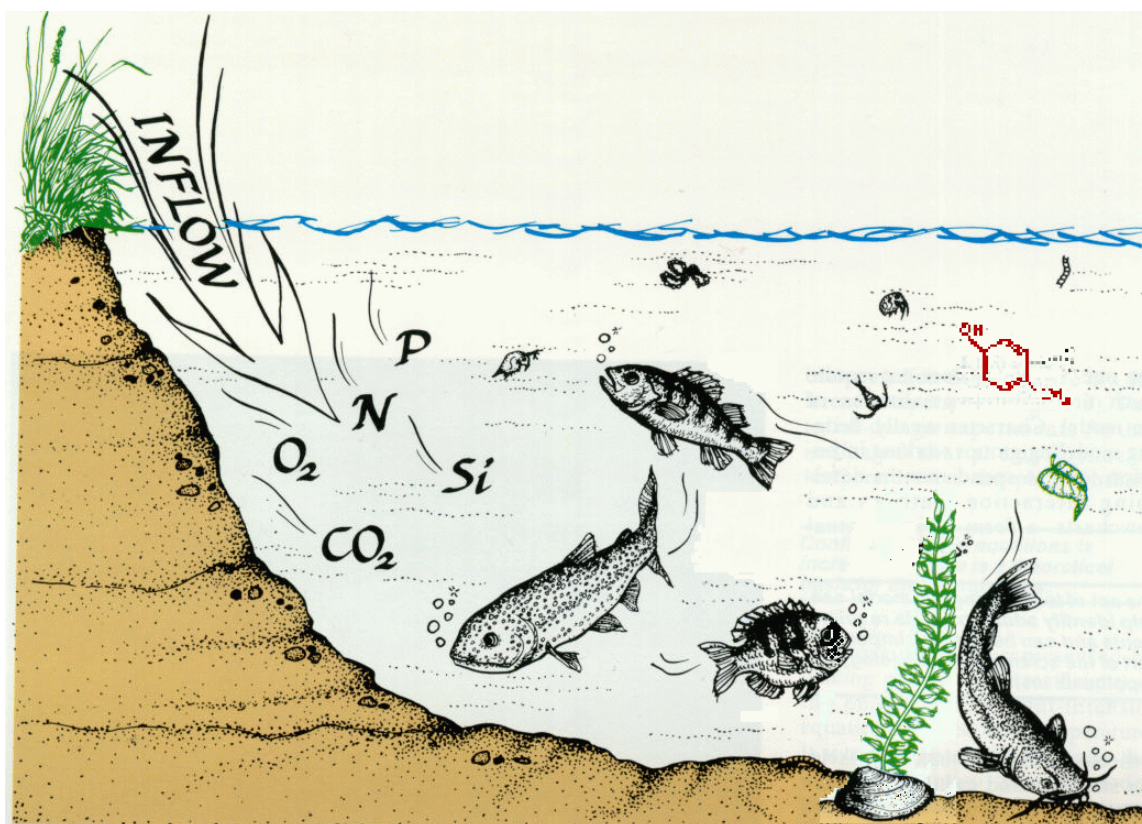




# AQUATOX.NET (RELEASE 1.0 alpha)

## MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS

### DRAFT VOLUME 1: USER'S MANUAL



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

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**Date TBD**

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OFFICE OF SCIENCE AND TECHNOLOGY  
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## Disclaimer

This document describes the interface of the aquatic ecosystem model AQUATOX.NET, Release 1.0 plus. 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.NET (RELEASE 1.0 alpha) 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. AQUATOX 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 2012 and includes a steady-state diagenesis model for sediments, updated ICE data (toxicity regressions), modified denitrification code, and many interface enhancements.
- AQUATOX Release 3.1 plus was completed in 2014 and includes the option to model nutrient limitation in plants based on internal rather than external nutrient concentrations.
- AQUATOX Release 3.2 was completed in 2017 and includes an update to the database management system, an ASCII input/output option, a command-line version, and nearshore-marine-environment modeling updates, as discussed in the 3.2 *Technical Documentation*.
- AQUATOX.NET Release 1.0 was completed in 2022. AQUATOX code was translated to C#. The interface is an

## Installation Considerations

- TBA at deployment time.

