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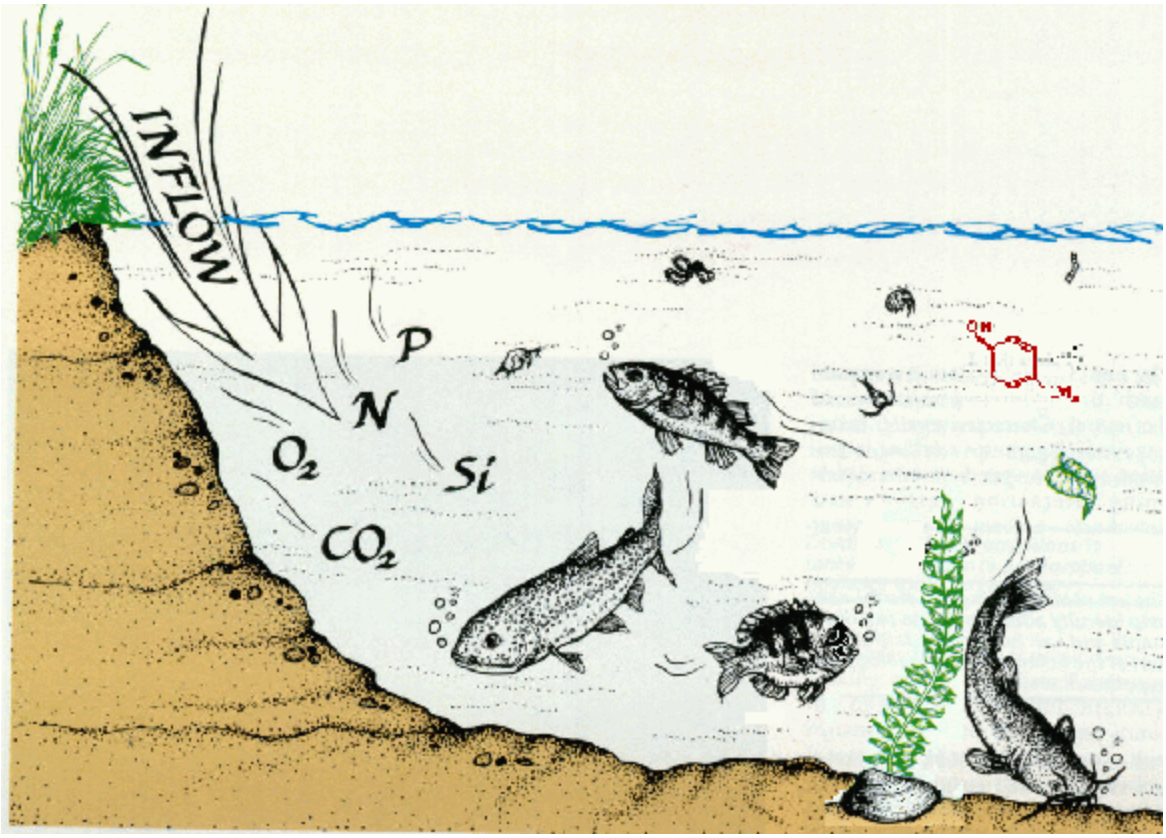
AQUATOX (RELEASE 2)

MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS

VOLUME 1: USER'S MANUAL



AQUATOX (RELEASE 2)

MODELING ENVIRONMENTAL FATE AND ECOLOGICAL EFFECTS IN AQUATIC ECOSYSTEMS

VOLUME 1: User's Manual

Richard A. Park,
Jonathan S. Clough,
and
Marjorie Coombs Wellman

JANUARY 2004

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF WATER
OFFICE OF SCIENCE AND TECHNOLOGY (MAIL CODE 4305T)
WASHINGTON DC 20460

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This document describes an aquatic ecosystem simulation model. It is not intended to serve as guidance or regulation, nor is the use of this model in any way required. This document cannot impose legally binding requirements on EPA, States, Tribes, or the regulated community.

ACKNOWLEDGMENTS

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PREFACE

The Clean Water Act— formally the Federal Water Pollution Control Act Amendments of 1972 (Public Law 92-50), and subsequent amendments in 1977, 1979, 1980, 1981, 1983, and 1987— calls for the identification, control, and prevention of pollution of the nation's waters. In the National Water Quality Inventory: 2000 Report (US EPA, 2002), 40 percent of assessed river lengths and 45 percent of assessed lake areas were impaired for one or more of their designated uses. The most commonly reported causes of impairment in rivers and streams were pathogens, siltation, habitat alterations, oxygen-depleting substances, nutrients, thermal modifications, metals (primarily mercury), and flow alterations; in lakes and reservoirs the primary causes included nutrients, metals, siltation, total dissolved solids, oxygen-depleting substances, excess algal growth and pesticides. The most commonly reported sources of impairment were agriculture, hydrologic modifications, habitat modification, urban runoff/storm sewers, forestry, nonpoint sources, municipal point sources, atmospheric deposition, resource extraction and land disposal. There were 2838 fish consumption advisories, which may include outright bans, in 48 States, the District of Columbia and American Samoa. Of these 2838 advisories, 2242 were due to mercury, with the rest due to PCBs, chlordane, dioxin, and DDT (US EPA, 2002). States are not required to report fish kills for the National Inventory; however, available information for 1992 indicated 1620 incidents in 43 States, of which 930 were attributed to pollution, particularly oxygen-depleting substances, pesticides, manure, oil and gas, chlorine, and ammonia.

New approaches and tools, including appropriate technical guidance documents, are needed to facilitate ecosystem analyses of watersheds as required by the Clean Water Act. In particular, there is a pressing need for refinement and release of an ecological risk methodology that addresses the direct, indirect, and synergistic effects of nutrients, metals, toxic organic chemicals, and non-chemical stressors on aquatic ecosystems, including streams, rivers, lakes, and estuaries.

The ecosystem model AQUATOX is one of the few general ecological risk models that represents the combined environmental fate and effects of toxic chemicals. The model also represents conventional pollutants, such as nutrients and sediments, and considers several trophic levels, including attached and planktonic algae, submerged aquatic vegetation, several types of invertebrates, and several types of fish. It has been implemented for streams, small rivers, ponds, lakes, and reservoirs.

AQUATOX Release 2 is described in these documents. **Volume 1: User's Manual** describes the usage of the model. Because the model is menu-driven and runs under Microsoft Windows on microcomputers, it is user-friendly and little guidance is required. **Volume 2: Technical Documentation** provides detailed documentation of the concepts and constructs of the model so that its suitability for given applications can be determined. **Volume 3: User's Manual for the BASINS Extension to AQUATOX** describes how AQUATOX can be run with site characteristics and loadings input directly from the BASINS data layers or from the HSPF and SWAT watershed models.

1 QUICK START

1.1 System Requirements

Minimum Requirements

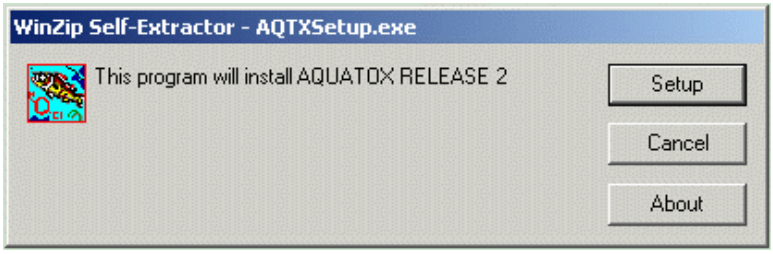
- PC Compatible, Pentium 133 MHz
- Microsoft Windows 95
- 64 MB RAM
- 30 MB free disk space

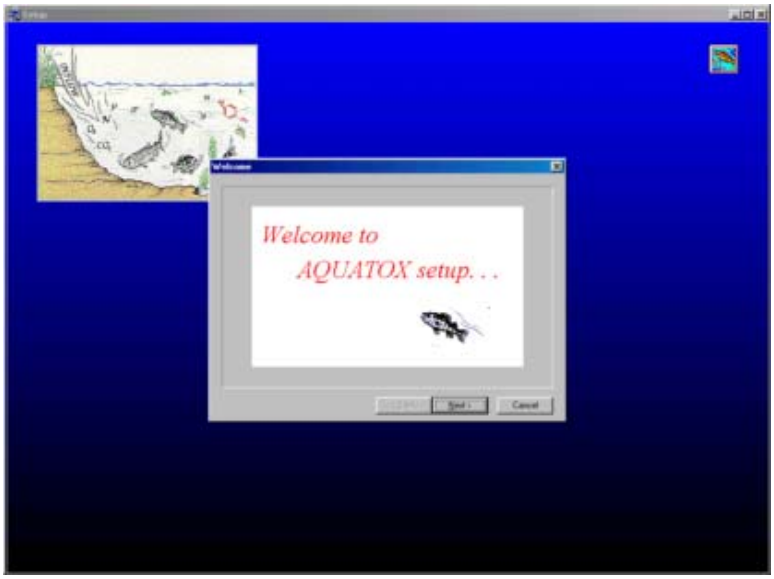
Recommended

- Pentium PC, 600 MHz or higher
- Microsoft Windows NT, 2000, or XP
- 128 MB RAM
- 75 MB free disk space

1.2 Installation

To install AQUATOX, run AQTXSetup.exe, the files will unzip, and InstallShield will lead you through the straightforward installation.

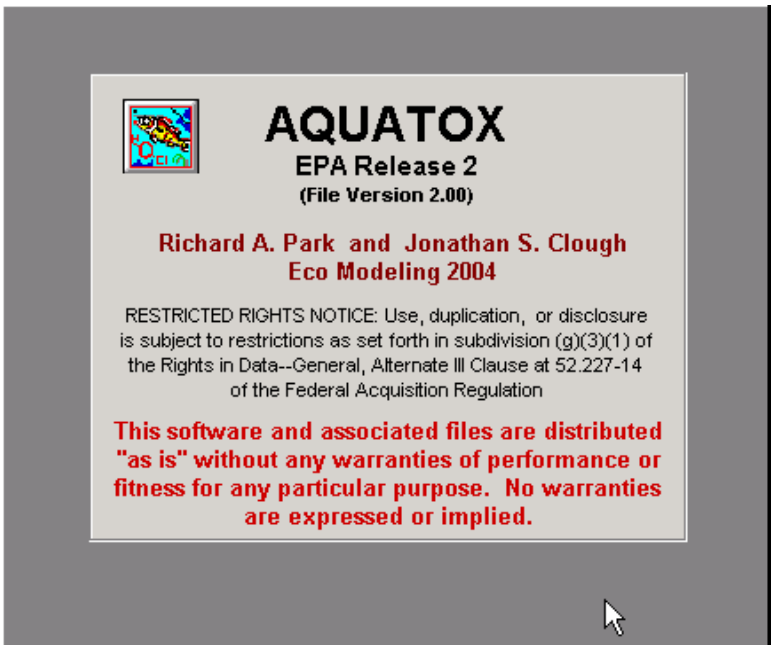




1.3 Starting

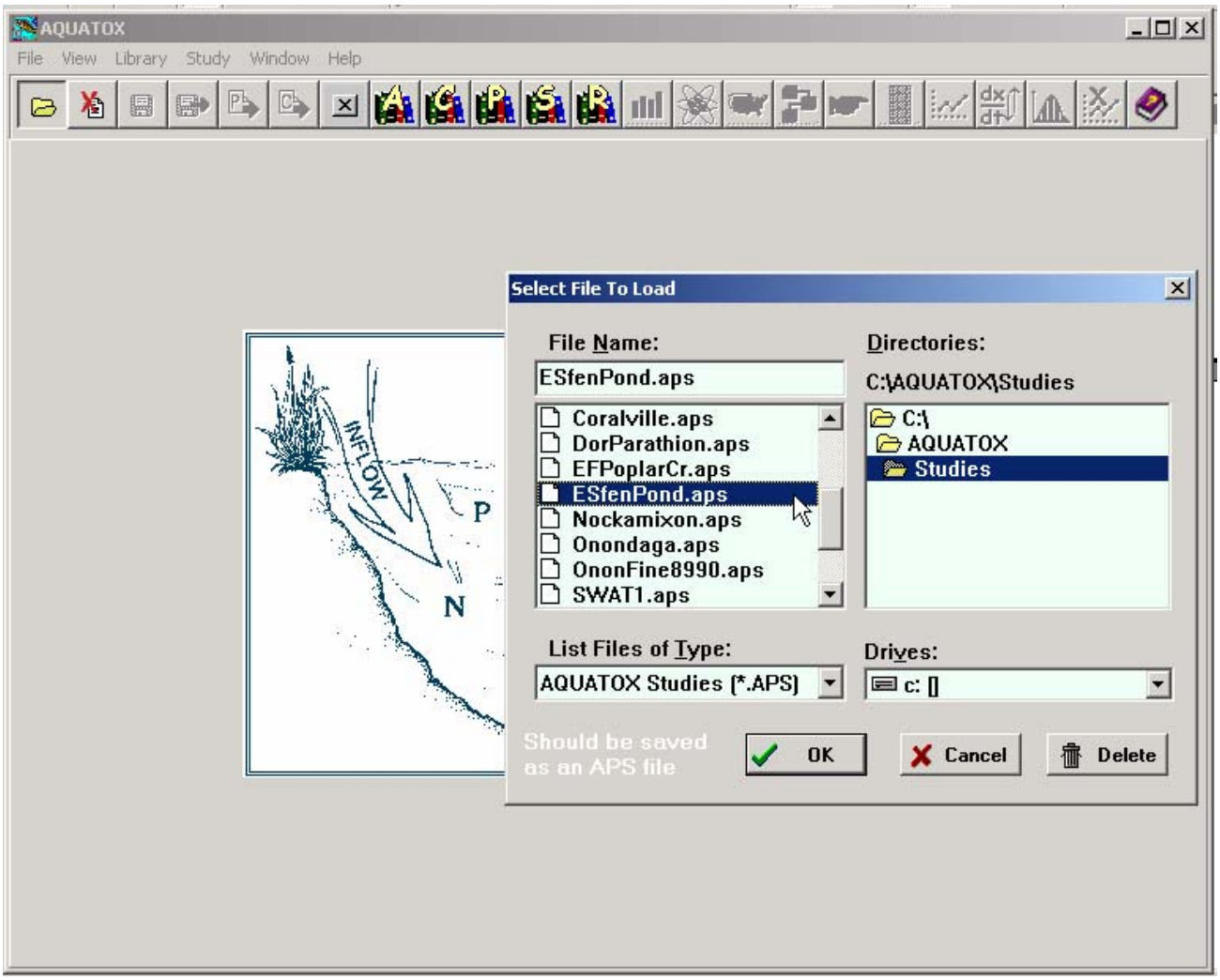
Double-click on the AQUATOX icon in Windows to open the program. Alternatively, you can double-click on a study file (with the suffix "aps") listed in Windows Explorer.

Then a "splash" window will open briefly, indicating that the model is still subject to modification and that, while the model is in the public domain, there are parts of the model interface that are proprietary.



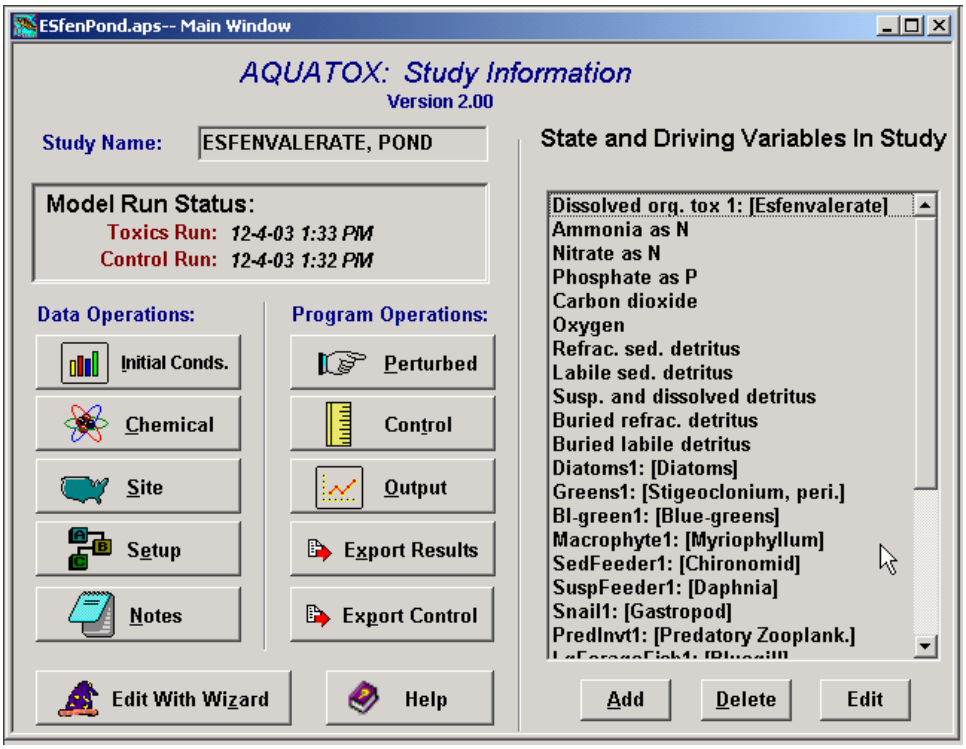
1.4 Loading a Study

The study 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. Usually we model one study at a time; however, a batch mode is described later. Click on **File** in the menu bar to get the pull-down file menu, and click on **Open**. You will then be given a choice of AQUATOX study files to load. For this example, we will choose **EsfenPond.aps**.

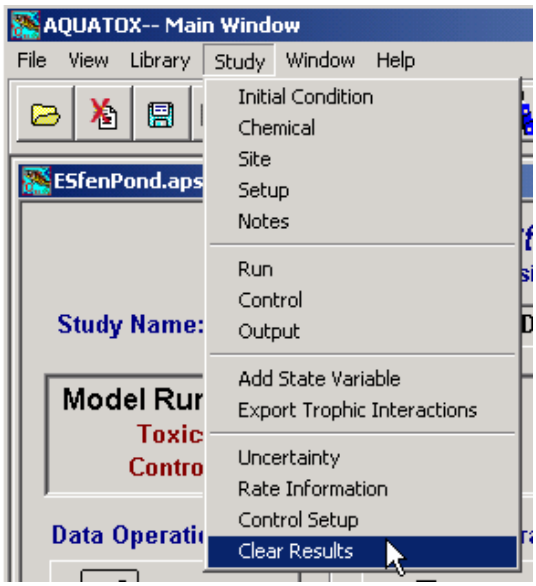


The main window will appear with the name of the study, the list of state variables used, and buttons from which to choose various operations. The **Study Name** can be edited; it is separate from the name of the file, which you loaded and which is displayed at the top of the screen. The study name is used as a title in graphical output, so is best capitalized. The **Status** window tells when the perturbed and control runs were made, and warns if they are incomplete. The **Initial Conditions** button brings up a screen with all the state variable values at the beginning of a simulation. The **Chemical** button brings up a list of organic chemicals in the study; selecting a particular chemical brings up the loading screen for that chemical, from which you can access the chemical parameter and toxicity screens. Double clicking on **Dissolved org. toxicant** at the top of the list of state variables and driving variables has the same effect. The **Site** button loads the site characteristic screen. **Setup** allows the user to set the dates of the simulation, and to specify various options such as the control setup, uncertainty analysis, and saving biologic rates. **Notes** provides a window for writing comments on the study. **Perturbed** starts the simulation with changed conditions, such as with a toxicant. **Control** starts a simulation without the stressor; the user can use **Control Setup** as mentioned above to specify what is changed and what is held constant. **Output** presents the results as a series of charts and

graphs. The output can be exported as database files by clicking on **Export Results** or **Export Control**. There also are **Help** and **Wizard buttons.**



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

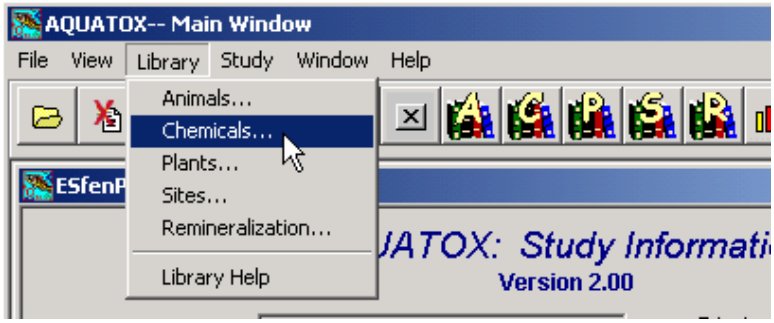


1.5 Loading a Library

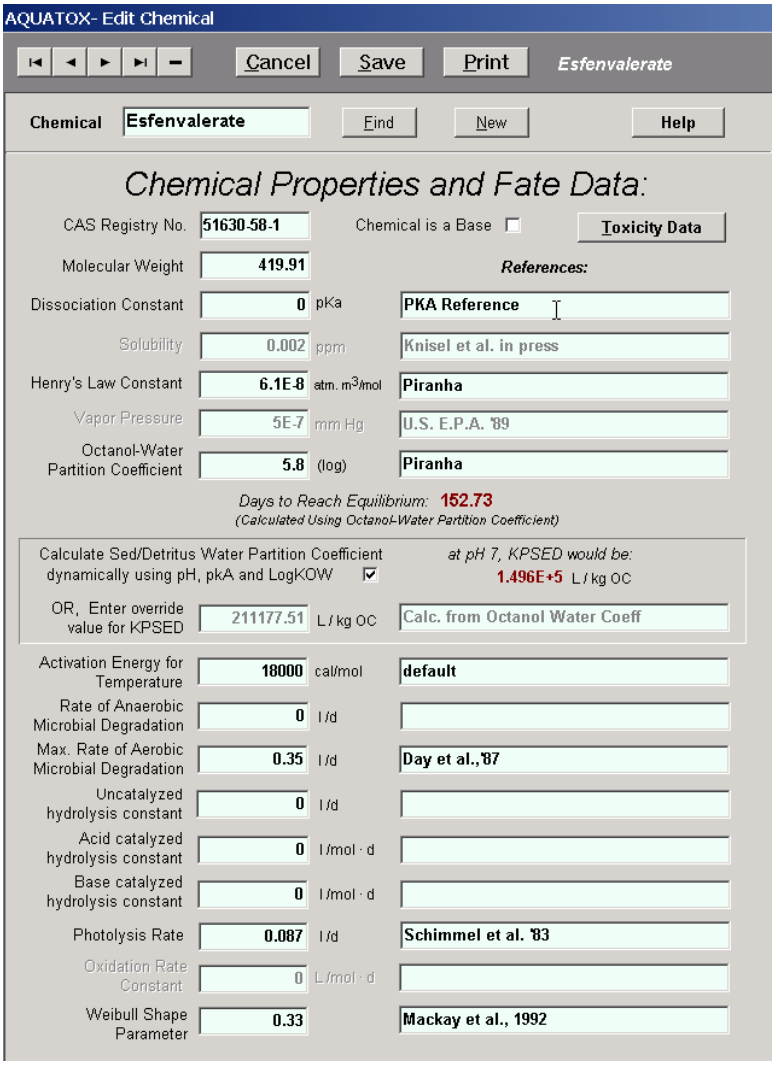
There is a basic dichotomy in working with AQUATOX. You have a choice of editing database files in the general library or of opening a particular study. Studies are self-contained files with all the information on a particular simulation, including initial conditions, loadings, parameter values, first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

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

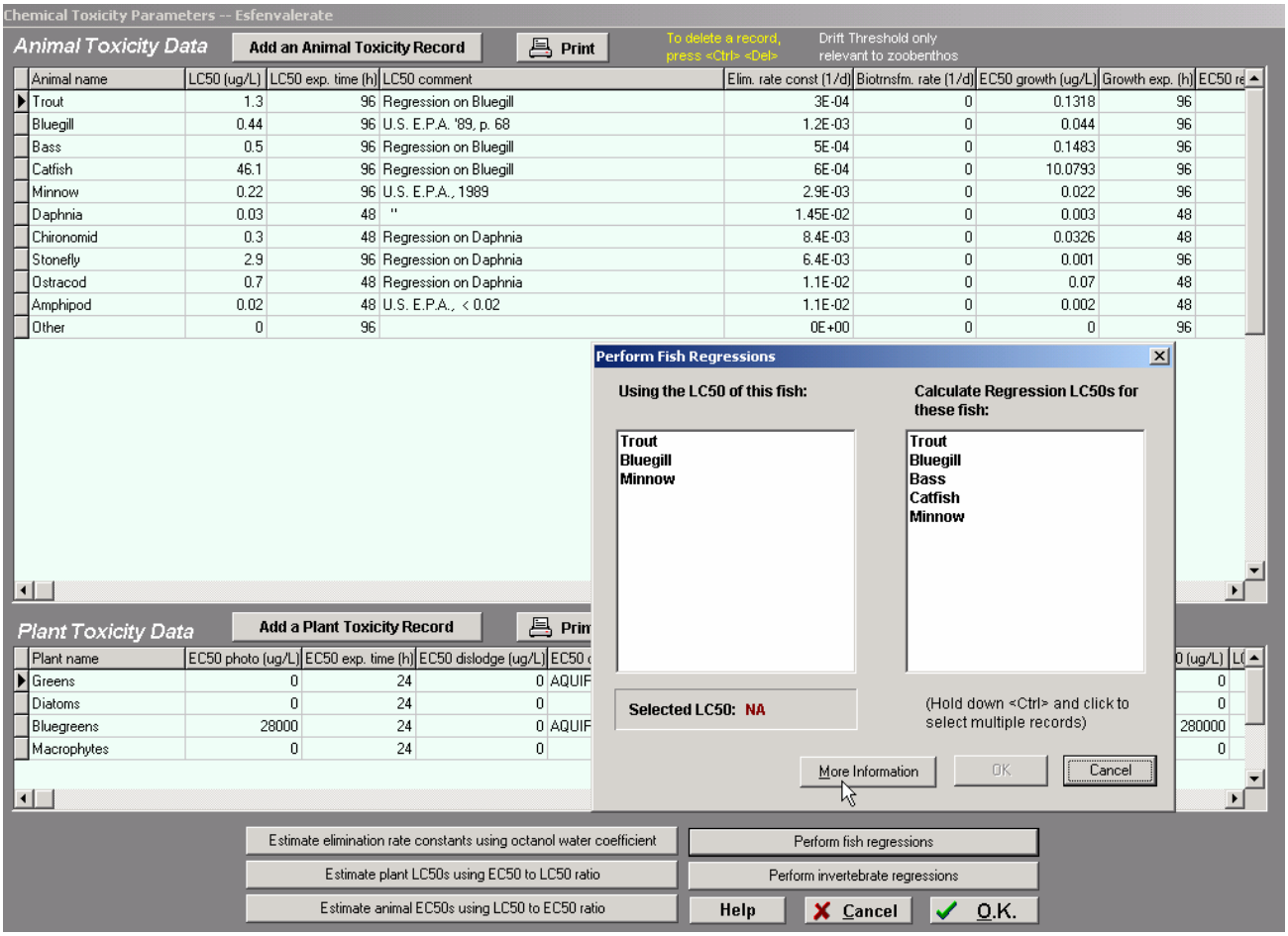
To create or edit a record for general use, click on **Library** in the menu bar. You can then click on the specific library from the pull-down menu. Alternatively, you can click on the appropriate library icon on the task bar (Animals, Chemicals, Plants, Sites, or Remineralization).



In this example we will choose **Chemicals** and **Default** in sequence. The first record is for 2,4-D Acid. We can click on the arrows in the upper left or can search for a particular name to move through the database. Use the arrow to move to Esfenvalerate. When you leave a database you will be asked whether you want to save it or lose any changes you might have made. The frequent requests for confirmation may be irritating, but they are for your protection. Any time you leave a record you may back out of a change by not saving it. There is no undo capability, so if you save a change, you are stuck with it, except by re-editing the entire record. It is easy to print a record, and you are encouraged to make a hard copy before you make extensive changes. Some variables are not used at this time and are so indicated by being grayed out.

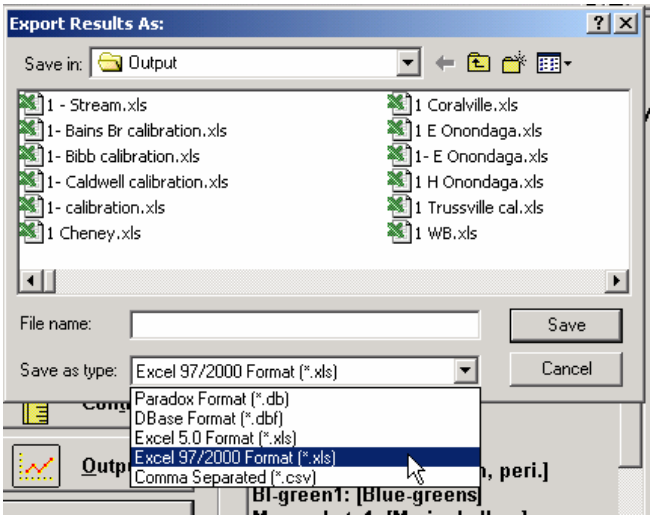


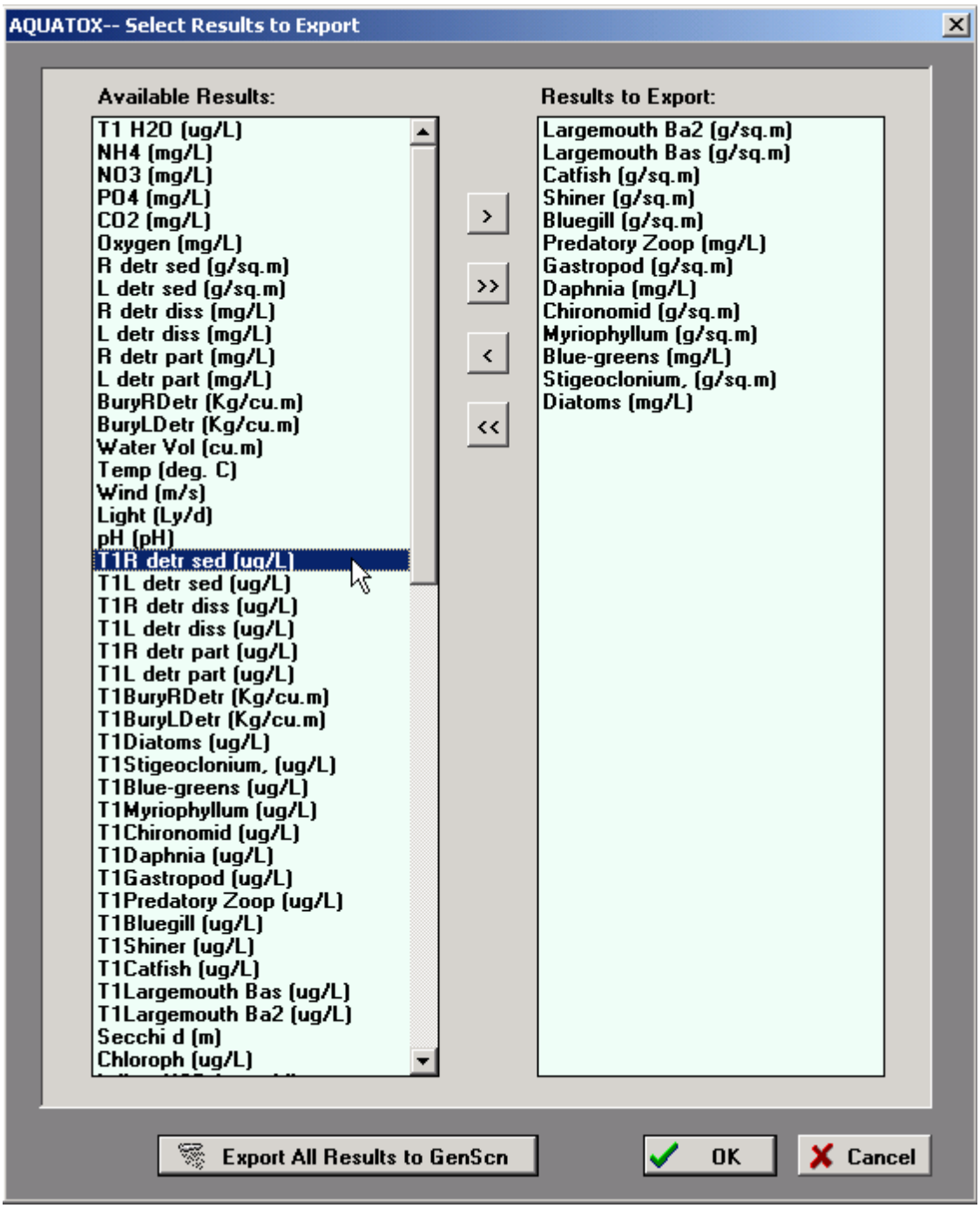
You can examine the toxicity data for the chemical, by clicking on the **Toxicity Data** button at the top right. Toxicity can be estimated for several organisms, given data for others indicated in bold type. For example, change the LC_{50} for trout from 1.3177 to 1.4 (or any other value). You will then get a window presenting you with other organisms for which the LC_{50} can be estimated. If any have zero values, they will be checked automatically. The estimation procedures were developed with pesticide databases (Mayer and Ellersieck, 1986, Suter et al., 1986), so they should be applied with caution to industrial chemicals.



