**.

### **Wizard: Step 11- Wind Loading**

Wind loadings can be constant, a time series can be entered, or a default time series can be used. The default is a 365-day record taken from the Buffalo NY airport. This series is represented by a Fourier series, with a mean value that can be specified by the user (the default is 3 m/s).

For more information about modeling wind in AQUATOX see **Wind Data**.

### **Wizard: Step 12- Light Loading**

Constant, time series, and annual mean and range may be given for light in Langleys/day.

When in a simulation, light loadings may be altered by double clicking on "Light" within the state variables list. This will bring you to the light loading screen.

### **Wizard: Step 13- Water pH**

The pH may be specified by the user, either as a constant or as a time series. It has various effects on simulations (see section 5.7 of the Technical Documentation).

When a time series is utilized the rules for dynamic loadings apply.

Alternatively, through the main pH entry screen, the user may specify that AQUATOX should calculate pH values using a simple semi-empirical formulation (this requires a Mean Total Alkalinity input, see section 5.7 of the technical documentation for more information.)

### **Wizard: Step 14- Inorganic Solids**

There are three options for simulating water-column inorganic solids within AQUATOX.

When the concentration of total suspended solids (TSS) is known, TSS can be input to provide a measure of inorganic solids. The model subtracts phytoplankton and detritus from the TSS to estimate the inorganic solids; therefore, care should be taken to use contemporaneous TSS and nutrient time series.

The second option, the sand-silt-clay model, is only relevant for streams. This option requires considerably more parameters and simulates the scour, deposition and transport of sediments and calculates the concentration of sediments in the water column and sediment bed within a river reach. More information about the sand-silt-clay model can be found in the section titled **Sand-Silt-Clay**.

The third option is to utilize the multi-layer sediment model, though this cannot be accessed through the AQUATOX wizard.

### **Wizard: Step 15- Chemicals**

AQUATOX can simulate as many as 20 different organic chemicals simultaneously. The assumption is that the toxic effects are additive. Initial concentrations for each toxicant are required for all associated state variables; as a check, the model calculates the total mass.

After a chemical has been selected for a simulation, you may specify initial conditions for that chemical in the water column and in all biotic and detrital compartments.

### **Wizard: Step 16- Inflow Loadings**

The Wizard compiles a list of all variables that may be loaded as concentrations in inflowing water. The units are sensitive to each given variable.

Click on one of the loadings from the "Inflow Loadings in Simulation" box and you will be able to select whether this is a constant or dynamic loading and edit the details about the loading.

### **Wizard: Step 17- Direct Precipitation**

The Wizard compiles a list of all variables that may be loaded as atmospheric deposition ("direct precipitation" and dry fall). The units are on an areal basis because deposition is on the surface of the water.

Click on one of the loadings from the "Direct Precipitation Loadings" box and you will be able to select whether this is a constant or dynamic loading and edit the details about the loading.

### **Wizard: Step 18- Point-Source Loadings**

Point-source loadings are entered as mass per day (g/d) to the water body.

Click on one of the loadings from the "Point-Source Loadings" box and you will be able to select whether this is a constant or dynamic loading and edit the details about the loading.

### **Wizard: Step 19- Nonpoint-Source Loads**

Nonpoint-source loadings are also entered as mass per day (g/d) to the water body.

Click on one of the loadings from the "Nonpoint-Source Loadings" box and you will be able to select whether this is a constant or dynamic loading and edit the details about the loading.

### **Wizard Data Incomplete**

This screen appears if the user originally selected to create a study from scratch. In order to do this, the user must populate all of the parameters within the model.

At this point you have selected to leave the wizard before providing all of the required parameters. You must go back and enter values for these parameters or accept default parameters provided by the program. The wizard progress screen can help you to determine in which areas you have not entered data. Arrows appear by the steps in which you have not entered information.

### **Exporting Parameters as Text**

In either linked mode or single-segment mode, a user may choose to "**Export Parameters as Text**" from the Study menu. This procedure will save all parameters and, optionally, all time-

series loadings that make an AQUATOX simulation unique. This procedure can be useful for several reasons:

- It makes all modeling choices transparent when documenting your model application, as an appendix, for example.
- Two AQUATOX simulations may be compared to determine how they differ, using a word-processor "compare documents" function. Any differences in parameters or loadings will be highlighted.

After this function has been selected, the user will be prompted as to whether to save time-series inputs to the file as well. This will increase the size of the text export, but will completely document the input variables that are driving simulation results. The file-name in which to save results will then be solicited. In linked mode, segment-specific parameters and initial conditions for all segments will be included in the text output.

### **Import Data from HSPF WDM**

This menu option (in the Study menu) allows a user to pass data from HSPF "WDM files" into AQUATOX. This compliments the existing BASINS HSPF-to-AQUATOX linkage, which required that the user work with WinHSPF and then ask WinHSPF to produce special time series used for the linkage. In some recent HSPF-to-AQUATOX linkage applications, the HSPF simulation produced the needed boundary conditions in a form not compatible with the previous WinHSPF-AQUATOX linkage. This required time-consuming manual linkages of time-series, something that this automated linkage attempts to avoid.

This linkage has AQUATOX import, as inflow loadings, "in-stream concentrations" as derived from HSPF as opposed to the boundary condition calculations passed in the original linkage.

There was some concern that HSPF and AQUATOX would both be calculating the same in-stream processes so there could be double counting. However, when passing average-daily loadings into short reaches with low retention times, the HSPF in-stream concentration and the AQUATOX in-stream concentration will be dominated by the inflow loadings rather than in-stream processes. Our testing has indicated that linking HSPF in-stream concentrations as AQUATOX in-flow loadings for such short reaches introduces negligible error.

Additionally, if one would like, they can design their study such that the AQUATOX boundary condition is represented by the end of, or outflow from, the HSPF reach being linked. This would eliminate any potential error from double-calculation of in-stream processes. The assumption would simply be that the well-mixed HSPF reach feeds directly into the AQUATOX reach being modeled below.

Specific Mechanics of the Linkage:

The steps taken by this linkage are summarized below:

1. The HSPF simulation must have been run and nutrients, organic matter and flow outputs must have been satisfactorily calibrated. The results must have been saved to an accessible WDM file.
2. From AQUATOX, the user selects the WDM file, and then the relevant location, and scenario to be linked using the "study" menu (select "import parameters from HSPF WDM").
3. The user selects the date range for the linkage. (Note that this changes the AQUATOX first day and last day of simulation but this can be changed after the linkage is complete.)

4. The user is presented with options for importing phosphate. The following HSPF P outputs may be input to maximize flexibility
  - a. TOTP -- Total Phosphorus in mg/L (Default is to link this to the AQUATOX Total P compartment, and AQUATOX will estimate Total Soluble P from Tot P)
  - b. Any combination of the below three compartments may be summed and imported as TP or TSP.
  - c. PO4-P -- Ortho P concentration as P in mg/L
    - i. PPO4 -- Adsorbed orthophosphate as P in mg/L
    - ii. TORP-- Total Organic Phosphorus in mg/L
5. The following items are loaded (Hourly data are converted to daily except for oxygen, CO2, organic matter, and nutrients.)
  - a. FLOW is read as AQUATOX "outflow water," units are checked to be CFS. If units are not specified the user is told that the assumption is that units are CFS. If different units are specified the user is prompted as to whether to continue or not. Units are converted to AQUATOX m3/d.
  - b. Average depth is read assuming the units are feet if unknown, converting, and prompting the user as above.
  - c. Ammonia, Phosphate, Oxygen, Nitrate, TOC/BOD, and TSS are imported in units of mg/L.
  - d. CO2 is set to the default value of 0.7 mg/L. This can be changed (or not set) if that is desirable.
  - e. Temperature is imported and converted to Deg. C. if required.
  - f. For QA/QC, these imports may be examined as compared to the WDM file results.
6. The linkage also imports as "external data" to plot against AQUATOX results (but not to drive the model) Chlorophyll a, Benthic Chlorophyll a, and BOD.

With regards to the units of data being imported, if units are not specified in the WDM file the log-file alerts the user that it assumes they are using a certain type of unit (general HSPF defaults). If units are specified and the linkage finds unexpected units it raises an error.

This new capability can link to BASINS as well as stand-alone HSPF, as all HSPF simulations can read from, and write their data/results to WDM files, which is the primary medium of this linkage.

Following successful linkage a log file describing all imported data and/or any errors encountered may be examined through the AQUATOX interface.

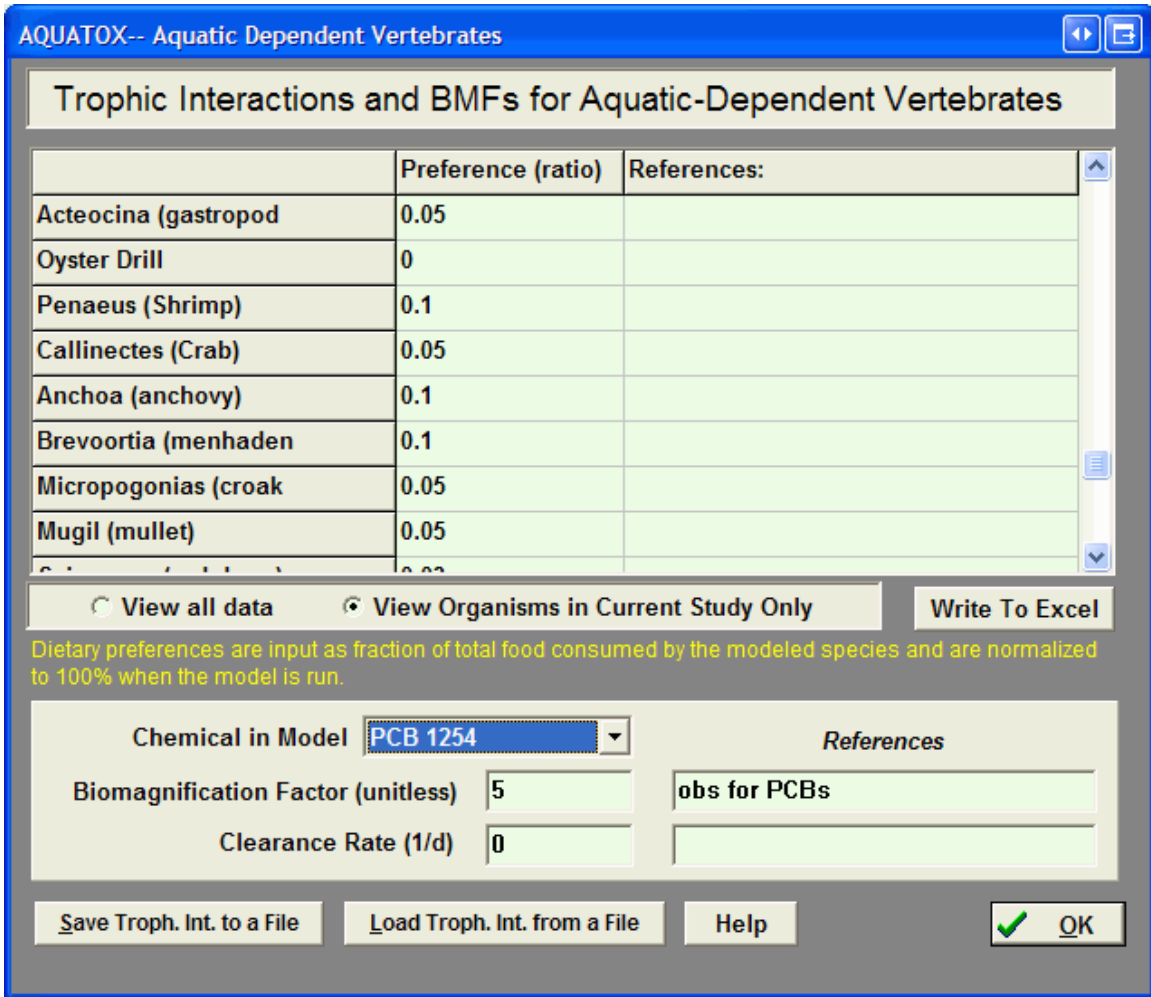
## **Aquatic-Dependent Vertebrates**

This simple submodel pertains to shorebirds and other terrestrial animals that feed exclusively from the water column. The model will estimate chemical concentrations in tissues based on dietary uptake from food-sources in the water column.

