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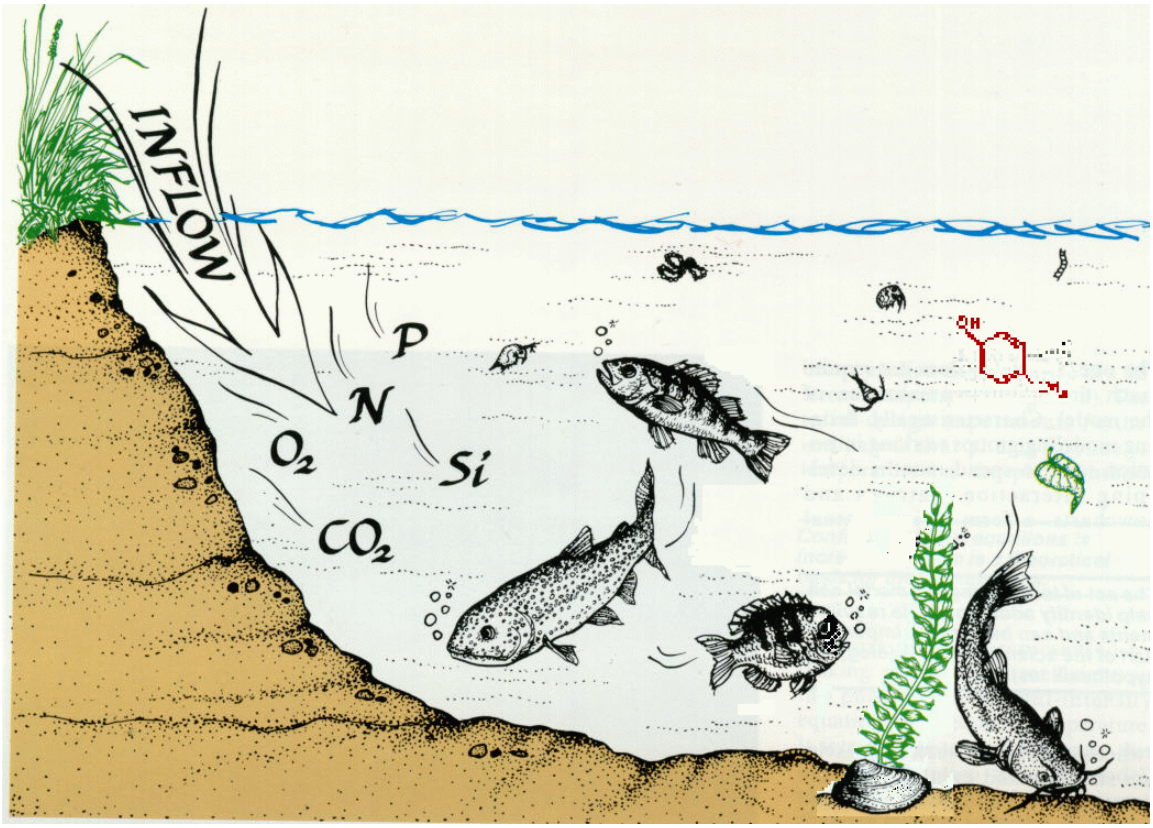
AQUATOX DOT NET (RELEASE 1.0 beta)

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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CENTER FOR EXPOSURE ASSESSMENT MODELING

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Disclaimer

This document describes the interface of the aquatic ecosystem model AQUATOX DOT NET, Release 1.0 beta. 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 DOT NET (RELEASE 1.0 beta) 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 the following: 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 the following: 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 DOT NET 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 its 3.2 *Technical Documentation* (U.S. Environmental Protection Agency. 2018).
- AQUATOX DOT NET Release 1.0 was completed in 2024 AQUATOX code was translated to C# in Microsoft Visual Studio. The interface was simplified to some degree, and a new multi-segment model capability is available that includes links to external model and data sources for stream networks, nutrients and sediment loadings, and water flows.

Installation Considerations

- TBA at deployment time.

Single-Segment Mode and Multi-Segment Mode

At the time of model startup, a user is prompted as to whether to run the model in single-segment mode or multi-segment mode.

Single-segment mode represents a single well-mixed compartment (0-D) in which to model nutrients, chemicals, and ecology. Multi-segment mode represents many 0-D segments linked together that are then run sequentially. In multi-segment mode, data may be imported from the NHD Plus, for stream-network information, the National Water Model for water flows and lake/reservoir volumes, and HAWQS/SWAT for nutrients, sediments, and water flows.

By returning to the initial splash screen and pressing one of the buttons again, Multiple single-segment or multi-segment mode windows may be opened at the same time. This enables multiple simulations to be running at the same time, or model outputs may be compared on adjacent windows.

Single-Segment Simulations

Loading a Simulation

For AQUATOX DOT 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 simulation files to load.

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

The Main window

The main window includes the name of the simulation, the list of state variables used, and buttons from which to choose various operations.

The **Name of Simulation** field (top center) can be edited; it is separate from the name of the JSON file you loaded, which is displayed in the pathway at the top of the screen.

The window buttons and labels moving from top to bottom down the left side are as follows.

The "**Load"** button was discussed in the previous section, Loading a Simulation.

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

Edit Setup allows the user to set the dates of the simulation, and to specify various options such as the saving of biologic rates.

The **Run** button starts the simulation. The date of this 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.