1.6 Running and Saving a Simulation

You can run both **Perturbed** and **Control** simulations to see the impacts of various stressors. They can be run concurrently by clicking on first one and then the other. The results can be exported in Excel, dBase, Paradox, or text formats. When you click on **Export** you will be given a list of output variables to choose among, or you may choose to export all to GenScn, the post-processor in BASINS (see **Volume 3**). The Output subdirectory is the default for saving the results, but you may choose some other directory.

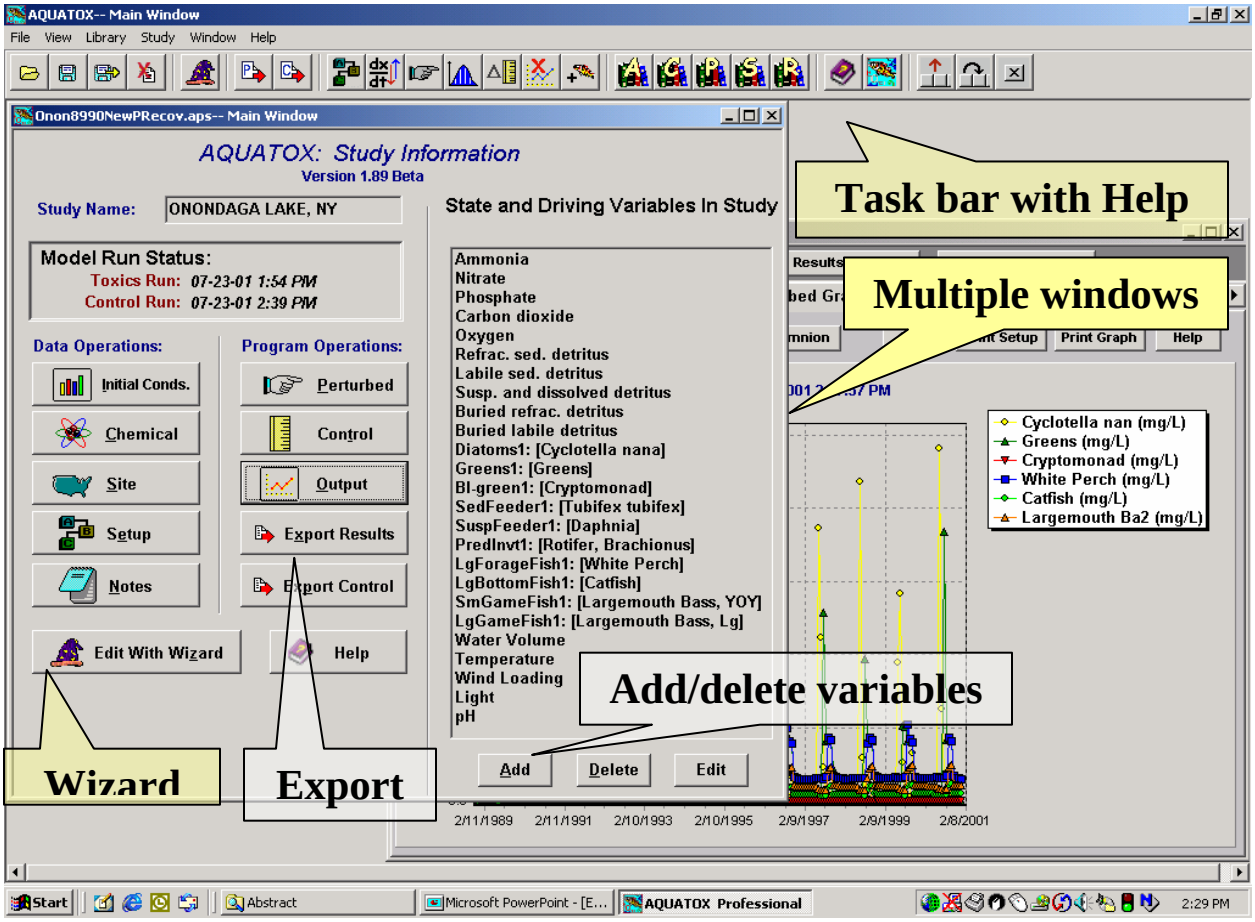

Export Results As:
Save in: Output
1 - Stream.xls
1- Bains Br calibration.xls
1- Bibb calibration.xls
1- Caldwell calibration.xls
1- calibration.xls
1 Cheney.xls
1 Coralville.xls
1 E Onondaga.xls
1- E Onondaga.xls
1 H Onondaga.xls
1 Trussville cal.xls
1 WB.xls
File name:
Save
Save as type: Excel 97/2000 Format (*.xls)
Cancel
Paradox Format (*.db)
DBase Format (*.dbf)
Excel 5.0 Format (*.xls)
Excel 97/2000 Format (*.xls)
Comma Separated (*.csv)
Bl-green1: [Blue-greens]



1.7 Overview of AQUATOX Release 2 Enhancements

Release 2 has been designed to be as user-friendly as possible, while providing greatly expanded analytical capability over Release 1. It follows MS Windows conventions in providing buttons on the Task Bar to give the user direct access to most functions. It supports multiple windows so that a user can edit parameters, plot previous results, and even run multiple

simulations simultaneously (although resources may be limited in earlier versions of MS Windows). It has a powerful Wizard and context-sensitive Help files to guide the user through an implementation.



The changes fall in three categories.

Enhanced Scientific Capabilities

The model is much more powerful and can better represent a variety of environments, especially streams and rivers compared to Release 1. Specific enhancements include:

- a large increase in the number of biotic state variables, with two representatives for each taxonomic group or ecologic guild;
- the addition of bryophytes as a special type of macrophyte;
- a multi-age fish category with up to fifteen age classes for age-dependent bioaccumulation and limited population modeling;
- an increase in the number of toxicants from one to a maximum of twenty, with the capability for modeling daughter products due to biotransformations;
- disaggregation of stream habitats into riffle, run, and pool;

- mechanistic current- and stress-induced sloughing, light extinction, and accumulation of detritus in periphyton;
- macrophyte breakage due to currents;
- computation of chlorophyll *a* for periphyton and bryophytes, as well as for phytoplankton;
- fish biomass is entered and tracked in g/m^2;
- entrainment and washout of animals, including fish, can occur during high flow;
- the options of computing respiration and maximum consumption in fish as functions of mean individual weight using allometric parameters from the Wisconsin Bioenergetics Model;
- respiration in fish is density-dependent;
- fish spawning can occur on user-specified dates as an alternative to temperature-cued spawning;
- elimination of toxicants is more robust;
- settling and erosional velocities for inorganic sediments are user-supplied parameters;
- uncertainty analysis now covers *all* parameters and loadings;
- biotic risk graphs are provided as an alternative means of portraying probabilistic results;
- limitation factors for photosynthesis are output along with the biotic rates; and
- AQUATOX is now an extension to BASINS, providing linkages to geographic information system data, and HSPF and SWAT simulations.

Additional User Interfaces

The model is even more user-friendly, taking full advantage of current Windows capabilities on modern high-speed personal computers. Capabilities include:

- a Wizard to guide the user through the setup for a new study;
- context-sensitive Help screens;
- multiple windows for simultaneous simulations and input and output screens;
- a task bar that can be customized by the user;
- enhanced graphics, including secondary Y axes; and
- a hierarchical tree structure for choosing variables for uncertainty analysis.

Corrected Errors

Several errors were discovered and corrected during the course of continuing model evaluation. Some of these may require recalibration of studies. The example studies provided with the software have been recalibrated, but users may wish to check their own calibrations in upgrading from various versions. The corrections include:

- a change in the bathymetric computations affecting the areas of the thermocline and littoral zone (Release 1);
- removal of an unnecessary conversion from phosphate and nitrate, assuming that all nutrient input is in terms of N and P; this could affect nutrient limitations (all versions);

- inclusion of an oxygen to organic matter conversion factor (a factor of 1.5) and inclusion of specific dynamic action in the allometric computation of fish respiration (Release 2 Beta Test only);
- adding a second-to-day conversion factor for inorganic sediment deposition; previously, deposition of suspended sediments was much slower than expected (all versions);
- adding a conversion factor for wind measured at 10 m height to wind occurring at 10 cm above the water surface in the volatilization computations; for some compounds this could result in a two-fold reduction in volatilization (all versions);
- nitrification is formulated to occur only at the sediment-water interface (Release 1); and
- bioaccumulation, and hence toxicity, are constrained by the life span of an animal (all versions).

At this point you may experiment with the various buttons and screens. You cannot hurt anything; just don't save the edited data or the study when you exit the screens and AQUATOX unless you **Save As** a different name. On the other hand, if you are more comfortable following directions, read on, doing the operations as you go.

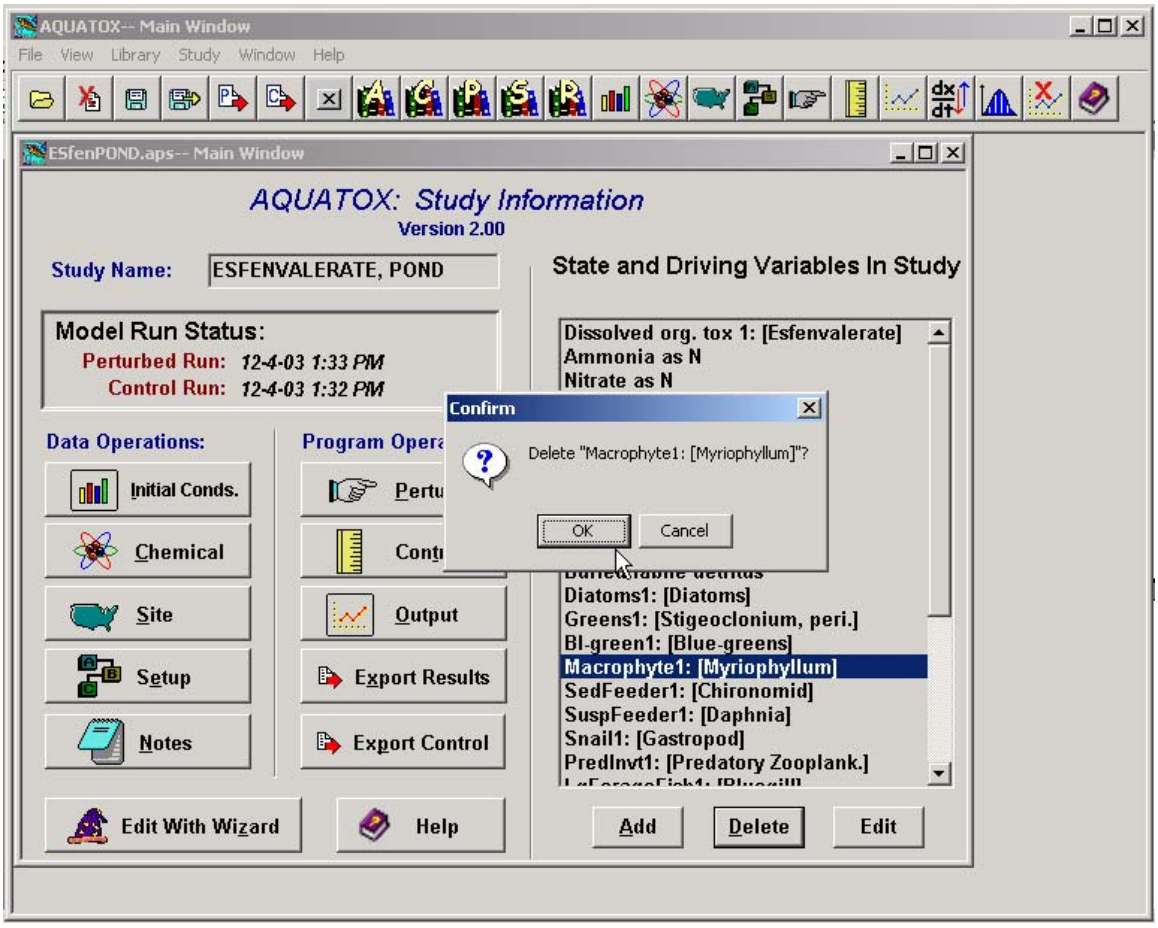
2 MODEL COMPONENTS

2.1 State Variables

Selection

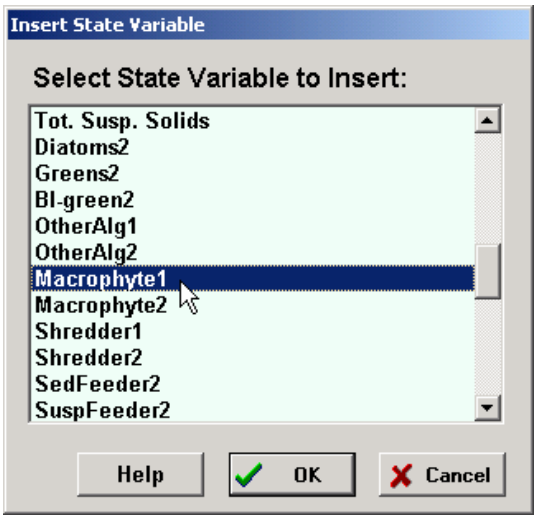
State variables are those ecosystem components that are being simulated. These include organism and detrital compartments and their associated toxicants (which are not listed in the **Study Information** window), nutrients, dissolved oxygen, and other variables traditionally considered driving variables, such as water inflow, temperature, pH, light, and wind.

AQUATOX is very powerful 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.

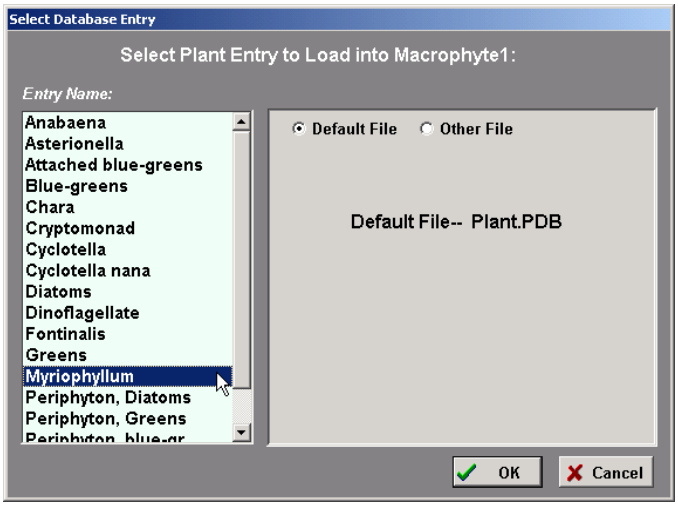


Open the file **Esfenpond.aps**, if it is not already open. We will remove the macrophyte compartment by highlighting it in the list, clicking on the **Delete** button, and confirming the deletion. When the change is made, you will see a small warning in the upper left corner of the main screen that the study has been modified.

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.



Note that the names of the taxonomic groups and ecologic guilds on the main study screen are followed by the names of the specific groups in brackets. We have to specify the type of macrophyte by highlighting **Macrophytes** and clicking on **Edit**, or by double-clicking on **Macrophytes**. That will give us a double screen representing both the macrophytes and the associated toxicant. Click on **Load Data** to load a specific plant record for macrophytes. In this example, *Chara* and *Myriophyllum* are the only macrophytes listed; we highlight *Myriophyllum* and click on **OK**. If there is no selection made you will receive an error message indicating that there is no data associated with the state variable **Macrophyte.**



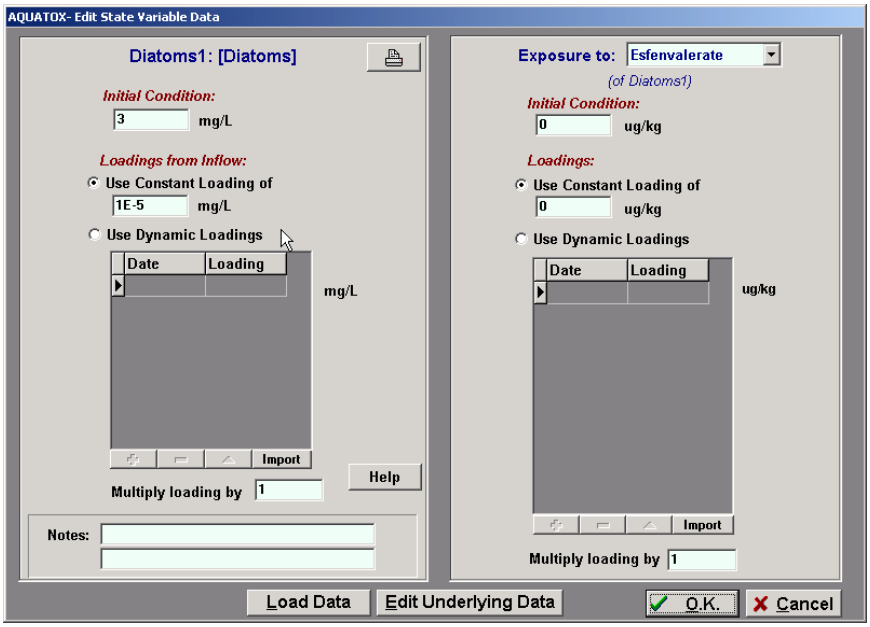
2.2 Initial Conditions, Loadings, and Parameters

Introduction

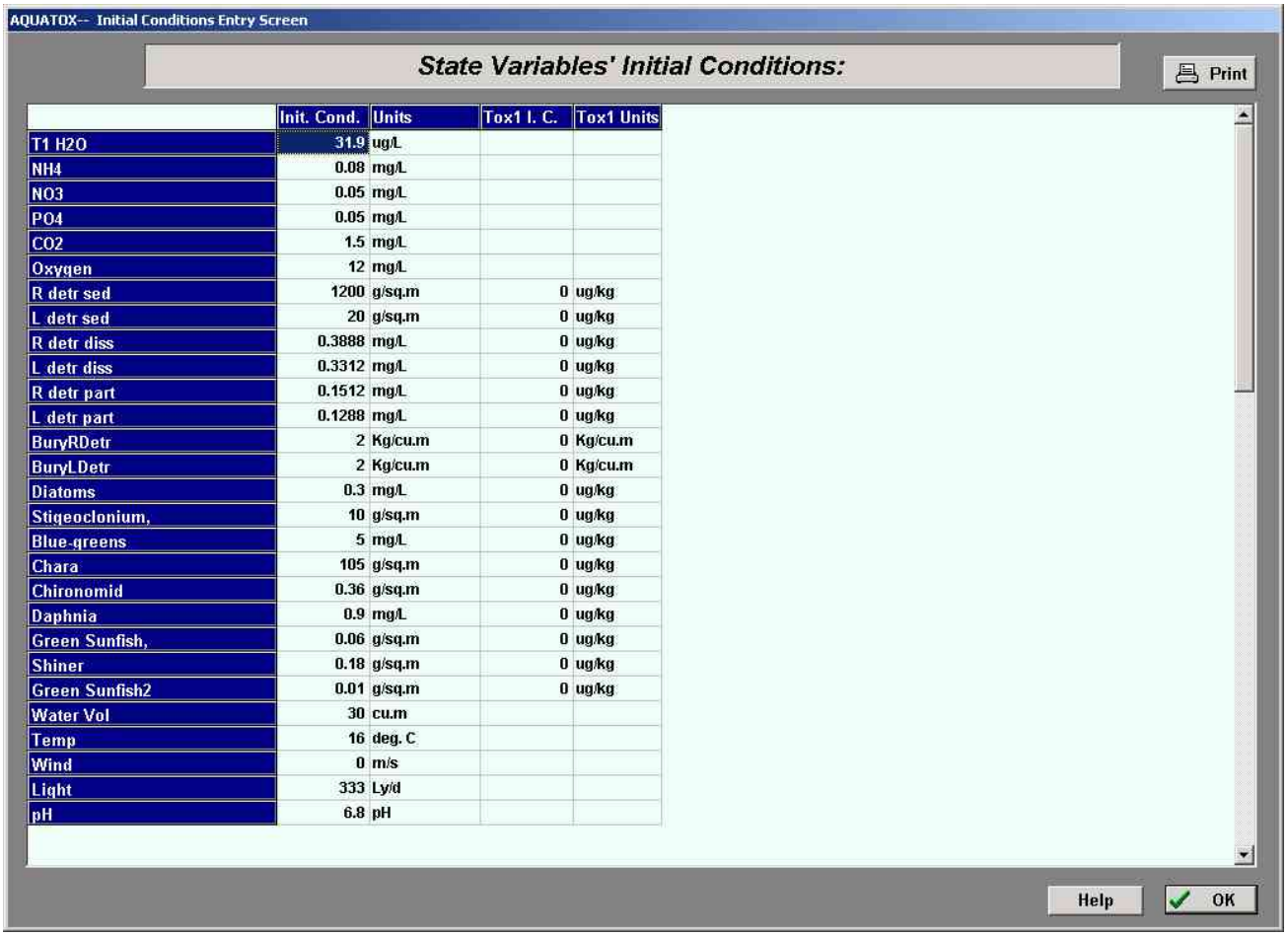
Initial values and loadings are needed for all the state variables or compartments simulated. These are input on the loadings screen. If one or more toxicants are modeled, then initial concentrations associated with the biota can also be specified. The initial condition will depend on when the simulation starts (which is specified in **Setup**). Initial conditions are often unknown. A useful procedure is to run a simulation for several repetitive years and then use the ending values as initial conditions, assuming steady state.

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, very small loading is appropriate. Likewise, macrophytes may die back in winter and sprout from rhizomes; because rhizomes are not explicitly modeled, a very small loading is the mechanism for reestablishing the population in the simulation.

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



Initial conditions can be displayed for all state variables in a summary screen, obtained by clicking on the **Initial Conds.** button on the main screen. In order to avoid conflicts with other windows, you cannot edit the initial conditions in this screen; that is reserved for the loading screens.



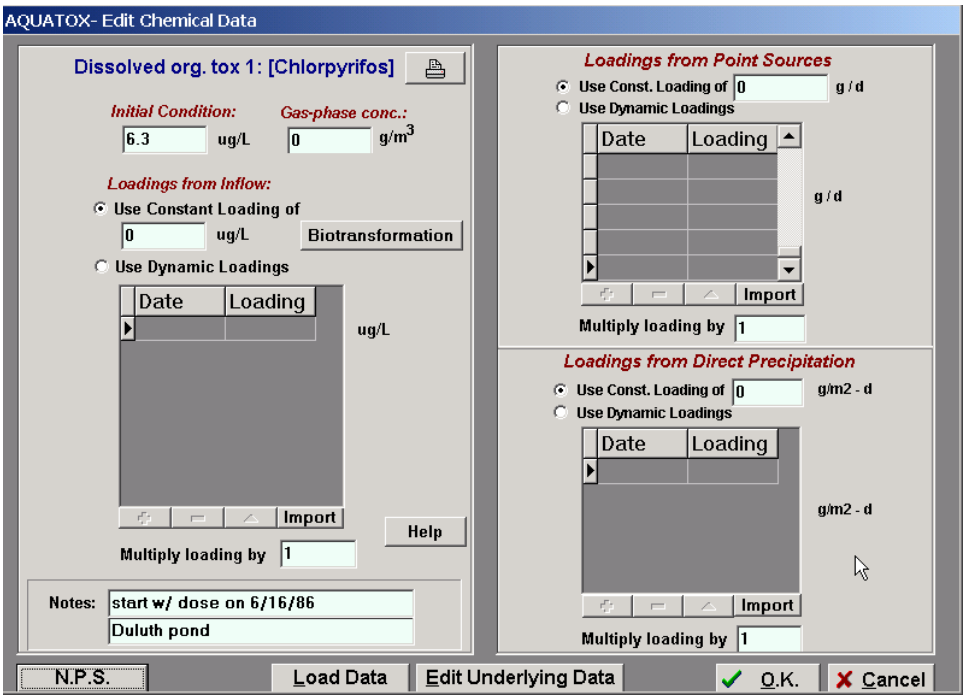
	Init. Cond.	Units	Tox1 I. C.	Tox1 Units
T1 H2O	31.9	ug/L		
NH4	0.08	mg/L		
NO3	0.05	mg/L		
PO4	0.05	mg/L		
CO2	1.5	mg/L		
Oxygen	12	mg/L		
R detr sed	1200	g/sq.m	0	ug/kg
L detr sed	20	g/sq.m	0	ug/kg
R detr diss	0.3888	mg/L	0	ug/kg
L detr diss	0.3312	mg/L	0	ug/kg
R detr part	0.1512	mg/L	0	ug/kg
L detr part	0.1288	mg/L	0	ug/kg
BuryRDetr	2	Kg/cu.m	0	Kg/cu.m
BuryLDetr	2	Kg/cu.m	0	Kg/cu.m
Diatoms	0.3	mg/L	0	ug/kg
Stigeoclonium,	10	g/sq.m	0	ug/kg
Blue-greens	5	mg/L	0	ug/kg
Chara	105	g/sq.m	0	ug/kg
Chironomid	0.36	g/sq.m	0	ug/kg
Daphnia	0.9	mg/L	0	ug/kg
Green Sunfish,	0.06	g/sq.m	0	ug/kg
Shiner	0.18	g/sq.m	0	ug/kg
Green Sunfish2	0.01	g/sq.m	0	ug/kg
Water Vol	30	cu.m		
Temp	16	deg. C		
Wind	0	m/s		
Light	333	Ly/d		
pH	6.8	pH		

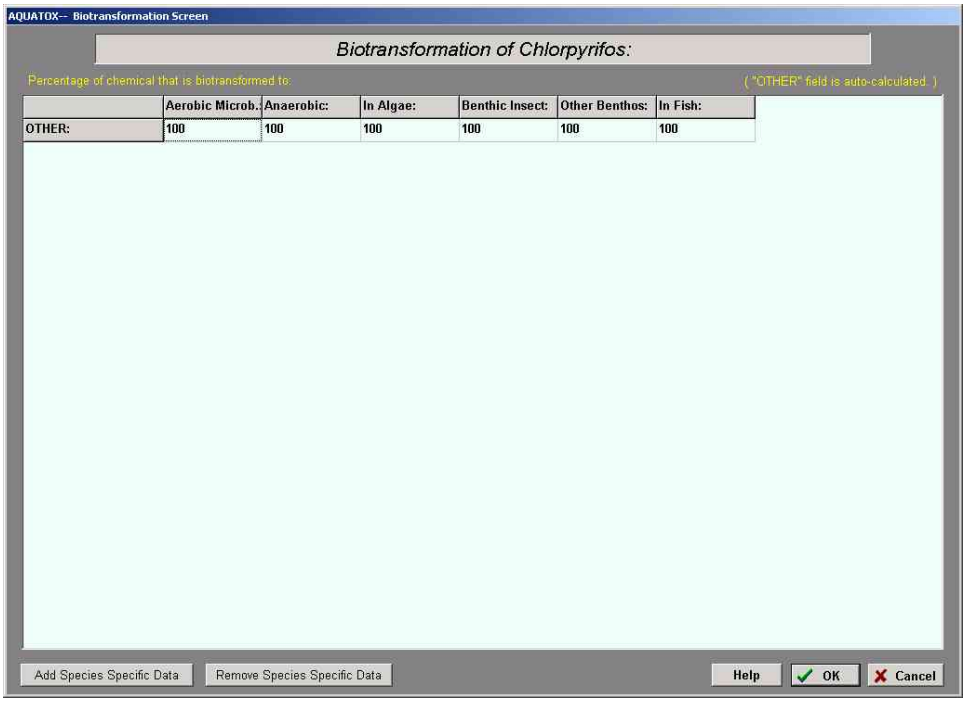
Parameters provide values for coefficients in the process equations. Although default values are given, the user has great flexibility in specifying values to represent site-specific species or groups. Parameters are available for editing and downloading from the general libraries; they also may be site-specific and associated with particular studies.

The following sections discuss loadings and parameters according to type of state variable.