## Loading a Study

For AQUATOX.NET a JSON text 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 the “**Load**” button in the upper left corner of the screen. In the “**Studies**” directory there is a choice of AQUATOX JSON study files to load.

When a study is opened, state variables are shown within the AQUATOX interface.

## 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. The window buttons moving from top to bottom are as follows.

The **Name of Simulation** 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 **Save** button allows the user to save the simulation and all archived results to a JSON file that can then be loaded with all parameters and driving time series.

The **Integrate** button starts the simulation. This date of the simulation run will be saved and a text description of the run can be added at the time of integration.

The Run Status label tells how many sets of archived results are included within the simulation at any time.



At the upper right of the interface is a panel showing **Databases of Parameter Values**. These databases are not attached to the JSON file and editing these databases will have no effect on the simulation unless a set of parameters is later loaded from the database into the simulation. More information can be found on this in [“Databases vs. Parameters in a Simulation.”](#) There are separate sets of parameters for Sites, Animals, Remin. Records (organic matter parameters), Chemicals, and Plants that can be edited via these buttons and then later brought into a simulation.

If you hit the **Help** button from the Main Screen, you will jump to this topic in the help screen. The **Help** button on other screens links to the appropriate subject in the help files.

The **Output** button brings up an interface to presents the results as a series of charts and graphs, or export archived results to comma separated format.

The **Multi-Segment Runs** button brings up an interface that allows a user to create and run multiple 0-D AQUATOX segments that have been linked together using data from the National Water Model.

In the center panel is a group of buttons to edit model parameters:

- **Setup** allows the user to set the dates of the simulation, and to specify various options such as the saving of biologic **rates**.
- The **Site** button loads the site characteristic screen for the current simulation.
- The **Org.Matter** button loads the remineralization record for the current simulation that can be edited by the user.
- **Plants** brings up an editable matrix of all plant parameters in the simulation.
- **Chemicals** brings up an editable matrix of all chemical parameters in the simulation.
- **Animals** brings up an editable matrix of all animal parameters in the simulation.
- **Diagenesis** brings up an editable set of parameters pertaining to the sediment diagenesis model (when relevant)
- **Food Web** brings up an editable matrix of trophic interactions for the study.

To the right of the center panel is a list of the state and driving variables in 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.

Clicking the “Edit” button, or double-clicking on any of the state or driving variables in this list will bring up the initial conditions and loadings associated with each of these state variables, and variable-specific parameters can also be edited from this window when relevant.

## Saving a Study

To save a file, click on the **Save** button at the upper left of the window.

## Working with Existing Simulations

### What is included in an AQUATOX JSON file?

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

- List of state variables and driving variables utilized and their loadings, 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";
- The graph library that has been produced for that simulation;

Databases of parameters are not included in the APS file, other than those parameters that have been "loaded" into a simulation and therefore have relevance to that simulation. There are separate JSON files that include databases (libraries) of parameters that can be loaded into a simulation as needed.

### Databases vs. Parameters in a Simulation

There is a basic dichotomy in working with AQUATOX. You have a choice of editing database JSON files 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.)

Sets of parameters that will be used repeatedly should be saved in the appropriate database. Each database in JSON format includes parameter values for a list of organisms, chemicals, or sites. Generally, editing of parameters should be done in the database 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.

It is the user's responsibility, though, to synchronize parameter values among studies. This can be done by saving a record to a database and then loading that record to each study.

See Also: [Types of Databases](#)

### 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 (on the opening screen after opening an APS file) 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 database.

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 by double-clicking on the name in the state variables list. 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 might 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 could be significant inputs to a reach or lake. These might 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 their 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.

Loadings associated with direct precipitation 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.

When working with a system with a relatively low retention time, such as a segment of a river, loading of floating biotic state variables such as phytoplankton can be important to properly characterize. These loadings are generally entered in units of milligrams per liter.

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

Also see the section titled "[Important Note about Dynamic Loadings](#)" describing how AQUATOX interpolates between data points.