If you hit the **Help** button from the Main window, you will jump to this topic in the on-screen version of this User's Manual. The **Help** button on other screens links to the appropriate subject in the on-screen version of this User's Manual.

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

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 "Parameters within Database Files vs. Parameters within in a Simulation." There are separate databases for Sites, Animals, Remin. Records (i.e., remineralization or organic matter parameters), Chemicals, and Plants, respectively that can be edited via these buttons and then later imported into a simulation.

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

- 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.
- The **Plants** button brings up an editable matrix of all plant parameters in the simulation.
- The **Chemicals** button brings up an editable matrix of all chemical parameters in the simulation.
- The **Animals** button brings up an editable matrix of all animal parameters in the simulation.
- The **Diagenesis** button brings up an editable set of parameters pertaining to the sediment diagenesis model (when relevant)

- The **Food Web** button brings up an editable matrix of trophic interactions for the simulation.

To the right of the center panel and below the Databases of Parameter Values is a list of the state and driving variables in the simulation. Variables can be added to or deleted from this list using the **Add** or **Delete** buttons, respectively, at the bottom of the list.

Clicking the "Edit" button below the list of state and driving variables, 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 the selected state variables. For animals, plants, and chemicals, parameters defining the state variable's characteristics can also be edited from this window.

You may also "Add" or "Delete" variables from this list. Note that the food web may need to be updated following this procedure.

Note: if no simulation has been loaded, several buttons/locations of information will not be displayed; only the following can be seen:

- Load, Save, Help, and Multi-Segment Runs buttons (on the left side)
- Run Status label but without detail (on the left side)
- Name of Simulation label and empty field
- Databases of Parameter Values panel with its five buttons (upper right side)

Saving a Simulation

To save a simulation to a JSON file, click on the **Save** button at the upper left of the window. The JSON saved will include all model parameters, driving time series, and sets of model results. The user will be prompted whether to overwrite the original parameters or save these parameters as a new file.

Working with Existing Simulations

What is included in an AQUATOX JSON file?

The AQUATOX JSON simulation file is the basic unit in which AQUATOX simulations are loaded and saved. Each JSON simulation 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 attached to the loaded JSON simulation file, and editing these databases will have no effect on the simulation unless a set of parameter values is later loaded from the parameter database into the simulation. These databases of parameters are provided as separate JSON files that include libraries of subject-specific parameters that can be loaded into a simulation as needed.

Parameters within Database Files vs. Parameters within in a Simulation

There are two approaches to working with parameters in AQUATOX.. You have a choice of editing specific (animals, plants, etc.) parameter database JSON files or of opening and editing a particular simulation file.

The parameter database files are stand-alone files that do not affect model results unless some or all of their contents are loaded into a simulation.

Simulation files are self-contained JSON files with all the information intended for a particular simulation, including initial conditions, loadings, parameter values, first and last dates for the simulation, and simulation results. Within the simulation file, parameter values can be edited, but those changes will apply *only* to that simulation. 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.

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 going to be used only for a single simulation, it may be desirable to create a unique set of parameters within the simulation.

It is the user's responsibility, though, to synchronize parameter values among studies. This can be done by saving a set of parameters to one of the existing databases and then loading that record to each simulation.

See also the section on parameters.

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 a JSON 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 window 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, the trophic interaction records will usually require modification. The best way to access trophic interactions is by selecting **"Food Web"** on the Main window.

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 conditions.

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 characterize properly. 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 Loadings

Loadings and other time series can be imported from Comma Separated Value (CSV) format files using the "Import from File" button below the list of loadings. 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 execution date of 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 on the day before and after the spike loading.

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 Release 3.2 technical documentation (U.S. Environmental Protection Agency. 2018).

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 **CBOD** (Carbonaceous Biochemical Oxygen Demand) and the model will make the necessary conversions. See the AQUATOX Release 3.2 technical documentation (U.S. Environmental Protection Agency. 2018) for more information about how the model converts organic carbon and CBOD loadings into organic matter.

By selecting the "Loading Type" dropdown, the type of variable input may be specified. 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 (µg/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^2, and the loadings are given as mg/L. Associated toxicants are given as µg/kg (ppb).

See section 5.1 of the release 3.2 technical documentation (U.S. Environmental Protection Agency. 2018) 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.

For more information on temperature modeling, see section 3.5 of the release 3.2 technical documentation (U.S. Environmental Protection Agency. 2018). 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 time series 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**.

For more information on wind, see section 3.7 of the release 3.2 technical documentation (U.S. Environmental Protection Agency. 2018).

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 on the site parameters screen.

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

See section 3.6 of the release 3.2 technical documentation (U.S. Environmental Protection Agency. 2018). 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 (U.S. Environmental Protection Agency. 2018) 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:

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

where:

Volume = site volume in cubic meters,
t = time in days, and
Inflow, Outflow, and Evaporation = fluxes in cubic meters per day.

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 **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 **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 **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.

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 **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.

To add a new database entry, add a new row 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 window 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 coefficients can be calculated dynamically or entered manually by the user. Sorption to inorganic sediments is relevant only when the multi-layer sediment model is incorporated.

Parameters on this screen govern the chemical fate processes of

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

A few of the parameters on this screen are "grayed 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** (U.S. Environmental Protection Agency. 2018) 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 (U.S. Environmental Protection Agency. 2018).

Chemical Bioaccumulation and Toxicity

This screen is where all of the chemical toxicity parameters are located. To get to this screen, use the "**Toxicity and Bioaccumulation**" 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). The radio buttons at the bottom of the animal and plant toxicity boxes allow the user to select which uptake and elimination model they wish to use.