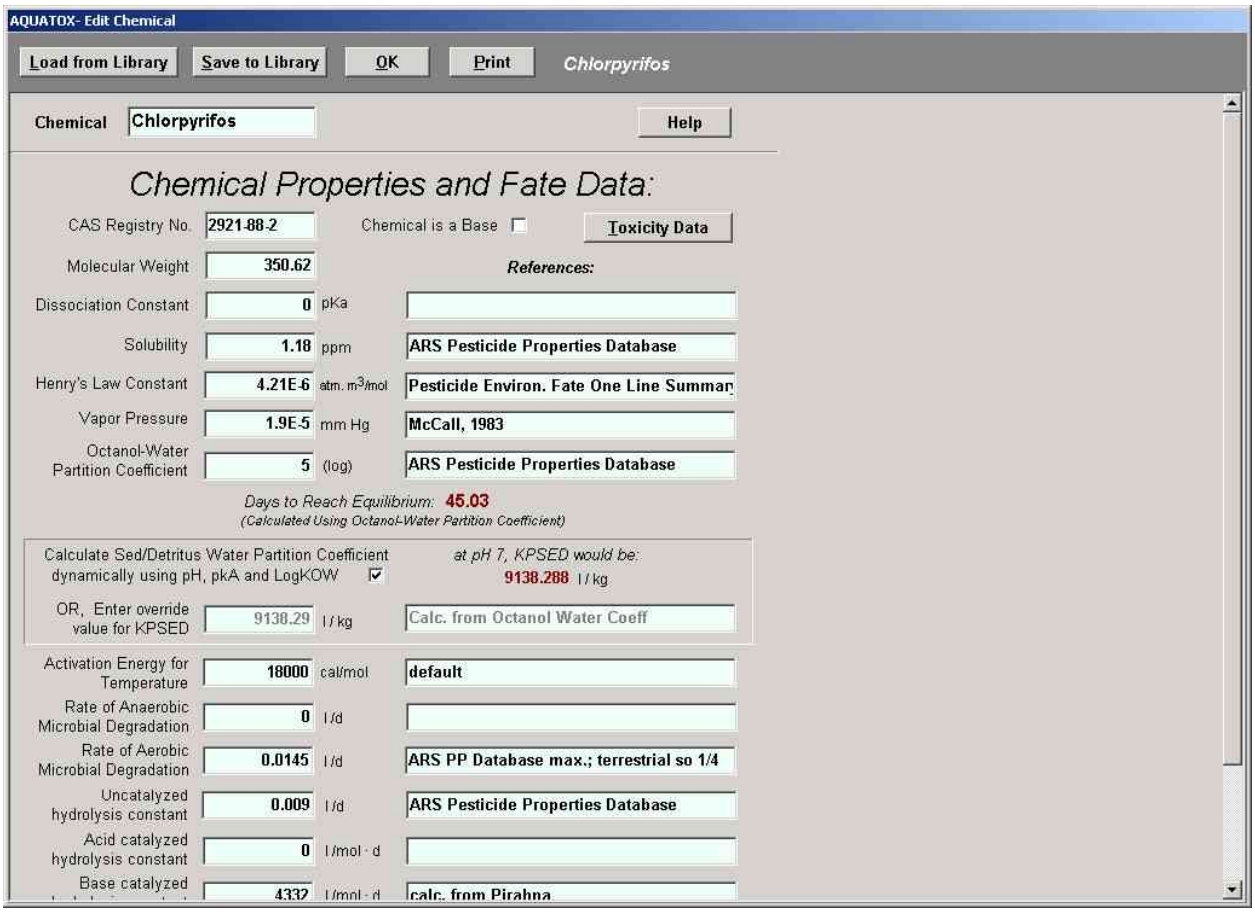
Dissolved Organic Toxicant

Organic toxicant initial conditions and loadings are relatively straightforward. New to Release 2 is the capability to indicate biotransformation to one or more daughter products, accessed by clicking on the **Biotransformation** button. To use this capability the daughter products have to be included as state variables. The biotransformation rate from one toxicant to another is specified by the user for each type of organism and is entered on the toxicity screen.

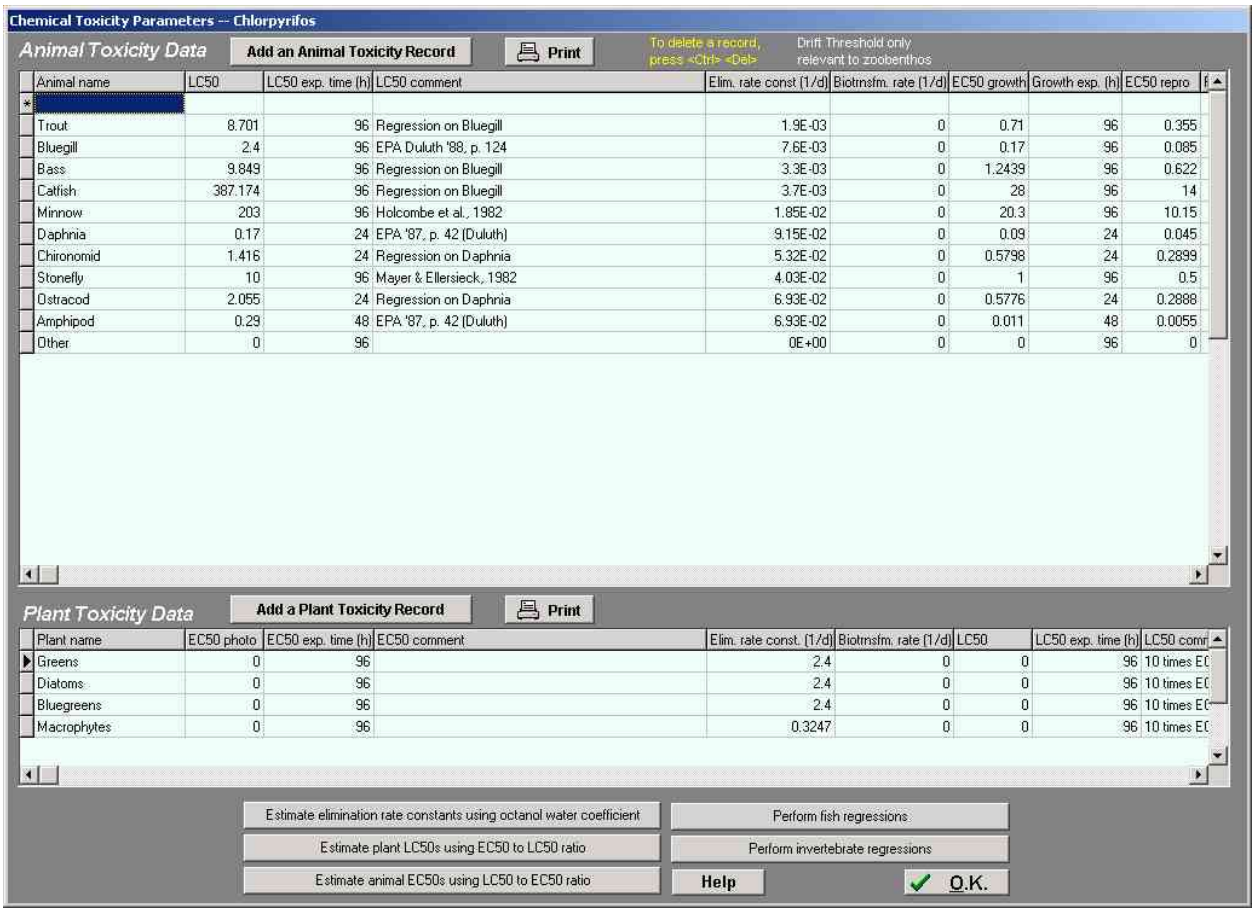




Clicking on the **Edit Underlying Data** takes one to the Chemical Properties and Fata Data screen. The only new feature on this screen is that the sediment/detritus and water partition coefficient can be calculated dynamically or entered manually by the user. The dynamic calculation is based on the octanol-water partition coefficient and the degree of ionization using Equation 212 as described by US EPA (2000b).



Clicking on the **Toxicity Data** button on the upper right portion of the screen takes the user to a large screen, requiring sideways scrolling, that provides entry and comment fields for animal and plant acute and chronic toxic effects. Minimal LC50 data are required; with a value for *Daphnia* one can click on **Perform invertebrate regressions** to obtain estimated LC50s for several groups. Likewise, with a value for minnows, bluegills, or rainbow trout one can click on **Perform fish regressions** to estimate LC50s for several fish species. Depuration or elimination rates are difficult to obtain, so usually one would want to click on **Estimate elimination rate constants using octanol water coefficient**. Chronic toxicity values may be available for only a subset of organisms; to extend those to other groups click on **Estimate plant LC50s using EC50 to LC50 ratio**, and **Estimate animal EC50s using LC50 to EC50 ratio**. Drift pertains only to zoobenthos; in the absence of good data, a fraction of the EC50 for growth or some other toxicological benchmark can be used. The lipid fraction flows from the organism parameter screen, but the mean weight (used in computing the elimination rate) is independent of the mean weight given in the parameter screen because it also can be parameterized in library mode when the animal screen cannot be accessed. The comment columns are skipped when the animal toxicity screen is printed in order to keep the font a legible size; the plant comment columns are printed because there are fewer columns.



Animal name	LC50	LC50 exp. time (h)	LC50 comment	Elim. rate const (1/d)	Biotrnsfm. rate (1/d)	EC50 growth	Growth exp. (h)	EC50 repro
Trout	8.701	96	Regression on Bluegill	1.9E-03	0	0.71	96	0.355
Bluegill	2.4	96	EPA Duluth '88, p. 124	7.6E-03	0	0.17	96	0.085
Bass	9.849	96	Regression on Bluegill	3.3E-03	0	1.2439	96	0.622
Catfish	387.174	96	Regression on Bluegill	3.7E-03	0	28	96	14
Minnow	203	96	Holcombe et al., 1982	1.85E-02	0	20.3	96	10.15
Daphnia	0.17	24	EPA '87, p. 42 (Duluth)	9.15E-02	0	0.09	24	0.045
Chironomid	1.416	24	Regression on Daphnia	5.32E-02	0	0.5798	24	0.2899
Stonefly	10	96	Mayer & Ellersieck, 1982	4.03E-02	0	1	96	0.5
Ostracod	2.055	24	Regression on Daphnia	6.93E-02	0	0.5776	24	0.2888
Amphipod	0.29	48	EPA '87, p. 42 (Duluth)	6.93E-02	0	0.011	48	0.0055
Other	0	96		0E+00	0	0	96	0

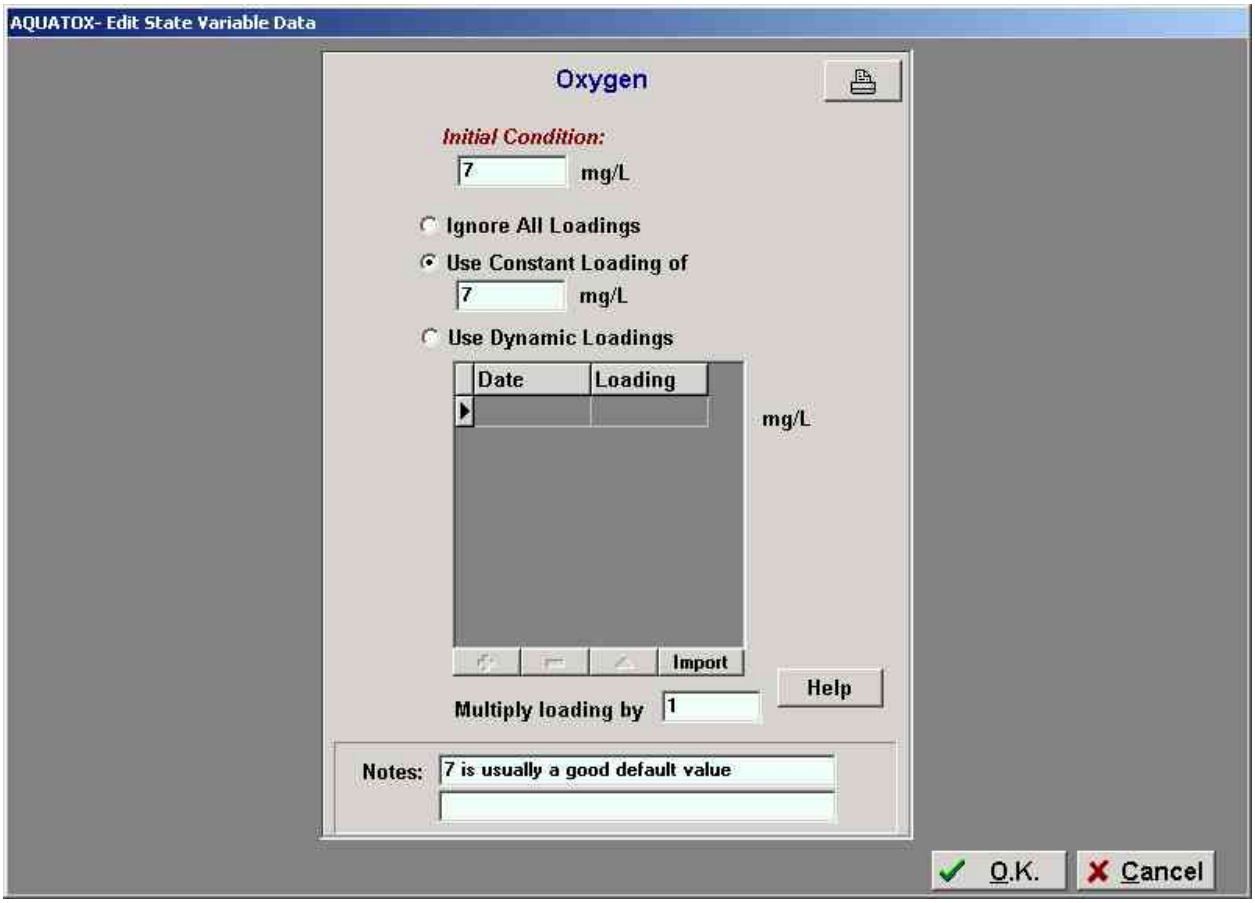
Plant name	EC50 photo	EC50 exp. time (h)	EC50 comment	Elim. rate const. (1/d)	Biotrnsfm. rate (1/d)	LC50	LC50 exp. time (h)	LC50 comr
Greens	0	96		2.4	0	0	96	10 times EC
Diatoms	0	96		2.4	0	0	96	10 times EC
Bluegreens	0	96		2.4	0	0	96	10 times EC
Macrophytes	0	96		0.3247	0	0	96	10 times EC

Chlorpyrifos Animal Toxicity Parameters

Animal name	LC50 (ug/L)	exp. time (h)	Elim. rate const (1/d)	Biotrnsfm. rate (1/d)	EC50 growth (ug/L)	Growth exp. (h)	EC50 repro (ug/L)	Repro. exp. time(h)	Ave. wet wt. (g)	Lipid Frac	Drift Threshold (ug/L)
Trout	8.701	96	3.485E-03	0	0.71	96	0.355	96	2410	0.11	0
Bluegill	2.4	96	6.197E-02	0	0.17	96	0.085	96	125	0.03	0
Bass	9.849	96	5.064E-03	0	1.2439	96	0.622	96	250	0.1	0
Catfish	387.174	96	5.57E-03	0	28	96	14	96	150	0.1	0
Minnow	203	96	5.428E-02	0	20.3	96	10.15	96	2	0.04	0
Daphnia	0.17	24	9.609E-01	0	0.09	24	0.045	24	0.0006	0.08	0
Chironomid	1.416	24	1.459E+00	0	0.5798	24	0.2899	24	0.0075	0.05	0.0289905
Stonefly	10	96	3.965E-01	0	1	96	0.5	96	0.03	0.05	0.05
Ostracod	2.055	24	6.82E+00	0	0.5776	24	0.2888	24	0.002	0.05	0.02888
Amphipod	0.29	48	6.82E+00	0	0.011	48	0.0055	48	0.002	0.05	0.00055
Other	0	96	4.169E-02	0	0	96	0	96	1	0.05	0

Oxygen, Nutrients

A simple input screen is used for oxygen; don't forget that oxygen dissolved in inflow water can be a significant loading. Likewise, 0 mg/L in a high flow loading can drive a stream reach anoxic.



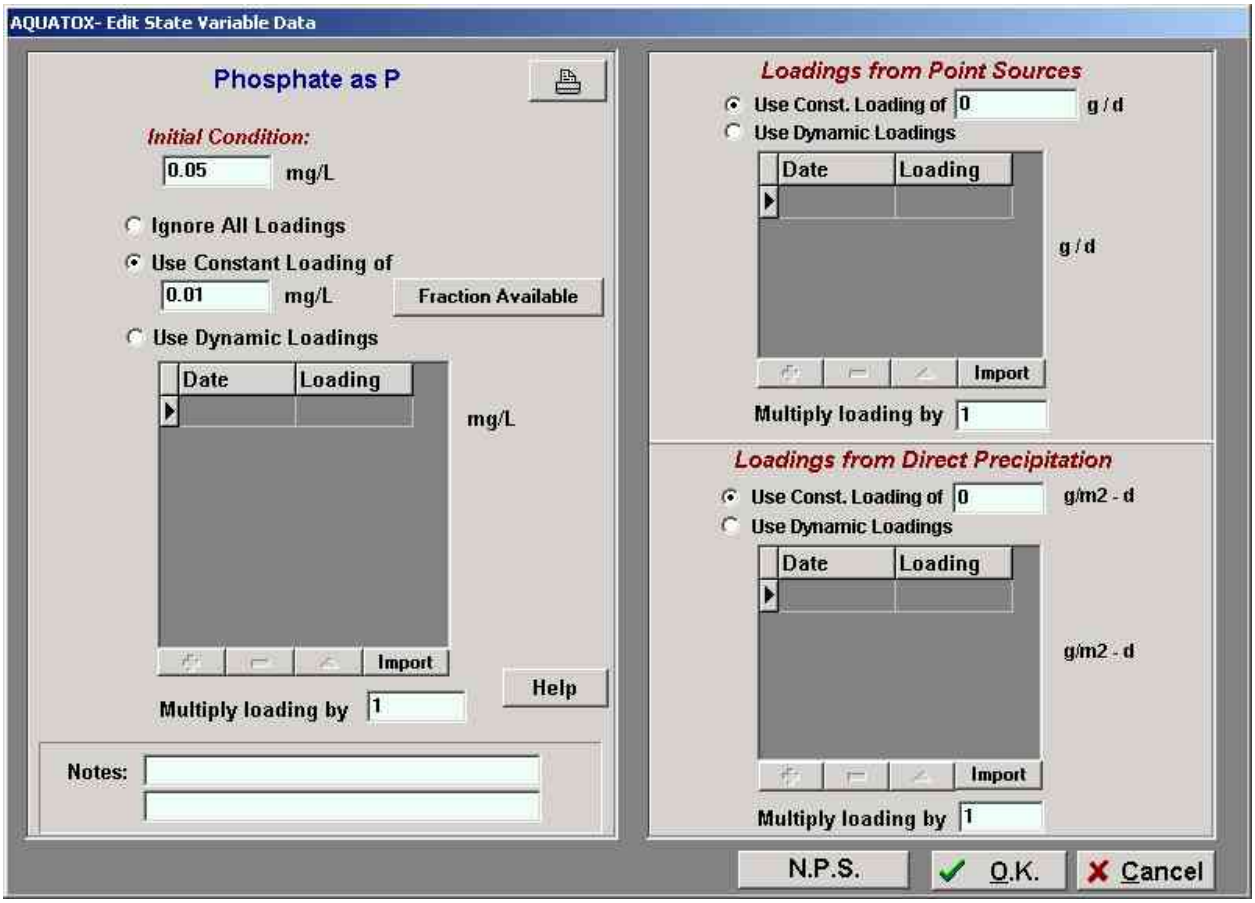
More complex input screens are used for nutrients. Loadings can be in concentrations (mg/L) in inflow water, in g/d from point sources (PS) and from non-point sources (NPS), and in g/m^2 d from direct precipitation (DP), including dry fall. A button at the bottom of the loading screen toggles between NPS and PS/DP. An additional button on the Phosphate loading screen enables the user to adjust the fraction available for each loading source; the default is 1.

Nutrient Conversions

Following limnological convention, nutrients are expressed in elemental form (such as phosphate as phosphorus and ammonia as nitrogen). Phosphate is treated as available or orthophosphate; if part of the phosphate loading is not available, the fraction available should be adjusted. Nitrate and nitrite are combined because nitrite levels are usually negligible. Organic nutrient loadings are considered part of the detrital loadings, with the simplifying assumption of constant stoichiometry, and are not considered separately.

If you have nutrient data in molecular form, use the following conversions:

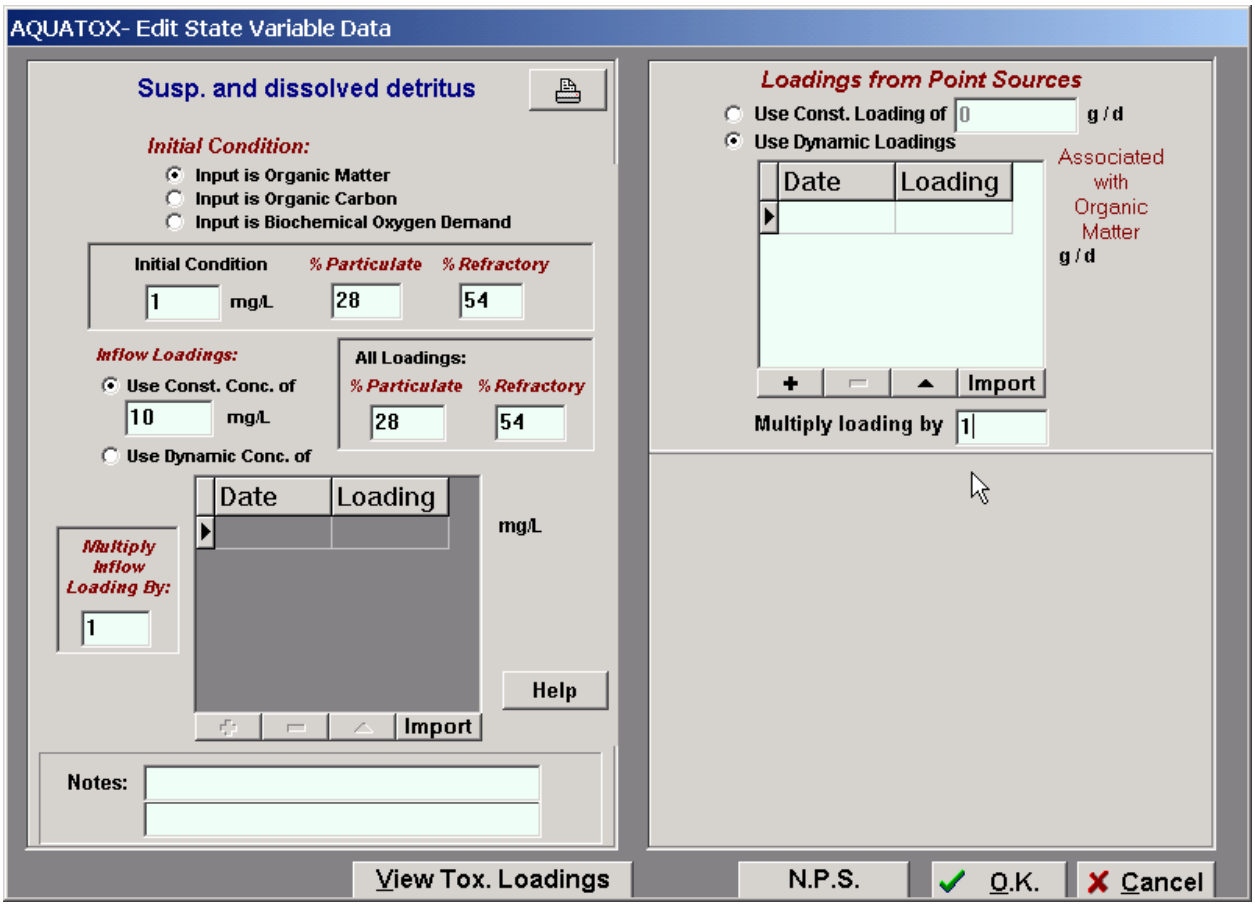
$$Phosphorus = phosphate \cdot 0.33$$
$$Nitrogen = ammonia \cdot 0.78$$
$$Nitrogen = nitrate \cdot 0.23$$



Detritus

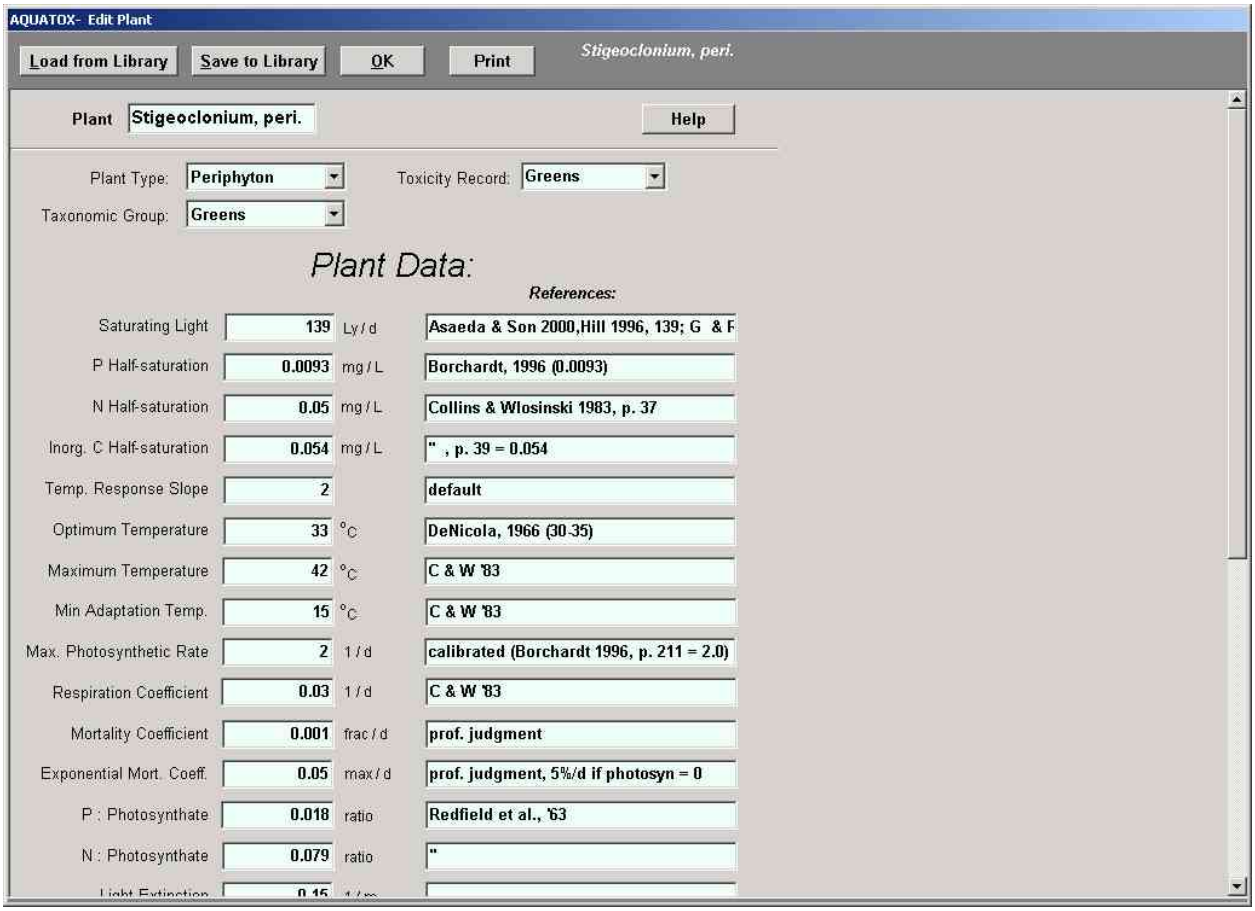
A complex loading screen is necessary for suspended and dissolved detritus. AQUATOX simulates **Organic Matter** (dry weight); however, the user can input data as **Organic Carbon** or **Biochemical Oxygen Demand** (BOD), and the model will make the necessary conversions. Suspended and dissolved detritus initial conditions and loadings are divided into four compartments: particulate refractory and labile detritus and dissolved refractory and labile organic matter. Initial conditions and loadings are parsed by specifying **% Particulate** and **% Refractory**. Loadings 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 (**:**g/kg).

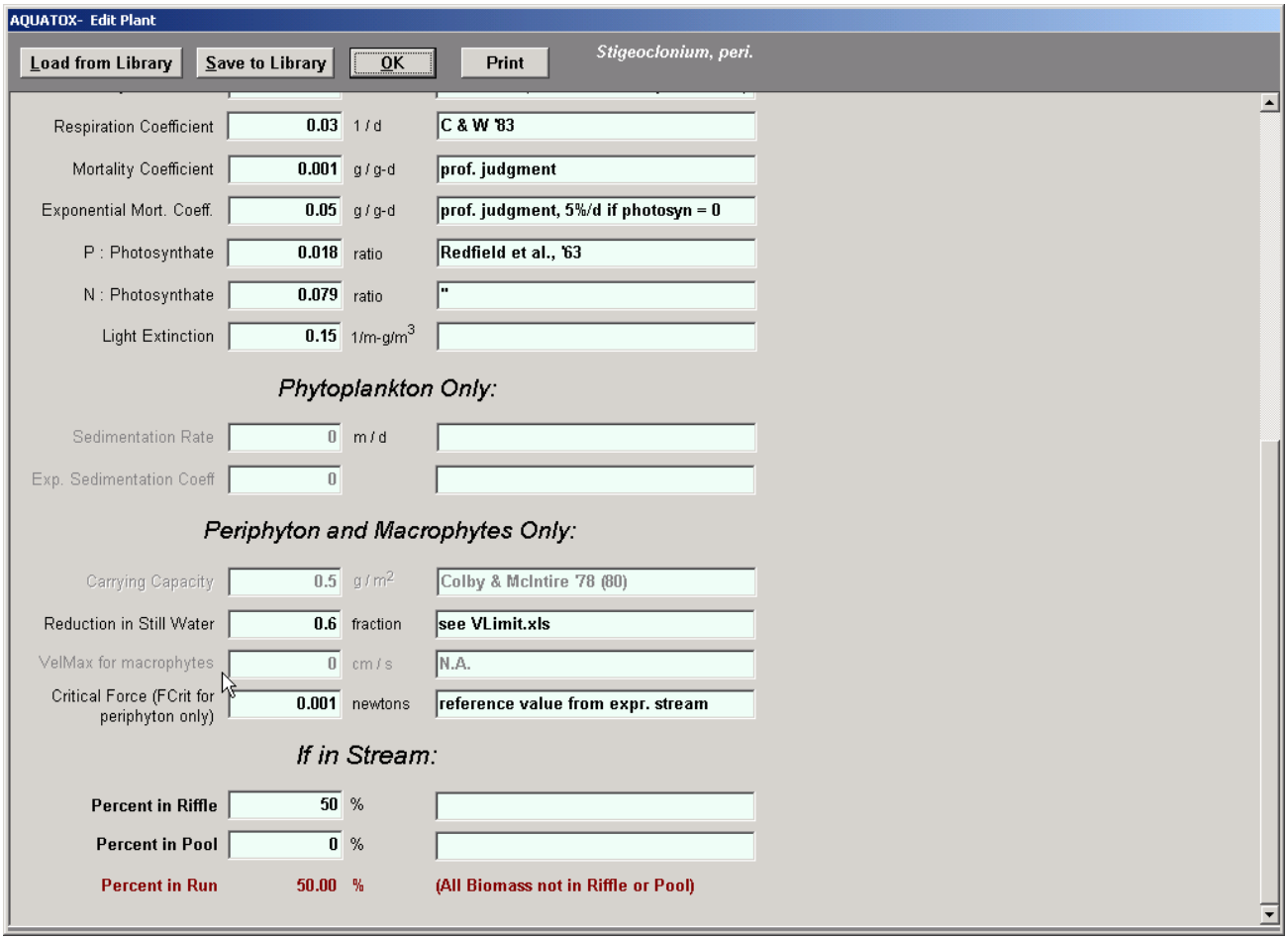
Separate screens are provided for refractory and labile organic sediments. The initial conditions are given as g/m^2, and the loadings are given as mg/L. Associated toxicants are given as **:**g/kg (ppm).