In this screen, the user can specify a biomagnification factor (BMF) for each chemical, and the preferences of the animal for various food sources so that alternate exposures can be computed. Dietary preferences will be normalized to 100% by the model if they do not sum to 100% within this screen.

The concentration of each chemical is based on the chemical concentration in prey at a given time-step. Uptake of toxicant is assumed to be instantaneous, but depuration of the chemical is governed by the user-input clearance rate.

After a run, when the aquatic-dependent vertebrates model is used, the list of model output will include one or more entries titled: "[Toxicant in] Birds etc. (ug/kg wet)."



## Batch Mode

There are applications where it is desirable to run a series of studies automatically. This can be done by creating a Batch subdirectory under the Study directory and placing studies with appropriately chosen options in it. The subdirectory should also contain a text file labeled "batch.txt" that lists the names of the studies to be run, one to a line. On the menu bar you should click on **Run Batch** on the pull-down **File** window. That will open a window that allows you to **Run in Batch Mode**. You also can save the BAFs and organic-matter partition coefficients (KOMs) to a comma-separated text file *batchout.csv*. (See chapter 8 in the Technical Documentation for discussion of bioaccumulation of organic toxicants, BAFs and KOMs.)

Batch mode automatically runs each simulation in "perturbed" mode. If "Run Control Simulations Too" is selected then control and perturbed simulations are both run (with differences reflecting the options selected in the **Control Setup Screen**.)

### Important Specifications for Batch Mode:

**To run a program in batch mode, you must have a subdirectory off of your Studies Subdirectory named "batch"**

In that "batch" subdirectory must be all studies you wish to run along with a file named "batch.txt".

The batch.txt file must include each study name that you wish to run on a separate line. No blank lines may be included.

The program will then execute each of the specified studies one by one and save them along with their results.

To output the last BAF datapoint for each organism in each of the batch files, select the Output button. This will open each study and write all of the BAF data from each study file into a CSV file named batchout.csv.

## Setting Up Simulation, Single Segment

Setting up a single segment simulation generally has the following types of steps

- Locate a surrogate simulation that can be modified.
- Produce a reasonable model of water volume for your site.
- Choose appropriate biotic state variables for your site.
- Examine the trophic interactions matrix to ensure that a reasonable food-web has been constructed.
- Use best available data to set initial conditions for nutrients, biota, sediment, and chemicals (optional).
- Use data to determine the external boundary condition loads for nutrients and, optionally, chemicals.
- Test the model and calibrate against observed chlorophyll *a*, biomass, and nutrients.
- Examine the effects of changing nutrient, sediment, or organic toxicant conditions.

## Data Requirements

Data requirements in AQUATOX depend considerably on the site-type that is being modeled and the goal of the modeling study. A modeling study to assess the effects of changing nutrient levels would benefit from an excellent accounting of nutrients in the water column and boundary-condition loadings of nutrients. On the other hand, a study that is primarily about chemical effects may not require such detailed nutrient information. In this case, a user may wish to produce the required nutrient environment for a stable food-web and then detailed information about chemical loadings can be applied to the simulation to assess effects.

Precise accounting of time-series loadings is especially important in rivers and streams. Due to low retention time, inflow loadings can be the dominant factor affecting water column conditions. For standing water, initial conditions may be more important than a perfect representation of daily loadings depending on both simulation time and retention time.

Here is a list of data requirements put together for a single-segment simulation project. This list is not necessarily exhaustive but contains what are generally the most important time-series inputs.

### LIST OF AQUATOX TIME-SERIES INPUTS

- Total N or Nitrate and Ammonia (inflow water, point source, non-point source)
- Total P or Bioavailable P, (inflow water, point source, non-point source)

- Chemical loadings (inflow water, point source, non-point source).
- Oxygen in inflow water
- TSS value in water
- Light Loadings (can be calculated based on latitude)
- BOD or Suspended Detritus Concs (organic matter inflow, point source, non-point source).
- Water Volume, Inflows, or Outflows (some flexibility here)
- Water Temperature (mean ranges can be used)
- Water Mean Depth (optional)

See **Additional Data Requirements for Linked Mode** for a more detailed list. Not all loadings are required to be precisely accounted for. However, it is useful to have at least some data for each of the various categories (nutrients, oxygen, organics, inorganic sediments or TSS, etc.)

A user will need to define the biotic state variables in each segment as well. Default parameterizations may be used for various organisms "Underlying Data" unless there's a pressing need to use your own site-specific parameters.

If a chemical is modeled, requirements include initial concentrations in biota, loadings from various sources, and toxicity data if you wish to model effects.

## Site Types

The site type may be set in the site data screen.

The following site-types are included.

- **Pond, Lake, Reservoir:** These standing-water types may stratify based on temperature inputs. These site-types may currently be used interchangeably but different site-types are provided for user clarification.
- **Stream:** Assumed to be moving water that will not stratify. Streams have the following additional characteristics
  - the sand-silt-clay model may be enabled;
  - Manning's coefficient may be used to model water volume;
  - dynamic temperature stratification is disabled;
  - periphyton scour and velocity limitation for plants is a function of water velocity;
  - oxygen reaeration is a function of stream velocity.
- **Enclosure:** An artificial experimental enclosure within a pond or lake. As noted in the technical documentation, the littoral fraction is modified based on the area of the enclosure's wall.
- **Estuary:** Assumed to be governed by permanent salt-wedge stratification. See **Estuary Version Notes**.
- **Tributary Input Segment:** This is a specialized segment for linked-mode only. See **Tributary Input Segments**.

## Estuary Version Notes

When an estuarine model is selected, the modeled segment is assumed to be composed of two well-mixed layers; stratification is governed by salinity. Water balance between the two layers is computed using a salt-balance approach. For this reason, the salinity in each layer at the mouth of the estuary must be specified as a constant value or as a time series. Time series of salinity is especially important for the upper layer as this will permit a reasonable and variable set of water flows to be derived.

Water-column salinity can have effects on animal mortality and gamete loss and algal photosynthesis, ingestion, respiration, and sinking. Estuary reaeration is also affected by salinity, especially through calculation of the level of saturation at which oxygen saturation occurs. Salinity can also affect the rate of volatilization of organic toxicants.

Various additional Tidal Range Model parameters are required at the bottom of the site "underlying data" screen to properly model the timing and extent of tidal amplitude (which especially affects salt-water intrusion). These parameters are generally available for download from NOAA databases on line.

Water volume is modeled on a daily basis, rather than an hourly basis; hourly tidal fluxes are not modeled. For this reason, the overall daily-average water volume of the estuary is assumed to remain constant. The simplifying assumption is that the water volume of the estuary is not sensitive to the fresh-water inflow. The water volume input screen is therefore different for the estuary model, with inflow water representing fresh-water inflow. Salt-water inflow is derived from the tidal range model as discussed above. The size and depth of the fresh and salt wedges then vary as a function of the tidal range and fresh-water flows.

Although Release 3.1 of AQUATOX can now run on an hourly basis, the estuary version of the model has not been set up to model tidal inputs and withdrawals on an hourly basis

### **Nutrient Inputs to the Lower Layer**

Nutrient concentrations in seawater flowing into the lower (saline) layer are set to temporally constant levels. The nutrients in seawater may be edited using a button available in the initial conditions and loadings screen for each relevant variable (Ammonia, Nitrate, Phosphate, Oxygen, and Carbon Dioxide).

Chapter 10 of the technical documentation covers the AQUATOX estuary model in detail.

### **Starting with a Surrogate Simulation**

When applying AQUATOX to a new site it is usually most efficient to find a surrogate site that best matches the characteristics of the site to be modeled. The user can then modify that site's characteristics so that it matches the modeled site with respect to Nutrients, Organic Matter, Turbidity, Biota, and Organic Chemicals (if relevant).

To assist in this process the file "**Study descriptions.pdf**" has been added to the STUDIES directory that describes the characteristics of each of the example model applications included with the model.

After the surrogate simulation has been loaded, the user should rename the file, and then examine the following components for compatibility with the site being modeled

- Physical characteristics (site-underlying data)
- Water volume setup (water volume loadings and initial condition screen.)
- Nutrients, organic loadings, and turbidity in the loadings and initial conditions screens
- Simulation time and other model setup
- Water temperature settings
- Biotic compartments included and food web (trophic interaction matrix)

Stepping through each step of the AQUATOX Wizard can be a useful method of examining the "key" parameters in a given simulation.

## Starting from Scratch

To start a simulation "from scratch" within AQUATOX, use the "**New Simulation Wizard**" in the file menu and then select "Create Simulation from Scratch" in Step 1 of the wizard.

Some users will want to enter each and every parameter and loading "from scratch" (that is to say, not to use a surrogate simulation). In some senses this may be the "safest" approach as the user is required to assess the appropriateness of each and every parameter in the model for their individual site. However, there are many parameters that can safely be assumed to be "global" within the model and the user will lose the benefit of having those parameters automatically brought in to their simulation. Because of this, the model creators suggest that users who are concerned about bringing in external parameters examine each and every parameter of the surrogate simulation closely.

## Water Volume Modeling Options

As noted in the Water Volume Data screen, there are many options as to how to compute or specify water volume; each requires a different set of input data. Often, the selected volume-modeling option is a function of the available data for the site being modeled.

Time series of stream volumes are quite rare whereas discharge data are more often available. For this reason, the Mannings Equation Method, which derives river volumes based on discharge, slope, and width data, is often used for streams.

Standing water volumes are sometimes assumed to be kept constant; alternatively time series of known volumes may be used. See the **Water Volume Data** section for more information about modeling water volume.

## Adding a State Variable

Chemicals and biotic state variables may be added to the model, either through the AQUATOX wizard or through the main interface screen (by clicking the "Add" button under the list of state variables). When adding fish, the wizard is especially useful as size-class and age-class linkages will be automatically produced through a user-friendly interface.

## Adding a Chemical

To add a chemical in AQUATOX select one of the 20 available toxicant compartments (usually "Dissolved org. tox 1"). You will then be prompted as to which chemical to load from the chemical library. Loading this chemical brings in "Underlying data" for the chemical and also animal and plant **toxicity databases**.

To properly model toxicity for the chemical, each and every animal and plant in the simulation must be properly linked to one of the rows in these toxicity databases. If any plant or animal lacks the link to toxicity data an error message will be returned. In the animal and plant underlying data records, toxicity data may be entered individually or "Edit All" may be selected, allowing you to link these organisms all at once.

## Adding a Plant

To add a plant in AQUATOX, select one of the available plant compartments (Diatoms, Greens, Blue-greens, Other Algae, or Macrophytes) and then choose the plant data you wish to load from

the plant library. Initial conditions for the plant and any external loadings must then be specified. A "seed" loading may be specified (generally as a constant load) to prevent permanent extinction from occurring. Seed loadings are generally very small loadings (e.g. 1e-5 mg/L) that allow for reintroduction of an organism after environmental conditions have improved to allow that organism to be viable in the system again. The Wizard interface may also be used to add plant variables.

### **Adding an Animal**

To add an animal in AQUATOX, select one of the available animal compartments (Shredders, Sediment Feeders, Suspended Feeders, Clams, Grazers, Snails, Predatory Invertebrates, Large and Small Forage Fish, Large and Small Bottom Fish, and Large and Small Game Fish) and then choose the animal data you wish to load from the plant library. Initial conditions for the animal, any external loadings, and trophic interactions within the food web must also be specified. Size-class fish may be specified using the **Animal Linkages** interface. A "seed" loading may be specified as a constant load to prevent permanent extinction from occurring. As mentioned above, the Wizard interface is especially useful for adding fish state variables.

### **Adding a Multi-Age Fish**

To add a multi-age fish, select "Multi. Age-Class Fish" from the bottom of the list of state variables. The user will be prompted for the number of age-classes to add and sources of parameters for the young of year (YOY) fish and all older fish. You will then be able to access the **Multi-Age Fish** interface by double-clicking on the "**Age-Class Fish**" item at the bottom of the state variable list.

### **Using Sediment Bed Models and Data Requirements**

There are four primary options for modeling the sediment bed within AQUATOX.

The simplest manner is to use the AQUATOX "default" sediment bed model in which organic matter is modeled in the sediment bed as a food source and toxicant-sorption site but inorganic matter in the bed is ignored.

In combination with the default sediment bed model, TSS concentrations may be entered as a time series to properly represent the light climate in the water column of the modeled system.

The sand-silt-clay model adds inorganic sediments to the default sediment bed model and also to the water column. Additional data are required to properly characterize boundary conditions and deposition and erosion parameters are required. This model is only relevant for streams and rivers.