- **Enter K2, Calc. K1 and BCF:** This is the default model formulation. The K2 elimination rate must be entered on the matrix, but K1 and BCF will be calculated using the model's equations.
- **Calc. BCF** (from K1 and K2): K1 and K2 must be entered by the user and the BCF will be estimated.
- **Calc. K2** (from K1 and BCF): K1 and BCF must be entered by the user and the elimination rate (K2) will be estimated.
- **Calc. K1** (from K2 and BCF): K2 and BCF must be entered by the user and the uptake rate (K1) will be estimated.

If the user has toxicity data for only a few species, an extensive library of regressions (Interspecies Correlation Estimation, or Web-ICE) may be accessed at https://www3.epa.gov/webice/.

The animal toxicity parameters are as follows:

Animal Name, must match the "toxicity data" record in the relevant Animal Data screen.

LC50, (µg/L), external concentration of toxicant at which 50% of population is killed

LC50 exp. time, (h), exposure time in toxicity determination

[Entered] **K2 Elim. Rate Const.**, (1/d), elimination rate constant

[Entered] **K1 Uptake Const.** (L/kg-d) optional uptake rate constant (dry weight)

[Entered] **BCF,** (L/kg) optional Bioconcentration Factor (dry weight)

Bio_rate_const, (1/d), Daily rate of biotransformation of this toxicant

EC50 growth, (µg/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., (µg/L), external concentration of toxicant at which there is a 50% reduction in reproduction

Repro exp. time, (h), exposure time in toxicity determination

Mean wet wt., (g), mean wet weight of organism

Lipid Frac, (g lipid/g organism), fraction of lipid in organism (wet weight)

Drift Threshold, (µg/L), concentration at which invertebrate drift is initiated

LC50 Slope, (species-specific slope at LC50 multiplied by LC50), LC50 slope factor for the external toxicity model. (Optional: if left blank or set to zero, the value from the chemical's underlying data is used.)

EC50 Growth Slope (species-specific slope at EC50 multiplied by EC50) EC50 slope factor for growth effects. (Optional: if left blank or set to zero, the value from the chemical's underlying data is used.)

EC50 Repro Slope (species-specific slope at EC50 multiplied by EC50) EC50 slope factor for reproduction effects. (Optional: if left blank or set to zero, the value from the chemical's underlying data is used.)

Note: there are several comment fields provided for documentation of parameter source citation or other notes.

The plant toxicity parameters are as follows

Plant Name, must match the "toxicity data" record in the relevant Plant Data screen.

EC50 photo, (µg/L), external concentration of toxicant at which there is 50% reduction in photosynthesis

EC50 exp. time, (h), exposure time in toxicity determination

EC50 dislodge, (µg/L), external concentration of toxicant at which 50% of algae is dislodged (not applicable for phytoplankton)

K2 Elim. Rate Const, (1/d), elimination rate constant

K1 Uptake Const. (L/kg-d) optional uptake rate constant (dry weight)

[Entered] **BCF,** (L/kg) optional Bioconcentration Factor (dry weight)

Biotrnsfm. rate const., (1/d), Biotransformation Rate

LC50, (µg/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)

LC50 Slope, (species-specific slope at LC50 multiplied by LC50), LC50 slope factor for the external toxicity model. (Optional: If left blank or set to zero, the value from the chemical's underlying data is used.)

EC50 Photo Slope (species-specific slope at EC50 multiplied by EC50) EC50 slope factor for photosynthesis effects. (Optional: if left blank or set to zero, the value from the chemical's underlying data is used.)

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 (U.S. Environmental Protection Agency. 2018) 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.

A 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 that 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 light extinction coefficient may need to be increased if algal growth is too strong—this coefficient may be the principal means of negative feedback, and can vary among algal groups.
- The sedimentation rate (phytoplankton only) should be small for streams and much larger for lakes.
- The Critical Force (FCrit. for periphyton and macrophytes only) for scour is quite important for periphyton.
- Salinity effects are relevant only 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** (U.S. Environmental Protection Agency. 2018) 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 (U.S. Environmental Protection Agency. 2018) 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 (U.S. Environmental Protection Agency. 2018).)

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 relevant only 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 (allometics).
- 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** (U.S. Environmental Protection Agency. 2018) 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 (i.e., 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 Parameters

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, U.S. Environmental Protection Agency. 2018). 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. This can also affect phytoplankton retention time in flowing systems as well as the calculation of cross-section area for velocity calculations.

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 (U.S. Environmental Protection Agency. 2018).

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 time period 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 National Oceanic and Atmospheric Administration (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; and
- 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 (U.S. Environmental Protection Agency. 2018) 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 method as described in section 2.1 of the technical documentation (U.S. Environmental Protection Agency. 2018). 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 step-sizes be precisely aligned. More information about this can be found in section 2.1. of the technical documentation (U.S. Environmental Protection Agency. 2018).

Output Storage Options

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

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 (U.S. Environmental Protection Agency. 2018) for more information about this optional model. Concentrations of internal nutrients will be output in units of µg/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

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

If you wish to compute steady-state Bioaccumulation Factors (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 (U.S. Environmental Protection Agency. 2018) 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 (U.S. Environmental Protection Agency. 2018).*

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 HighLt_LIM is equal to the overall light limitation and "low light limitation" is set to 1.0.