AQUATOX- Edit State Variable Data
Susp. and dissolved detritus
Initial Condition:
Input is Organic Matter
Input is Organic Carbon
Input is Biochemical Oxygen Demand
Initial Condition
% Particulate
% Refractory
1
mg/L
28
54
Inflow Loadings:
Use Const. Conc. of
10
mg/L
Use Dynamic Conc. of
All Loadings:
% Particulate
% Refractory
28
54
Date
Loading
mg/L
Multiply Inflow Loading By:
1
Import
Help
Notes:
Loadings from Point Sources
Use Const. Loading of
0
g / d
Use Dynamic Loadings
Date
Loading
Associated with Organic Matter
g / d
Import
Multiply loading by
1
View Tox. Loadings
N.P.S.
O.K.
Cancel

Plants

The plant initial condition and loading screens are sensitive to the types of plants. Phytoplankton units are mg/L, and periphyton and macrophytes are given as g/m^2. Toxicants associated with biota are given as **:** g/kg (ppm). Related parameter files can be accessed by clicking on **Edit Underlying Data**. Some parameters are not used; those will appear grayed out on the screen.

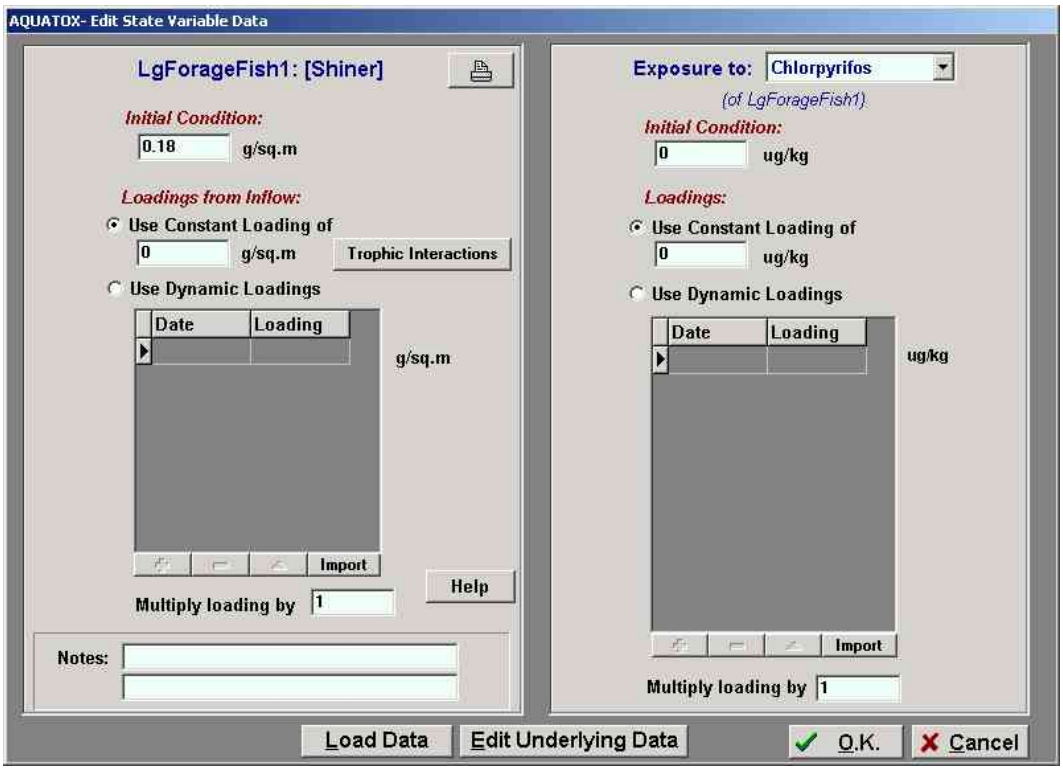


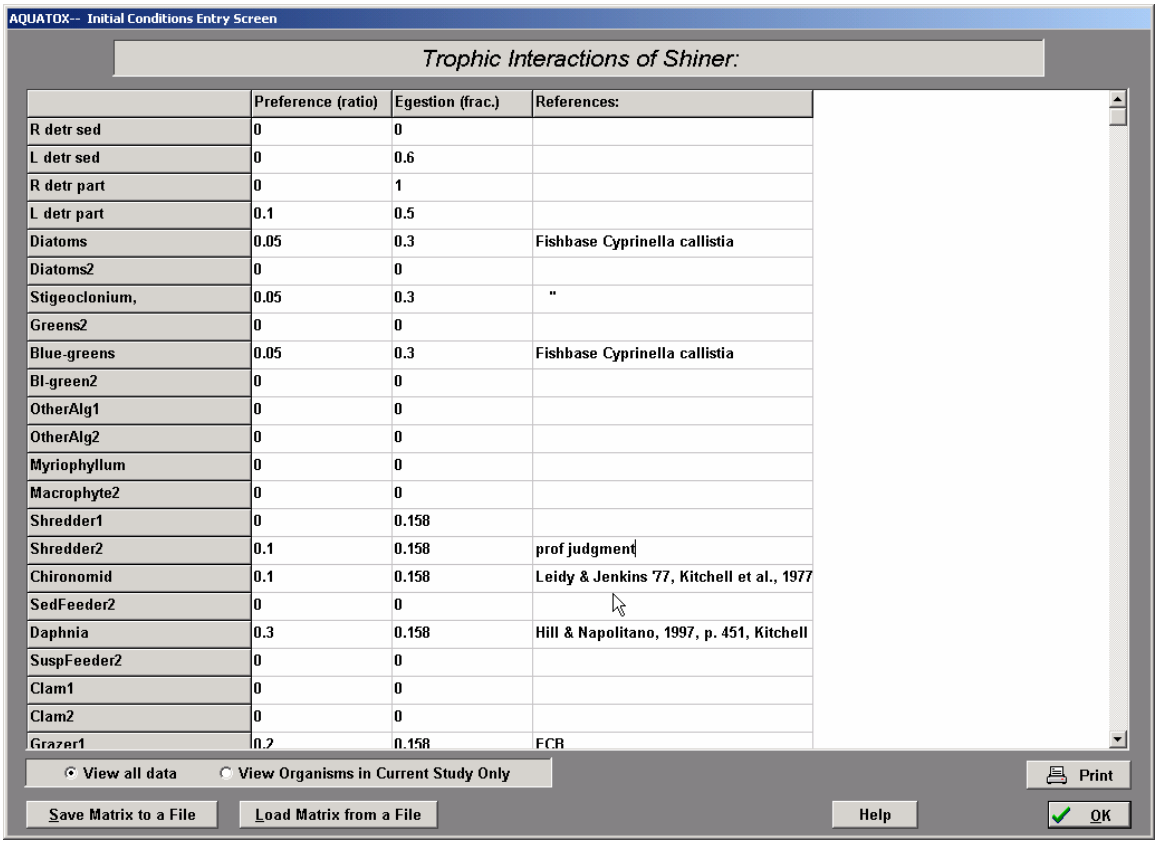


Animals

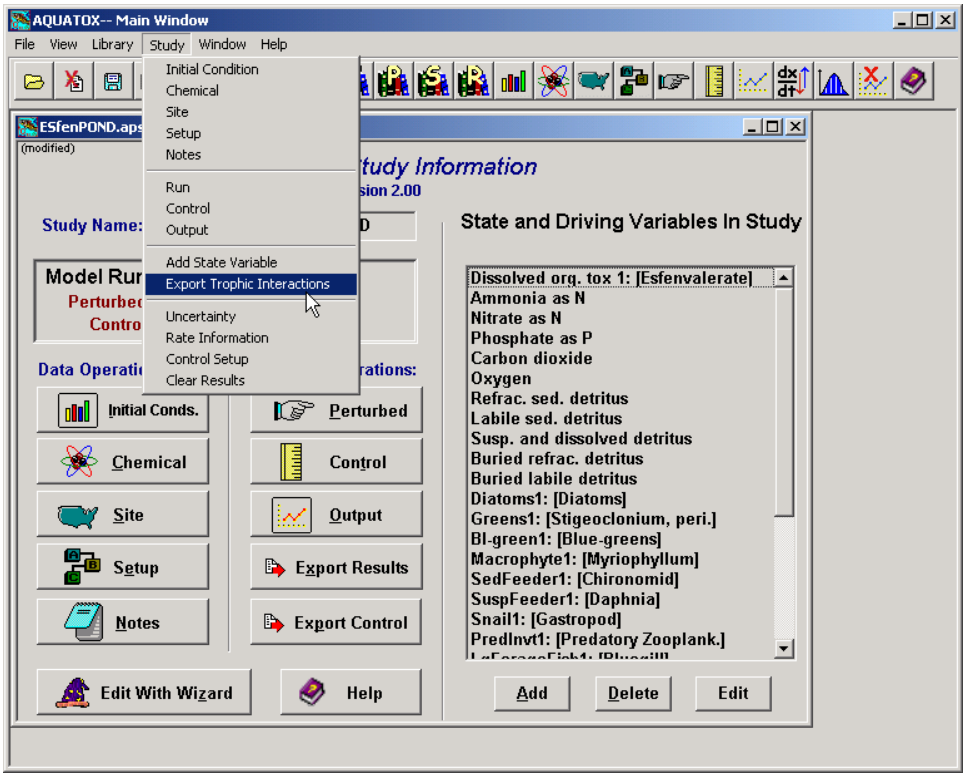
The animal initial condition and loadings screens are sensitive to animal type. Zooplankton are given in units of mg/L; zoobenthos and fish are given in units of g/m^2. As always, toxicants associated with biota are given as **:**g/kg (ppm); loadings of associated toxicants can be thought of as body-burden sources due to immigration.

By clicking on **Trophic Interactions** one can access a separate screen with feeding preferences and egestion coefficients. The entire trophic interaction record can be displayed or just the organisms simulated in the present study. The program normalizes preferences during execution so that they sum to 1.0, facilitating the addition or deletion of state variables without the user having to recalculate the preference values. The matrix can be imported or exported, providing considerable flexibility in defining organisms. However, the format is internal to AQUATOX, so the matrices should be prepared in the context of the parameter screen for an organism in either a study or library. The actual values used at the beginning of a simulation can be determined by clicking on **Study**, then **Export Trophic Interactions**; it will create a text file with the matrix.

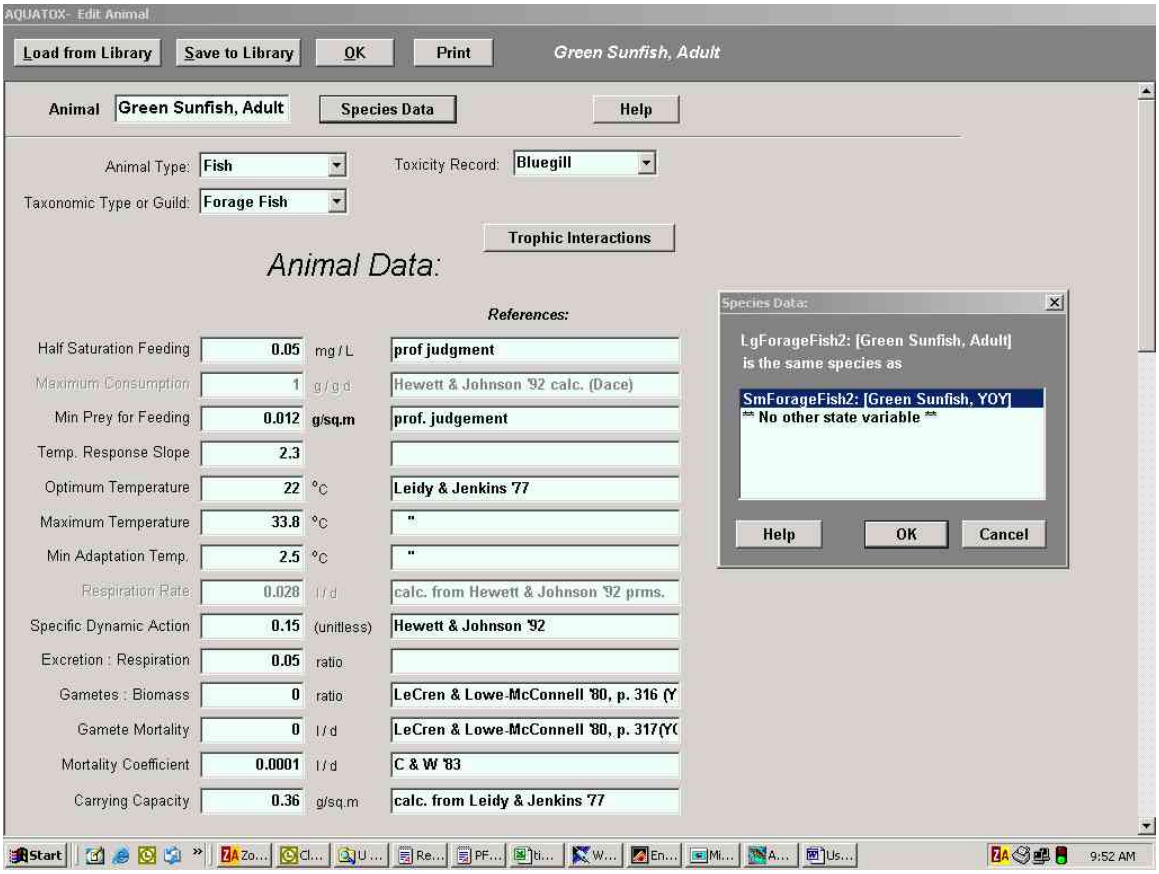




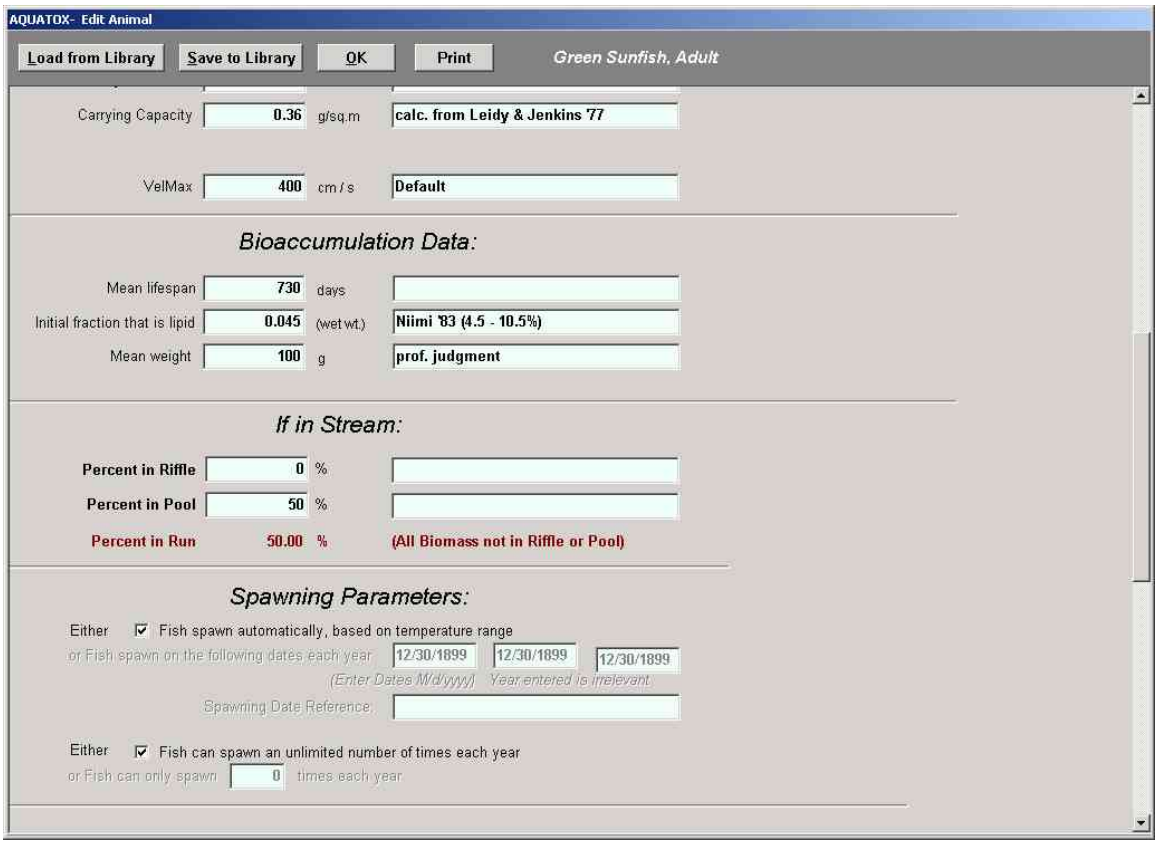
	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	0	
L detr sed	0	0.6	
R detr part	0	1	
L detr part	0.1	0.5	
Diatoms	0.05	0.3	Fishbase Cyprinella callistia
Diatoms2	0	0	
Stigeoclonium,	0.05	0.3	"
Greens2	0	0	
Blue-greens	0.05	0.3	Fishbase Cyprinella callistia
Bl-green2	0	0	
OtherAlg1	0	0	
OtherAlg2	0	0	
Myriophyllum	0	0	
Macrophyte2	0	0	
Shredder1	0	0.158	
Shredder2	0.1	0.158	prof judgment
Chironomid	0.1	0.158	Leidy & Jenkins '77, Kitchell et al., 1977
SedFeeder2	0	0	
Daphnia	0.3	0.158	Hill & Napolitano, 1997, p. 451, Kitchell
SuspFeeder2	0	0	
Clam1	0	0	
Clam2	0	0	
Grazer1	0.2	0.158	FCB



Clicking on Edit Underlying Data can access related parameter files. Release 2 can model two size classes for each fish species and up to fifteen age classes for one species. Records for different size classes are linked by clicking on **Species Data** and choosing the correct record from the list given. In the example, "Green Sunfish, Adult" is linked with "Green Sunfish, YOY." Two different species can be modeled instead of two size classes, in which case "No other state variable" should be chosen in the Species Data window.



Scrolling down through the window, we find several parameters that are new to Version 2. *VelMax* is the maximum velocity that the organism can experience without being swept downstream. Preferences for stream habitats can be specified; the default is 100% for the run; if the site is not a stream, the habitat preferences are ignored. Fish spawning dates can be specified as an alternative to being cued by temperature preferences.



Allometric Parameters

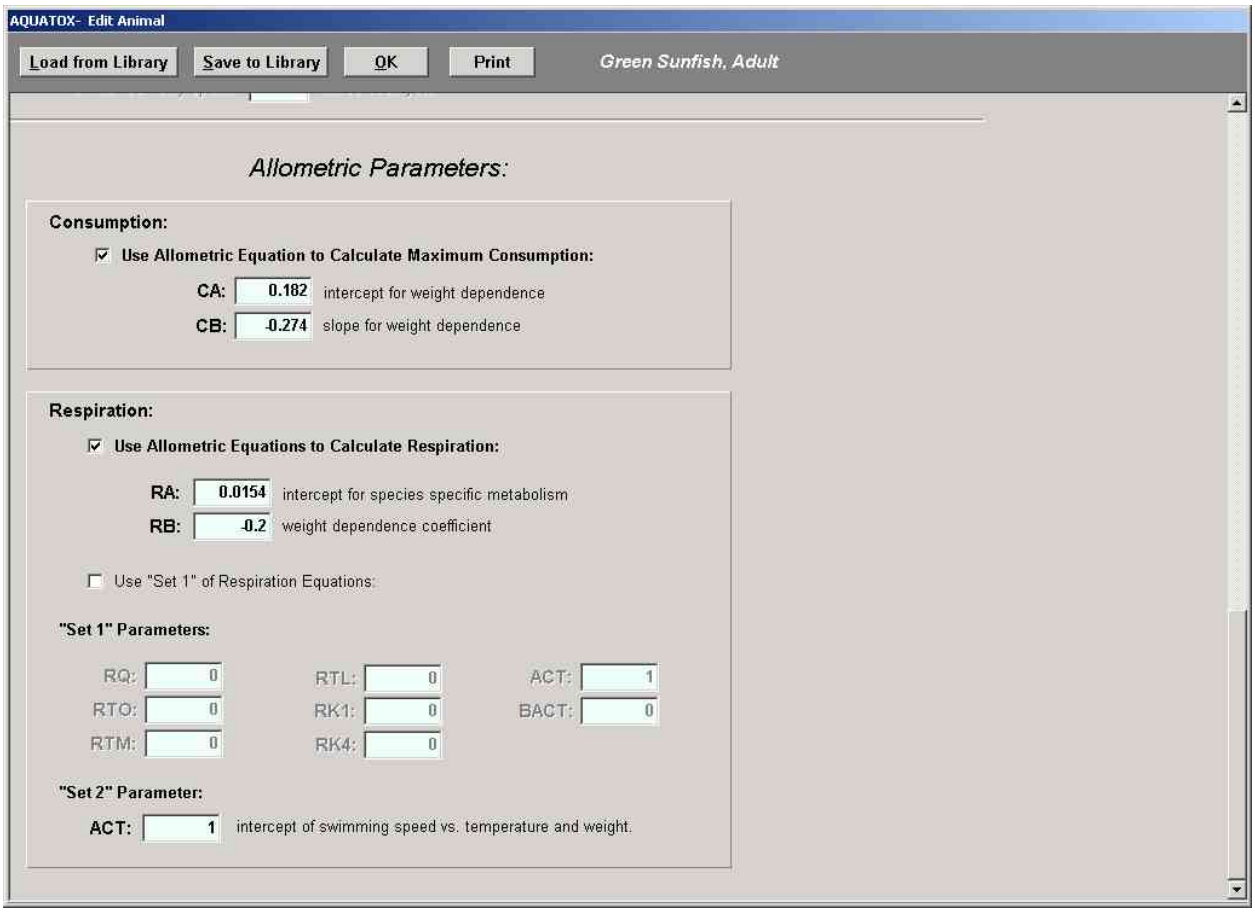
The allometric parameters permit computation of maximum consumption rates (*CMax)* and respiration rates based on size using parameter values available from documentation of the Wisconsin Fish Bioenergetics Model (Hewett and Johnson, 1992); we do not recommend using these without reference to that document. To facilitate use of this source of parameters, the parameter names are the same. *CA* is the intercept of the allometric consumption function, and *CB* is the weight exponent:

$$CMax = CA \cdot Wt^{CB}$$

The maximum respiration rate (*RMax*) is computed from the intercept of the allometric respiration function (*RA*), the weight exponent (*RB*), and an activity factor (*Activity*):

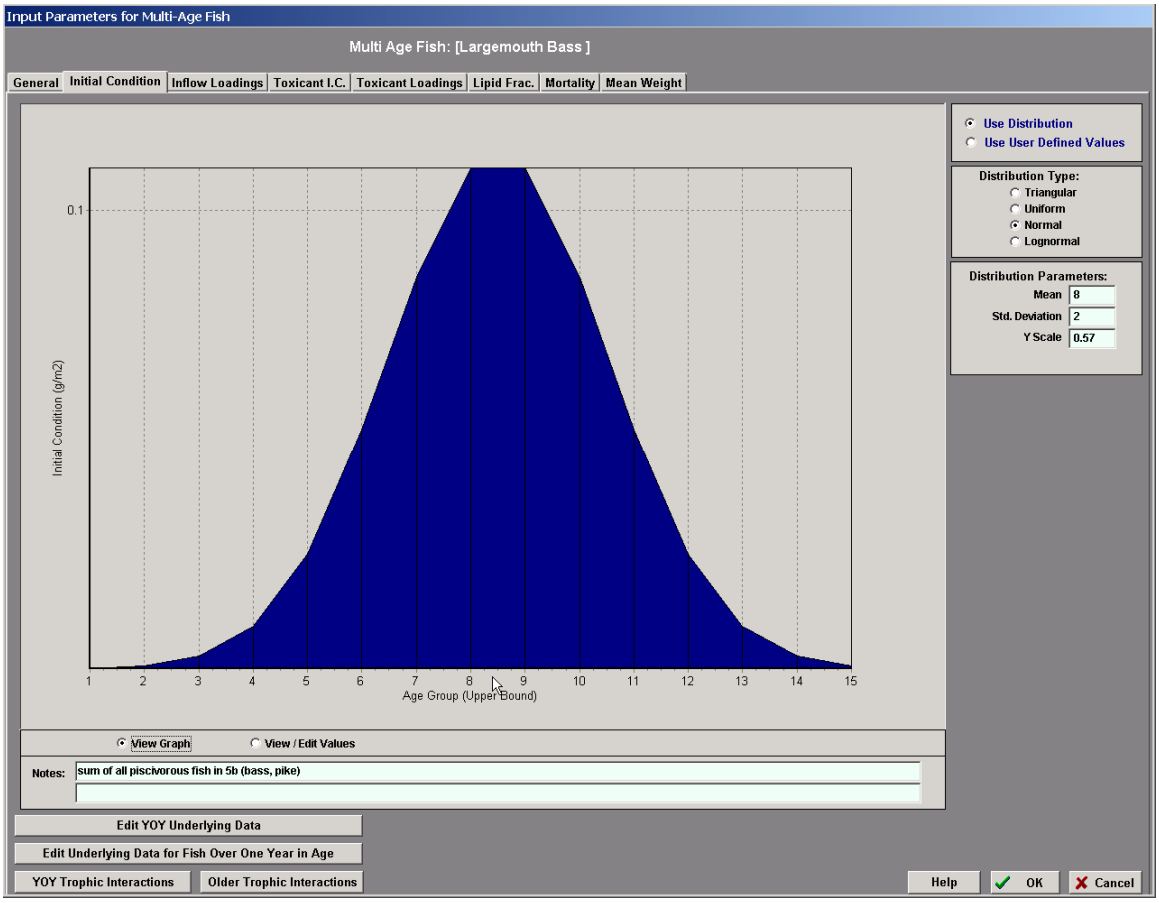
$$RMax = RA \cdot Wt^{RB} \cdot Activity$$

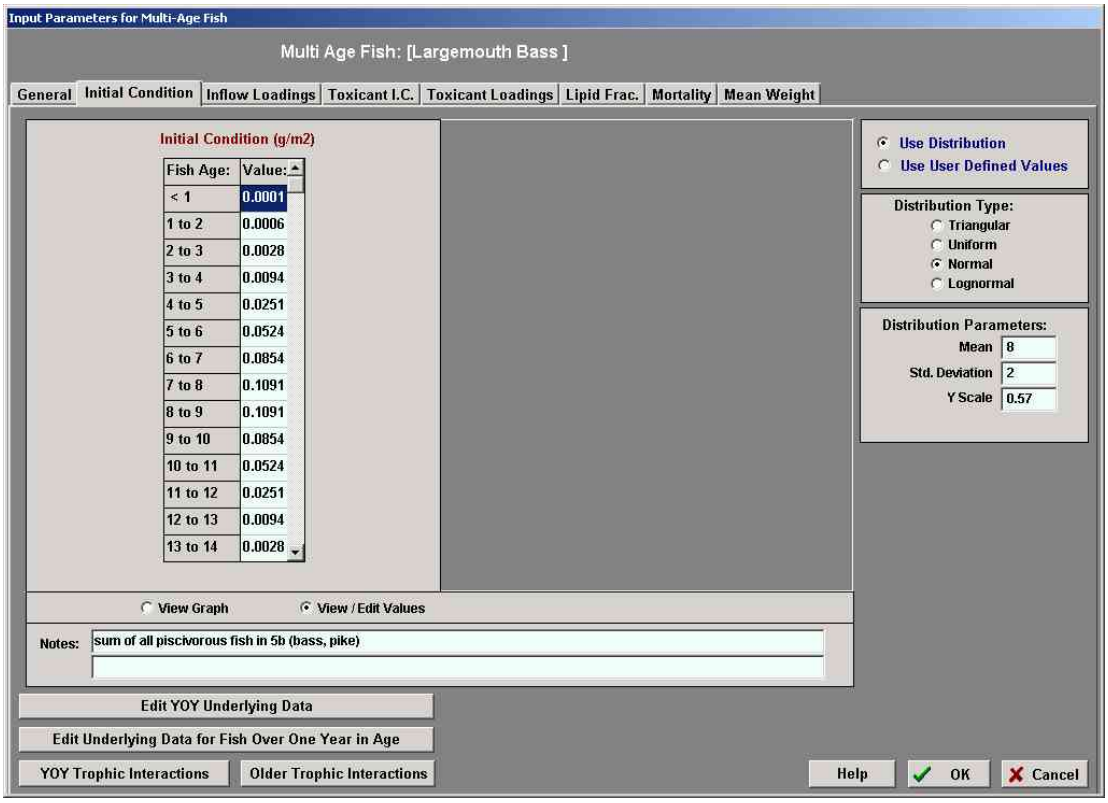
Computation of the activity factor can be a complex function of swimming speed with several parameters (Set 1). Briefly, these are the Q10 (the increase per 10E C, *RQ*), the optimum temperature (*RO*), the maximum temperature (*RM*), the temperature above which swimming speed changes (*RTL*), the intercept for swimming speed above *RTL* (*RK1*), the weight exponent for swimming (*RK4*), the intercept for swimming speed below *RTL* (*ACT*), and the temperature dependence of swimming speed below *RTL* (*BACT*). Otherwise, the Set 2 activity parameter (*ACT*) is used as a multiplier.