## Importing and Exporting Loadings

Loadings and other time series can be imported from Comma Separated Value (CSV) format. The date should appear in the first column and the numerical value in the second column of the file.

### 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.

## Nutrient Loadings

To access this screen double-click on "Total Ammonia as N," "Nitrate as N," or "Total Soluble P" in the state variables list in the main window.

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, and other loadings are entered as Total N, by selecting the "Nitrate inputs represent Total N" radio button, model inputs are located in the "Nitrate" initial conditions and loadings screen and loadings on the ammonia screen 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

To access this screen double-click on the "Susp. and dissolved detritus" in the state variables list in the main window.

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 Carbonaceous **Biochemical Oxygen Demand** (CBOD) and the model will make the necessary conversions. See the technical documentation for more information about how the model converts organic carbon and CBOD 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 the section titled ["Important Note about Dynamic Loadings."](#)

### Temperature Data Screen

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

The annual mean and range in temperature from the site parameters screen can be used or a 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.

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** in 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 may be 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 from the ground surface 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, visible when "**Use Default Time Series**" is chosen.

For more information on wind, see section 3.7 of the technical documentation.

### Light Loadings Screen

To access this screen double-click on "Light" in 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 Langleys/day. If annual mean and range are used, these parameters must be filled-in in the site parameters screen.

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

Conversions into Langleys 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 the section titled "[Important Note about Dynamic Loadings](#)."

### pH Screen

To access this screen double-click on "pH" in 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 "Water Volume" 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 might 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 rate can be input as an annual evaporation rate on the site parameters screen or using a time-series import available on the site-type screen. When available, a known time series can be entered or imported.

### **Water Volume Modeling Notes:**

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

The **Manning's 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 parameters 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:

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

## 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 **databases** of parameter values that may be loaded into a simulation. These databases can be reached by clicking on the Sites, Animals, Remin., Chems, and Plants buttons available at the upper right of the main AQUATOX interface..

The **Chemical Database** 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 **Parameters**. See also: [Chemical Data Screen](#).

The **Animal Database** 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 **Parameters**. See also: [Animal Data Screen](#).

The **Plant Database** 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 **Parameters**. See also [Plant Data Screen](#).

The **Site Database** 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 **Parameters** button that appears. See also [Site Data Screen](#).

The **Remineralization Database** 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.

To add a new database entry a new row may be added to the bottom of the matrix.

When you are editing the parameters that apply to a simulation, you can load those parameters from the library file by clicking on the **Load** buttons at the top right of the screen.

## Chemical Properties and Fate Data Screen

This screen can be accessed by clicking on the "Chemical" button on the main screen or double-click on "Dissolved org. tox." on the state variables list in the main window.

Required chemical 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

A few of the parameters on this screen are “greyed out” as they are not currently utilized by the model (e.g. “Solubility” and “Vapor Pressure”). These parameters have not been completely suppressed so that data in the database are not lost and in case these parameters become useful in the future.

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 Parameters”** as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this way, a user can use this appendix as a reference to search the technical documentation and find all equations and related parameters. 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.

## Plant Data Screen

To access this screen double-click on a plant name in the state variables list in the main window and choose Parameters or by accessing the plant library.

Several fields near the top of the screen require explanation. If you click on the drop-down 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.

If a plant is “surface floating” it is assumed reside in the top 0.1 m of the system unless wind distributes it to the top 3 m based on Langmuir circulation. The averaging depth for surface floating plants, when calculating plant concentrations (mg/L), is assumed to be the top three meters to more closely correspond to monitoring data.

The capability to model internal nutrients in algae was added just prior to release of AQUATOX 3.1plus. Consequently, there was limited time to calibrate the enhancement. The user must consciously choose to model internal nutrients by checking that option in the Setup screen. However, to ease the transition, six parameters that are unique to modeling internal nutrients are populated with default values taken from the documentation of WASP7 (Ambrose et al. 2006).