Run Button (running the model)

To run an AQUATOX simulation, click the "Run" 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 Window

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

At the upper left of the window, the user may select which set of Saved **Simulation Results** that will be graphed or exported. A set of 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. The results of an individual graph can be exported using the **CSV** button to the right of the screen.

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.

Once a graph is created you may choose to **Draw a box to zoom.** In this case, clicking and dragging a box on the graph will zoom into a particular set of dates or values. Alternatively, **clicking on the graph to show date and value** will display the time and value if a line on the graph is clicked on. You may toggle a log scale at the lower right (excluding graphs with zero values or negative values, of course).

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 and two Y axes. Use the "**<**" and "**>**" buttons to move results into and out of a particular axis's 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 outputs.
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.

Below 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.

- 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 may currently be used interchangeably but different site-types are provided for user clarification.
- **Stream:** Assumed to be moving water, streams have the following additional characteristics
    - Manning's coefficient may be used to model water volume;
    - 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 (U.S. Environmental Protection Agency. 2018), 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 (U.S. Environmental Protection Agency. 2018).*

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_AQUATOX DOT NET.pdf"** has been added to the STUDIES directory and 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 JSON 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)

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 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).
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 database as well as 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 with 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.

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.

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 DOT 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.

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

Note, the Multi-Layer Sediment Model was not brought forward into AQUATOX DOT 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 two approaches 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/m2 dry);
- Refrac. Sed. Detritus (Refractory Detritus in the Sediment bed) (g/m2 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 (U.S. Environmental Protection Agency. 2018).

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 to the left 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).
- Particulate Organic Matter (POM) variables:
  - **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.
- **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 relevant for only depositional regimes. No direct scour of sediment from the sediment bed is modeled.

AQUATOX DOT 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 (U.S. Environmental Protection Agency. 2018).

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, except for 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, and 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 (U.S. Environmental Protection Agency. 2018).

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 the way 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 a re-specification 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 (U.S. Environmental Protection Agency. 2018) 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 one of the following:

- New time-periods,
- New sites and exposure conditions, or
- 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 (U.S. Environmental Protection Agency. 2018).

Multi-Segment and Data-Linkage Mode

AQUATOX DOT NET can model multiple 0-D segments linked together. In this case, water, nutrients, and biota will flow through pre-defined (NHDPlusV2) river and lake networks within the continental US. It can also pull data from HAWQS/SWAT or the National Water Model for single segment simulations of hydrologic drainage basins or lakes and reservoirs defined within the NHDPlusV2 data set.

Modeling options are as follows:

- **Stream networks** based on NHDPlus flow lines linked together. These stream networks can include lakes and reservoirs as defined as an NHDPlusV2 waterbody. Stream segments are based on USGS COMIDs[1]
    - Water flows and time-series water volumes can be automatically imported from the national water model.

[1] COMIDs are "Common Identifiers" from NHDPlus data model version 2.1

    - Water flows, nutrient and sediments from boundary conditions and overland flows, water temperature, chlorophyll *a*, and dissolved oxygen can be imported using runs of the HAWQS/SWAT modeling system.
- **A single HUC** (Hydrologic Unit polygon boundaries) may be modeled as a segment.
    - Water flows, nutrient and sediments from boundary conditions and overland flows, water temperature, chlorophyll *a*, and dissolved oxygen can be imported using runs of the HAWQS/SWAT modeling system.
- **A single lake or reservoir** (NHDPlusV2 waterbody)
    - Water flows and water volumes can be automatically imported from the national water model

When working within the multi-segment window, all model files are saved in a single working directory. To start a new simulation, select **New Project.** This will bring up the below. After the spatial and temporal domain of the simulation has been set up, and the base simulation selected, clicking "OK" will exit this screen. AQUATOX will then ask for a directory in which the new simulation will be stored. Either a new folder can be created and selected, or an existing folder where there is no simulation, or a folder in which the user does not mind overwriting the existing AQUATOX simulation.

You can also toggle between a list of the most recent project directories using the "Recent Projects" pull-down menu.

Once a new project has been created a map of the simulation will be shown. A user can toggle between a log console and the map using the radio buttons below the map. Once the model has been run, a summary of model results across segments can be selected with the "Show Graph" button.

When the map is displayed, a user can zoom and pan by using the mouse wheel or dragging across the map with the mouse cursor. The "Reset Map" button will re-center and zoom the map to show the selected model domain. Different layers may be selected for view selecting the layers icon at the upper right of the map that looks like stacked papers. Other mapping options include:

- Show HUC14s—this displays the smallest size drainage basin included in the model. HUC14s are the native size for a HAWQS/SWAT simulation that will be linked to stream-segment results.
- Show Boundary Conditions – icons will be displayed that show boundary condition stream inputs. Green icons represent upstream boundary conditions and a single red icon represents the pour-point for the simulation.
- Labels – when selected this will display the COMIDs on the map.
- Show Non-Run Segments – when there is a lake or reservoir within a simulation some COMID stream segments are superseded by the larger lake/reservoir polygon. These segments are plotted when "show non-run segments" is selected.

Once the domain has been selected, the user can then follow the following steps to execute a simulation. In general, the workflow moves from the upper left of the screen to the lower left:

1. **Base JSON:** Choose a template 0-D AQUATOX segment to form the basis for the multi-segment simulation. **This is usually completed through the New Simulation Window, but can be modified here if that is desired.**

   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 the JSON in the multi-segment interface. The state variable list must be the same in all modeled segments to simplify the passage of

data. (Biotic state variables that are irrelevant in one segment may be set to zero in that segment, however.)

a. **Choose Template** (optional)**:** this button brings up the "below Simulation" interface that shows most of the relevant AQUATOX simulations that can form the basis of this new model.