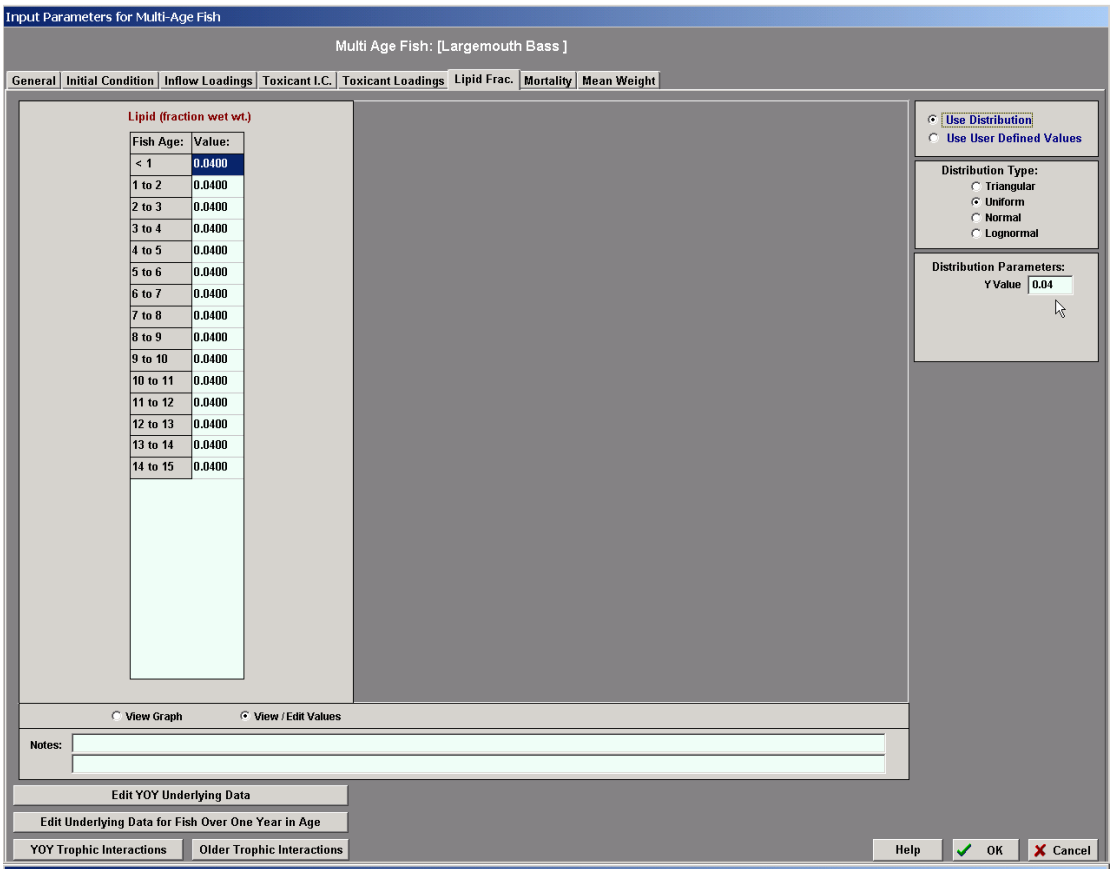


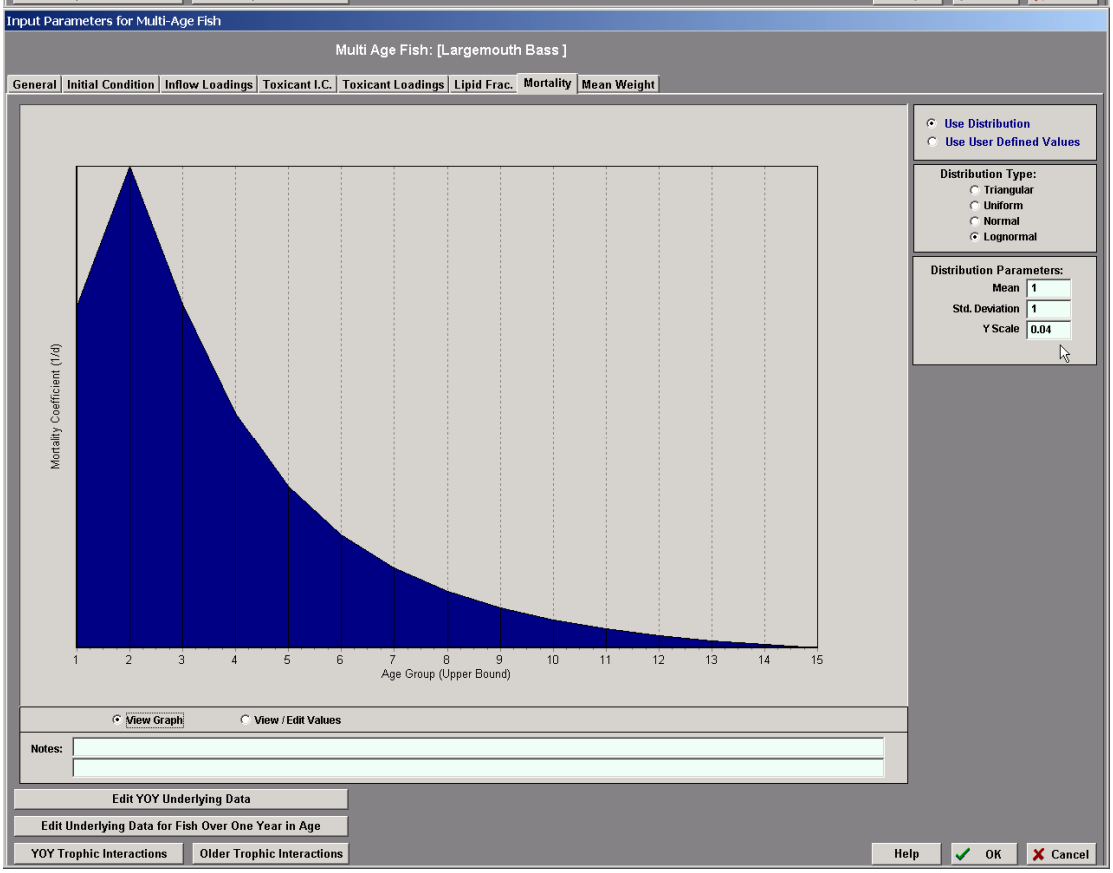
As mentioned previously, Release 2 also can model one species as having multiple age classes. Tabs indicate the different input screens, including General (fish name and age at which sexually mature), Initial Conditions, Inflow Loadings (from upstream), Toxicant I.C. (initial conditions), Toxicant Loadings, Lipid Fractions, Mortality coefficients, and Mean Weights. For each, the user can enter values for each age class or can choose one of several distributions, characterized by user-supplied statistics. The values can be graphed as well. Parameter screens and trophic interaction screens can be accessed for young-of-the-year (YOY) and older fish.

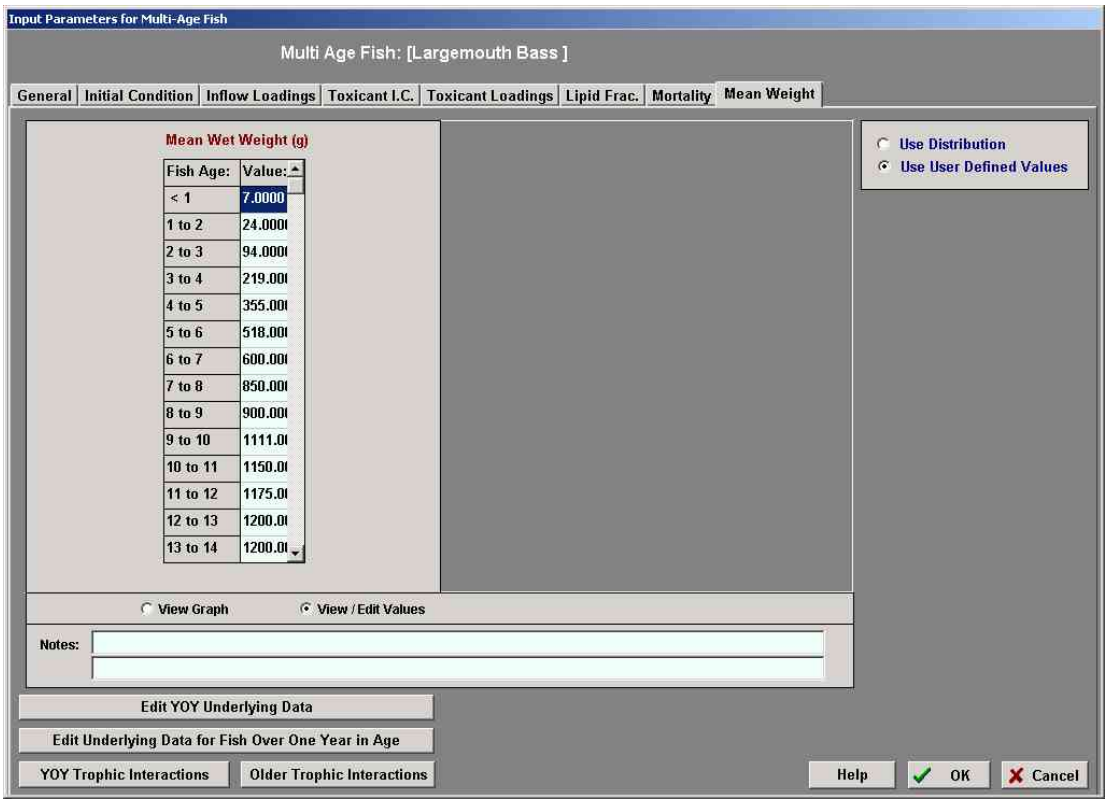
Entering values for each category can be tedious. Initial biomass in each age class can be entered using a normal distribution. The "Y Scale" value is the total biomass, and the mean is the most important age class in terms of biomass. This is best seen by selecting **View Graph**; values can be seen by selecting **View/Edit Values**—but, contrary to the label, you cannot edit them in that mode. By selecting **Use User Defined Values**, you can make any changes you wish to individual age class values. Distributions are not as useful for other categories; one might use a uniform distribution to populate the age classes with a constant value for lipid fraction or a log normal distribution to obtain an initial distribution of values for mortality. You could then modify individual values. Caution: if you switch to **Use Distribution** from **Use User Defined Values**, the manually entered values will be lost! Mean weights are very important because they determine the maximum consumption and respiration rates, using the allometric equations. There is no way to use a distribution to get meaningful mean weights.


Input Parameters for Multi-Age Fish
Multi Age Fish: [Largemouth Bass]
General
Initial Condition
Inflow Loadings
Toxicant I.C.
Toxicant Loadings
Lipid Frac.
Mortality
Mean Weight
Use Distribution
Use User Defined Values
Distribution Type:
Triangular
Uniform
Normal
Lognormal
Distribution Parameters:
Mean 8
Std. Deviation 2
Y Scale 0.57
0.1
Initial Condition (g/m2)
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
Age Group (Upper Bound)
View Graph
View / Edit Values
Notes: sum of all piscivorous fish in 5b (bass, pike)
Edit YOY Underlying Data
Edit Underlying Data for Fish Over One Year in Age
YOY Trophic Interactions
Older Trophic Interactions
Help
OK
Cancel


Input Parameters for Multi-Age Fish
Multi Age Fish: [Largemouth Bass]
General
Initial Condition
Inflow Loadings
Toxicant I.C.
Toxicant Loadings
Lipid Frac.
Mortality
Mean Weight
Initial Condition (g/m2)
Fish Age: Value:
< 1 0.0001
1 to 2 0.0006
2 to 3 0.0028
3 to 4 0.0094
4 to 5 0.0251
5 to 6 0.0524
6 to 7 0.0854
7 to 8 0.1091
8 to 9 0.1091
9 to 10 0.0854
10 to 11 0.0524
11 to 12 0.0251
12 to 13 0.0094
13 to 14 0.0028
Use Distribution
Use User Defined Values
Distribution Type:
Triangular
Uniform
Normal
Lognormal
Distribution Parameters:
Mean 8
Std. Deviation 2
Y Scale 0.57
View Graph
View / Edit Values
Notes: sum of all piscivorous fish in 5b (bass, pike)
Edit YOY Underlying Data
Edit Underlying Data for Fish Over One Year in Age
YOY Trophic Interactions
Older Trophic Interactions
Help
OK
Cancel

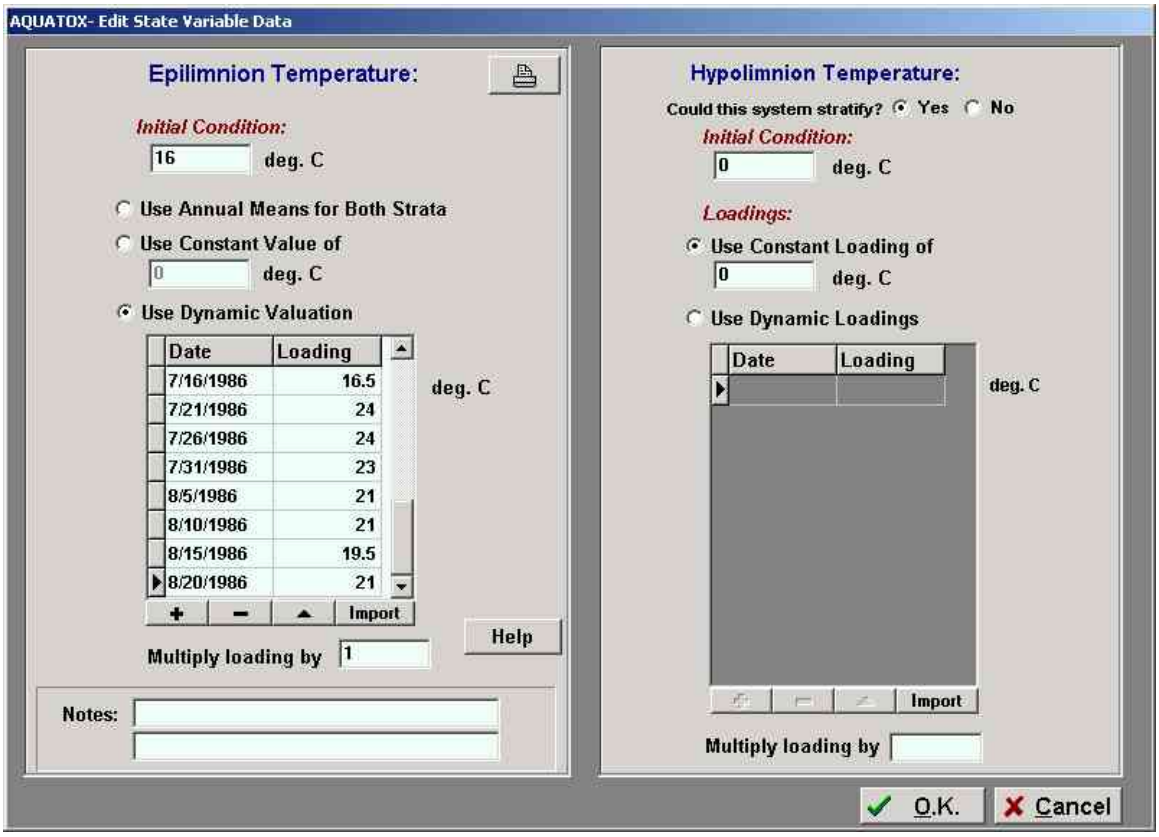

Input Parameters for Multi-Age Fish
Multi Age Fish: [Largemouth Bass]
General
Initial Condition
Inflow Loadings
Toxicant I.C.
Toxicant Loadings
Lipid Frac.
Mortality
Mean Weight
Lipid (fraction wet wt.)
Fish Age:
Value:
< 1 0.0400
1 to 2 0.0400
2 to 3 0.0400
3 to 4 0.0400
4 to 5 0.0400
5 to 6 0.0400
6 to 7 0.0400
7 to 8 0.0400
8 to 9 0.0400
9 to 10 0.0400
10 to 11 0.0400
11 to 12 0.0400
12 to 13 0.0400
13 to 14 0.0400
14 to 15 0.0400
Use Distribution
Use User Defined Values
Distribution Type:
Triangular
Uniform
Normal
Lognormal
Distribution Parameters:
Y Value 0.04
View Graph
View / Edit Values
Notes:
Edit YOY Underlying Data
Edit Underlying Data for Fish Over One Year in Age
YOY Trophic Interactions
Older Trophic Interactions
Help
OK
Cancel


Input Parameters for Multi-Age Fish
Multi Age Fish: [Largemouth Bass]
General
Initial Condition
Inflow Loadings
Toxicant I.C.
Toxicant Loadings
Lipid Frac.
Mortality
Mean Weight
Mortality Coefficient (1/d)
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
Age Group (Upper Bound)
Use Distribution
Use User Defined Values
Distribution Type:
Triangular
Uniform
Normal
Lognormal
Distribution Parameters:
Mean 1
Std. Deviation 1
Y Scale 0.04
View Graph
View / Edit Values
Notes:
Edit YOY Underlying Data
Edit Underlying Data for Fish Over One Year in Age
YOY Trophic Interactions
Older Trophic Interactions
Help
OK
Cancel


Input Parameters for Multi-Age Fish
Multi Age Fish: [Largemouth Bass]
General
Initial Condition
Inflow Loadings
Toxicant I.C.
Toxicant Loadings
Lipid Frac.
Mortality
Mean Weight
Mean Wet Weight (g)
Fish Age:
Value:
< 1
7.0000
1 to 2
24.000
2 to 3
94.000
3 to 4
219.00
4 to 5
355.00
5 to 6
518.00
6 to 7
600.00
7 to 8
850.00
8 to 9
900.00
9 to 10
1111.0
10 to 11
1150.0
11 to 12
1175.0
12 to 13
1200.0
13 to 14
1200.0
Use Distribution
Use User Defined Values
View Graph
View / Edit Values
Notes:
Edit YOY Underlying Data
Edit Underlying Data for Fish Over One Year in Age
YOY Trophic Interactions
Older Trophic Interactions
Help
OK
Cancel

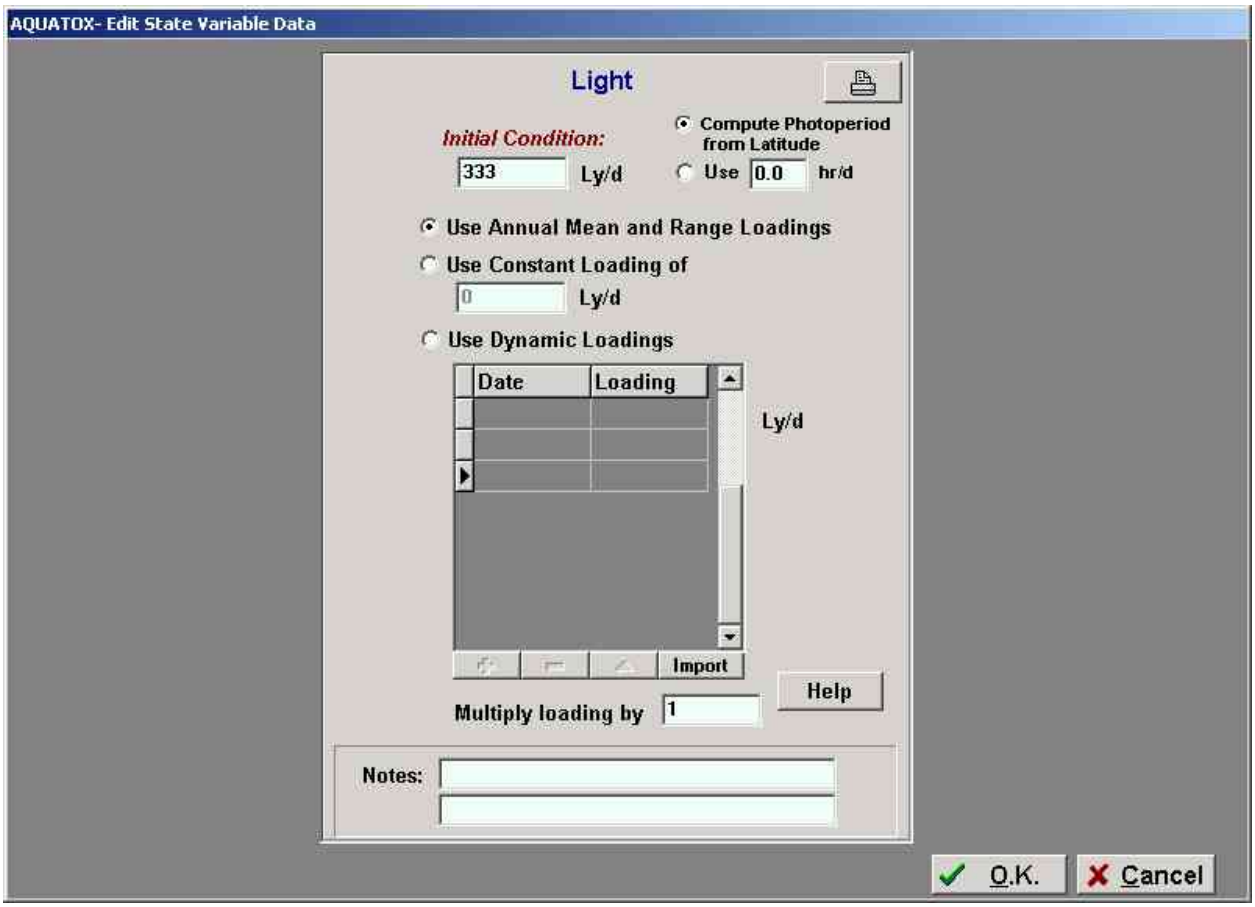
Temperature

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



Light

Annual mean and range values for light are input in the site screen and may be used to estimate daily incident solar radiation at the surface of the water in Langleys/day (Ly/d). Dynamic loadings are especially useful for areas where light intensity is not a simple sinusoidal relationship, such as areas with seasonal coastal fog and streams where there is seasonal riparian shading. Ordinarily the photoperiod is computed from the latitude; but occasionally, such as with indoor experimental streams, it may be desirable to set a constant photoperiod.



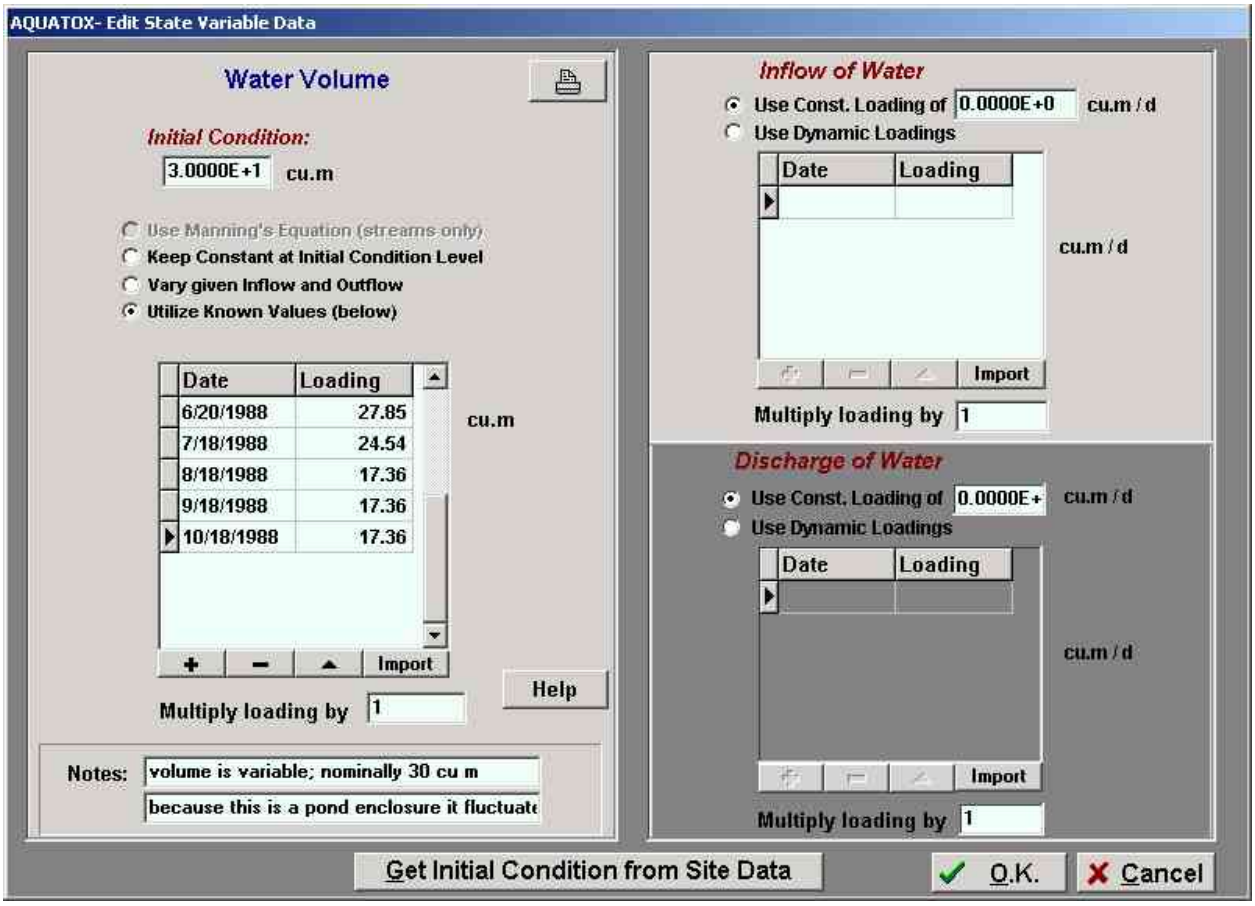
Light Conversions

Approximate conversions are:
1 Ly/d = 10 Kcal/m^2 = 5.2 Einsteins = 2764.46 Joules/m^2 d.

Water Volume

Considerable flexibility exists to compute or specify water volume. Depending on the method chosen, inflow or discharge values may be required. The Manning's equation can be

used to compute changing volumes in a stream. The simplest procedure is hold volume constant at the initial condition. Volume can be computed dynamically using both inflow and discharge, which are input on this screen; however, it also uses the annual evaporation rate, which is input on the site screen. When available, a known time series can be entered or imported. Flow data can be imported in several formats, including USGS tab-delimited; however, recent changes in the USGS format, including variable header material, makes this prone to problems. If the data do not appear in the preview window then the flow data will have to be converted in a spreadsheet from cfs to m^3/d, and the date column and flow column then exported as a tab-delimited or comma-separated file suitable for importing into AQUATOX.



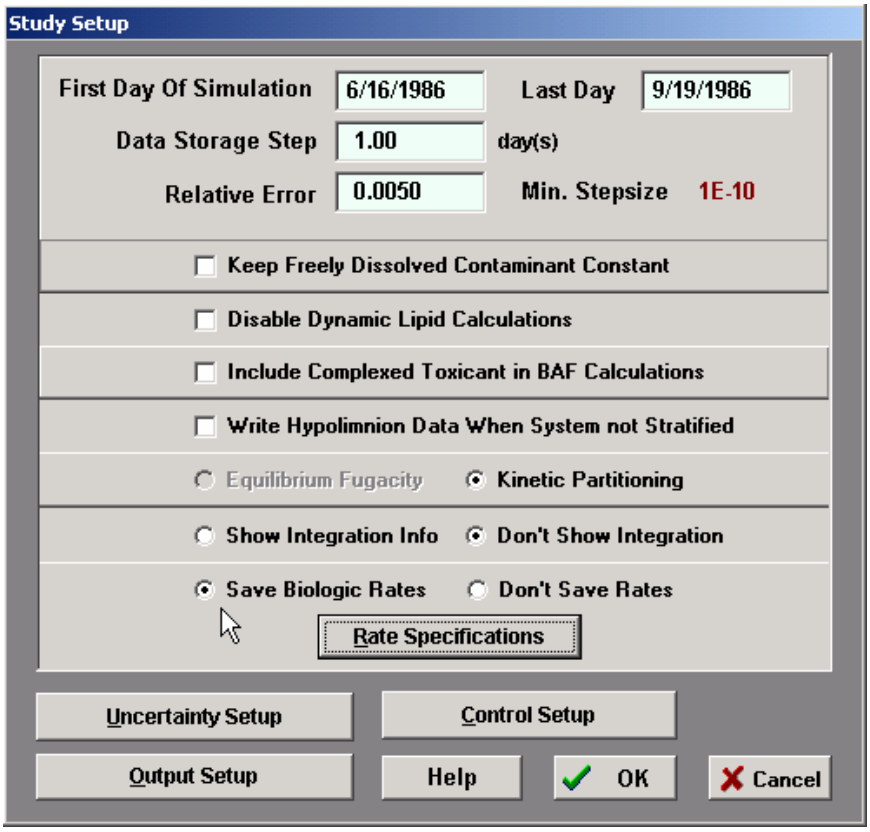
pH

AQUATOX does not compute pH as a state variable at present. Therefore, it is important to enter a reasonable constant value or provide an observed time series. This variable is especially important in computing hydrolysis of toxic chemicals. Extreme values (below 5 and above 9) can affect microbial degradation.

Setup

By clicking on **Setup** in the Main screen, the user can set some simulation variables and several important procedures. At the top of the setup screen, you can modify the first and last

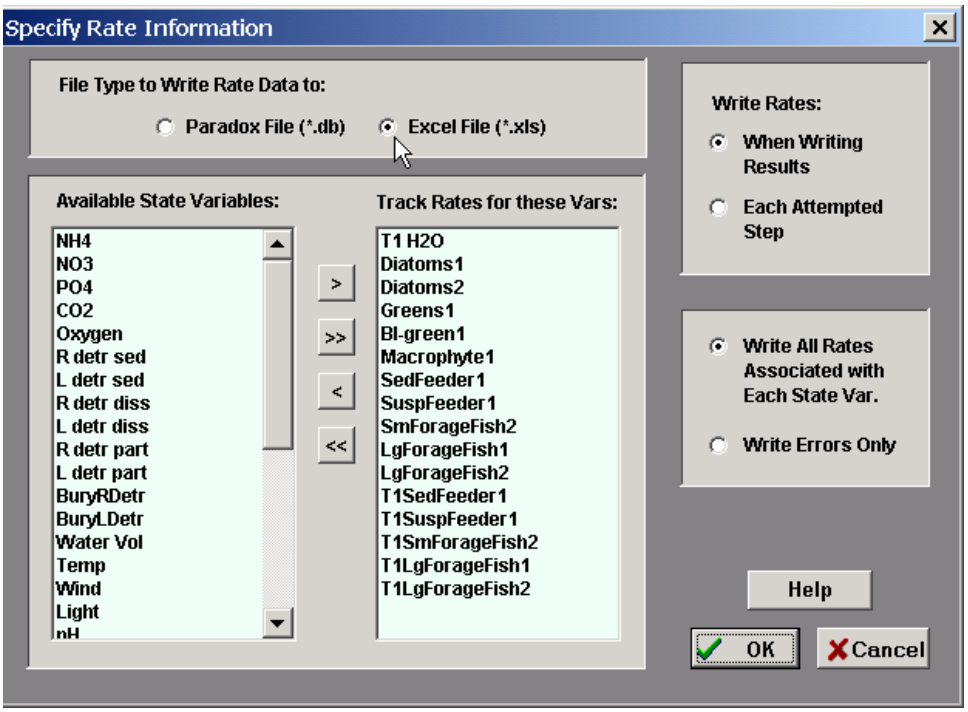
days of the simulation. Use a 4-digit year designation to avoid any confusion between the years 1900 and 2000; the model will interpret "/00" as "/2000." The Data Storage Step defines how often the results are saved; it is usually one day, but can be varied to save space or show high frequency results. AQUATOX interpolates variable-step output to obtain the desired interval. The Relative Error is the acceptable error in the simulation; if it is not achieved in a particular time step, the variable Runge-Kutta routine decreases the step size and tries again. If the relative error is too large, the results may be erroneous; if it is too small, the run time may be too long. Usually a value between 0.005 and 0.0005 is appropriate, but you may wish to experiment for a particular application.



What follows are three choices for computing bioaccumulation factors (BAFs) and a choice for saving output. If you are computing steady-state BAFs, you may wish to hold the freely dissolved contaminant constant. AQUATOX calculates time-varying lipid fractions in fish, but those calculations can be disabled and default or user-supplied initial values can be used. The older literature often did not distinguish between freely dissolved contaminants and those complexed with dissolved organic matter. You may choose to include the complexed contaminant in computing BAFs so that the results are directly comparable with the older literature values. In plotting output for stratified systems, it is usually more pleasing to plot continuous values for the hypolimnion, even when the system is not stratified. This is done by duplicating epilimnion values for the hypolimnion when the system is well mixed; however, that takes additional storage, so you may choose not to duplicate those data points.