The effects of modeling internal nutrients were investigated for all studies supplied as examples with the AQUATOX installation. As might be expected, the nutrient-poor sites exhibited the greatest response to luxury uptake of nutrients, but default parameters cannot be used as-is and require the most recalibration. Where there were sufficient observed data to evaluate the results,

the applicability of the internal-nutrient submodel is noted. In general, the following sites benefited from modeling internal nutrients: Cahaba River AL, Evers Reservoir FL, Lake Onondaga NY, Tenkiller Reservoir OK, and Rum River MN. The following sites showed a tendency to over-predict algal biomass (and dissolved oxygen): Blue Earth River MN, Crow Wing River MN, DeGray Reservoir AR, and Lake Jesup FL.

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 drop-down 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 phytoplankton mortality coefficient can be adjusted for a particular site;
- The exponential mortality coefficient (which increases the mortality for suboptimal conditions) might 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.
- The sedimentation rate (phytoplankton only) should be small for streams and much larger for lakes;
- The Critical Force (FCrit) (periphyton and macrophytes only) for scour is quite important for periphyton; and
- 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 Parameters"** as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this way, 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.

## Animal Data Screen

This screen displays all of the relevant parameters for the animal that has been selected. To access this screen double-click on an animal name in the state variables list in the main window

and choose Parameters.

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.

AQUATOX can model two size classes for each fish species. Records for different size classes are linked by clicking on **Size-Class Links** (under the Animal Name towards the top of the screen) and choosing the correct record from the list given.

As was the case in the Plant Data Screen, the choice of **Animal type** is important because different animal 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 4.7 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. (These parameters are not on the chemical toxicity screen since they are not organic-toxicant specific.)

If an organism resides in a stream, the habitat-type within the stream should be specified using the **percent riffle**, **percent pool**, and **percent run** parameters. This affects the water velocity the organism is exposed to and also potentially excludes the organism from some water segments on the basis of habitat availability.

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, maximum consumption and endogenous (basal) 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);
- The minimum prey for feeding affects the efficiency of foraging behavior;
- The optimum temperature can have a significant effect on biomass computations;
- Intrinsic mortality rate ("mortality coefficient") is often a site-specific response and is therefore subject to calibration;
- Allometric means the change in metabolic rate in relation to the size of the organism; allometric parameter values can 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 Parameters**" as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this way, 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.

#### **Trophic Interaction Matrix Screen:**

This screen is accessed from the "Food Web" button on the "Main" screen.

The matrix 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 model is executed.

#### **Site Information**

This screen displays all of the relevant parameters for the site. To access this screen, click on the "Site" button on the main window.

At the upper left is a panel that allows a user to select which site type is being simulated. Six site types are available: pond, lake, stream (creek or river), reservoir, and (experimental) enclosure, and marine.

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:

- Manning's coefficient may be used to model water volume;
- periphyton scour and velocity limitation for plants is a function of water velocity;

Additionally, a user may edit a **site's parameters** from this screen.

Parameters that may be edited on this screen in a time series or constant manner are accessed by the pull down menu labeled "Site Time Series" at the center top of this screen.

- "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 site parameter record is not relevant.
- "Fraction of site that is shaded." See [modeling shade](#).

## 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 **Parameters** in the **Site Data** window, or they can be loaded from the **Database**. 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 (see equation 8 in the Technical Documentation). 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. This can also affect phytoplankton retention time in flowing systems as well as the calculation of cross-section area for velocity calculations.

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, in the **Light Screen**, if 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** on the Site Data screen, 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, although 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 might 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 "Site Length" 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** panel on Site screen) the **Stream Data** button in the upper right is enabled. Clicking this button displays a series of important stream parameters regarding site morphometry, and habitats represented.

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 Parameters**" as well as their manner of referral in the equations of the technical documentation (often a shorter variable name). In this way, 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. These parameters are accessed from the "Remineralization" button at the lower left of the screen.

Many of the parameters on the remineralization screen can be assumed to remain constant from one simulation to another. A few highlights may be worth examination because they can both be site-specific and can affect some types of model results:

- Maximum degradation rates: These rates should be modified if site-specific data are available.
- Detrital Sedimentation Rate (KSed): This rate 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 multiple Remineralization records included in the model:

- 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.

If your site has very different characteristics governing remineralization, you can edit one of the existing records or create your own.