2. **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.

   Note: When water flow and velocity data are read from the National Water Model, the dates specified in the setup record will be used to read time series inputs. Therefore, if the setup record dates change after "create linked inputs" is selected, the "create linked inputs" step will need to be repeated to query the correct time period. The interface creates a warning in this case.

3. **Choose your data source:**

   HAWQS Simulation: This will enable the user to set up and run a HAWQS/SWAT simulation to provide data about water flows, nutrient and sediments from boundary conditions and overland flows, water temperature, chlorophyll *a*, and dissolved oxygen

   NWM (flows only): This will import flows and water volumes from the national water volume, but the user must specify boundary conditions

   Note, when modeling 0-D HUC simulations, NWM data are not spatially aligned and therefore not relevant. Similarly, when modeling 0-D lakes and reservoirs, HAWQS/SWAT data are not spatially compatible, so NWM data is the only option.

4. (NWM chosen) **Create Linked Inputs:** This button reads water flows and water velocities from the National Water Model (NWM) and also saves a separate JSON input simulation for each COMID in the stream network in the base directory (named AQT_2D_[COMID].JSON).

   Water flows from one reach to another are imported based on NWM flow data. **Note:** This process may take several minutes depending on the number of segments in the model and the number of days in which water-flow data needs to be read from the web service.

   For lake segments, volume, inflows, and outflows are read from the National Water Model.

   For stream segments, a time-series volume for each COMID is specified based on the length of the COMID and the NWM flow and velocity.

   volume (m^3) = flow(m^3/s) / velocity(m/s) * sitelength (km) * 0.001 (m/km)

   After linked inputs are created, parameters for individual segments may be edited by clicking on the waterbody on the map. Initial conditions, point-source, and non-point-source loadings may be edited within the interface before executing the network in step five below.

At the inflow boundary of the stream network, boundary condition of nutrients or other state variables should be specified. (Inflow loadings for downstream segments will be overwritten when the stream-network is executed as these data will be passed from the upstream segment.)

5. (NWM Chosen) **Overland Flows:** Optional, and stream-network only. 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. If specified, these inputs will overwrite any other non-point source loadings in a segment before model execution.

4. (HAQS Simulation Chosen) **Run HAWQS:** This button will first identify the relevant domain for the HAWQS simulation and will then display a dialog that shows the HAWQS API parameters as documented here. For the most part, these parameters do not need to be changed and should only be changed by users familiar with the HAWQS/SWAT modeling system. The user must also input a HAWQS API Key that will be required to run the HAWQS model. To get an API key, contact TBA. Following this, the status of the HAWQS run will be shown on a progress bar in the Model Execution window. If the HAWQS run completes successfully, model results will be saved in the project directory and the model is ready for linkage.

6. (HAWQS Simulation Chosen) **Link HAWQS Data:** This button reads all of the HAWQS linkage data for water flows, nutrients, and sediment from the completed HAWQS simulation. This button will saves a separate JSON input simulation for each COMID in the stream network in the base directory (named AQT_2D_[COMID].JSON).

   For lake segments, volume, inflows, and outflows are read from the National Water Model.

   After linked inputs are created, parameters for individual segments may be edited by clicking on the waterbody on the map. Initial conditions, point-source, and non-point-source loadings may be edited within the interface before executing the network in step five below.

5. **Execute Network:** This button will start the simulation's execution.

   For stream networks, 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.

6. **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 export a comma-separated value matrix of model results that may be exported into spreadsheet software for further analysis.

Once a run has been completed, if "Click to Outputs" is selected, clicking on a stream line or waterbody will bring you to the output window that pertains to the segment selected.

New Simulation Window

Three types of simulations can be specified via the new simulation window.

Stream Network (with lakes): A stream network based on NHDPlusV2 flow lines that optionally includes lakes or reservoirs can be simulated. In this case, water flows and volumes can be specified from the National Water Model or the HAWQS/SWAT model linkage in which case nutrient, sediment, and other simulation data will also be available. Because HAWQS/SWAT does not explicitly model lakes and reservoirs, if a lake/reservoir is in the model domain the national water model will be used to estimate those water flows and volume calculations.

A **0-D** (zero dimensional) **lake or reservoir** may be simulated in which case inflows, outflows, surface area, and water volumes for the waterbody will be available from the national water model. (HAWQS/SWAT data are not available for this simulation type.)

One HUC: A single drainage basin (HUC or hydrologic unit code) of varying sizes. HUC8 is the largest size and HUC14 is the smallest. HAWQS/SWAT data will be used to estimate average conditions within the primary reach of the basin.

First, select which type of simulation you wish to model using the radio buttons at the top of the screen. Then you will select the geographic domain for the model.

If you are working with a **stream network model**, zoom the map close enough that the NHDPlusV2 stream segments start to render. These shapes are loaded to the interface via web service so it may take a moment for all of the shapes to be loaded. Click on the pour point (downstream) COMID to be modeled or enter the COMID number (if known) into the COMID entry box in "Parameters to Read Network." You must then specify an up-stream COMID, for a single stream segment, or a number of kilometers upstream, to capture all tributaries to the selected pour point (within that number of river kilometers). Then click "Read Network." If valid inputs have been specified, the selected stream network for the model will be rendered as red lines. The total number of stream segments in the model will be displayed under "Selected Model Domain."