The multi-layer sediment model was designed to model long-term sequestration or exposure of chemicals within a sediment bed. It is a complicated model with considerable additional data requirements.

The sediment diagenesis model implements Di Toro's sediment diagenesis model as presented in *Sediment Flux Modeling* (2001). This model tracks the decomposition of organic matter in the sediment bed with more precision and predicts nutrient flux based on this decomposition (and the oxygen climate in the water column). This model is best suited to represent predominantly anaerobic sediments in eutrophic lakes.

A non-reactive active layer may also be modeled, which allows the user to specify the concentrations of toxicants in pore-water and sediments for uptake into biota. This model would generally only be useful when linking model results from a linked sediment model. The non-reactive layer may not be run in combination with the sand-silt-clay, multi-layer, or sediment diagenesis models.

### **Default Sediment Bed Model**

The default sediment bed model includes the following components

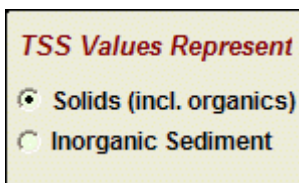
- Labile Sed. Detritus (Labile Detritus in the Sediment bed) (g/m<sup>2</sup> dry);
- Refract. Sed. Detritus (Refractory Detritus in the Sediment bed) (g/m<sup>2</sup> dry);
- Toxicants sorbed to both of those compartments (ug/kg dry);

These detrital compartments are assumed to be located in the active layer and available for consumption, and sorption of chemical from (and desorption of chemical to) the water column. Through long-term deposition, these compartments may become deeply buried and join the buried detritus state variables. Nutrients within these detrital compartments are subject to release to the water column when the organic matter decomposes. For more information about this model, please see section 5.1 of the AQUATOX technical documentation.

Data requirements for this model are rather minimal, primarily being the initial condition of detritus in the sediment bed. Setting the initial condition for these state variables may be facilitated by using an Excel spreadsheet (**AQUATOX\_Sed\_Bed\_Inputs.xls**) that is included in the Studies directory. This spreadsheet will convert data about the fraction organic carbon, depth, sediment density, and fraction labile into initial conditions for these two state variable compartments.

### **TSS**

AQUATOX allows a user to input time-varying concentrations of TSS so that the light climate of the system being modeled may be accurately represented. TSS may represent either total suspended solids or total suspended sediments. A user can choose which of these options is being specified using the radio buttons on the upper right portion of this screen (accessed by double-clicking TSS on the state variable list):



If total suspended solids are chosen, AQUATOX will subtract phytoplankton and detritus loadings from the TSS loadings to estimate the inorganic solids loadings, therefore, care should be taken to use synoptic TSS and nutrient time series.

When TSS is included in the model, it is a driving variable that is not in any way linked to the sediment bed unlike the inorganic sediments in the Sand-Silt-Clay model.

## **Sand-Silt-Clay Model**

The sediment transport component of AQUATOX simulates scour, deposition and transport of sediments and calculates the concentration of sediments in the water column and sediment bed within a river reach. For running waters, the inorganic sediment model within AQUATOX is based primarily on Hydrologic Simulation Program in Fortran (HSPF, US EPA 1991). Within river or stream simulations, sediment is divided into sand, silt, and clay. Wash load (primarily clay and silt) is deposited or eroded within the channel reach depending on the daily flow regime. Sand transport is also computed within the channel reach. Inorganic sediments in standing water are computed based on total suspended solids loadings, and not by means of the sand-silt-clay model.

Within AQUATOX, inorganic sediment concentrations affect the extinction coefficient for water, and therefore change the light climate for algae. Chemicals are assumed not to sorb to inorganic sediments within the AQUATOX sand-silt-clay model but chemicals sorbed to organic matter are assumed to scour and deposit with the same characteristics as the inorganic silt within the model. The fraction of detritus that is being scoured or deposited within a river reach is assumed to equal the fraction of silt that is being scoured or deposited.

There are additional data requirements for this model. AQUATOX requires loadings information for each of the inorganic sediment categories as well as an initial condition. The initial fraction in bed sediments must also be specified. Additional parameters for the inorganic sediment model are found in the site underlying data (stream data) or can be found in Step 14 of the setup Wizard. These parameters include

- Critical shear stress for scour for silt & clay
- Critical shear stress deposition for silt & clay
- Fall velocity for silt & clay

To add the Sand-Silt-Clay model to a simulation, select to "**Add**" a state variable from under the state variable list and select Sand, Silt, or Clay from the list of variables (directly under the chemicals) or use Step 14 of the AQUATOX Wizard.

## **Multi-Layer Sediment Model**

AQUATOX also includes a complex multiple-layer sediment model. This model can simulate up to ten bottom layers of sediment. Within each sediment layer, the state variables consist of inorganic solids, pore waters, labile and refractory dissolved organic matter in pore waters, and sedimented detritus. Each of these state variables can also have up to twenty organic toxicant concentrations associated with it.

Data requirements for this model are significant

- Thickness of each layer;
- Densities of organic matter and inorganic matter in the sediment bed;
- Pore water quantities and initial toxicant concentrations;
- Organic matter initial conditions and initial toxicant concentrations;
- Inorganic matter initial conditions;
- Deposition and Scour may be inputs or the Sand-Silt-Clay model may be used (with its own data requirements);
- Boundary condition loadings of inorganic sediments in the water column.

This model was designed primarily to capture the long-term sequestration or release of chemicals from the sediment bed. As such, linkage to a complex model of sediment scour and deposition may be warranted. For more information on this model, please see section 6.2 of the AQUATOX technical documentation.

To add the Multi-Layer Sediment model, select "**Add Multi-Layer Sediment**" from the AQUATOX **Sediment** menu. It cannot be added with the AQUATOX Wizard.

### **Sediment Diagenesis Model**

Di Toro's model assumes a small aerobic layer (L1) above a larger anaerobic layer (L2). For this reason, it is best to apply this optional submodel in sites where anoxic sediments are prevalent, otherwise the assumption of a very thin aerobic layer may not be appropriate.

The additional 22 state variables added when the sediment diagenesis model is enabled are as follows:

- **POC** (Particulate Organic Carbon) in sediment: three state variables to represent three reaction classes in the anaerobic layer.
- **PON** (Particulate Organic Nitrate) in sediment: three state variables to represent three reaction classes in the anaerobic layer.
- **POP** (Particulate Organic Phosphate) in sediment: as with POC, three state variables to represent three reaction classes in the anaerobic layer. The third modeled component of POM.
- **Ammonia**: two state variables to represent two layers (Layers 1 and 2).
- **Nitrate**: two state variables (in Layers 1 and 2).
- **Orthophosphate**: two state variables (in Layers 1 and 2).
- **Methane**: modeled in Layer 2
- **Sulfide**: two state variables (in Layers 1 and 2).
- **Bioavailable Silica**: modeled in Layer 2.
- **Non Biogenic Silica**: two state variables (in Layers 1 and 2).
- **COD**: Driving variable for chemical oxygen demand in the water column that affects the flux of sulfide to the water column.

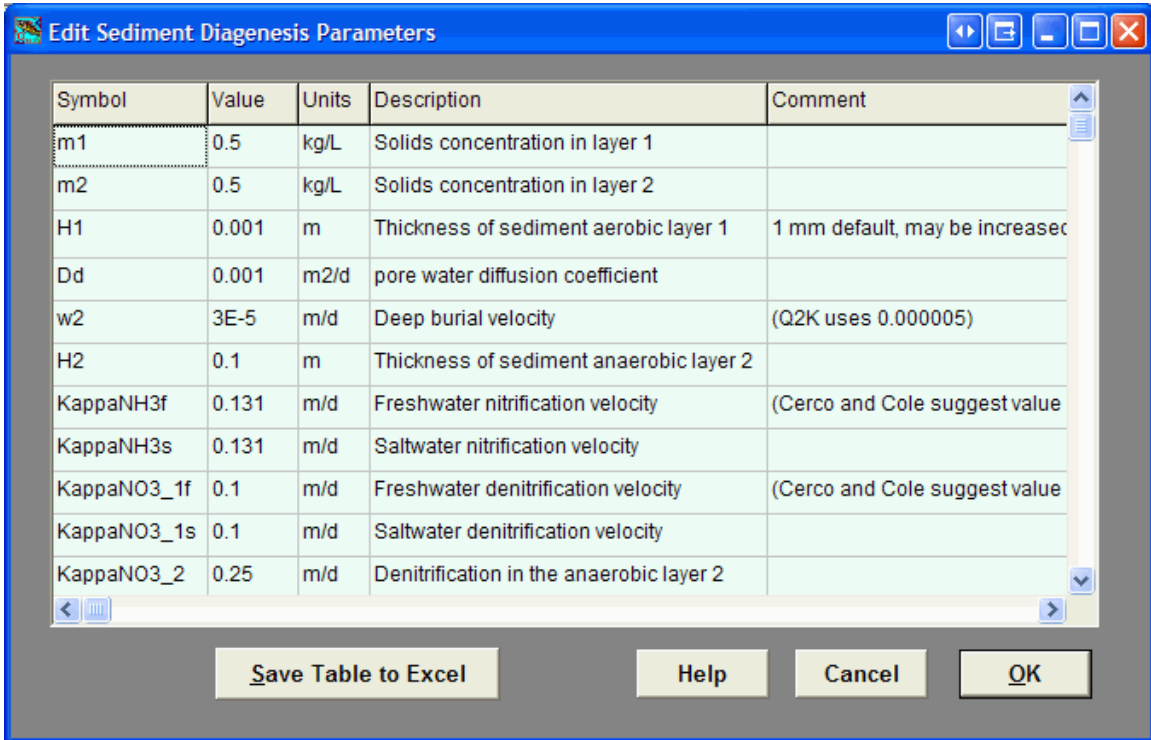
The sediment diagenesis model is only relevant for depositional regimes. No direct scour of sediment from the sediment bed is modeled.

Release 3.1 includes a new option to "**Model Diagenesis Layer 1 as Steady State.**" When this is selected, state variables in the upper-layer (between Layer 2 and the water column) are all modeled using the assumption of steady-state. This is the "native mode" of Di Toro's sediment diagenesis model. As noted in the interface, this process significantly speeds model execution (by up-to a factor of 10), but may have an effect on the mass balance of nutrients. Effects on overall model results are generally quite minor, however. More information about this option is available in Chapter 7 of the *Technical Documentation*.

Data requirements for this model are moderate. Initial conditions for all variables specified above are required but most rapidly become a function of organic matter deposition and may be derived by "spinning up" the model (running the model with arbitrary initial conditions and then setting the initial conditions based on model results which are a function of organic matter deposition).

A large set of "**Diagenesis Parameters**" govern the behavior of the model as well. Most of these may be kept constant from site-to-site but Di Toro suggests a few parameters are site-specific. Partitioning to phosphorus, in particular, is subject to considerable site specificity (*kdPO42*

and *dKDPO41f*). For reporting and archival purposes, parameters may be saved to Excel using a button on this screen.



Setting the initial condition for the organic matter sediment diagenesis state variables may be facilitated by using an Excel spreadsheet (**AQUATOX\_Sed\_Bed\_Inputs.xls**) that is included in the Studies directory. This spreadsheet will convert data about the fraction organic carbon, depth, sediment density, fraction labile and nonreactive sediment, as well as stoichiometry assumptions, into initial conditions for these three state variable compartments (POC, PON, and POP).

For more information about the equations and concepts within the Sediment Diagenesis model, please see chapter 7 of the Technical Documentation.

To add the Sediment Diagenesis model, select "**Add Sediment Diagenesis**" from the AQUATOX **Sediment** menu. It cannot be added with the AQUATOX Wizard.

### Non-Reactive Active Layer

In some cases, it may be worthwhile to see the effects of different sediment chemical concentrations on the modeled set of biota. This would usually only be relevant when working with linked models (to provide a time-series of chemical concentrations in the sediment bed). By selecting to model a "**Non-Reactive Active layer**" under the "Sediment" menu, toxicants within pore water and organic matter in the active layer of sediment may be input as a time series and biotic uptake and toxic effects will be calculated as a result. Uptake equations from the multi-layer sediment model are used, but chemical concentrations in the sediment bed are externally forced rather than calculated.

### Model Calibration

Model calibration is the process of modifying model parameters within their range of uncertainty (reasonable ranges as defined by literature if possible) such that model results match observed data or observed conditions.