## Modeling Shade

Shade can be an important limitation to light, especially in riparian systems. A user input "**Fraction of site that is Shaded (canopy covered)**" 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** checked on the Site Parameters screen, the mean depth calculation is irrelevant. In this case, mean depth is volume divided by surface area.

## Setup Parameters

The "Simulation Setup" screen specifies important parameters about the simulation itself (as opposed to any of the components of the simulation.) To access this screen, click on the **Setup** button on the main window.

### Simulation Time and Relative Error

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

Default model behavior is to use a variable step size Runge Kutta as described in section 2.1 of the technical documentation. 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 might wish to experiment for a particular application.

A **fixed step size** may also be selected with time step varying from one tenth to one hundredth of a day. This may be useful when a user is precisely comparing "control" and "perturbed" runs and so wishes to have their stepsizes be precisely aligned. More information about this can be found in section 2.1. of the technical documentation.

### Output Storage Options Parameters

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

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.

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 uncheck this box (output predictions that occur exactly at a given time-step).

### Biota Modeling Options Parameters

Selecting the option to **Model Nutrients Internally** will populate the model with additional state variables that track changes to internal nutrient concentrations (N and P) in non-rooted plants. See *Internal Nutrients* in section 4.1 of the AQUATOX Technical Documentation for more information about this optional model. Concentrations of internal nutrients will be output in units of ug/L or the "N to org" and "P to org" ratios may be viewed as they change over time. Some additional plant parameters are required, see the section on the ["Plant Data Screen"](#) in this document.

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.

### Chemical Options Parameters

This panel is accessed using the collapsible "show" or "hide" button.

If you wish to compute steady-state BAFs, you might want 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.

The chemical concentration in bottom-sediment organic matter can become a driving variable when **"Tox. in Sed. Detr. is driving var."** is checked. This allows the user to specify a time-series of sediment chemical concentrations to drive the model and examine the extent of bioaccumulation and effects on the ecosystem.

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.

If **"T1 is an aggregate of all other toxicants in study"** is checked, then the organic chemical in compartment T1 is used to aggregate all of the other chemicals being modeled as discussed in section 8.14 of the Release 3.2 *Technical Documentation*.

## Rate Output

In the Setup Screen, choose the **Save Derivative Rates** radio button. 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.

Two light limitation outputs 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 1.0. When photoinhibition is occurring then the HighLtLIM is equal to the overall light limitation and "low light limitation" is set to 1.0.

## Integrate Button (running the model)

To run an AQUATOX simulation, click the "Integrate" 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 can use the output button to view the model results.

## Multiple Archived Simulations

A powerful feature of AQUATOX is that it can run paired simulations for perturbed and control conditions.

## Output Screen

The "Output" screen is accessed from the Output button on the **main screen**.

At the upper left of the window, the user may select which set of **Saved Simulation Results** that should be graphed or exported. Individual archived results sets may be deleted by selecting them from the pull-down box and then selecting **Delete**. A full set of archived state variable results may also be exported to comma-separated value output using the **Save CSV** button.

## Viewing Existing Graphs

To determine which graphs have been produced for the given archived simulation, click on the drop-down box under **Saved Graphs**. If there is more than one graph included, a drop-down list

of graphs will be shown. The user can select a graph within this list and it will update on the chart canvas below.

To add a new graph to the list of graphs in the graph library select the "**New Graph**" button. To edit the existing graph, select the "**Edit**" button. The selected graph may also be deleted using the "**Delete**" button.

### Setting Up a New Graph

When the "**New**" button is pressed, a user will get to the **Graph Setup** window. By clicking on the "**Edit**" button above a graph, one can also get to this 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 the topic [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.

#### 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
- Sediment diagenesis state variables
- Toxicant PPB
  - T1-T20 (PPB) in organic matter, plants, invertebrates, and fish
- State Variable Rates
  - These include limitations to photosynthesis

The user can 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 that all variables on the same axis should have the same units.

### Selecting from a List of Output

The list of outputs is initially populated with state variable results. These can be limited to **Animals** and **Plants** variables by selecting those check boxes.

When "**Include Rates**" is selected, there are potentially hundreds of output variables associated with each simulation, as individual components of each state variable's derivatives are output.