For a **lake or reservoir model**, use the map to zoom into the waterbody of interest. You may use the mouse wheel or the "plus minus" icon at the top left of the map to change the zoom level. All waterbodies available in NWM are shown by default. Hovering the mouse cursor over one of the waterbodies will show its name or COMID. To select a lake or reservoir for your model, click on one of the waterbodies. It will turn red and the map will zoom into that shape. The simulation name may then be edited. The surface area of the shape is displayed and will be read into AQUATOX parameters once the simulation is set up.

For a **HUC simulation**, select the HUC size to display using the radio buttons above the map. HUC14 segments are smallest so you must zoom in to see those rendered. To select a single HUC for your model, click on one of the polygons. It will change color and the map will zoom into that shape. The simulation name may then be edited.

Once the domain for either type of model has been selected, the user can specify a template segment for the simulation and also the start and end date for the simulation. Clicking on the "Choose Template" button will show all of the relevant AQUATOX simulations that can form the basis of this new model. If the user wishes to select a different existing AQUATOX simulation file (JSON) than is contained in the matrix, the **Browse** button next to the choose template button may be chosen to select the file.

Following the template selection, the **Start Date** and **End Date** of the simulation may be edited as well using the calendar inputs at the lower left of this window.

If you click "OK" you will be prompted for a directory in which to store your simulation data.

Select Surrogate Simulation

Clicking "Choose Template" brings up a matrix that shows all of the available lake, reservoir, and stream segment files that can serve as a template for the multi-segment simulation being created, (or the 0-D lake/reservoir simulation). At this time, all state variables in each segment must be the same, so a single 0-D AQUATOX simulation will form the basis of this simulation.

This matrix shows the name, location, type of waterbody, and summaries of plants, and animals in each simulation. Clicking on the column headers will sort the matrix by that column. Clicking on one of the rows of the matrix will highlight that row and that simulation will form the basis of the multi-segment simulation that is being created, once the user selects "OK".

Tutorial

Simple Tutorial for a 0-D simulation

This tutorial introduces basic concepts and gets a user started with the AQUATOX interface.

Tutorial-- Step 1: Deleting and Adding a Plant

Open the file **Farm Pond MO Esfenval**. (See Loading a Simulation)

This study represents a generic pond built to USDA specifications. Esfenvalerate loadings are the worst-case scenario using runoff from an adjacent corn field.

First remove the macrophyte compartment (**Macrophyte1: [Myriophyllum])** by highlighting it in the list, and clicking on the **Delete** button. 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 be prompted as to which database you will load parameters from. Select the "default database" which is called "**PlantLib.JSON**. You will then see another dialog box allowing you to select from a list of plant-parameter datasets. This relates to the fact that the names of the taxonomic groups and ecologic guilds on the state variables list (on the main window) 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**.

Next, Setting an Initial Condition

Tutorial-- Step 2: Setting an Initial Condition

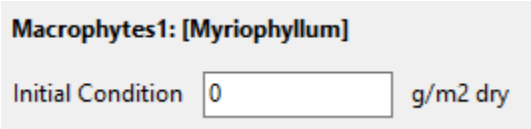
To continue with our macrophyte example, we should enter a value for the biomass of macrophytes present at the beginning of the simulation; if the value is left as 0 and there is no

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^2, which is appropriate for *Myriophyllum* in a temperate pond at the beginning of the growing season.

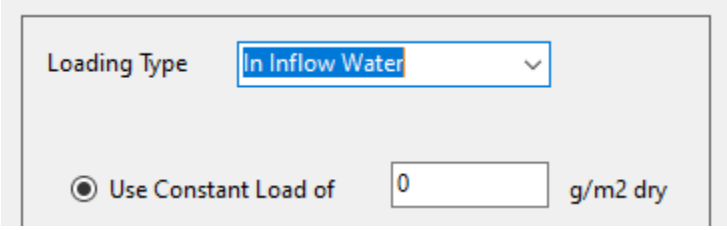
Double click on the state variable list on "Macrophytes1: [Myriophyllum]."

The Loadings Form is then displayed. There are three things we are looking at in this screen. First, the initial condition for the state variable is shown at the top left of the window. Ongoing plant loadings from up-river are shown in the panel below that. The drop-down list specifying Loading Type can be changed to view chemical concentrations within the macrophyte. For now, leave the Loading Type as "In inflow Water."

Enter 0.1 into the initial condition (in g/m2 dry weight).



You may also enter a loading in inflow water 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.

To add this "seed" loading add the value of 1E-5 g/m^2 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.

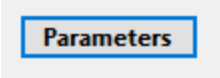
See Also: Initial Conditions and Loadings.

Next, Viewing Parameters in a Simulation

Tutorial-- Step 3: Viewing Parameters in a Simulation

In the following examples, we will examine the parameters associated with the animals, plants, and chemicals in this simulation. Parameters can be loaded from databases of parameters when adding a state variable as we did above (when we loaded *Myriophyllum*). Records can also be loaded from a **database** by choosing **Read from DB** when looking at parameters associated with the animal, plant, and chemical state variables.

We will examine first the plants parameters associated with *Myriophyllum*. From the loadings form, select the **Parameters** button at top of the screen.