The **Import Observed Data** function is quite useful for model calibration as all external data that is relevant to model output may be imported into the model and compared to model results. The graph gallery can be filled with plots of model results compared to observed data, and then parameters can be modified to best match all available data sets.

Parameters will have a varying degree of uncertainty depending on how measurable a parameter is, variability in field measurements, and uncertainty in lab equipment. Parameters will also have a varying degree of sensitivity depending on how much model outputs change as a function of the parameter changing. Within AQUATOX, parameter sensitivity may be ascertained through an automated **sensitivity analysis**. "Calibration Parameters" might be defined as those parameters that simultaneously have some range of uncertainty and to which important output endpoints are sensitive.

Calibration can be like trying to solve a puzzle. It requires creative thought and a real understanding of why the model is behaving like it is.

The first step in AQUATOX model calibration is often to ensure that the food-web is stable and matches current conditions. This may be quantitative if biomass data exists for a site or it may be qualitative. For example, if the user knows that largemouth bass exist at the modeled site but this category does not persist in model results then some type of respecification of the trophic interactions (or the lower portions of the food-web) will be required. Once the food-web is stable and reasonable then calibration to organic toxicant data may be undertaken.

It is recommended that the user start by trying to specify all of the important components of the food-web simultaneously. Calibrating the primary producers alone might be misleading as this model would not include grazing pressures from higher in the food web. Next, produce a plot of all the plants and animals and ensure that there are no inappropriate crashes or expansions of biomass beyond what would be supported by observed data or, lacking that, common sense.

#### **Some notes about calibrating plants:**

- Algae are differentiated on basis of:
  - nutrient half-saturation values (P half-saturation and N half-saturation)
  - light saturation values (Light Saturation or Adaptive Light option), and
  - maximum photosynthetic rate (PMax).
- Phytoplankton sedimentation rates differ between running and standing water.
- Some parameters are fairly site-specific, probably due to adaptation by the algae: these include critical force for periphyton scour (FCrit) and optimum temperature (TOpt).
- AQUATOX biotic state variables are quite sensitive to temperature parameters. These parameters include "optimal temperature," "maximum temperature," and "temperature response slope."
- "Percent lost in slough event" is a sensitive parameter for periphyton biomass.

#### **Some notes about calibrating animals:**

- The trophic interaction matrix is usually subject to uncertainty; proper specification of feeding preferences is critical.
- Simpler food-web models are more sensitive to effects from food-web interactions (less dietary substitution is possible resulting in more intense indirect effects).

- Biomass predictions are sensitive to "Maximum Consumption" rate and "Endogenous Respiration" rates when not calculated based on weight (allometrics); when allometric formulations are used, the model is sensitive to those parameters.
- Mortality is often a site-specific response and is therefore subject to calibration;
- The optimum temperature can have a significant effect on biomass computations;
- The minimum prey for feeding affects the efficiency of foraging behavior;

Additional information about model calibration may be found in the following document:

[EPA, 2009. \*AQUATOX Technical Note 1, A Calibrated Parameter Set for Simulation of Algae in Shallow Rivers\*, EPA-823-R-09-003 February 2009](#)

Also see Section 2.6 on "Calibration and Validation" in the AQUATOX Technical Documentation and Section 2.4 on Sensitivity Analysis.

## **Model Validation**

Model validation is a numerical cross-examination of the model against new data sets. By definition, a calibrated model is effective given conditions it was calibrated against, but there is uncertainty as to whether it will correctly model changing conditions. If the model can be tested against a different data set than was used for calibration, this increases confidence that the model has the capability to effectively capture alternative scenarios.

Model validation can consist of extrapolating the model

- to new time-periods,
- to new sites and exposure conditions, or
- to different chemicals.

Model validation exercises are often defined by, or limited by, the data available for validation.

If a model validation is not successful then the user can go back to the model calibration and seek an alternate calibration that will adapt to changing conditions more successfully. The model calibration and validation data sets may be combined for a more robust calibration, but at the expense of the loss of the validation data sets.

Also see Section 2.6 on "Calibration and Validation" in the AQUATOX Technical Documentation.

## **Working with a Linked Simulation**

A linked AQUATOX simulation is essentially a series of single segment simulations that are linked together with flow-fields. All linked segments must have an identical set of state variables. (State variables that do not occur in an upstream segment may be set to zero there.) State variables can pass from segment to segment through active migration, passive drift, diffusion, or bedload transport. Mass balance of all state variables is maintained throughout a multi-segment simulation.

Linked AQUATOX simulations have a file extension of \*.ALS. When a linked simulation is loaded, and **show segment data** is checked, all segments are displayed in a list. Double clicking any of the segments will bring the user into the Main Window for viewing that particular segment. Segment-specific parameters and output may be viewed through that window.

Clicking on **Show Link Data** will provide the user with a list of water-flow linkages between modeled segments. Double clicking on any of the linkages will bring a user to the **Edit Linkage Between Segments** window.

**Linked Output** brings a user to a screen that will provide graphical or tabular output for all segments simultaneously.

For reference, an optional bitmap **map** may be attached to the simulation, though this map will have no practical interface functionality.

Another option, within Linked mode, is to run several single-segment simulations together without any linkages to one another. This is an efficient way of calibrating several single-segment simulations with the same set of parameters; it can be used to calibrate across sites or experiments (such as artificial streams). In a linked simulation, changing a biotic parameter in one segment changes that parameter for all segments. Therefore, if it is desirable to test parameter changes over several simulations, loading these simulations into a "linked simulation" but specifying no water linkage between the segments may be possible. However, linked mode also requires that so the state variable list is identical in every segment.

For more information on linked simulations, see section 3.8 in the Technical Documentation.

## **Viewing and Editing Linkages**

There are two types of linkages that may be specified between individual segments: "cascade links" and "feedback links." A cascade link is unidirectional; there is no potential for water or state variable flow back upstream. Segments that are linked together by cascade linkages are solved separately from one another moving from upstream to downstream. This is particularly useful when modeling faster flowing rivers and streams.

"Passive" state variables such as nutrients and organic chemicals dissolved in water and plankton, move between segments as a function of water flow and diffusion. Benthic state variables and fish are assumed to stay in the reach in which they were initiated with the exception of specified fish migration and specified bed-load between segments (for benthic state variables).

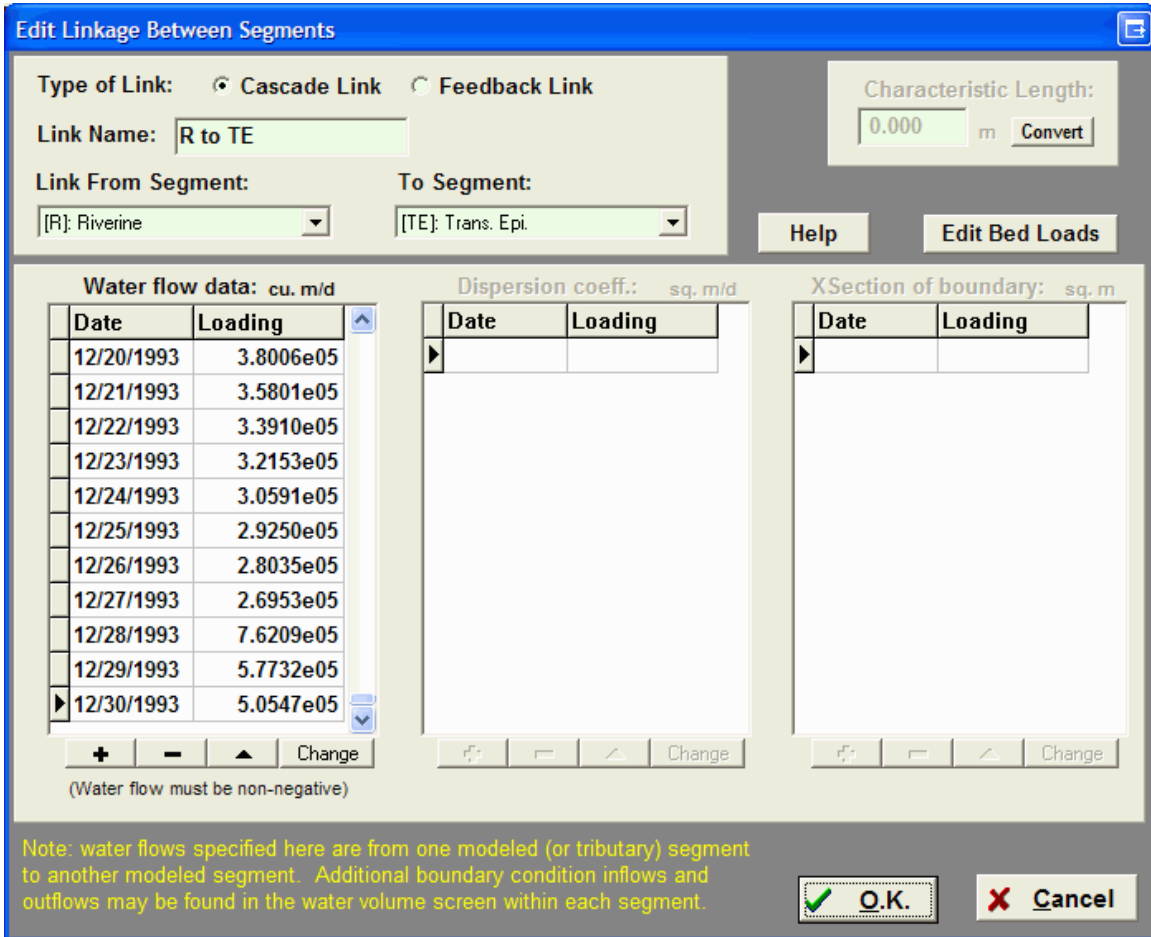
A feedback link allows for water or state variables to flow in both directions. For bookkeeping purposes, water flows are required to be unidirectional (i.e. entered water flows over a feedback link must not be negative). However, two feedback links may be specified simultaneously (in opposite directions) to allow for bidirectional water flows. Segments that are linked together by feedback links are solved simultaneously. There may only be one contiguous set of segments linked together by feedback linkages within a simulation but there is no limit on the number of segments that may be linked together in this manner.

Each segment's water volume inflow is a function of any boundary condition loadings that are specified in the **water volume screen**, and water from one or more linked segments. Each segment's water volume outflow is a function of any boundary condition outflows, as specified in the water volume screen, and outflow of water to one or more linked segments.

Feedback linkages also allow for passive diffusive exchange of state variables between segments. To model this type of state variable movement, the dispersion coefficient for each interface must be specified along with the cross section area and the characteristic length.

Finally bed loads for inorganic sediments may be specified over a given linkage if the multi-layer sediment model is included in time series of g/d.

Linkages between segments should be assumed to be horizontal unless two segments have been specified as a stratified pair in which case vertical linkage is possible.



### Examining Linked Output

The linked output window displays results from all linked segments simultaneously.

As in the single-segment output window, a library of graphs may be specified and observed data may be plotted against them. The only difference between the single-segment and linked output screens is that every segment is plotted simultaneously, differentiated by segment ID.

To observe results from a single segment only, go into a specific segment by double-clicking on the list and then go into the output window from there.

Currently there is no way to specify a sub set of linked segments, and the graph-setup window is disabled in linked-output mode.

The tabular data in this screen will also display all segments' results simultaneously.

### Examining a Single Segment

When a linked AQUATOX simulation (\*.ALS) is loaded, and **show segment data** is checked, all segments are displayed in a list. Double clicking any of the segments will bring the user into the Main Window for viewing that particular segment. Segment-specific parameters and output may be viewed through that window.

### **"Local" and "Global" Parameters**

Double-clicking on any of the state variables in the state variable list will display segment-specific initial conditions and segment-specific inflow loadings. Inflow loadings are associated with inflow boundary conditions as specified in the water volume screen. Inflow loadings from another modeled segment are a function of the internal processes in that segment and the flow of water over the linkage between segments.

Moving into underlying data for any of the state variables shows parameters that are global to all the animals, plants, or chemicals in a simulation. Changing any of these parameters will change the parameters for all segments in the system. Similarly, if a state variable is added or removed when the model is run in Linked-Mode, that change to the state variable list will occur within every modeled segment.

On the other hand, going into the **site type screen** within a linked segment will show parameters that are unique to the given segment. Site underlying parameters, remineralization parameters, water velocity, shade, and water depth information are all unique to the segment being modeled.