Equilibrium Fugacity is grayed out because the model only represents kinetic partitioning now. If you click on **Show Integration Info.**, you will be able to see what time steps are used in solving the differential equations and what rates and associated relative errors are causing the integration to slow down while the model is running. The progress screen also will show when periphyton sloughing is occurring in a stream simulation.

You may save biologic (and chemical) rates for examination with a spreadsheet program. Choose **Save Biologic Rates** and click on **Rate Specifications** to designate those state variables for which you want the additional output. Don't save rates for all state variables or the output will be voluminous! Usually you would save rates for each output step, by choosing "When Writing Results." However, you can save rates for each step in the solution of the differential equations, that is, "Each Attempted Step". You also can choose to save just the errors associated with each state variable. These latter choices are useful only if you are concerned with the details of the numerical analysis. Unless you have Paradox or Quattro, choose to save as an **Excel File (*.xls)**.



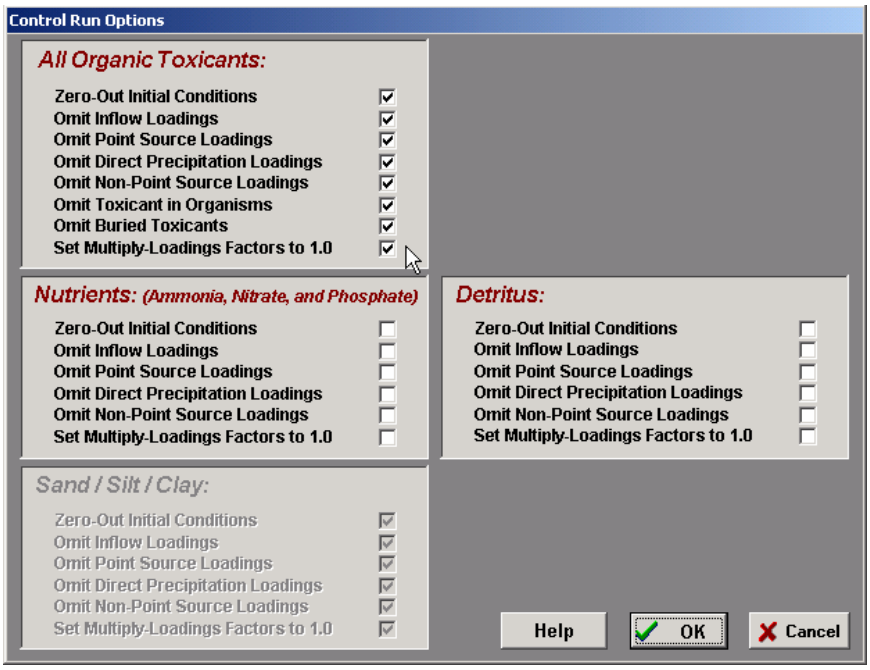
Uncertainty, Control and Output setups are complex and are covered below.

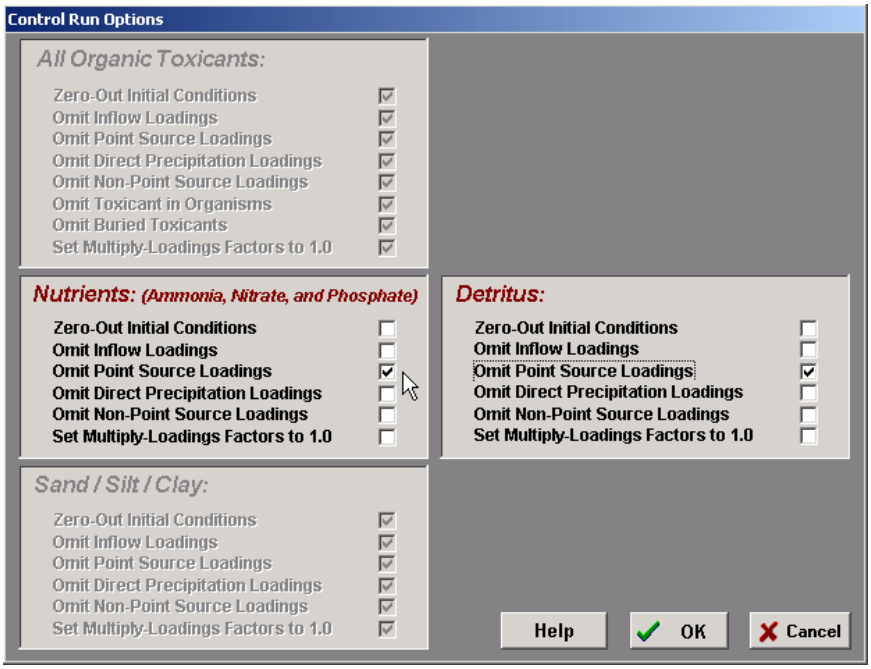
Control Setup

A powerful feature of AQUATOX is that it can run paired simulations for perturbed and control conditions. The default is for the control simulation to have all organic toxicants zeroed out or omitted. However, there is considerable flexibility in setting up the control run. For example, toxicants can be kept and point-source nutrients can be omitted in the control run. In fact, it is possible with a few judicial choices to set up a factorial analysis to determine the effects of various combinations of pollution control scenarios. Click on **Control Setup** to check

which options should be used in the Control simulation. Most are self-explanatory; however, **Set Multiply-Loadings Factors to 1** deserves some explanation. Each loading screen has a field labeled "Multiply loading by" with a default value of 1. A loading can be perturbed easily by changing the factor to a fraction less than 1 (decreasing the loading) or to a value greater than 1 (increasing the loading). These perturbations can be negated in the control screen by setting them to 1. Also, note that "Direct Precipitation" includes both wet and dry fall.

Two examples are given: the first zeroes out all organic toxicants in the control. In the second, there are no organic toxicants (indicated by the grayed out box), and the only change in the control simulation is that the point sources for nutrients and detritus are omitted.

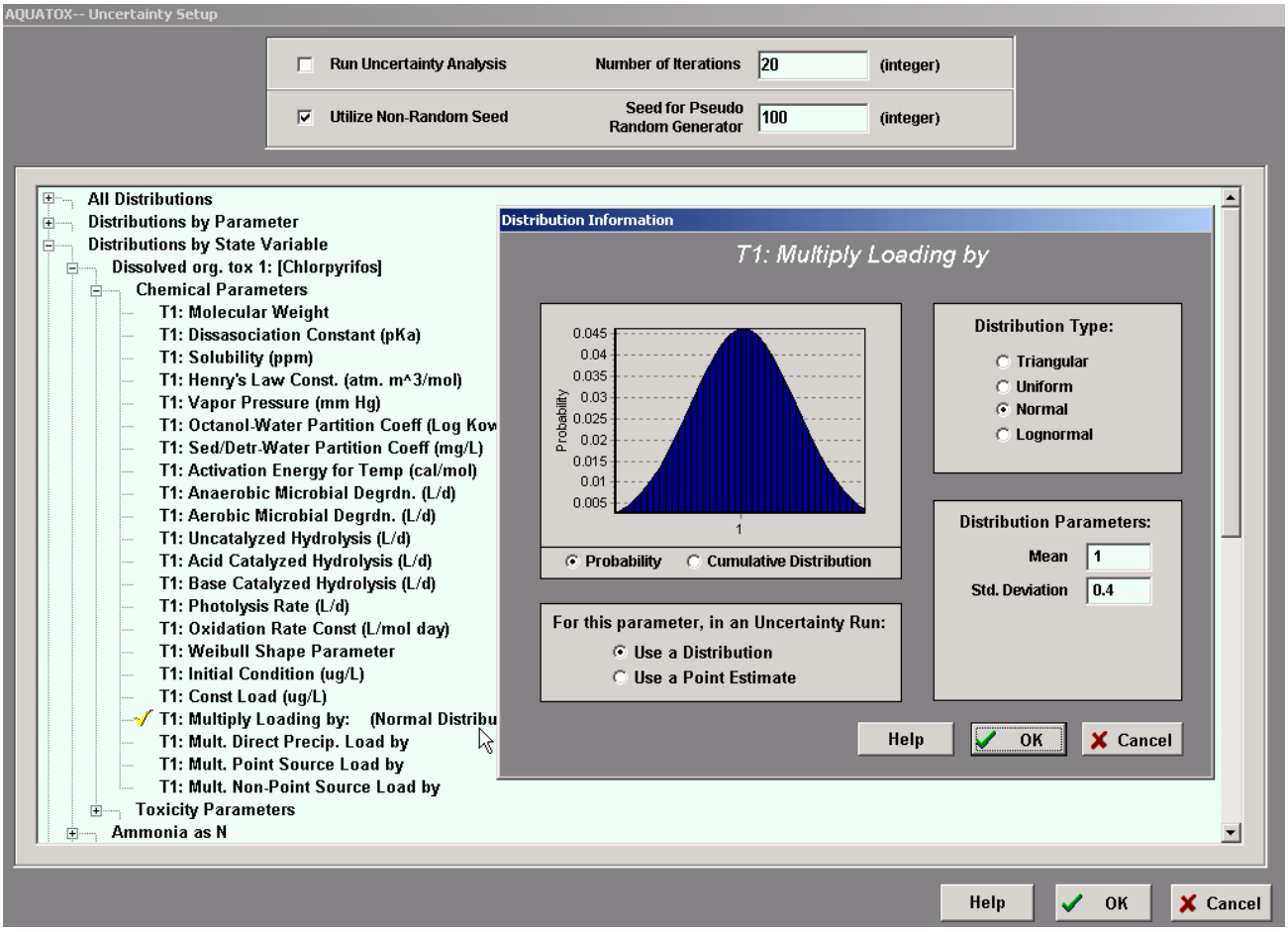




Uncertainty Setup

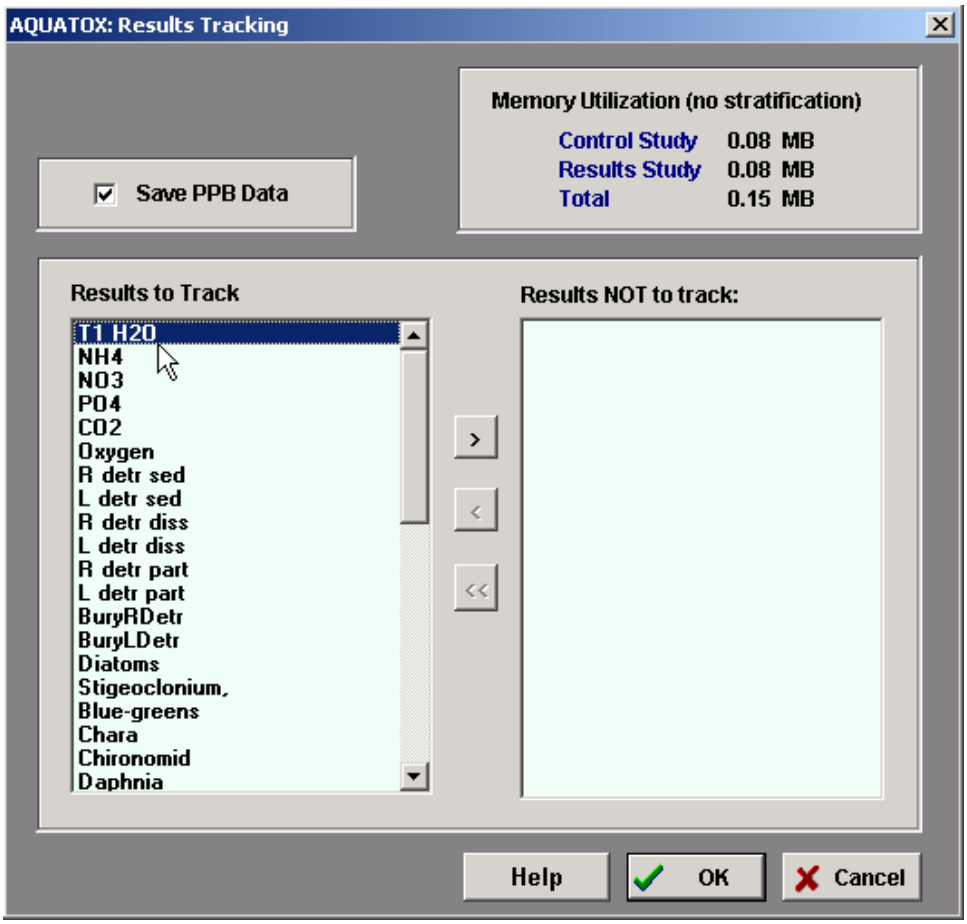
Another powerful feature of AQUATOX is that it can perform uncertainty or sensitivity analysis to provide probabilistic results. Latin hypercube sampling is performed, ensuring that all parts of the chosen distribution are sampled. Therefore, the number of iterations can be kept to a minimum, which is important because each iteration is a complete simulation. Twenty iterations is the default, meaning that the distribution is divided into 20 segments for purposes of sampling, and that often may be more than sufficient to obtain an adequate sample.

Any and all parameters and loadings can be chosen, either singly or in combination (although linked distributions or covariances are not modeled). By double-clicking on a variable one can access the corresponding distribution information. The default is a normal distribution with a mean of the point or parameter value and a standard deviation of 60% that value. Often loadings are well represented by lognormal distributions. If less is known about the distribution, but minimum and maximum values and some central tendency can be defined, then a triangular distribution may be appropriate. If only minimum and maximum values are known, then a uniform distribution may be sufficient, and the number of iterations can be decreased. A separate section will discuss Uncertainty Analysis in more detail.



Output Setup

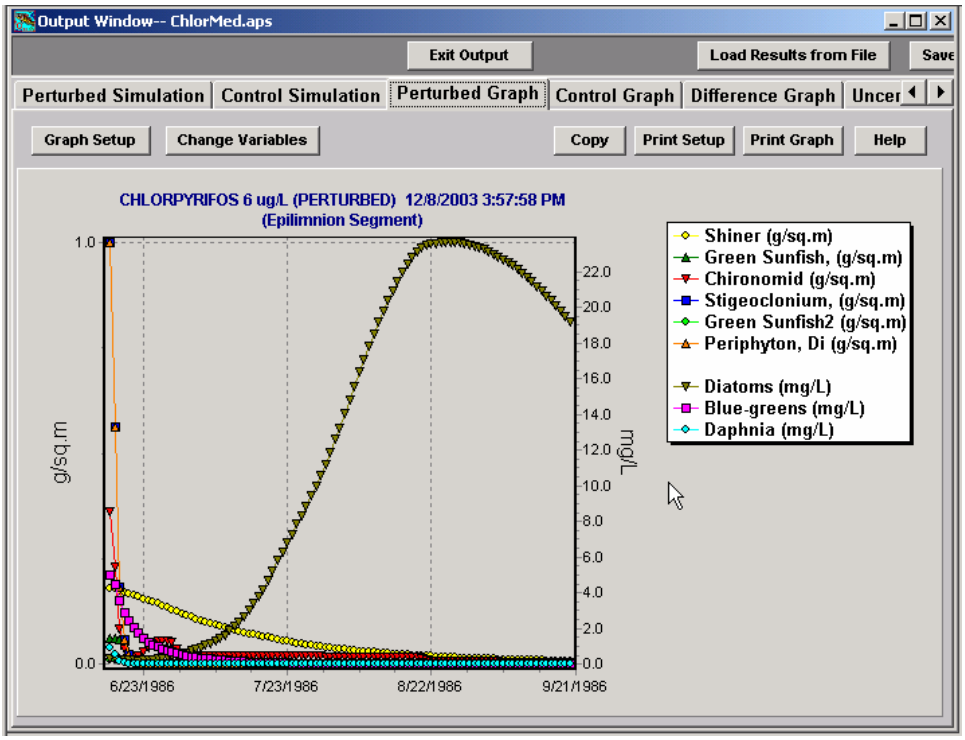
Because Release 2 has the potential for modeling so many state variables, the user has the option of not saving given state variables, thus decreasing the memory requirements. Click on **Output Setup** to access the **Results Tracking** window. By removing the check mark from **Save PPB Data** any toxicant concentration results can be discarded; this is useful, for example, if an ecosystem calibration is being performed prior to calibrating the toxicants.

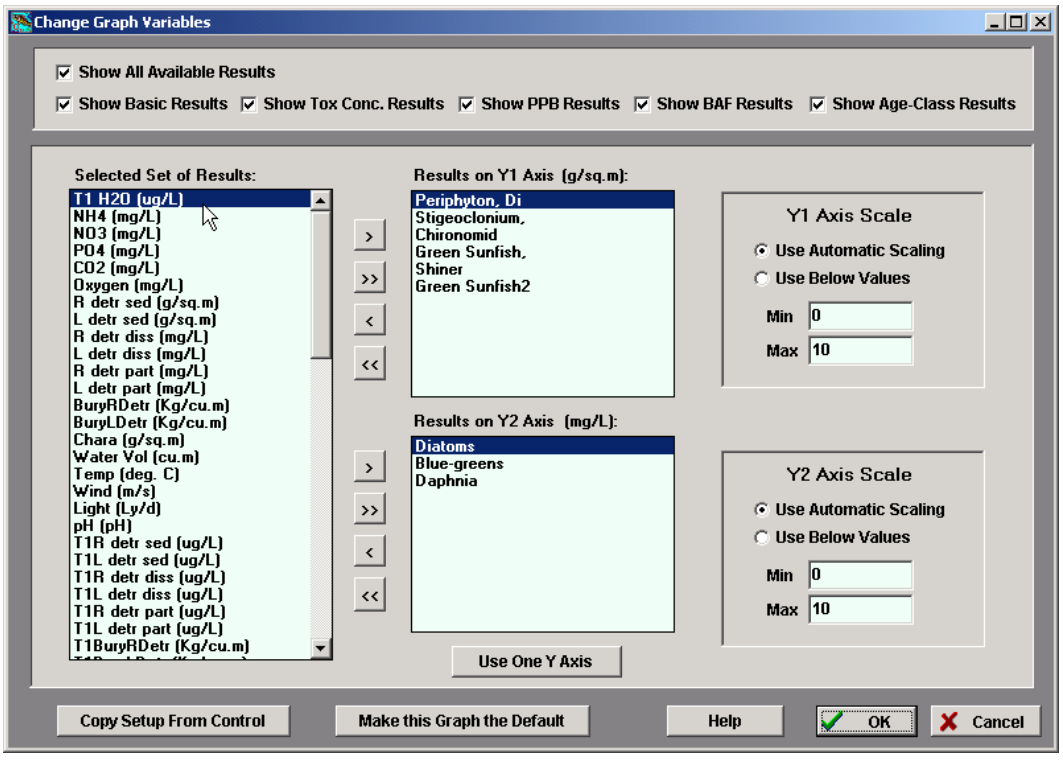


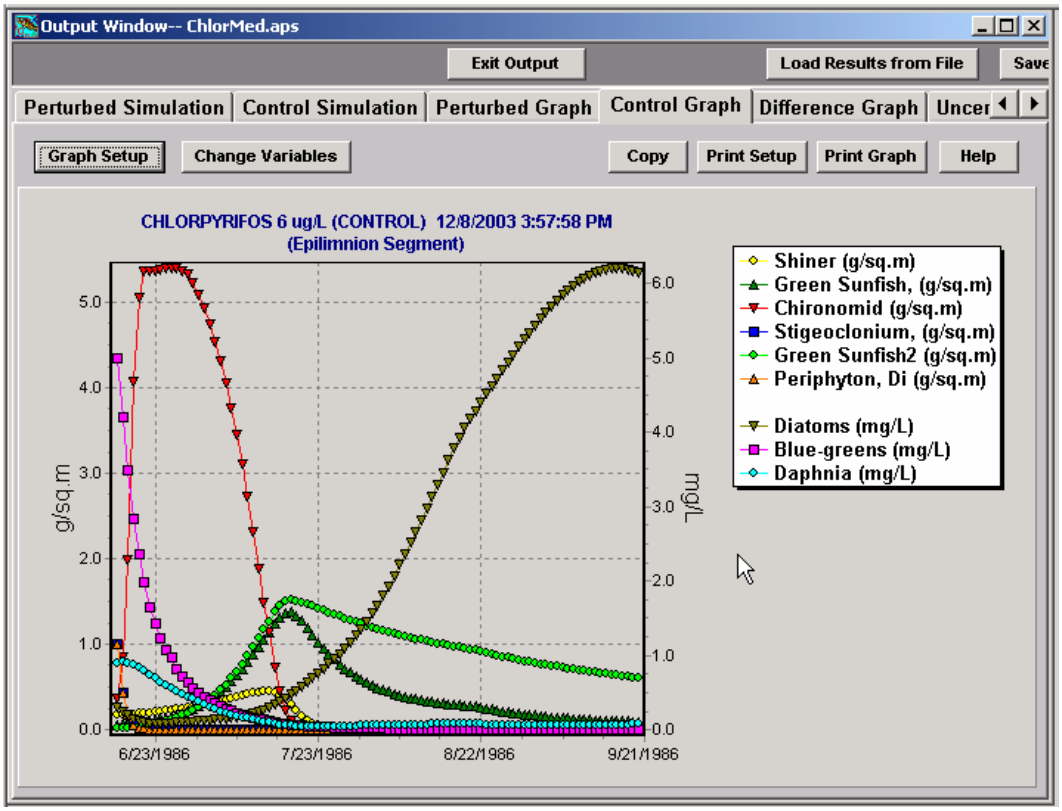
2.3 Displaying Output

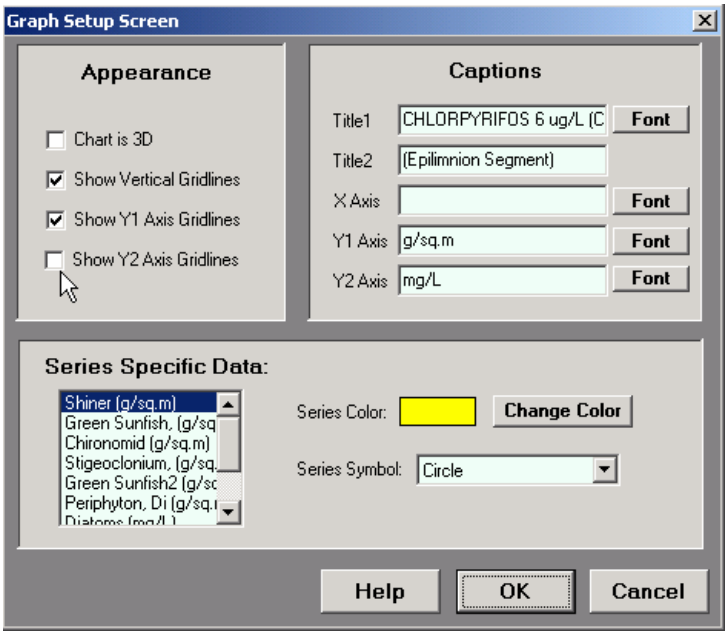
Graphs

AQUATOX has extensive capabilities for graphical and tabular output. By clicking on **Output** on the main screen one can access the Output Window. There are six tabs, each representing a different form of output. Graphical output has a title that is input on the main screen, and a time and date stamp to facilitate record keeping, especially if the graph is printed out. Two different sets of variables can be plotted with separate scales on the Y1 and Y2 axes. Variables are chosen by clicking on **Change Variables** to access the Graph Setup screen. The model will only allow variables with the same units to be plotted together. One or two Y axes with separate scales can be specified. It is often useful to **Copy Setup From Perturbed** or to **Copy Setup From Control** so that results can be compared easily. Either automatic scaling or user-specified scaling can be used. By clicking on **Graph Setup** the user can access a screen that controls the appearance of the graph.

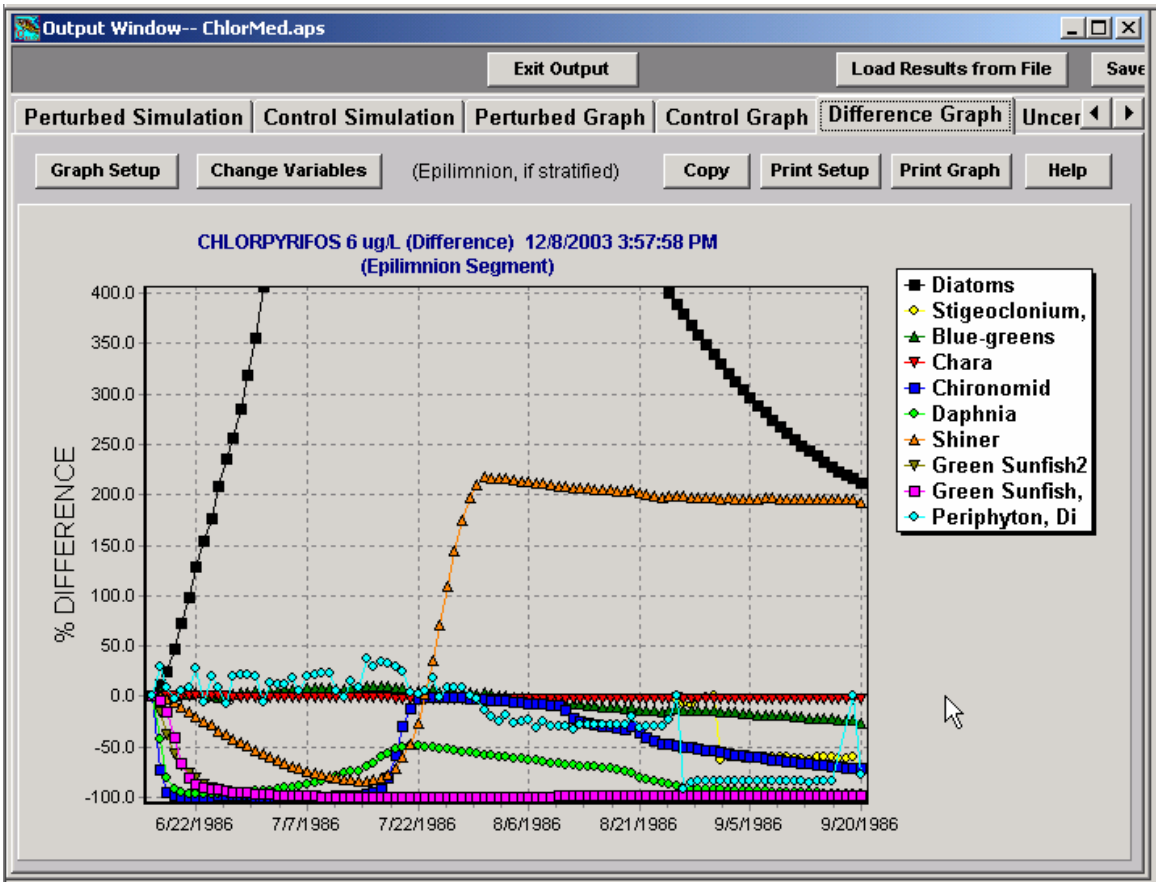

Output Window-- ChlorMed.aps
Exit Output
Load Results from File
Save
Perturbed Simulation
Control Simulation
Perturbed Graph
Control Graph
Difference Graph
Uncer
Graph Setup
Change Variables
Copy
Print Setup
Print Graph
Help
CHLORPYRIFOS 6 ug/L (PERTURBED) 12/8/2003 3:57:58 PM
(Epilimnion Segment)
g/sq.m
mg/L
1.0
0.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
0.0
6/23/1986
7/23/1986
8/22/1986
9/21/1986
Shiner (g/sq.m)
Green Sunfish, (g/sq.m)
Chironomid (g/sq.m)
Stigeoclonium, (g/sq.m)
Green Sunfish2 (g/sq.m)
Periphyton, Di (g/sq.m)
Diatoms (mg/L)
Blue-greens (mg/L)
Daphnia (mg/L)


Change Graph Variables
Show All Available Results
Show Basic Results
Show Tox Conc. Results
Show PPB Results
Show BAF Results
Show Age-Class Results
Selected Set of Results:
T1 H20 (ug/L)
NH4 (mg/L)
NO3 (mg/L)
PO4 (mg/L)
CO2 (mg/L)
Oxygen (mg/L)
R detr sed (g/sq.m)
L detr sed (g/sq.m)
R detr diss (mg/L)
L detr diss (mg/L)
R detr part (mg/L)
L detr part (mg/L)
BuryRDetr (Kg/cu.m)
BuryLDetr (Kg/cu.m)
Chara (g/sq.m)
Water Vol (cu.m)
Temp (deg. C)
Wind (m/s)
Light (Ly/d)
pH (pH)
T1R detr sed (ug/L)
T1L detr sed (ug/L)
T1R detr diss (ug/L)
T1L detr diss (ug/L)
T1R detr part (ug/L)
T1L detr part (ug/L)
T1BuryRDetr (Kg/cu.m)
Results on Y1 Axis (g/sq.m):
Periphyton, Di
Stigeoclonium,
Chironomid
Green Sunfish,
Shiner
Green Sunfish2
Results on Y2 Axis (mg/L):
Diatoms
Blue-greens
Daphnia
Use One Y Axis
Y1 Axis Scale
Use Automatic Scaling
Use Below Values
Min 0
Max 10
Y2 Axis Scale
Use Automatic Scaling
Use Below Values
Min 0
Max 10
Copy Setup From Control
Make this Graph the Default
Help
OK
Cancel