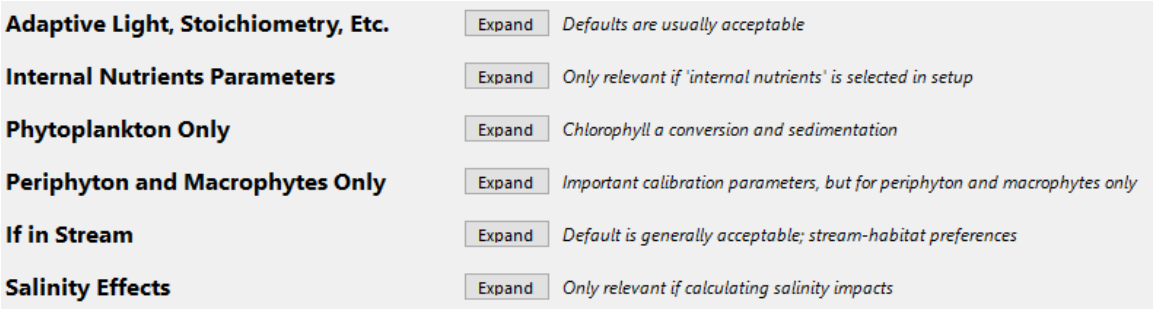


Plant parameters for *Myriophyllum* will then appear. Two fields near the top of the screen require explanation. If you click on the drop-down menu to the right of **Plant type**, you will be given a choice. The choice of **Plant type** is important because different types have different physical or 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 this modeled organism record with one of the limited number of organisms that have some toxicity data or procedures for estimating toxicity. In this instance, if you choose **Macrophytes** the model will utilize the toxicity data (e.g., EC50) for Esfenvalerate that is labeled as "Macrophytes."

Parameter values within the model's databases are provided to get you started; if you have more appropriate or locally measured values, you should use them.

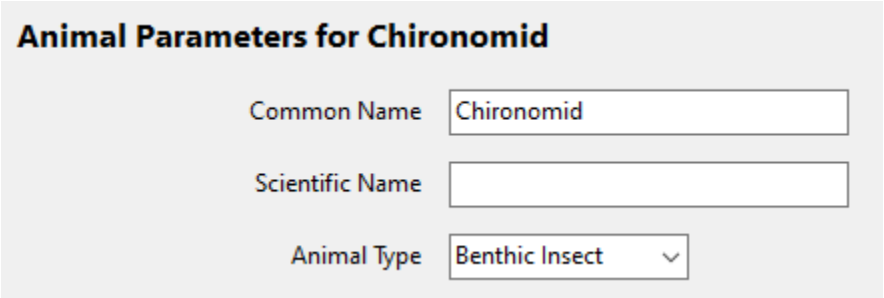
The primary parameters are shown on the input window by default, but the screen can be modified to display other subsets of parameters by selecting the "Expand" button next to each subheading.



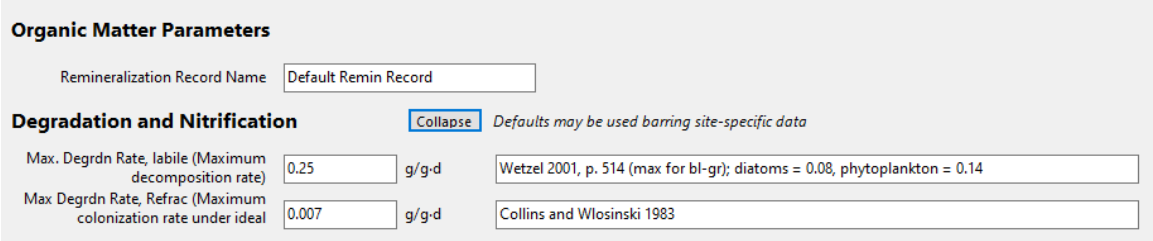
Next, we will locate the parameters for the Chironomid (DepFeeder1) within the simulation. Hit **Cancel** to leave the plant parameters screen and then select OK to return to the main window and save your changes to the organism's initial condition and loadings.

Double click on the Chironomid about 2/3 of the way down the state variable list and again, select "Parameters."

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



Finally, we will examine the parameters pertaining to organic matter for this simulation. To do this, return to the main window, and select the **Org. Matter** button. 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. If you have site-specific nutrient decomposition data, or wish to alter the sinking rate for suspended organic matter, those model parameters would be found here. For more information about the three different types of Remineralization records included with AQUATOX see the section titled Remineralization**.**



After you have viewed the organic matter parameters, select OK or Cancel to return to the main simulation window. At the upper right of the main simulation window are buttons that will take you to matrices that show the available databases site, animal, organic matter (remin.), chemical, and plant parameters that are included with the AQUATOX model. Unless these parameters are loaded into a simulation, as discussed above, they will have no impact on a model's result. (See also "Parameters within Database Files vs. Parameters within in a Simulation.")