### **Exporting All Graphs to Word (Linked)**

When the main linked interface is shown (map and list of segments) a user may export all of the graphs associated with the simulation into Microsoft Word at the same time, by going to the Study menu and selecting "**Export All Graphs to MSWord**". AQUATOX will step through each and every graph in the graph library of every linked segment and paste those graphs into MSWord in Windows Metafile format.

This can be a powerful tool if summary graphs and graphs of observed data vs. model results are available in each segment. The selection of a single menu item will enable a graphical summary of the entire system.

### **Tributary Input Segments**

For the linked version of AQUATOX "**Tributary Inputs**" are available as a site-type. State variables are not solved within this type of segment, rather, loadings of nutrients, organic matter, and biota to this type of segment are loaded directly into the directly modeled system.

In the single-segment formulation, point sources and non-point source loadings have no water associated with them, and loadings are given in grams per day. The tributary input segment allows a user to enter a set of nutrient, organics, toxicants, and/or biotic loadings as concentrations in water that are associated with a water flow. The loadings are entered **as loadings to the tributary input segment itself**. The water flows that those loadings are associated with are entered **as linkages** from the tributary input segments into the modeled segment.

Tributary inputs may be used to model tributaries, point sources, non-point sources, and even groundwater inputs into the modeled system.

Because tributary input segments are "dummy" segments, output from these segments are not included in the linked output screen, or when linked results are exported.

Tributary input segments provide the user with considerable flexibility for playing "what-if" games regarding a given source of loadings. For example, if a management practice could conceivably reduce both the amount of water released and the concentrations of pollutants within that water from a point-source, the effects of this change can be directly modeled.

## Setting Up a Linked Simulation

### Additional Data Requirements for Linked Mode

The primary data requirements difference between linked mode and single-segment mode is that a water volume and water movement model for the entire linked system must be specified and input as a combination of boundary condition loadings, boundary condition withdrawals, and movement of water from segment to segment. This model may be derived from an external model or through simple assumptions and Manning's equation for linked streams. Additionally, initial conditions and boundary conditions are required for the entire modeled system rather than a single modeled segment.

The overall data requirements for a linked project are represented by the following list. For each segment modeled, the following time series may be required:

- Water Flow (m<sup>3</sup>/day)
  - Boundary Condition Inflow (Tributary / main stem flow into first segment, m<sup>3</sup>/day)
  - Boundary Condition Outflow (Withdrawals m<sup>3</sup>/day)
  - Flow from One Modeled Segment to Another (m<sup>3</sup>/day)
- Nitrogen (TotN, or Ammonia & Nitrate)
  - Nitrogen Boundary Condition Inflow (Tributary / main stem 1st, mg/L)
  - Nitrogen Point Source Loadings (g/d)
  - Nitrogen Nonpoint-Source Loadings (g/d)
- Phosphate (TotP, or TSP)
  - Phosphate Boundary Condition Inflow (Tributary / main stem 1st, mg/L)
  - Phosphate Point Source Loadings (g/d)
  - Phosphate Nonpoint-Source Loadings (g/d)
- Oxygen Loadings
  - Oxygen Boundary Condition Inflow (Tributary / main stem 1st, mg/L)
  - Oxygen Point Source Loadings (g/d)
  - Oxygen Nonpoint-Source Loadings (g/d)
- Organic Matter Loadings (BOD, OC, or Organic Matter)
  - Organic Matter Boundary Condition Inflow (Tributary / main stem 1st, mg/L)
  - Organic Matter Point Source Loadings (organic matter, g/d)
  - Organic Matter Nonpoint-Source Loadings (organic matter, g/d)
- pH or Total Alkalinity in Each Reach (pH or ueq CaCO<sub>3</sub>/L)
- TSS Concentration (optional) in Each Reach (mg/L)
- Water Temperature in Each Reach (deg C)
- Boundary Chlorophyll a loadings (mg/m<sup>3</sup> = ug/L)
- Mean Depth Time Series (m)
- Fraction Shaded (Const. or Time Series)
- Water Velocity (Optional, in cm/s)
- Sand / Silt / Clay Loadings, Optional (separated for each sediment category, TSS not required if SSC used)

- Sand / Silt / Clay (optional) Boundary Condition Inflow (Tributary / main stem 1st, mg/L)
- Sand / Silt / Clay (optional) Point-Source Loadings (g/d)
- Sand / Silt / Clay (optional) Nonpoint-Source Loadings (g/d)
- Toxicant boundary condition loadings and initial conditions (ug/L, optional)

Note, this list is fairly exhaustive and includes many optional items so the user should not be put off by it-- there are many ways to fill these parameters using observed water quality data. In some cases, point-source and nonpoint-source loadings may not be required.

## Using a Template Segment

To create a new linked simulation, a user must first select an existing single-segment AQUATOX simulation to serve as a template for the rest of the simulation. This will be the first segment in the linked system. The state variable list within this segment must be matched by any additional segments that are added. However, state variables may be added and subtracted in linked-mode; they will simply be added or removed from all linked segments simultaneously.

## Excel Template Import Capability

Using the AQUATOX interface to set-up or modify a large linked-mode AQUATOX simulation can be very time-consuming. This process is also not “auditable,” that is to say, it is very difficult to ascertain whether a mistake was made in the time-consuming click-intensive process. The wrong loadings could be imported to the wrong segment and the only way of knowing this would be by clicking into the loadings for that segment or carefully examining the “text output” of AQUATOX parameters.

To facilitate the process of setting up large simulations and understanding the parameters that go into them, a function to import loadings and parameters from an “Excel template” was added to the linked mode of AQUATOX. This enables a user to perform the following tasks:

- Create a multi-segment simulation from a single template segment;
- Modify site-specific parameters that are likely to change between segments;
- Input or modify state-variable loadings within each segment of the simulation, including non-detects handling;
- Input or modify water-flow linkages between segments;
- Define tributary or groundwater inputs into the linked-mode system;
- Import observed data that can be used to compare against model results;
- A log of all simulation modifications is written including warnings and errors.

The Excel template function can be utilized when first setting up a linked simulation (the user is prompted when selecting “File, New Linked Simulation”). In this case, the user will need to specify an existing single-segment simulation to reproduce as multiple segments of the new simulation. Alternatively, a template can be used to modify an existing linked simulation (“Add Time series from Excel” in the “Study” menu). The user will need to provide the file name and location of the Excel template in either case.

AQUATOX reads from the Excel template on a column by column basis. Depending on the type of input being read, and whether non-detects are included, each model input can be from one to three columns in width. The first column (column “A”) of each worksheet is not read from; it usually contains a “cheat-sheet” of allowed template input strings (for reference only). This “cheat-sheet” is included in the AQUATOX “STUDIES” directory as “import\_template.xls.” In cell “B1” of the spreadsheet is the first “command” to AQUATOX and it explains what type of model

input is located in its columns (and potentially in the next one or two columns to the right). After those columns have been processed, AQUATOX reads the top row (Row "1") of the next column to obtain its next input or command.

	A	B	C	D	E	F	G
1	<b>Addition Type</b>	NewSeg	NewSeg	Inflow	<-----	NewLink	<-----
2	<b>Addition Name (ND Flag?)</b>	Seg 1	Seg 2	FALSE		S1 to S2	
3	<b>Seg/Link ID (seg ID from)</b>	S1	S2	S1		S1	
4	<b>Length km</b> <i>(seg ID to) (comment1)</i>	4.50	13.03	<i>Upstream Boundary</i>		S2	
5	<b>Vol IC m<sup>3</sup></b> <i>(link type) (comment2)</i>	113,231	243,304	<i>Boundary Condition</i>		Cascade	
6	<b>SARA m<sup>2</sup></b> <i>(time series header)</i>	289,620	456,152	Date:	Flow (m3/d)	Date:	Flow (m3/d)
7	<b>Mean Depth m</b> <i>(time series)</i>	2.558	1.875	1/1/1998	604,304	1/1/1998	605,408
8	<b>Max Depth m</b>	3.837	2.812	1/2/1998	594,518	1/2/1998	594,241
9	<b>Slope m/m &lt;or blank&gt;</b>	0.0023	0.0024	1/3/1998	596,964	1/3/1998	597,518
10	<b>Manning's N &lt;or blank&gt;</b>	0.043	0.043	1/4/1998	592,071	1/4/1998	591,794
11				1/5/1998	594,518	1/5/1998	593,965
12	<b>(set inflow, disch to zero)</b>			1/6/1998	599,411	1/6/1998	598,860
13	<b>(calc dynamic)</b>			1/7/1998	604,304	1/7/1998	605,131
14				1/8/1998	596,964	1/8/1998	596,413
15							

The type of model inputs, their parameters, and their effects on a linked simulation are documented below.

- “NewSeg” (One column in width) : This command either creates a new segment or, if the Segment ID already exists, overwrites relevant parameters for the segment with those in the spreadsheet. If there is no segment with the given Segment ID, the template segment is copied to a new segment and the parameters listed below are used to populate the segment. The rows below the header contain the following parameters:
  - Row 2: Segment Name (string)
  - Row 3: Segment ID (string)
  - Row 4: Length of Segment in km (number)
  - Row 5: Initial Condition Volume in cubic meters (number)
  - Row 6: Surface Area in square meters (number)
  - Row 7: Mean Depth of segment in meters (number)
  - Row 8: Maximum Depth of segment in meters (number)
  - Row 9: Optional, Slope of segment in m/m (number)
  - Row 10: Optional, Manning’s N in s/m<sup>1/3</sup> (number)
  
- “NewLink” (Two columns in width): This command creates or modifies a water-flow linkage between two existing segments.
  - Row 2: Linkage Name (string)
  - Row 3: Segment ID, water volume from (string)
  - Row 4: Segment ID, water volume to (string)
  - Row 5: Link Type, “cascade” or “feedback”
  - Row 6: Time-series header. Strings to help provide context within the template. Usually “Date” in the first column and “Flow in m3/d” in the second column.
  - Rows 7-End: Dates in the first column and flows in m3/day in the second column. AQUATOX will read downward until it finds the first empty cell.
  
- “NewTrib” (Two columns in width): This command creates or modifies a tributary input into the AQUATOX simulation. The tributary segment will not be a modeled segment but

any loadings into the tributary are loaded directly into the relevant modeled segment. Any water volume linked from the tributary input into the modeled segment will also be added to the modeled segment. This command specifies the water loading and the linkage to the modeled segment but other loadings (nutrients, chemicals, etc.) must be specified later using the nutrient input format documented below.

- Row 2: Tributary Name (string)
  - Row 3: Tributary Segment ID (string)
  - Row 4: Segment ID to link tributary to (string)
  - Row 5: Link Type, irrelevant, must be "cascade."
  - Row 6: Time-series header. Strings to help provide context within the template. Usually "Date" in the first column and "Flow in m3/d" in the second column.
  - Rows 7-End: Dates in the first column and flows in m3/day in the second column. AQUATOX will read downward until it finds the first empty cell.
- "Inflow" or "Disch" (Two columns in width): This command creates or modifies a boundary condition inflow or boundary condition discharge from an existing segment.
    - Row 2: Non-Detect Flag, generally "false" for water flows (Boolean)
    - Row 3: Segment ID, water volume to or water volume from (string)
    - Rows 4 and 5: Optional comment fields that will be loaded into the AQUATOX "Notes" fields.
    - Row 6: Time-series headers. Strings to help provide context within the template. Usually "Date" in the first column and "Flow (m3/d)" in the second column.
    - Rows 7-End: Dates in the first column and flows in m3/day in the second column. AQUATOX will read downward until it finds the first empty cell.
- Nutrient Import / Parameter Valuation Format (two or three columns in width): This is relevant to
    - "NO3:" Nitrate loadings in mg/L;
    - "NH4:" Ammonia loadings in mg/L;
    - "TSP:" Total Soluble P loadings in mg/L;
    - "OM:" Organic Matter loadings in mg/L
    - "BOD:" Biochemical Oxygen Demand loadings in mg/L;
    - "O2:" Oxygen loadings in mg/L;
    - "TP:" Total P in mg/L;
    - "TN:" Total N in mg/L;
    - "pH:" pH values in water;
    - "TSS:" Total Suspended Solids within segment water, mg/L;
    - "Temp:" Temperature of segment water, degrees C;
    - "ZMean:" Mean Depth of segment, meters;
    - "Shade:" Percent shaded for segment, (0-100);
    - "WaterVel:" Water velocity of segment, cm/s;

Loadings or valuations are added to the linked simulation or modified if they already exist. Loadings in water are relevant to boundary conditions only, as nutrients moving from modeled segment to modeled segment are internally calculated. As noted above, loadings applied to unmodeled "tributary input" segments will be passed directly through to the modeled segment that the tributary is linked to.