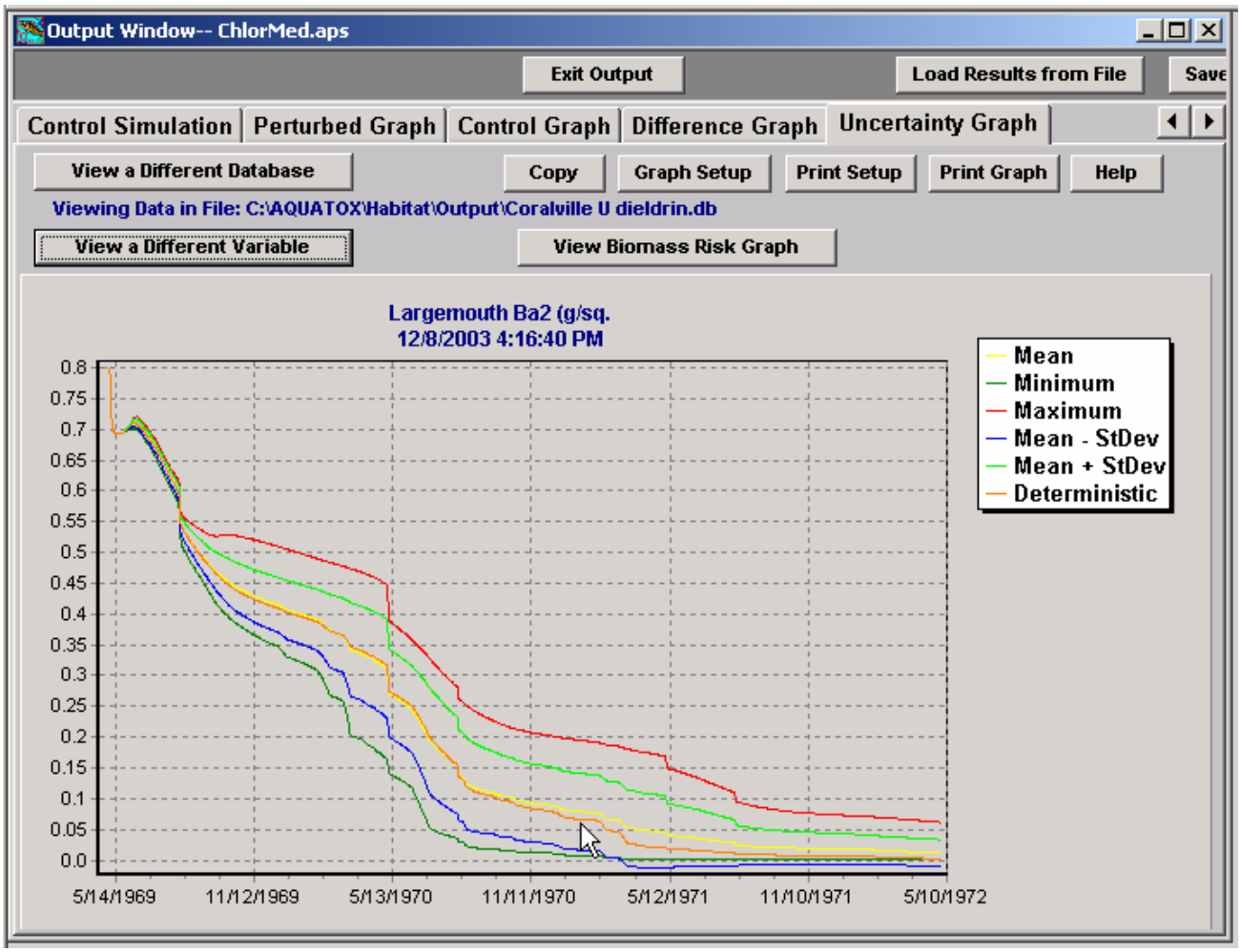




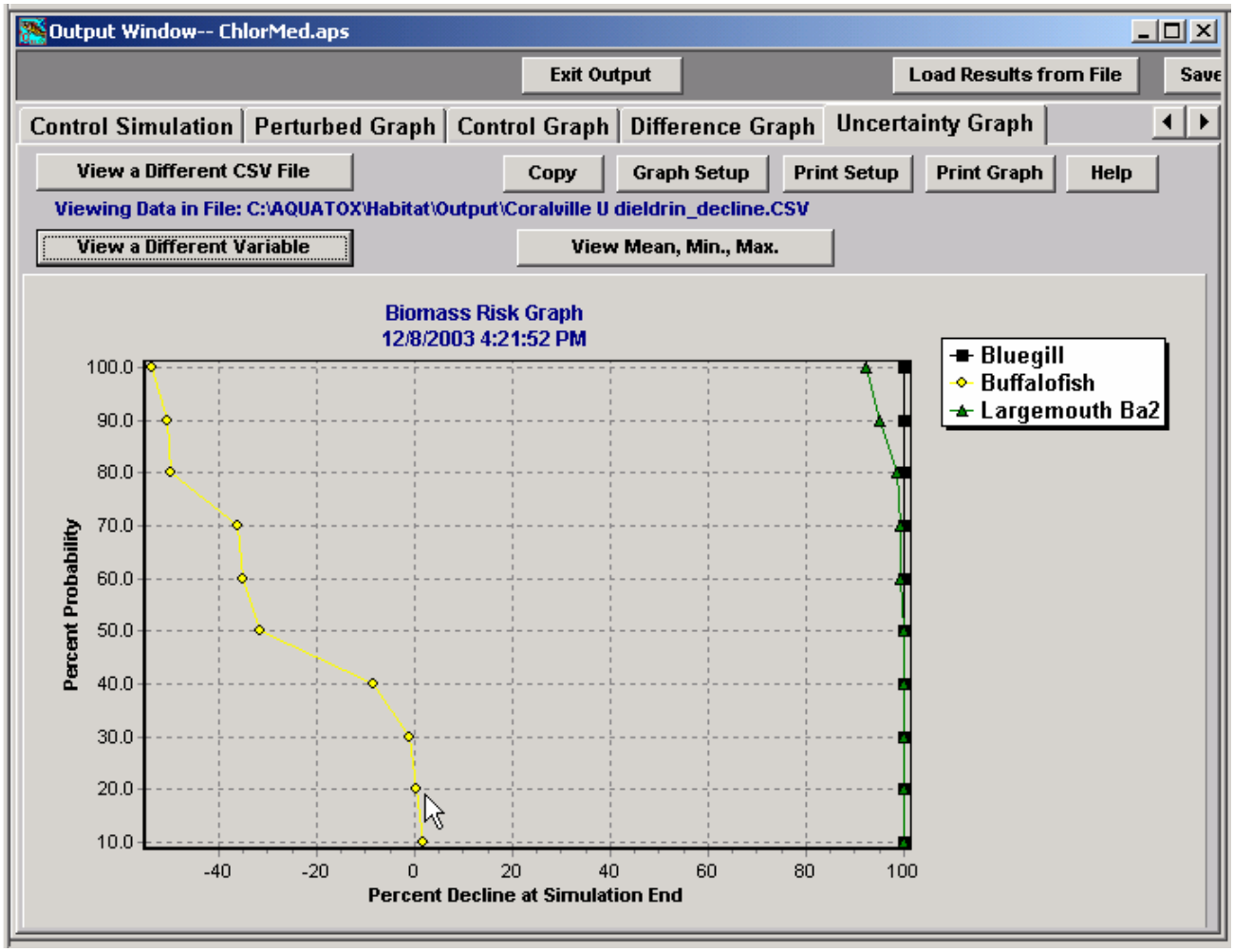
One of the most useful forms of output is the **Difference Graph**, which plots the results of the perturbed simulation minus the control simulation as percent differences. The default minimum and maximum percentages are 400% and -100% (complete loss). However, these can be changed by accessing the Change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



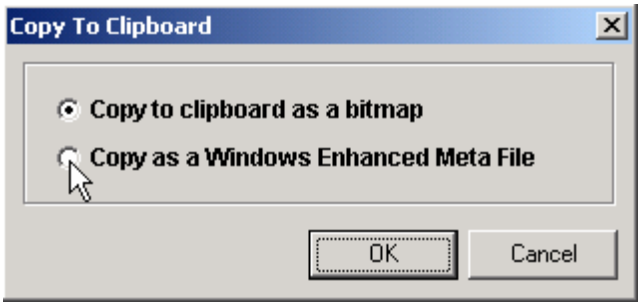
Another powerful form of graphical output is the **Uncertainty Graph**. If an uncertainty analysis has been performed the results can be potted as a series of lines representing the mean, minimum, maximum, mean - 1 standard deviation, mean + 1 standard deviation, and deterministic results. Only one variable can be viewed at a time, so click on **View a Different Variable** to view another. With a large number of variables, it may be necessary to split the output into two files. If you do not see all the results that you wish to plot, such as bioaccumulation factors (BAFs), click on **View a Different Database** and load another file with the same name but with the suffix "2."



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



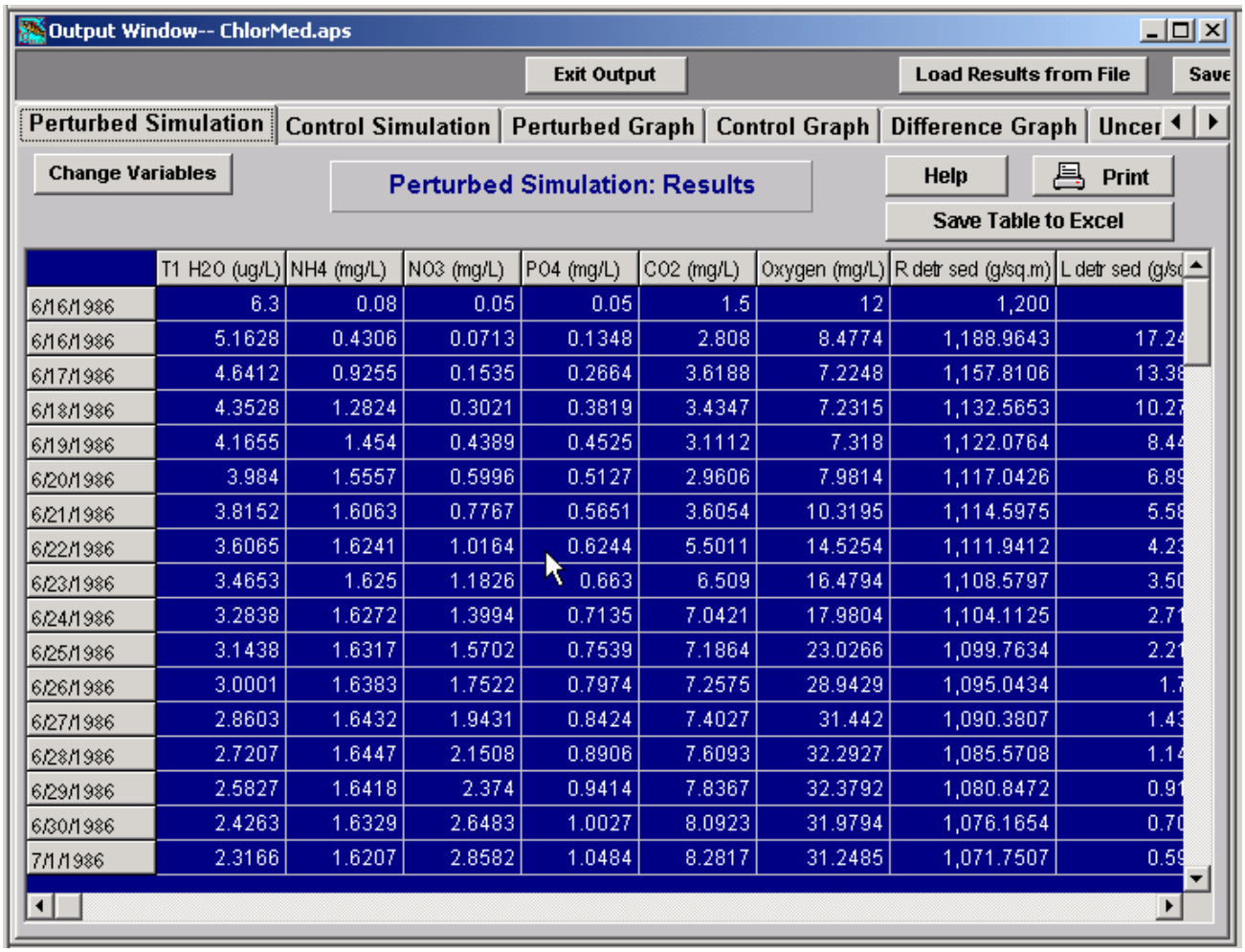
By clicking on **Copy** a graph can be saved to the Windows clipboard as a bit map (bmp) or Windows enhanced meta file (emf) for insertion in a document or graphical presentation. Bit maps are raster files with every pixel being saved; meta files are usually vector files with instructions being saved to replicate the image. A typical AQUATOX graph saved as a bit map is 2,716 kb compared to 46 kb for an enhanced meta file, and the results are virtually identical! The only reason for saving a graph as a bit map is that not all programs support enhanced meta files.



Because Release 2 can support multiple windows, output from another study can be loaded (by clicking on **Load Results from File**). This can be useful for comparing results from two or more simulations saved as separate studies.

Tables

Tables can be obtained for both perturbed and control runs. The user can specify what variables are to be tabulated. The results can be saved to an Excel file.



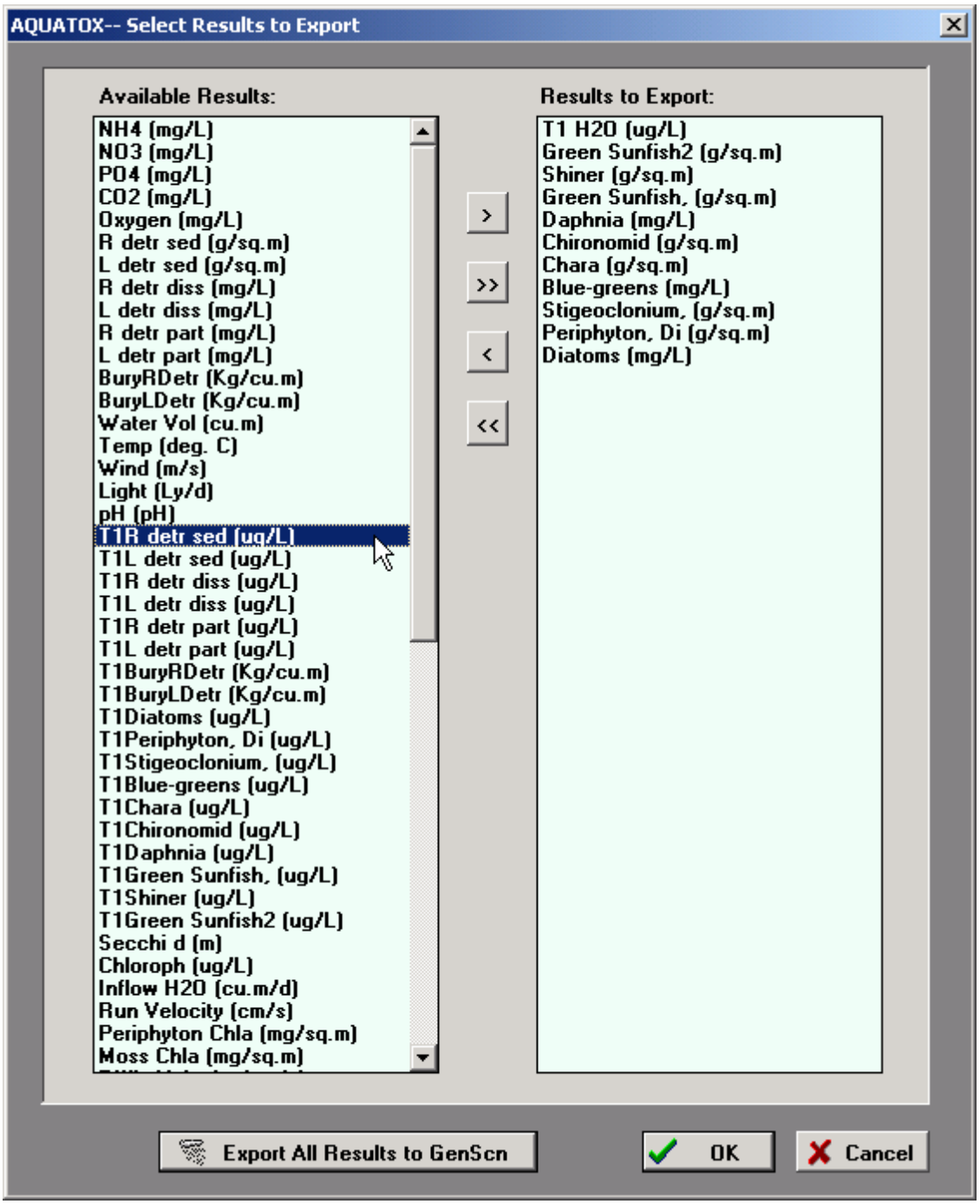
	T1 H2O (ug/L)	NH4 (mg/L)	NO3 (mg/L)	PO4 (mg/L)	CO2 (mg/L)	Oxygen (mg/L)	R detr sed (g/sq.m)	L detr sed (g/s
6/16/1986	6.3	0.08	0.05	0.05	1.5	12	1,200	
6/16/1986	5.1628	0.4306	0.0713	0.1348	2.808	8.4774	1,188.9643	17.2
6/17/1986	4.6412	0.9255	0.1535	0.2664	3.6188	7.2248	1,157.8106	13.3
6/18/1986	4.3528	1.2824	0.3021	0.3819	3.4347	7.2315	1,132.5653	10.2
6/19/1986	4.1655	1.454	0.4389	0.4525	3.1112	7.318	1,122.0764	8.4
6/20/1986	3.984	1.5557	0.5996	0.5127	2.9606	7.9814	1,117.0426	6.8
6/21/1986	3.8152	1.6063	0.7767	0.5651	3.6054	10.3195	1,114.5975	5.5
6/22/1986	3.6065	1.6241	1.0164	0.6244	5.5011	14.5254	1,111.9412	4.2
6/23/1986	3.4653	1.625	1.1826	0.663	6.509	16.4794	1,108.5797	3.5
6/24/1986	3.2838	1.6272	1.3994	0.7135	7.0421	17.9804	1,104.1125	2.7
6/25/1986	3.1438	1.6317	1.5702	0.7539	7.1864	23.0266	1,099.7634	2.2
6/26/1986	3.0001	1.6383	1.7522	0.7974	7.2575	28.9429	1,095.0434	1.7
6/27/1986	2.8603	1.6432	1.9431	0.8424	7.4027	31.442	1,090.3807	1.4
6/28/1986	2.7207	1.6447	2.1508	0.8906	7.6093	32.2927	1,085.5708	1.1
6/29/1986	2.5827	1.6418	2.374	0.9414	7.8367	32.3792	1,080.8472	0.9
6/30/1986	2.4263	1.6329	2.6483	1.0027	8.0923	31.9794	1,076.1654	0.7
7/1/1986	2.3166	1.6207	2.8582	1.0484	8.2817	31.2485	1,071.7507	0.5

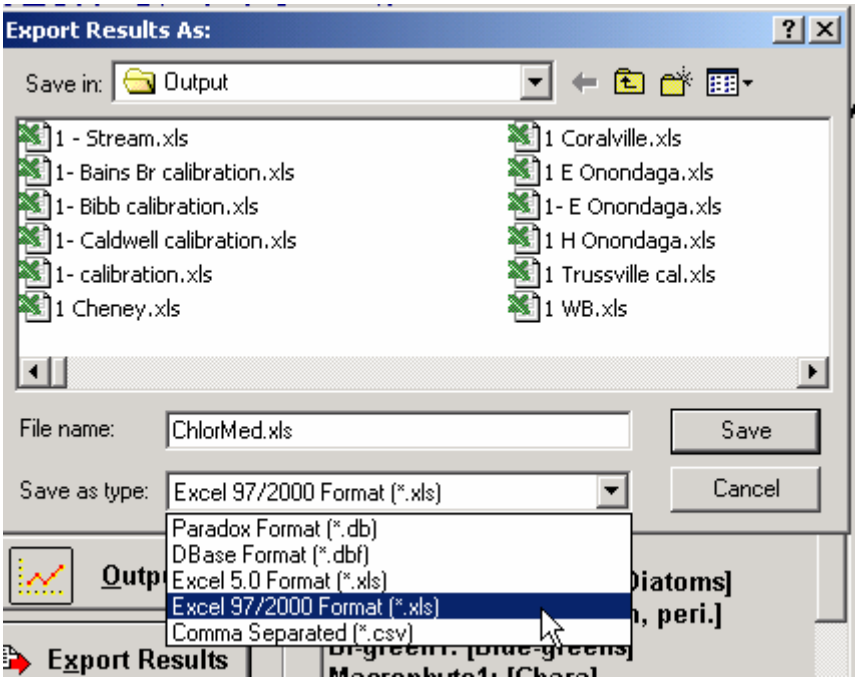
2.4 Exporting Results

All results can be exported in Paradox, dBase, Excel, or comma-separated values by clicking on **Export Results** (perturbed) or **Export Control**. Results also can be exported to GenScn if it has been installed as part of the BASINS implementation (see **Volume 3**).

Two Ways to Export Results

Results also can be exported from a table in Output. However, at this time, exporting from the main screen as described here is the faster procedure. For a long simulation with numerous state variables, the difference is appreciable!





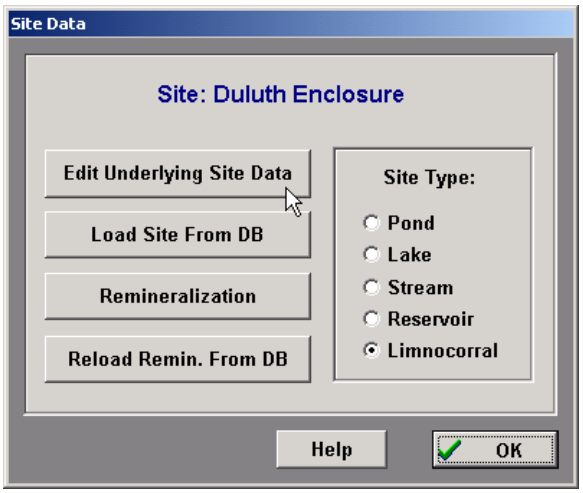
2.5 Site Information

Click on **Site** on the main screen to access site information. Five site types are available: pond, lake, stream (creek or river), reservoir, and limnocorral (an experimental enclosure).

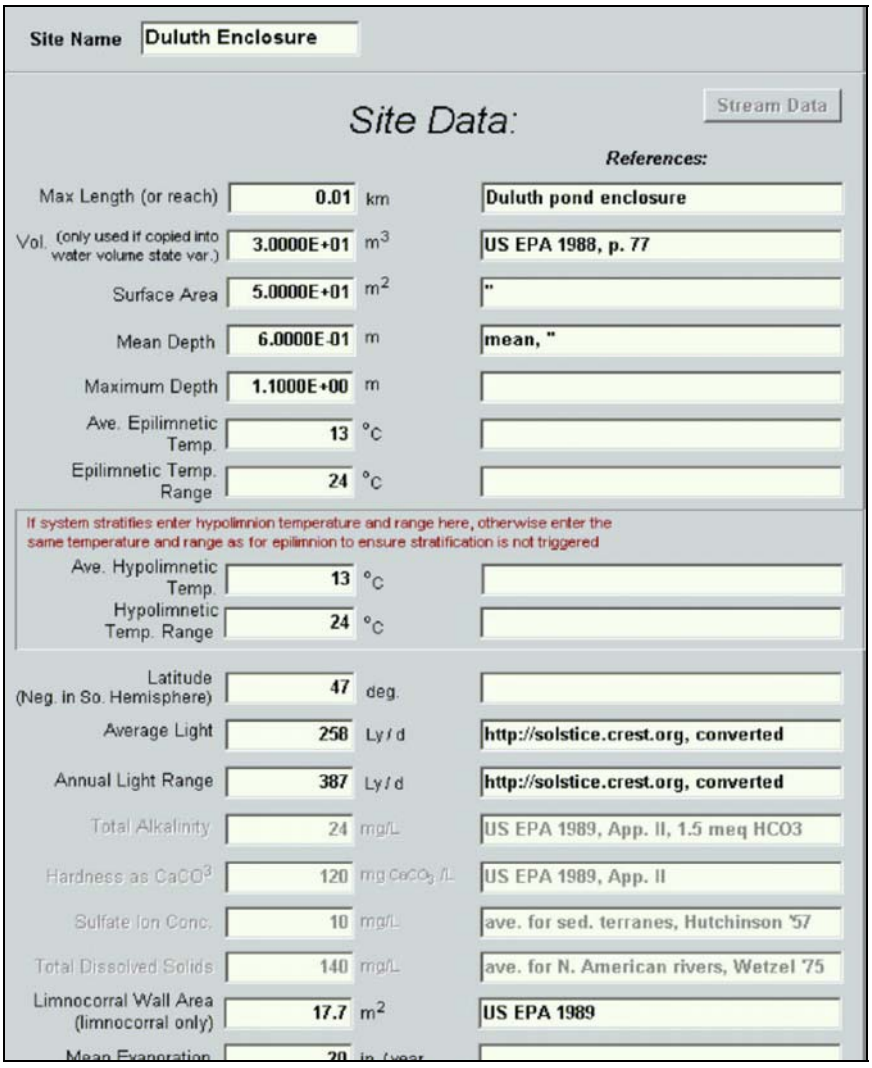
Site Types

There are five types of sites. Lakes, reservoirs, and ponds are treated similarly in AQUATOX; only the default extinction coefficients for water differ. However, their implementation is often quite different. Limnocorrals differ because the area of the enclosure wall is specified and enters into the computation of area available for colonization by periphyton. Streams differ even more in that they have an additional screen for entry of data on slope, roughness (Manning's coefficient), and percent habitat distribution. Implementation considerations are given below.

Type	Discharge	Plants	Invertebrates	Detritus	Stratified
Pond and Limnocorral	unimportant	periphyton, macrophytes	zoobenthos, zooplankton	autochtho-nous	no
Lake	site-specific	phytoplankton	zooplankton	autochth. +/- allochth.	often
Reservoir	important	phytoplankton	zooplankton	allochtho-nous	often
Stream/river	v. important	periphyton bryophytes	zoobenthos	allochtho-nous	no

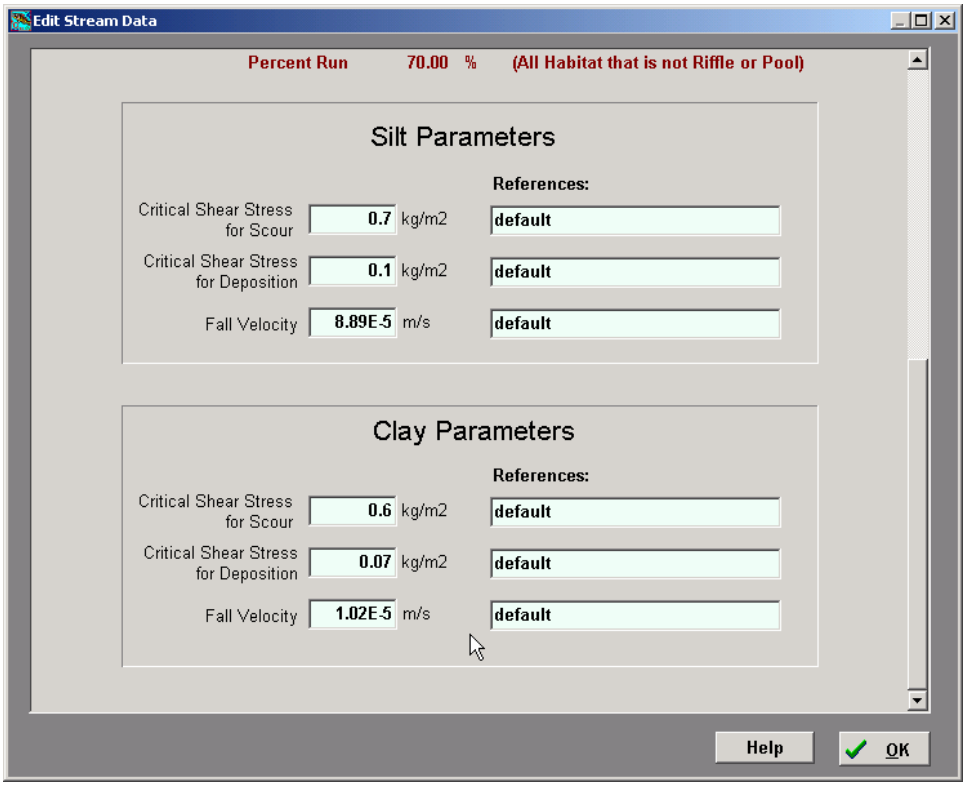


A limited number of sites can be loaded from the database, but ordinarily one would **Edit Underlying Site Data**, to modify a default site to represent a new site. The site data screen is for entry of site characteristics. If a site does not stratify, enter the same temperature values for "hypolimnion" as for "epilimnion." Several characteristics such as alkalinity are not used at this time, so they are grayed out.

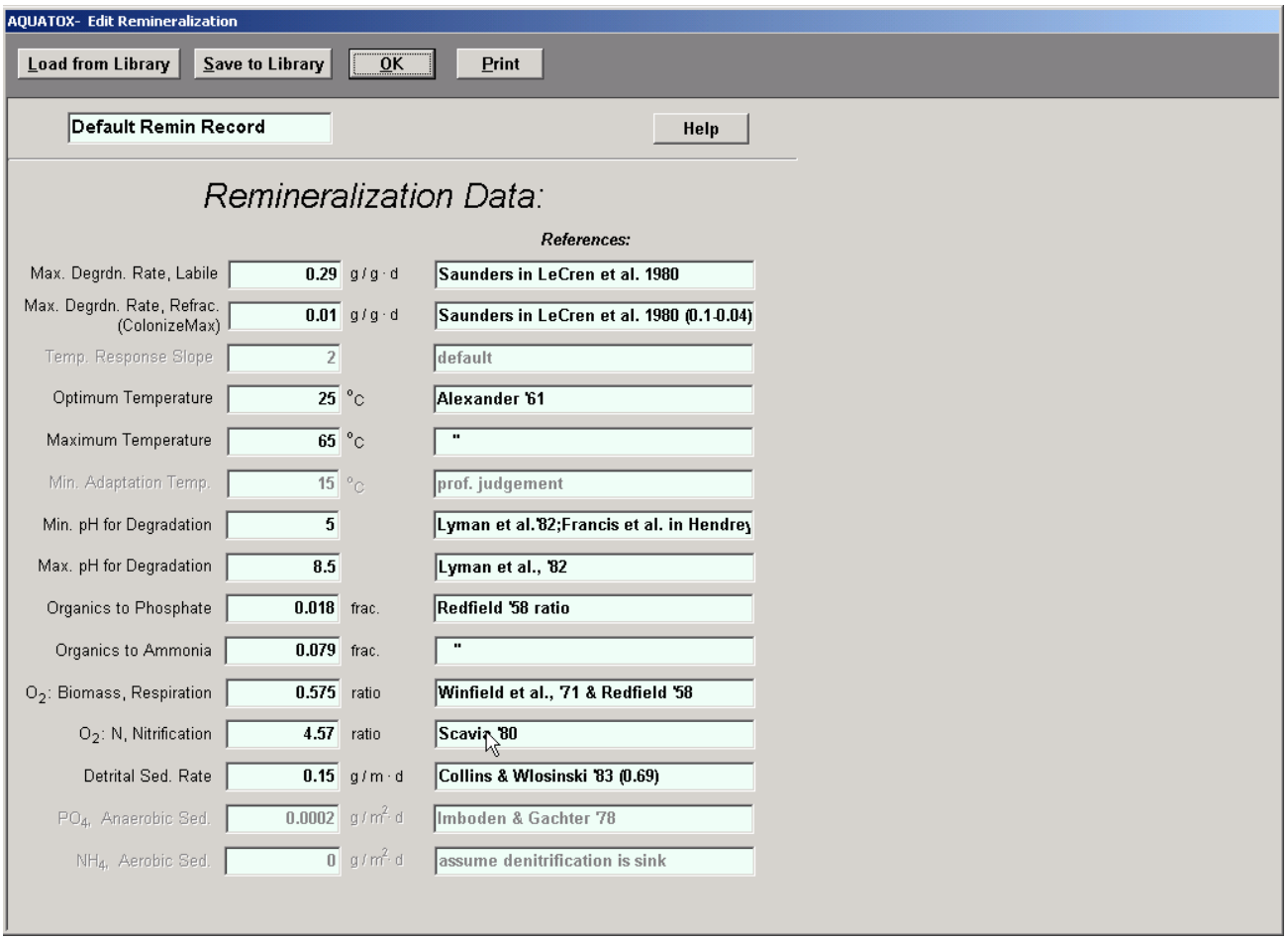


If the site is a stream, one can click on **Stream Data** to edit site characteristics such as the channel slope, the Manning's roughness coefficient, and percent habitats. If inorganic sediments are being simulated, the user also can enter site-specific parameters for critical shear stresses and fall velocities.