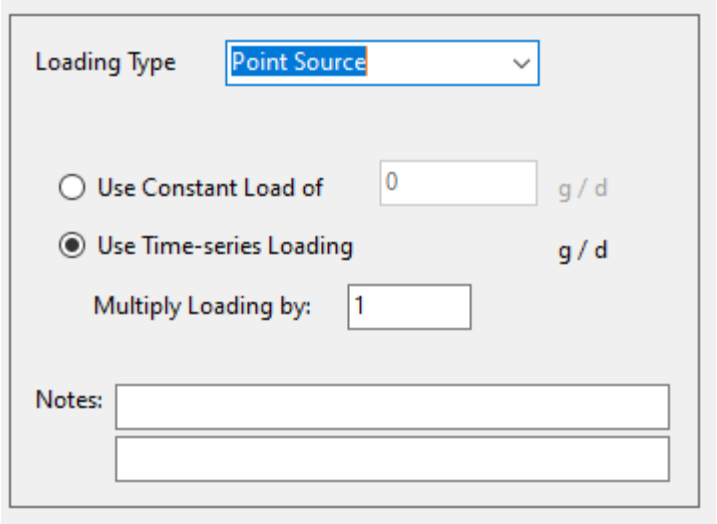
Next, Viewing Toxicant Loadings

Tutorial-- Step 4: Viewing Toxicant Loadings

Following the tutorial to this point, we should still have **FarmPond MO Esfenval.aps** loaded from back in **Step 1**.

In the "State and Driving Variables" list, double-click on **Dissolved org. tox 1** to bring up the loadings form for the chemical, and to examine the 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.

Click on the Loading Type drop down box to toggle between loadings types.



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 loadings 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 with loadings data from only one or a few years. Sporadic loadings, which could be expected only in one particular year might 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 simulation using the **Import** button. See also Importing Loading.

Another potential pollution loading source is from direct precipitation. These loads are given as g/m2 day because AQUATOX does not explicitly model the addition of water to a system via precipitation.

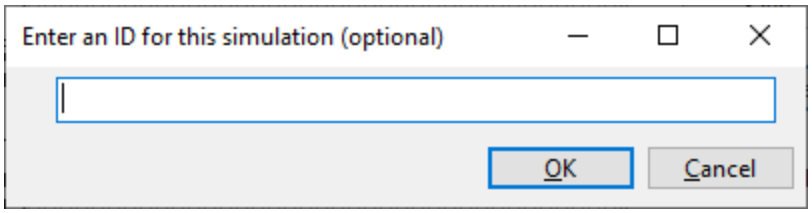
Next, Running the Simulation

Tutorial-- Step 5: Running the Simulation

To change the time period of a simulation or other integration options, click the **Edit Setup** button to the upper left of the main window. The most important inputs from this screen are the start and end of model simulation, which sets the simulation time. (This should be compatible with the time period of any time-series model loadings you have entered previously.) For other options, see the Setup Parameters section of this manual.

To run the simulation, select the **Run** button to the left of the main window.

You will be asked for an optional text string to define the run. Multiple runs can be saved within each AQUATOX JSON and then can be compared graphically or have their results compared within the output window. The date of each simulation will be also saved.



A progress bar will appear showing the status of the model run. This run should take a minute or two.

Next, Viewing Output

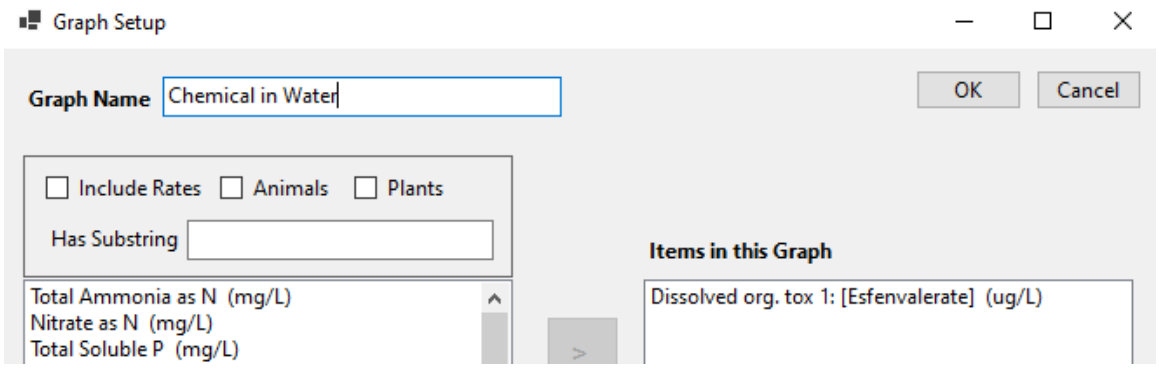
Tutorial-- Step 6: Viewing Output

When a simulation has been executed, results for various state variables are stored in memory. These results will be saved as an updated JSON if the simulation is saved. After the simulation has completed the **Output** window will pop up. (To view the output at another time, select the "Output' button on the main window.)

By selecting "**Save CSV**," model results may be exported to a comma-separated text-file format for import into spreadsheet or database software.

By selecting "**New Graph**," a set of model results can be created.

- To see the chemical concentration in water, name the graph "Chemical in Water", and then use the arrow buttons to move "Dissolved org tox 1:" to the box on the right.



After selecting OK you will see a graph of predicted water-column concentrations of Esfenvalerate given the PRZM based inputs.

- To see results for all the animals in a simulation, click "New Graph" again, name the graph "Animals," click on the "Animals" check box on top of the output list, and use the double right arrow to move all of the animals onto the graph.

Clicking on any of the results in the graph will identify the state variable and provide a snapshot of its concentration in time. Also, items on the graph may be toggled by clicking the colored rectangles within the legend.

For more information about the output window see: Output Window.

You have now seen the basic building blocks for an AQUATOX model. You should have an initial exposure to state variables, parameters, external loadings, available databases of parameters, running a model and viewing model output.

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