- Row 2: Non-Detect Flag. If "false," two columns will be input with the first column holding date and the second column holding loadings values. If "true," three columns will be input with the first column holding the date, the second column holding the non-detect flag, and the third column holding the loading in the proper units. If the non-detect column is not empty, the sample is assumed to be a non-detect and the loading is set to one half of the loading in the third column (detection limit).

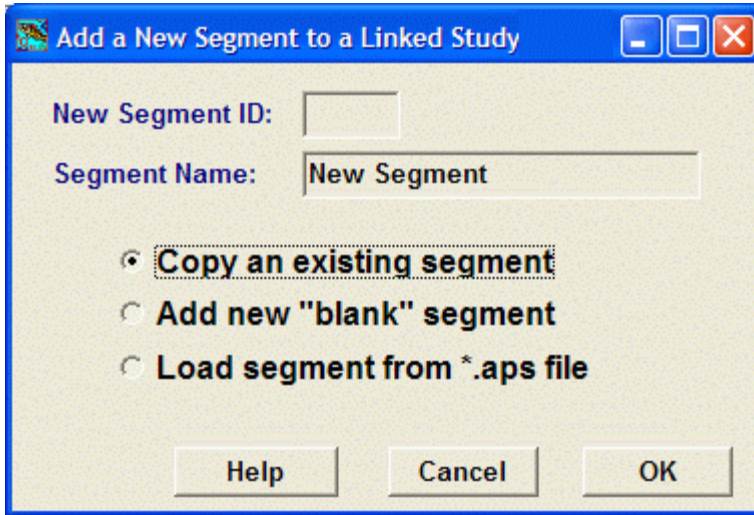
- Row 3: Segment ID or Tributary Segment ID to load nutrients into (string)
  - Rows 4 and 5: Optional comment fields that will be loaded into the AQUATOX “Notes” fields.
  - Row 6: Time-series headers. Strings to help provide context within the template. Usually “Date” in the first column and “Loading / Value” in the second column. Alternatively “Date” in the first column, “Non-Detect Flag” in the second column and “Loading / Value” in the third column.
  - Rows 7-End: Dates in the first column and loadings or valuations in the appropriate unit in the second column. AQUATOX will read downward until it finds the first empty cell.
- “Chla” (two or three columns) Chlorophyll a in ug/L: Chlorophyll a is processed the same as are nutrient loadings above with two exceptions. To convert chlorophyll a data to biomass units, the “multiply loading by” field within AQUATOX is set to 0.0532 (mg/L biomass to ug/L chla). Secondly, the chlorophyll a data must be assigned to a particular phytoplankton species within the simulation. The import template first looks for an assignment in the second column of Row 2 (to the right of the non-detect flag). The following strings are valid:
    - “diatoms1” to “diatoms6”
    - “greens1” to “greens6”
    - “blgreens1” to “blgreens6”
    - “otheralg1” to “otheralg2”

If no valid assignment is found in this cell, the software finds the phytoplankton compartment highest on the list of state variables. If there are no phytoplankton compartments in the simulation, the linkage raises an error.

- “Observed” (Two or three columns in width): This command creates or modifies external data imported into AQUATOX for use in graphing model results against observed data..
  - Row 2: Non-Detect Flag. If “false,” two columns will be input with the first column holding date and the second column holding loadings values. If “true,” three columns will be input with the first column holding the date, the second column holding the non-detect flag, and the third column holding the loading in the proper units. Non-detects are plotted as red arrows.
  - Row 3: Segment ID, observed data is relevant to this segment (string)
  - Row 4: Description of data and source (string)
  - Row 5: Units for data (string) in first column, optional reference in second column.
  - Row 6: Time-series header. Strings to help provide context within the template. Usually “Date” in the first column, “Non-Detect flag” if relevant in the second column, and “Value” in the column that follows.
  - Rows 7-End: Dates in the first column, non-detects in the second column, if relevant, and values in the second or third column. Non-detects are assumed “lesser than” unless a “>” is used as the non-detect flag in which case it is assumed “greater than” (e.g. the denominator of a normalized data field is non-detected).
- “NextPage” Command to move to column B in the next Excel worksheet (next tab in the spreadsheet). Used when the user runs out of rows in the given sheet.
- “End” Command to stop processing the Excel spreadsheet.

## **Adding a New Segment**

To add a new segment to an AQUATOX linked simulation, the **"Add"** button may be used on the main linked study screen when "show segment data" is selected.



A dialog box will appear that allows the user to specify a segment ID (which is used organizationally, and to label output), a segment name (which describes each segment), and three options as to how to add a segment. The Segment ID must be four characters or less.

- An existing segment may be copied, in which case initial conditions, loadings, and site-specific data will then need to be modified to match the new segment to be modeled.
- A "blank" segment may be added, in which case initial conditions and inflow loadings are set to zero.
- A segment may be loaded from another single-segment mode simulation \*.APS (single-segment mode) file. In this case, all state variables must match the existing segments in the linked simulation or the study won't be loaded.

## Linking Segments Together

To link two segments together, the two segments must first be included in a simulation. Then **"Show Link Data"** must be selected in the main linked interface window. When **"Add"** is then selected, the Edit Linkage window will be visible which will enable the user to specify a "cascade" or "feedback" linkage and also to enter water flows and other relevant parameters and time series. For more information on editing linkages see **"Viewing Linkages."**

## Adding "Tributary" Inputs

To add a tributary input (which can also be used to model point and non-point sources and groundwater inputs) a new segment must first be added. Adding a "blank" segment will work fine. Then, the site type must be designated as a "tributary input" within the site-type input screen.

Within this tributary-input segment, initial conditions, site underlying data, and boundary-condition water volume inflows and outflows should all be ignored as these are not relevant. Instead, the user should focus exclusively on the nutrient, oxygen, biota, and chemical loadings *into* the new tributary segment. These loadings will be passed right through this tributary segment and into the modeled segment that it is linked to. For this reason, a linkage of the tributary input into the modeled segment must also be added. Add a new linkage from the tributary input segment to the

modeled segment and specify an associated water flow. This linkage must be a "cascade" linkage, as no feedback to the tributary input is possible.

On a given date, the water flow of the linkage multiplied by the concentration of the loadings specified into the tributary-input segment will provide an accounting of the mass of the loading to the modeled segment. The volume of water specified, of course, will also be added into the modeled segment.

Tributary inputs can also be added through the Excel Template Import, which can simplify the process. For more information about tributary inputs see "**Tributary Input Segments**"

### **Setting up Linkages, Complex Systems**

Setting up linkages in truly complex systems can be a time-consuming process. For this reason, the Excel Template Import Capability is especially powerful for these systems. This allows complex linkages to be set up in an auditable fashion and also allows these linkages to be modified and re-imported. Alternatively, boundary-condition loadings may be modified in the Excel template and then the template may again be re-imported to test alternative scenarios.

It is important to remember that inflow water for each segment is governed by two sources of model input:

- Boundary-condition inflows as specified in the water volume screen.
- Inflows from other linked segments as specified in the list of linkages.

Similarly, the outflow water for each segment has two sets of loadings:

- Boundary-condition outflows or withdrawals as specified in the water volume screen.
- Outflows to other linked segments as specified in the list of linkages.

### **Water Balance Considerations**

New users of the AQUATOX linked-mode often have difficulties with water volumes going to zero, or water volumes going to unreasonably high levels.

Other than evaporation (which is often set to zero in linked-systems for simplicity sake), AQUATOX linked segments are modeled as "closed systems" where no water enters or leaves the system unless it is specifically accounted for. The *outflow* for each segment is defined as "*Inflow - d Volume + inputs - withdrawals.*" The *inflow* of the next segment may be defined as the *outflow* from the previous segment.

For systems that take a long time to run, any changes to the water balance model may be tested by first saving the simulation, then saving the simulation to a different name, then removing all state variables and ensuring that the water volumes are behaving as required before returning to the version with all of the biotic state variables.

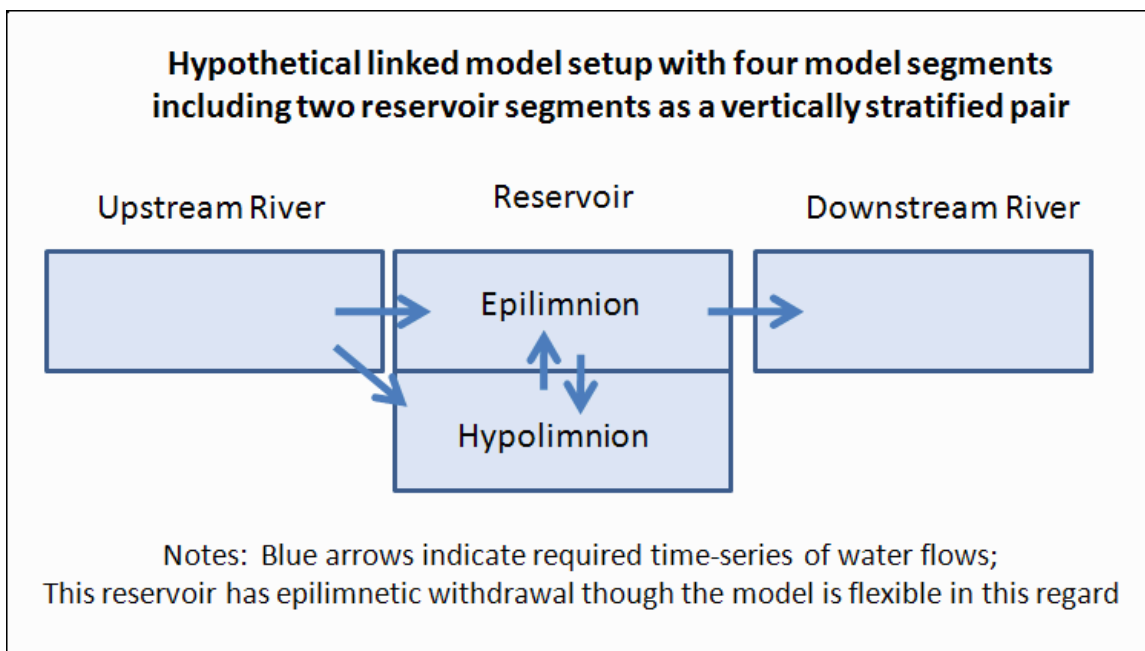
An external "closed system" accounting of water flow is often quite useful for the use of the linked-mode model, whether it be a complex hydrological model or a simple spreadsheet model.

### **Stratification in a Linked System**

“Dynamic stratification” does not apply to the multi-segment model. Instead, a user must specify two unique linked segments as a vertically stratified pair. In this case, the segments must be linked together with a feedback linkage. A stratification screen within each segment’s main interface allows a user to specify whether a segment is part of a vertically stratified pair and, if so, whether it is the epilimnion or the hypolimnion segment. (The model needs to know if one segment is located "on top" of another segment so that sinking organic matter and plants are routed to the lower segment rather than moving directly to the sediment bed. This also affects light climate in the lower segment.)

Unlike the single-segment model, water flows must be specified between the two segments. Overturn may be specified by a high degree of mixing between the two segments whereas periods of stratification will have considerably lower flow.

When two segments are set up as stratified together, the thermocline area is defined by the user-entered cross section between them. As noted above, annual cycles of stratification and overturn may be specified using the time-varying water flows and dispersion coefficients. As was the case in the dynamic stratification model, fish automatically migrate to the epilimnion in the case of hypoxia in the lower segment. Sinking phytoplankton and suspended detritus in the epilimnion segment pass into the designated hypolimnion segment. The light climate of the bottom segment is limited to that light which penetrates the segment defined as the epilimnion.



## Tutorials

### Simple Tutorial

This basic tutorial introduces basic concepts and gets started using the AQUATOX interface.

### Tutorial-- Step 1: Deleting and Adding a Plant

Open the file **FarmPond MO Esfenvalerate.aps** . (see **Loading a Study** )

First remove the macrophyte compartment by highlighting it in the list, clicking on the **Delete** button, and confirming the deletion. The variable will disappear from the state variable list.