To help the user pick out relevant variables to be graphed, the "**Has Substring**" edit box 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.

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.

## 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 might not require such detailed nutrient information. In this case, a user might 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 the 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 might 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 IMPORTANT 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)
- CBOD 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)

Not all loadings need to be precise. 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 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 might 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.
- **Marine:** Selecting this option primarily has effects on nitrification, denitrification, reaeration, and water-freezing temperature. See section 3.9 of the Release 3.2 *Technical Documentation*.

## 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 site morphometry, nutrients, organic matter, suspended sediments, 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 save the APS file to a new name and then examine the following components for compatibility with the site being modeled

- Physical characteristics (site parameters)
- 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 (i.e. without using a surrogate simulation) 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. In some senses this might 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 Manning's Equation, 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 can 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, which brings up the "Insert State Variable" screen and its list of available state variable compartments). When adding fish, the wizard is especially useful as size-class and age-class linkages will be automatically set up through the user interface.

If you are modeling an animal, chemical, or plant state variable for which there are no database parameters available, you will first need to create a new set of parameters for your state variable in the relevant AQUATOX database. Often it is best to use an existing database record most

similar to your new addition and modify as necessary. See the section on [parameters](#) for more instructions on adding a new database entry.

### Adding a Chemical

To add a chemical in AQUATOX select one of the 20 available toxicant compartments (usually "Dissolved org. tox 1") on the "Insert State Variable" screen. You will then be prompted as to which chemical to load from the chemical database. Loading this chemical brings in parameters 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 parameters, the toxicity linkages may be entered individually by choosing the appropriate group in the dropdown in the "Toxicity Record" field 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) on the "Insert State Variable" screen and then choose the plant data you wish to load from the plant database. 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) on the "Insert State Variable" screen and then choose the animal data you wish to load from the animal database. 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. The Wizard interface is especially useful for adding fish state variables.

### Using Sediment Bed Models and Data Requirements

Inorganic sediments can have significant effects on light climate and inorganic sediment effects on biota can also be explicitly modeled. AQUATOX.NET contains two options for inorganic sediment submodels:

1. TSS Model: The TSS option is a simple model based on a regression relationship between sediment deposition and total suspended sediments. This option also ensures that the effects of inorganic sediments on the light climate of the water column are properly represented. This approach should be used when the only inorganic sediment data available are TSS. This option also assumes that TSS does not undergo any degradation or other reactions while within the AQUATOX reach. Add the "TSS" state

variable to use this option.

2. **Sediment Diagenesis Model:** The sediment diagenesis model implements the sediment diagenesis model as presented in *Sediment Flux Modeling* (Di Toro, 2001). This model provides a more sophisticated accounting of the decay of organic matter and remineralization in an anaerobic sediment bed and the effects on sediment oxygen demand and nutrient flux into the water column. The diagenesis model assumes a depositional environment; scour of sediments is not incorporated. This model is best suited to represent predominantly anaerobic sediments in eutrophic lakes. This model may be selected under the sediment menu by choosing "Add Sediment Diagenesis." This action adds the "Sed Layer(s)" button to the main screen, which can be used to access the sediment diagenesis parameters.

*Note, the Sand-Silt-Clay Model was not brought forward into AQUATOX.NET at this time.*

*Note, the Multi-Layer Sediment Model was not brought forward into AQUATOX.NET at this time..*

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. The model will utilize this option if none of the four models above have been added to a simulation. The model will always track the remineralization of organic material within the sediment bed and the water column.

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

These detrital compartments are assumed to be located in the active layer and available for consumption and sorption-desorption of chemical from-to the water column. Through long-term deposition, these compartments may become deeply buried and join the buried detritus state variables. Buried detritus is considered to be non-reactive. Nutrients within the sediment 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 can 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 can 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.

### Sediment Diagenesis Model

Di Toro's (2001) 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 might not be appropriate.

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

- **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).
- **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.
- **COD:** Driving variable for chemical oxygen demand in the water column that affects the flux of sulfide to the water column (optional, and to be differentiated from carbonaceous "CBOD").