Likewise, state variables can be added by clicking on the **Add** button and choosing from the list. Let's add macrophytes back to the list of state variables.

Click on the Add Button and scroll down the list until you see the **Macrophyte1** to **Macrophyte6** compartments. AQUATOX has the capacity to model up to six unique macrophyte species. Select **Macrophyte1** and click on OK.

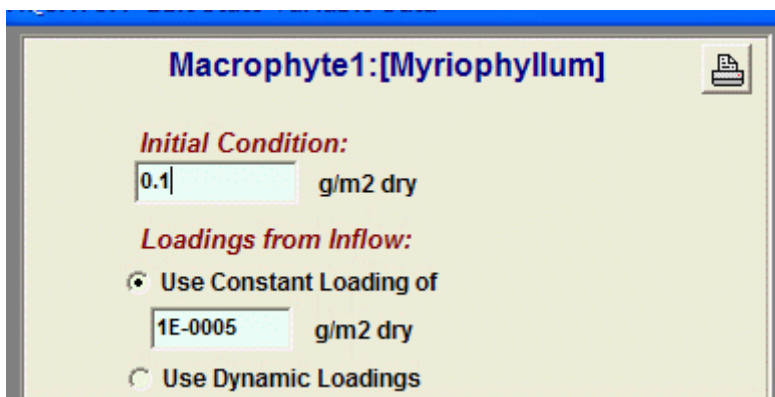
You will then see another dialog box open asking you to "**Select Plant Entry to Load Into Macrophyte1.**" Note that the names of the taxonomic groups and ecologic guilds on the main study screen are followed by the names of the specific groups in brackets. We therefore have to specify the type of macrophyte we are adding. Select *Myriophyllum* on the list at the left and click on **OK**. If you do not select a species when you run the simulation you will receive an error message indicating that there is no data associated with the state variable **Macrophyte**.

next, Setting an Initial Condition

## **Tutorial-- Step 2: Setting an Initial Condition**

To continue with our macrophyte example, we should enter a value for the biomass of macrophytes present at the beginning of the simulation; if the value is left as 0 and there is no loading, then macrophytes would not be simulated. The initial condition will depend on when the simulation starts (which is specified in **Setup**). In this example we will enter a value of 0.1 g/m<sup>2</sup>, which is appropriate for *Myriophyllum* in a temperate pond at the beginning of the growing season.

Double click on the state variable list on Macrophyte1: Myriophyllum. Enter 0.1 as shown below.



As you can see from the picture above, AQUATOX also automatically entered a loading of 1e-5 (0.00001) for macrophytes in this simulation. Ordinarily we think of loadings as pertaining only to chemicals and freely moving organisms such as plankton and fish. However, it is usually desirable to enter a small constant loading to serve as a "seed" if the population or group is killed off entirely by a toxicant or adverse environmental conditions. The "seed" will allow the biota to recover, or recolonize if and when conditions become favorable. This is especially important for macrophytes that suffer winter die-back

For all biota, AQUATOX uses a value of 1E-5 g/m<sup>2</sup> as a constant loading. This is small enough that it will not affect the results during the growing season, but it is large enough to prevent extinction.

Click the OK button to return to the Main screen.

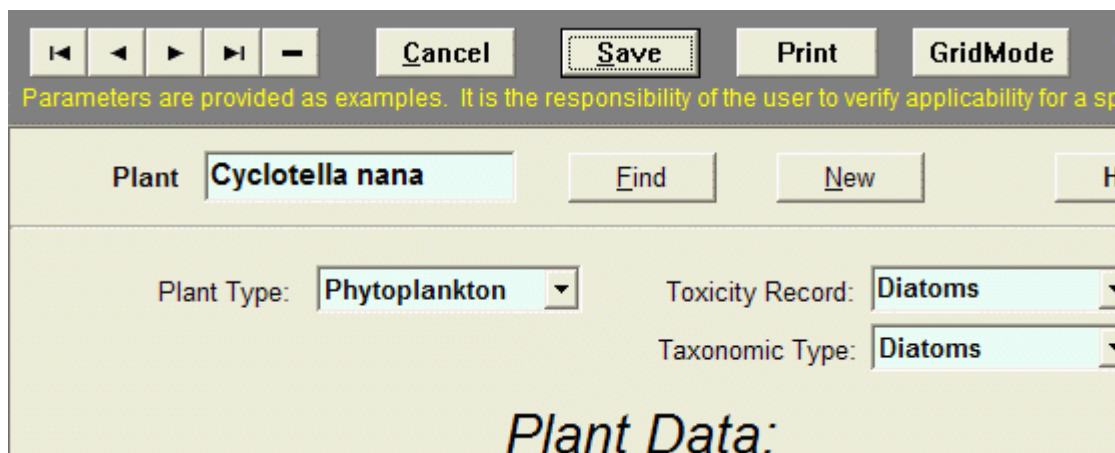
See Also: **Initial Conditions and Loadings**

next, Viewing Parameters

### Tutorial-- Step 3: Viewing Parameters

In the following examples we will examine a record from each of the other libraries. A record can be down-loaded into a study from a **library** by choosing **Load data** on the Edit State Variable Data screen.

We will examine first the parameter screen for plants. From the main screen, choose **Plants** from the **Library** menu at the top of the screen (or click on the big button "P" on the toolbar), view the default library file, then move to *Cyclotella nana* by clicking on the arrows at the top left of the screen. We are now moving through a database of parameters that is provided with AQUATOX. These parameters are not necessarily associated with the study file that has been loaded, but can be loaded into the simulation. (To see the parameters associated with the given study, double-click on any of the animals or plants in the state variable list and then click the "**Underlying Data**" button.)



Two fields near the top of the screen require explanation. If you click on the triangle to the right of **Plant type**, you will be given a choice. The choice of **Plant type** is important because different types have different physical or biological processes that apply to them. For instance, phytoplankton are subject to sinking, but not periphyton, which are attached to a surface. Conversely periphyton are limited somewhat by very slow current velocity; but not phytoplankton, which are adapted to still water.

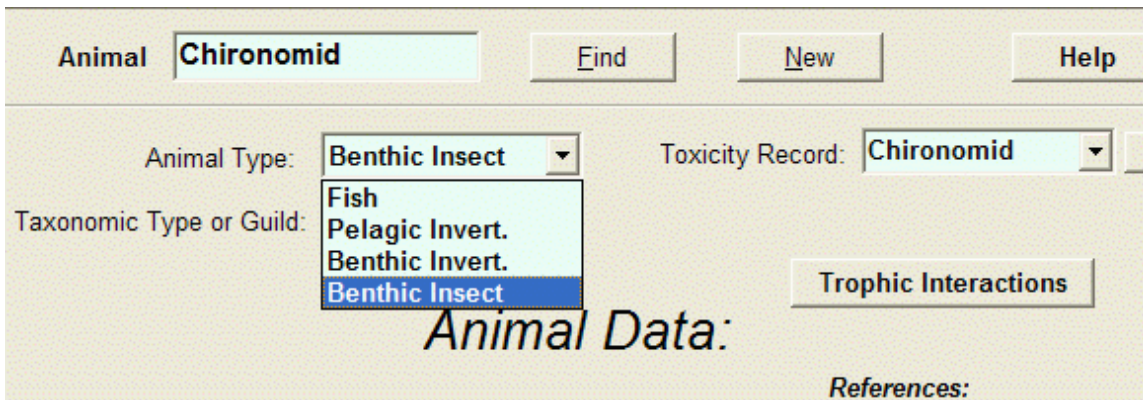
Less obvious is the **Toxicity Record**; again, clicking on the arrow to the right of the field will give you several choices. The intent is to associate the organism record with one of the limited number of organisms for which there might be toxicity data or procedures for estimating toxicity. In this instance, if you choose **Diatoms** the model will utilize the toxicity data (e.g., EC50) for Esfenvalerate to Diatoms, as listed on the **Toxicity Record** portion of the **Chemical Properties** screen.

The given parameter values are provided to get you started; if you have more appropriate values, you should use them. Those parameters that do not pertain to phytoplankton are dimmed. If you

try to enter a value for **Reduction in still water**, for example, you will find that the field cannot be edited.

Next we will locate the record for Chironomid from the Animal Library. Hit **Cancel** to leave the plant screen and again go through the **Library** menu to get to the animal library. (Alternatively you can select the "A" for animal on the toolbar.) Again, scroll using the arrow buttons to find the Chironomid record or you can click the **find** button and enter "Chironomid."

Click on **Animal Type** to see the pull-down menu. Chironomids have aquatic larvae, so **Benthic insects** is chosen; this is important because emergence is simulated by AQUATOX for insects as a loss term, but does not apply to other animals.



Click the button to see the associated trophic interaction table. The trophic interaction table is important because it defines the food-web relationships and assimilation efficiencies. Here we see that Chironomids primarily feed on labile detritus, and that they assimilate 70% of it. See also **Trophic Interactions**.

After exiting the trophic interactions screen, click on the scroll bar to the right to see the rest of the Animal screen. The **Bioaccumulation Data** section contains parameters relevant to bioaccumulation of organic toxicants, only one of which (**Fraction that is Lipid**) is sensitive in insects. The model is not sensitive to the longevity of the insects because emergence is a function of growth rate, which depends on local, seasonally varying conditions. Likewise, mean weight can only be approximate across all instars because it will vary greatly during the growing season.

Finally, we will examine the remineralization screen for this study. To do this, return to the main screen, select the **Site Button** and then select the **Remineralization** button from within that dialog. Many of the parameters on this screen are global and there is little need to change them for a site, unless the organic material is quite different or there is some reason that the microflora might have adapted to abnormal conditions, such as a thermal spring or acid mine drainage. For more information about the three different types of Remineralization records included with AQUATOX see the section titled **Remineralization**.

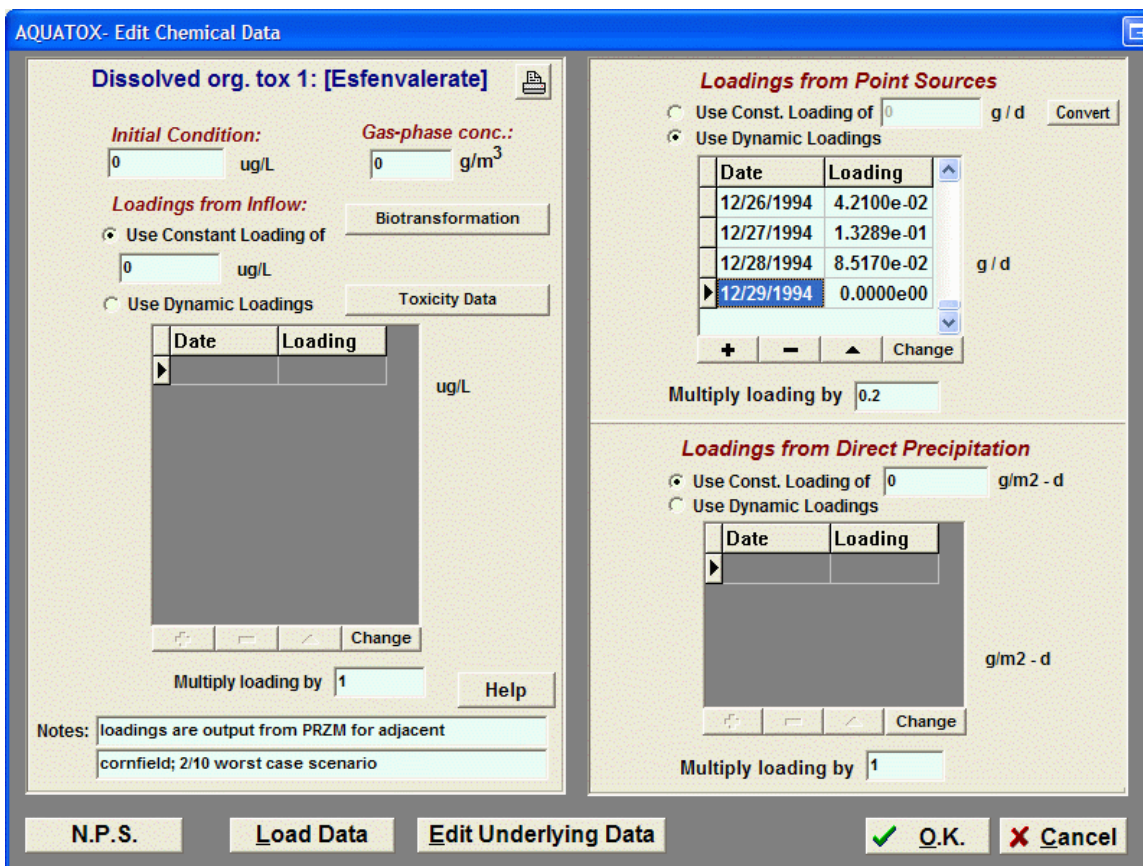
<b>Default Remin Record</b>		<b>Find</b>	<b>New</b>	<b>Help</b>
<i>Remineralization Data:</i>				
<i>References:</i>				
Max. Degrdn. Rate, Labile	<input type="text" value="0.25"/>	g / g · d	<input type="text" value="Wetzel 2001, p. 514 (max for bl-gr); diato"/>	
Max. Degrdn. Rate, Refrac. (ColonizeMax)	<input type="text" value="0.007"/>	g / g · d	<input type="text" value="Collins and Wlosinski 1983"/>	
Optimum Temperature	<input type="text" value="25"/>	°C	<input type="text" value="temperature at which measured"/>	
Maximum Temperature	<input type="text" value="65"/>	°C	<input type="text" value="Alexander '61"/>	

Next, Viewing Toxicant Loadings

#### **Tutorial-- Step 4: Viewing Toxicant Loadings**

Following the tutorial to this point, we should still have **FarmPond MO Esfenvalerate.aps** loaded from back in **step 1**. Return to the main screen.

Double-click on **Dissolved org. toxicant** or click on the **Chemical** button on the main screen to bring up the **Edit Chemical Data** screen, and to examine the various options for loadings to the system. Pollutant loadings can be entered as constant or dynamic loadings in several different forms. The pollutant can be entered as a concentration in the dissolved phase (or loosely bound to suspended sediment); the water inflow and the site volume are then used by the model to compute the loading per unit volume. The gas-phase concentration is used to compute atmospheric exchange; ordinarily concentration in the atmosphere can be considered to be 0, although some pollutants such as PCBs may have significant atmospheric concentrations.



Point-source loadings are mass per day (g/d) for the entire site; they are divided by the site volume to obtain the loading per unit volume. In this example, dynamic loadings from a point discharge as calculated by the PRZM model are entered. Note that the dynamic loadings are interpolated, so if the intent is to represent a spike such as from storm runoff on a particular day, then the loading should be bracketed by "0" loadings. The model assumes that the loadings "wrap around" with an annual cycle and that the last loading can be interpolated to the first loading as if it were in the succeeding year. Exercise caution when modeling multiple years, but only have loadings data form one or a few years. Sporadic loadings, which would only be expected in that one particular year may inappropriately be repeated in successive years. If you do not wish loadings to be repeated, enter values ("0" or otherwise) for the first and last days of the simulation. The dynamic loadings in this example were entered by hand; an excellent alternative is to download or prepare a file external to the model and import it into the study using the **Import** button. See also: Dynamic loadings.

Another potential pollution loading source is from direct precipitation. These are given as g/m<sup>2</sup> day because AQUATOX does not explicitly consider precipitation. Click on **N.P.S.** to toggle to the non-point source screen, which is in g/d.

Next, Running the Simulation

### Tutorial-- Step 5: Running the Simulation

To run the simulation, select the **Perturbed** or **Control** buttons from the main screen.

Depending on the control setup selected, a control run will omit toxicants or nutrients from the run.

### **Tutorial-- Step 6: Viewing Output**

When a study has been executed, results for various state variables are stored in memory. To view this output, you must either export the output to an appropriate file-type using the **Export** buttons on the main screen or select the **Output Button** from the main screen. The **Output Button** will spawn an additional output window which will allow you to view output in graphical or tabular format.

Also See: Viewing Graphical Output

### **Stream Tutorial**

This tutorial uses the AQUATOX Wizard to make a number of changes to a "template" study. This is the usual approach taken when applying the model.

#### **Stream Tutorial-- Step 1: Selecting an Existing Study as a Template**

An existing study that is as close as possible to the site you are trying to model should be chosen. In this case, open the file **Rum R MN.aps** (see **Loading a Study**), save as **LBR Middleton ID.aps**.

It is best to immediately save the template study with a new name so that you do not overwrite the original with your changes.

#### **Stream Tutorial-- Step 2: Modifying the Study with the AQUATOX Wizard**

Click on large **Use Wizard** button on main screen

Step 1: Change the study name to "L. Boise Middleton" This will be the heading for output.

Step 2: Change the simulation period to 1/1/2000 to 12/31/2001.

Step 3: Keep the nutrient initial conditions; stream simulations are not sensitive to nutrient initial conditions but rather to loadings

Step 4: Also keep the sediment detrital initial conditions for lack of better data and keep the water-column BOD (you can change this after importing loadings)

Step 5: Keep the following algal state variables and initial conditions; generally these will be applicable to any stream; however, remove the macrophyte *Fontinalis*, which is a moss. To do this click "Next >>" until you reach the "Macrophytes" screen.

Step 6: Keep the invertebrates without change until "Pred Inverts" when you should drag Stonefly to the simulate column on the right. Keep the initial conditions, but use 0.01 for Stonefly

*(Note, any changes that are made in the wizard may be undone using the "cancel" button. However, any changes made in any single wizard session must be undone at the same time. Therefore you may wish to periodically click on "finish" to save your partial changes and then reenter the wizard. You may jump to whatever screen is appropriate by double clicking on that step on the Wizard Progress window.)*

Step 7: Although plant and invertebrate groups do not vary appreciably over large geographic areas, fish are often restricted to specific drainage basins; therefore, you will need to make numerous changes. First, select and remove: **Bluegill, Smallmouth Bass (YOY and Lg) and Walleye.**

Next add:

Single compartment, small forage fish **Chiselmouth and Dace**;  
Single compartment, large forage fish **Pikeminnow**; and  
Size-class gamefish **Largemouth Bass, Mtn Whitefish, and Rainbow Trout** (Use YOY data record for small size class).

*When adding a size-class fish, you are first prompted to load parameters for the small or young-of-year fish. Then you are asked if you wish to use the same parameter record for the large fish or not. In this tutorial, load a different parameter set for the large size-class fish.*

Change all fish initial conditions to 0.1; we will let the model adjust these during iterative simulations.

Step 8: Change the site name; enter

**5 km** for length (arbitrary);  
surface area = **1.8e5 m<sup>2</sup>** based on 36 m width determined from Google Earth;  
mean depth = 0.42 m;  
max depth = 0.63 (1.5 X mean depth);  
evaporation = 0 (is not important for a short stream reach);  
latitude = 43.57.

Keep channel slope = 0.002  
Keep Manning's coefficient estimated based on natural stream;  
Riffle = 47% and pool = 0% based on site observations and pebble count.

Step 9: Continue to Use Manning's Equation for simulating water volume and select "Next."

For initial volume use **7.56E4 m<sup>3</sup>** based on mean depth of 0.42 and surface area given earlier; discharge data should be entered by clicking on **Change** and **Import** and choosing **Midd discharge.xls**, which is based on USGS data from the Middleton gage converted from cfs to cu m/d.

*Note: All Excel files to be imported in this tutorial may be found in the "Tutorial" directory off of the AQUATOX "Studies" directory. Whenever one time-series is imported over another, the original data is deleted prior to the import.*

Step 10: Select to use time-varying temperature and then use time series imported from **Midd temp.xls**; these observed data are almost a year in length and are from a later period, but they represent the variable nature of temperature and are interpolated by the model. The initial temperature for January 1 may be set to 5 degrees based on the imported data.

Step 11: Wind is not important for a stream, so keep it constant at 1 m/s

Step 12: Select "Annual Mean and Range" then use observed mean = 380 Ly/d and range = 516 Ly/d; Internet sources for these data change frequently. One research approach would be to Google the nearest airport and "solar" to try to find approximate values (which may require units conversion).

Select to compute photoperiod from latitude.

- Step 13: Import observed pH from **Midd pH.xls**; keep initial pH at 8, which is approximate for January 1 based on the imported data.
- Step 14: Sporadic observed TSS values are available from the USGS NWIS for the Middleton gage; a regression was obtained for TSS as a function of discharge (see **Midd discharge TSS.xls**), but there was no significant relationship, so the raw observed values in **Midd TSS.xls** should be imported.
- Step 15: No toxic chemicals will be simulated.
- Step 16: Ignore loadings for ammonia; import nitrate loadings from **Midd TN.xls** and P from **Midd TP.xls** (you will have an opportunity to verify that these are specified as TN and TP later); keep CO<sub>2</sub> loadings constant at 0.7; For oxygen, import **Midd DO.xls**; import suspended and dissolved detrital loadings from **Midd BOD.xls** (here too you will check later to make sure it is specified as BOD); all the biotic loadings are seeds to prevent a group from becoming extinct and should be 1 -E5.
- Step 17: Direct precipitation is unimportant to a stream such as this, so all values should be either 0 or ignored.
- Step 18: Point-source loadings are unimportant for this reach and should be 0; these would be set for effluent such as from a wastewater treatment plant.
- Step 19: Nonpoint-source Loads are also unimportant and should be 0 for this reach.

### **Stream Tutorial-- Step 3: Additional Study Modifications and Running**

You have now finished changing state variables, site constants, and loadings with the Wizard. Now check to make sure that N is as TN, P as TP, and Suspended and Dissolved Detritus as BOD by double-clicking on each in the state variable list in the main screen ("Nitrate," "Total Soluble P," and "Susp. and dissolved detritus.") In the last of these three screens, the % refractory and % particulate detrital allocations are 20% and 10%, which do not need to be adjusted; however, they could be quite different if a factor such as leaf fall were important.

Click on **Site** and then **Edit Underlying Site Data** to review and change other site constants. Altitude should = 760 m; Total Length for Phytoplankton Retention = 63 km (distance to Diversion Dam). This last parameter is located toward the very bottom of the screen.

Click on **Setup** and choose **Run model in spin-up mode** so that the biotic end conditions will be used as the initial conditions in the next simulation. (Turn this off when you have a fully calibrated model.) Also, unless storage space is a problem, choose all the state variables for saving rates (click on **Save Rates** and **Rate specifications** and then on >> to move all variables into the save column).

Be sure to save the study! Then click on **Control** to run the model. You will get a reminder that it is in spin-up mode, which you should ignore; you will also get a warning that there is zero habitat for adult largemouth bass—cancel, double-click on bass in the state variable list, and set % Pool = 50%. The once again click on **Control**.

### **Stream Tutorial-- Step 4: Examining Model Output and Importing External Data**

When run is complete, click on **Output**. The observed data from Rum River will still display, so choose **External Data** from the pull-down menu in the upper right corner of the screen. Delete "Obs. chlorophyll a" and select "Obs. periphyton chl a" (we will keep the title and units). Click on **Import Data** and choose "Mid peri chl norm.xls." You may wish to open the file first in Excel to make sure where the data are located; in this case the default sheet 1, row 1, columns a and b are satisfied, so choose **Import** and overwrite data. When the data are plotted the simulation results will span only a short period compared to the observed data. Click on **Edit** and **Graph**

**date range reset** (in the upper right corner). By choosing **Statistics from Graph** in the pull-down menu, you can get the statistics for the plotted variables. Also, from the pull-down menu (or right-clicking on the graph itself) you can **Copy, Print**, and alter the graph (using **Graph Setup**).

Click on **New**, choose **Custom Graph** and then label as "Depth" and select "Zmean (Dynamic)" to plot depth. You will see that a constant, initial depth is used. This is not realistic for a stream that is hydraulically regulated for purposes of seasonal irrigation. Therefore we will change the way that mean depth is modeled.

Exit Output and click on the large **Site** button and **Show Mean Depth Panel**; choose **Import and Change**, then **Import** "Midd Depth.xls" and re-run simulation (perhaps saving results as "perturbed" to help see the effects of this change). "Midd Depth.xls" was created using Manning's equation with observed discharge in an Excel spreadsheet originally calibrated for the Glenwood Bridge site on the Lower Boise River (Glenwood Depth Discharge calibration.xls). The new model result fits the sparse periphyton data equally well, but is more defensible.

You may wish to run the simulation over again to obtain better initial conditions for the animals due to spin-up mode. Remember to turn off spin-up mode when you have obtained a calibrated model.

Also, click on the "save-as" icon often to save the study. Saving iterative versions of the model under different names along with a log file that describes changes between versions is recommended.