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

AQUATOX.NET includes the option to "**Model Diagenesis Layer 1 as Steady State.**" When this option 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 (2001) sediment diagenesis model. As noted in the interface, this process significantly speeds model execution (by up-to a factor of 10), but might have an effect on the mass balance of nutrients. However, effects on overall model results are generally quite minor. 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 rapidly become a function of organic matter deposition and can 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). Initial conditions for the variables, with the exception of COD, are entered on the Diagenesis Model Setup screen.



Selecting the Edit Diagenesis Parameters button on the Diagenesis Model Setup screen brings you to a large set of "**Diagenesis Parameters**" that also govern the behavior of the model. Most of these may be kept constant from site-to-site but Di Toro (2001) 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 can be saved to Excel using a button on this screen.

Setting the initial condition for the organic matter sediment diagenesis state variables can 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.

## 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.

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 change in parameter value.

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 might be quantitative if biomass data exists for a site or it might 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 can be undertaken.

The user should 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 generally 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 the 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 could be combined for a more robust calibration, but at the expense of the loss of the validation data sets; this combined approach should be avoided if possible.

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

## Multi-Segment Runs

AQUATOX.NET contains the capability to link multiple segments based on COMIDs and stream-flow networks and using water flows from the national water model. The sequential process of running a multi-segment model is as follows.

1. **Base JSON:** Choose a template 0-D AQUATOX segment to form the basis for the multi-segment simulation. This template segment should contain all the state variables that the user wishes to model (in every segment of the simulation). State variables should be added or removed from the 0-D segment prior to specifying that JSON in the multi-segment interface. The state variable list must be the same in all modeled segments.
  - a. **Choose Template** (optional): this button brings up a check-box interface that allows the user to select which elements they wish to include in the base JSON and then selects an appropriate base JSON for the simulation. For the *alpha* version of the model, only nutrients and organic matter are included in template segments.
2. **Output Dir:** Choose a directory in which JSONS regarding individual segments, stream-network information, and the master-setup record will be stored.
3. **Read Stream Network:** By specifying the COMID that will be the end-point for the simulation and selecting an up-river span or an (optional) upper-limit COMID and then selecting **Read Network**, the stream network of COMIDs will be read from web service and saved to the output directory as a JSON. (If a StreamNetwork.JSON file already exists in that directory it will be overwritten.)
4. **Master Setup:** This brings up the setup record indicating the start date, end date, and integration options for the linked system. This setup record will be read from and used each time the model is executed.
5. **Create Linked Inputs:** This button reads water flows and water velocities from the national water model (NWM) and creates a separate JSON simulation for each COMID in the stream network. Water flows from one reach to another are imported based on NWM flow data. The time-series volume of each COMID is specified based on the length of the COMID and the NWM flow and velocity.

$$\text{volume (m}^3\text{)} = \text{flow(m}^3\text{/s)} / \text{velocity(m/s)} * \text{sitelength (km)} * 0.001 \text{ (m/km)}$$

After linked inputs are created, individual JSONs will be found in the output directory labeled with COMID. These JSONs may be loaded into the single-segment interface. Initial conditions, point-source, and non-point-source loadings may be edited within these files before executing the network in step seven below. At the inflow boundary of the stream network, boundary condition inflow loadings should also be specified. (Inflow loadings for downstream segments will be overwritten when the stream-network is executed.)

6. **Overland Flows:** Optional. This button allows the user to specify non-point-source loadings for each segment in a constant g/d for nutrients and organic matter through a matrix input.
7. **Execute Network:** This button will start the simulation's execution. Each AQUATOX simulation will be run in the order specified in the stream network file—multiple segments will be run in parallel when possible. The water-quality components from upstream segments will automatically be added as loadings to downstream segments. After the

simulation is run, model results will be saved in new JSONS in the output directory labeled AQT\_RUN\_{COMID}.JSON. These segments may be examined, run, and output graphs may be produced in the main AQUATOX interface.

8. **View Outputs:** By selecting a state variable from the SV Index drop down box, graphs of all segments over time will be produced. The CSV button will display a comma-separated value matrix of model results that may be exported into spreadsheet software for further analysis.

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