Edit Stream Data
Stream Parameters:
Reference:
Channel Slope
0.004
(m/m)
from #2 to #3
Maximum Channel Depth Before Flooding
4
m
Default
Sediment Depth
5
m
Default
Mannings Coefficient:
Estimate based on Stream Type:
or
use the below value:
natural stream
0
s / m1/3
River Habitats Represented
Percent Riffle
15
%
Percent Pool
15
%
Percent Run
70.00
%
(All Habitat that is not Riffle or Pool)
Help
OK

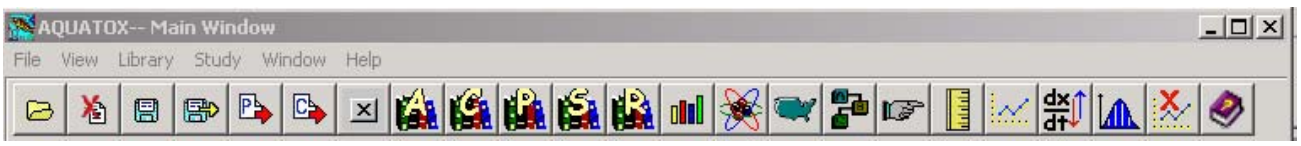

Edit Stream Data
Percent Run
70.00
%
(All Habitat that is not Riffle or Pool)
Silt Parameters
References:
Critical Shear Stress for Scour
0.7
kg/m2
default
Critical Shear Stress for Deposition
0.1
kg/m2
default
Fall Velocity
8.89E-5
m/s
default
Clay Parameters
References:
Critical Shear Stress for Scour
0.6
kg/m2
default
Critical Shear Stress for Deposition
0.07
kg/m2
default
Fall Velocity
1.02E-5
m/s
default
Help
OK

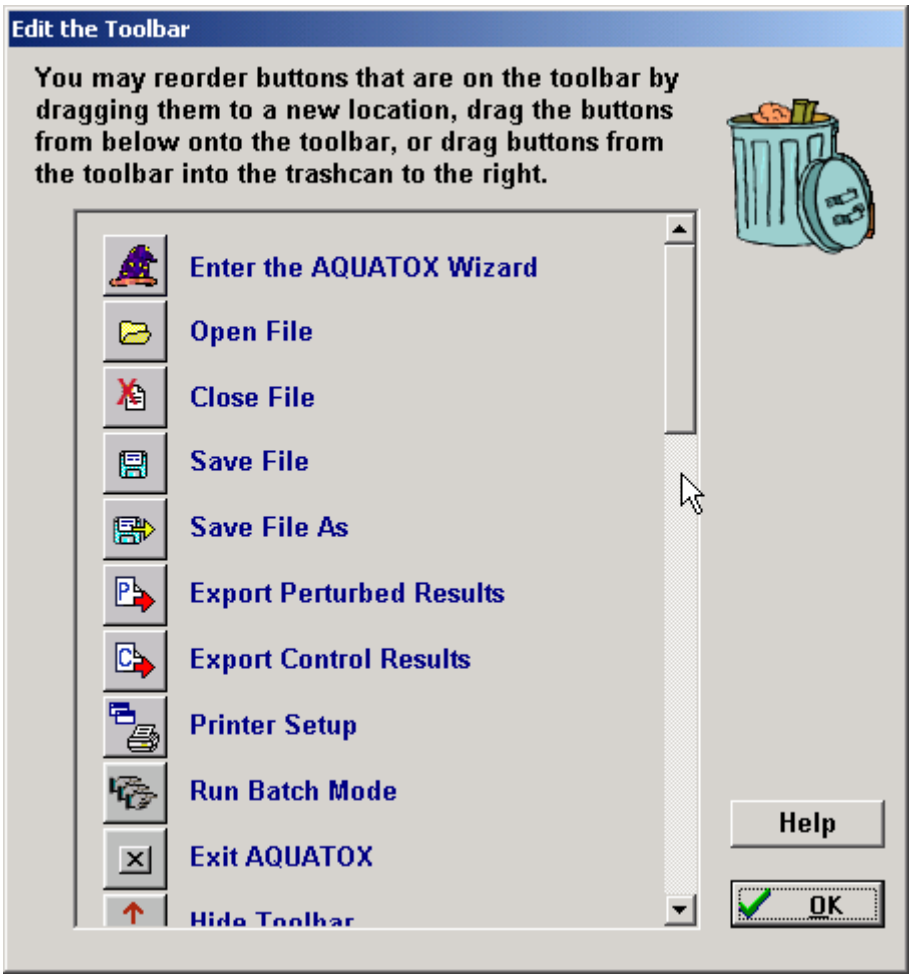
The **Remineralization** parameter screen can be accessed; but these are global parameters that usually would not be changed for a particular site.



2.6 Using the Toolbar

Virtually every function in AQUATOX can be accessed by clicking on the applicable icon on the toolbar. For the experienced user they provide a quick way to bring up a particular screen or to perform a function, such as saving a simulation, without going through several layers of options in the menu bar or the "big buttons." (The big buttons can be suppressed entirely through the **View** menu option.) The icons can be added, deleted, or moved by clicking on **Edit Toolbar** under the **View** menu option. This is also a good way to learn the functions of the icons. There are 32 icons that are listed and can be used, compared to the 24 icons shown on the default toolbar. One can also use dividers to visually group icons representing similar functions.





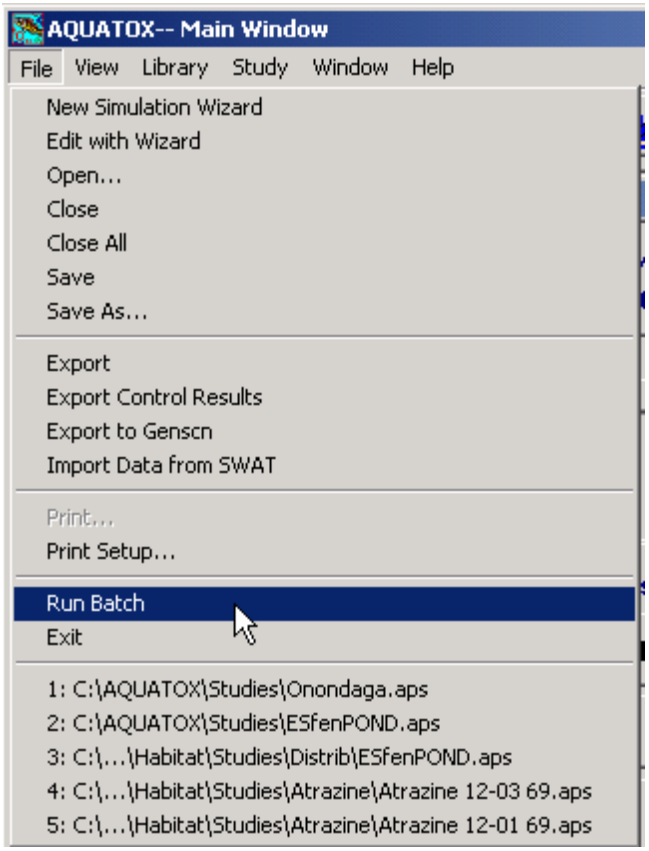
2.7 Running Batch Mode

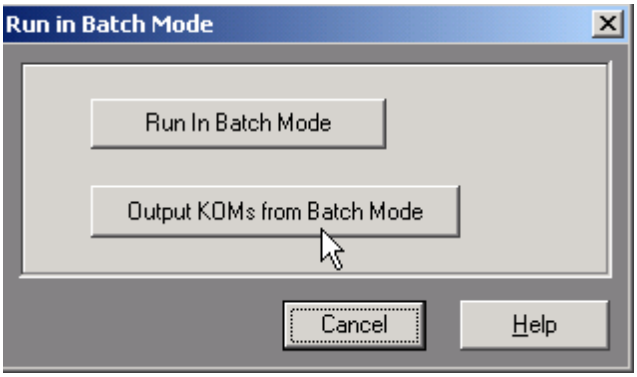
There are applications where it is desirable to run a series of studies automatically. This can be done by creating a Batch subdirectory under the Study directory and placing studies with appropriately chosen options in it. The subdirectory should also contain a text file labeled "batch.txt" that lists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

Important Specifications for Batch Mode:

- To run a program in batch mode, you must have a subdirectory under your Studies Subdirectory named "batch."

- In that "batch" subdirectory must be all studies you wish to run along with a file named "batch.txt."
- The batch.txt file must include each study name that you wish to run on a separate line. No blank lines may be included.
- The program will then execute each of the specified studies one by one and save them along with their results.
- To output the last BAF datapoint for each organism in each of the batch files, select the Output button. This will open each study and write all the BAF data from each study file into a CSV file named batchout.csv.



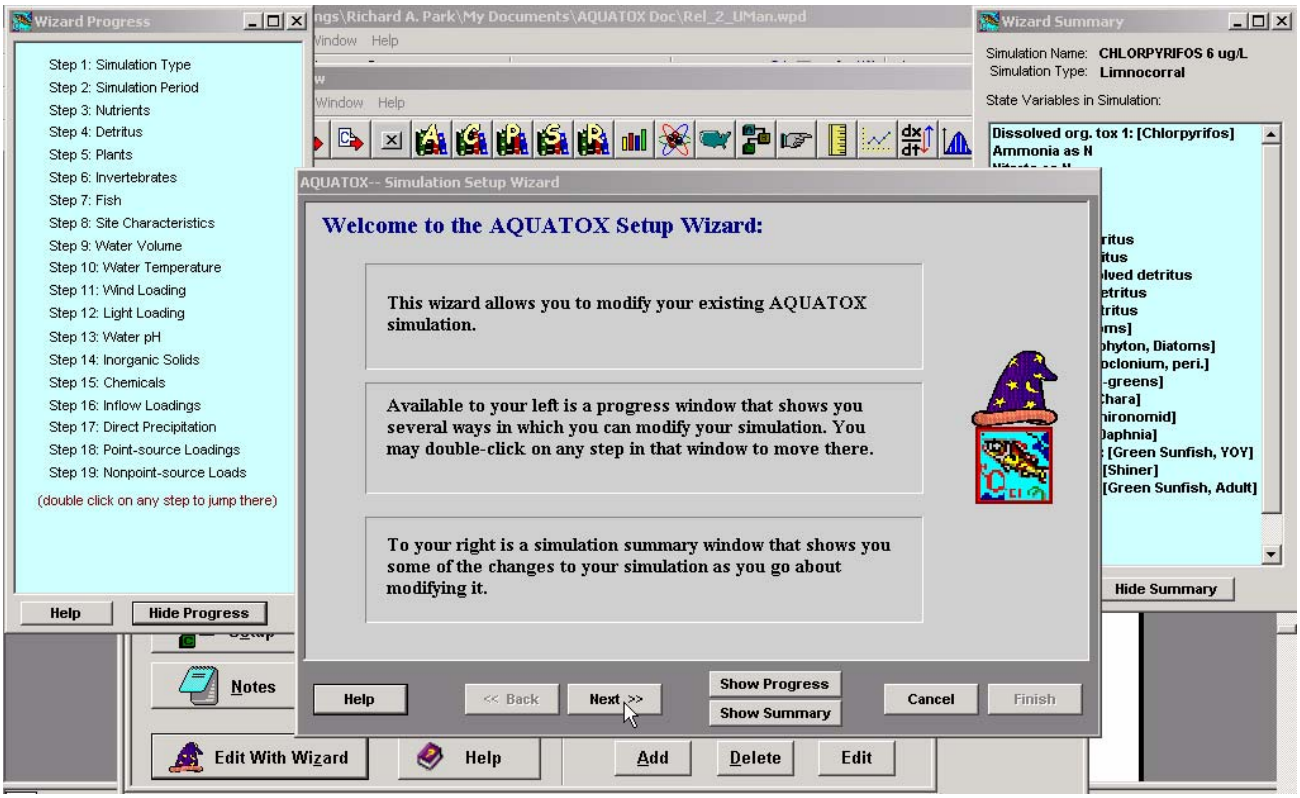


2.8 The Wizard

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

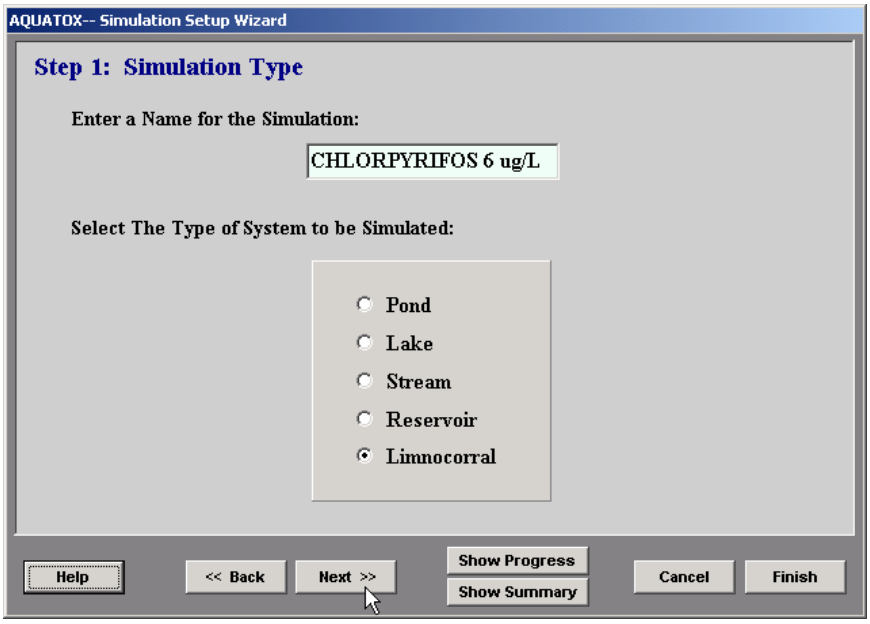
The **Progress Screen** lists the steps and shows which step is currently active. It also provides a means of skipping from one step to another by double-clicking on any step in order to move there.

The **Summary Screen** lists the state and loading variables as they are changed while going through the Wizard.



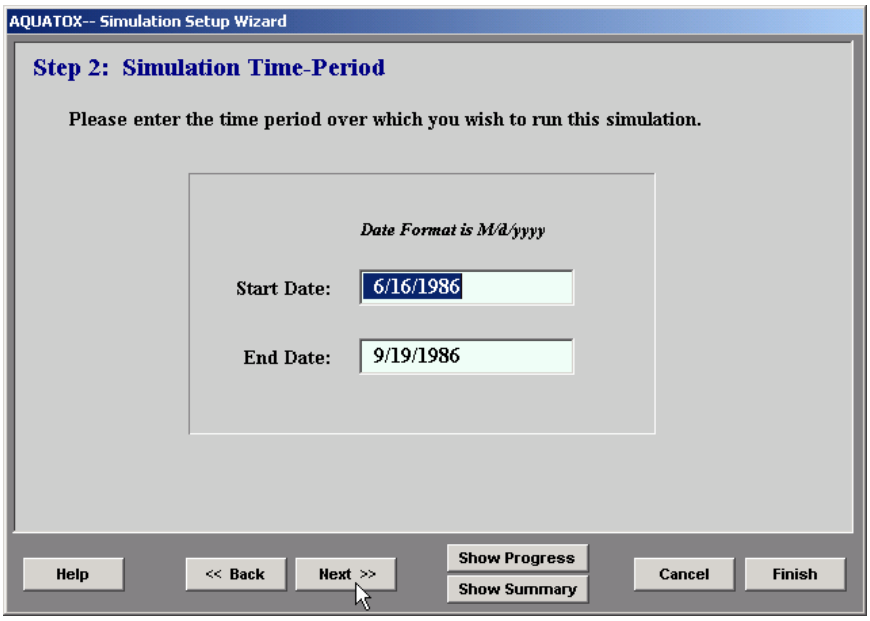
Step 1: Simulation Type

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



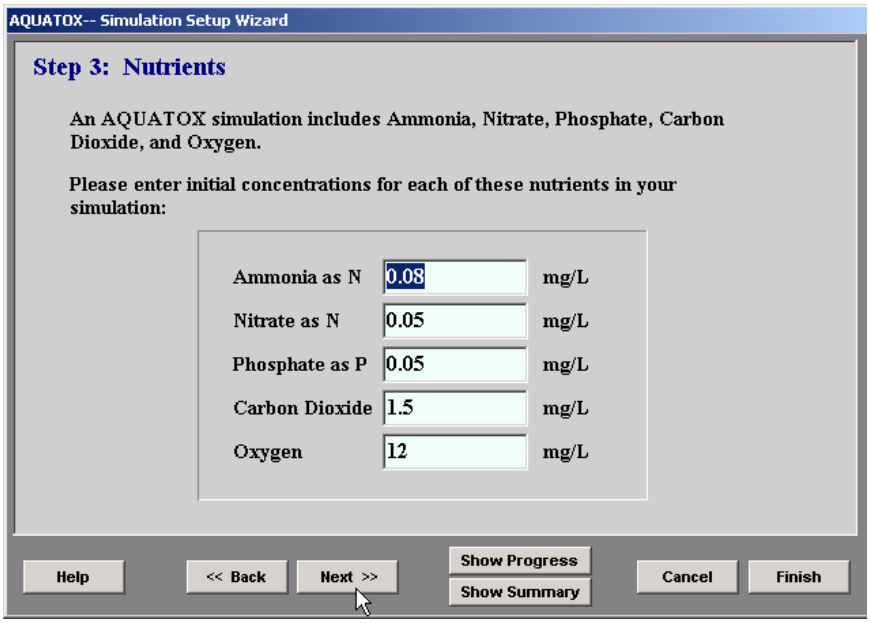
Step 2: Simulation Time Period

The time period for the simulation may be a few days, corresponding to an experiment, or a year, or even several decades. The time period does not have to correspond to the loadings, because the loadings can be interpolated automatically. However, it is advisable to consider the correspondence between the start date and the initial conditions; if the initial conditions are poorly known then a start date in the middle of winter may allow the simulation to "spin up" before going into the growing season. Years have to be entered as four digits.



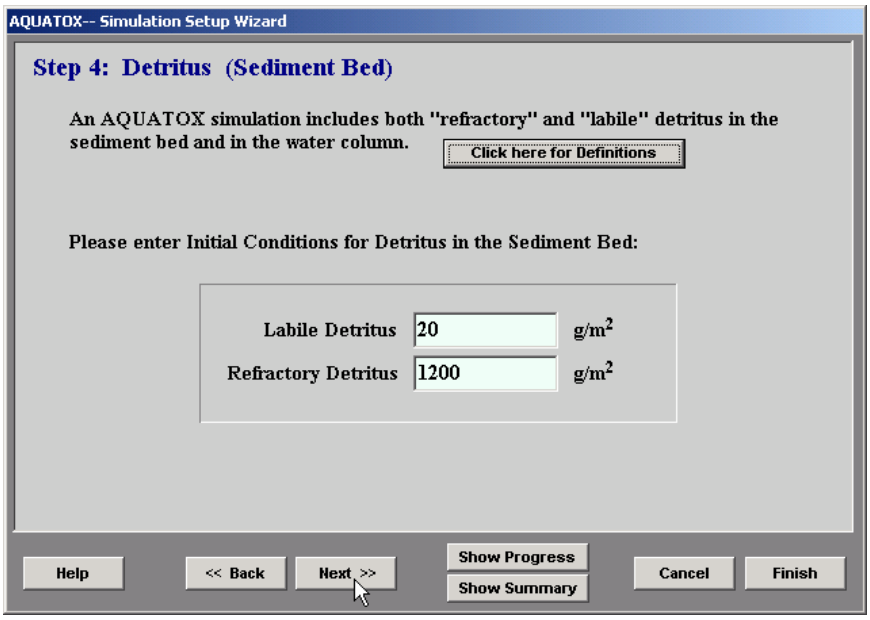
Step 3: Nutrients

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

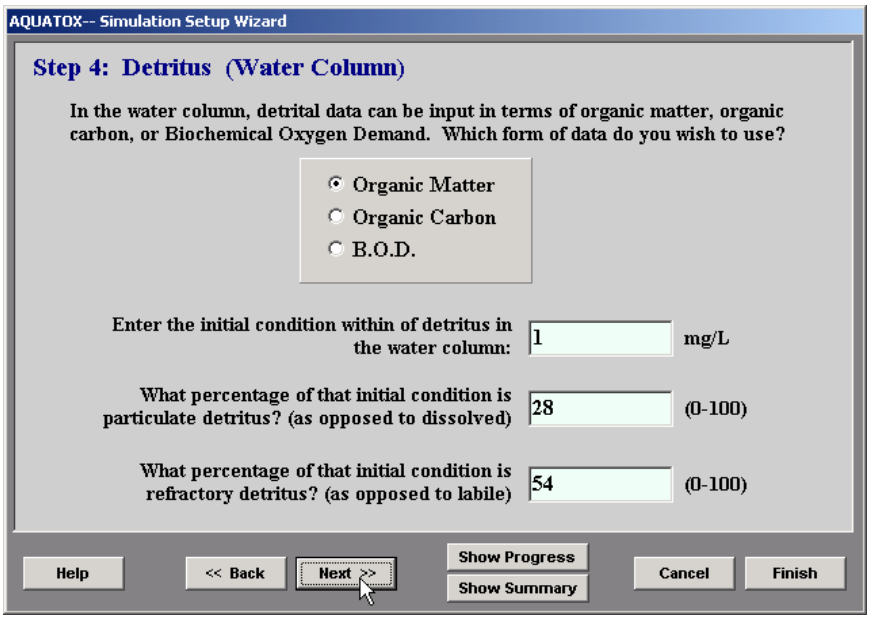


Step 4: Detritus

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

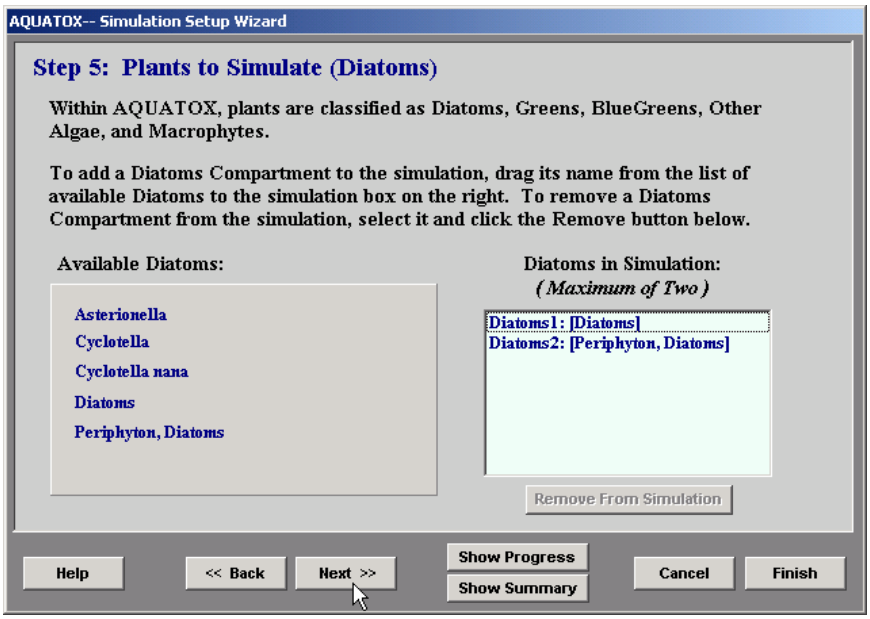


Initial conditions and loadings of detritus in the water column can be input as Organic Matter (dry weight), Organic Carbon, or Biochemical Oxygen Demand (BOD) and the model will make the necessary conversions. Suspended and dissolved detritus initial conditions and loadings are divided into four compartments: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

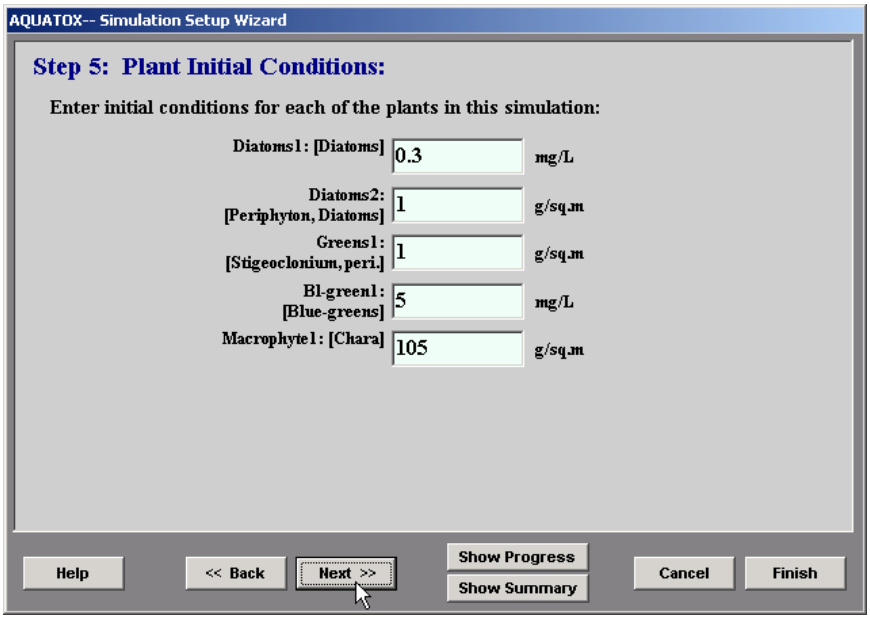


Step 5: Plants to Simulate

The user is provided with a list of plants for each taxonomic group from which to choose. These reflect the organisms that are in the current data libraries.

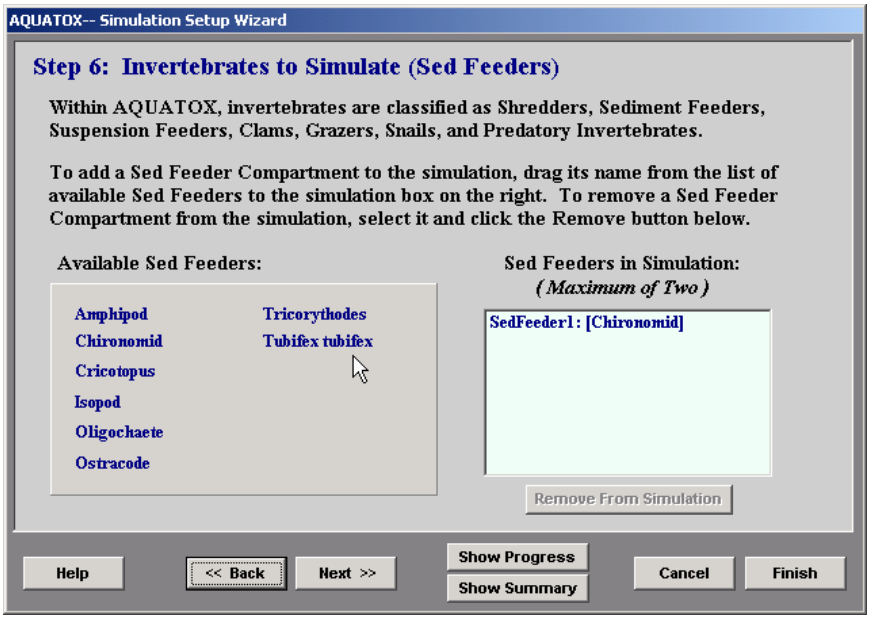


Initial conditions should be entered for each plant group; as with any biotic group, a value of "0" coupled with 0 loadings will keep the group from being simulated. Note that the units are sensitive to whether the plant is planktonic or benthic.



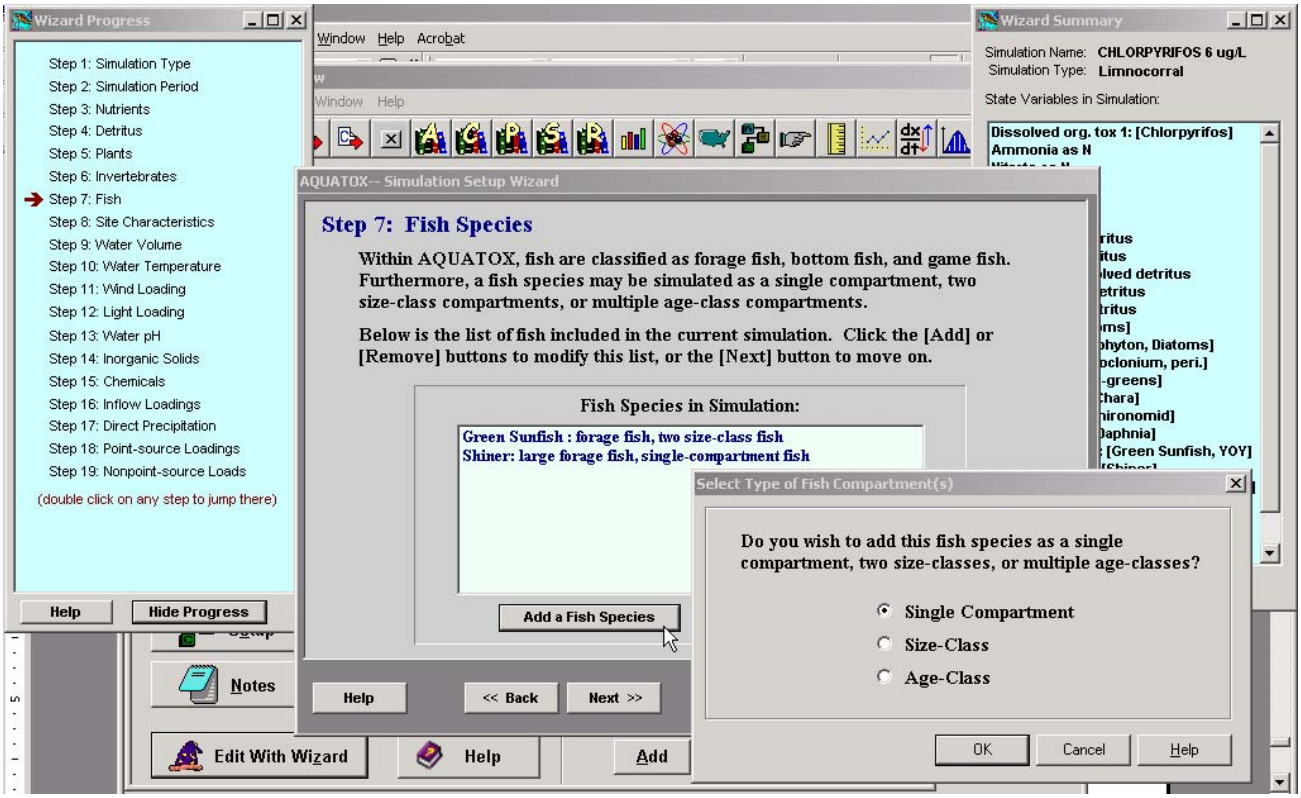
Step 6: Invertebrates to Simulate

The user is presented with a list of invertebrates for each ecological guild from which to choose. As with the plants, this list reflects the organisms currently in the data libraries. Some are general taxonomic groups and some are genera and species. The initial conditions are either mg/L or g/m^2, depending on the mode of life (pelagic or benthic).

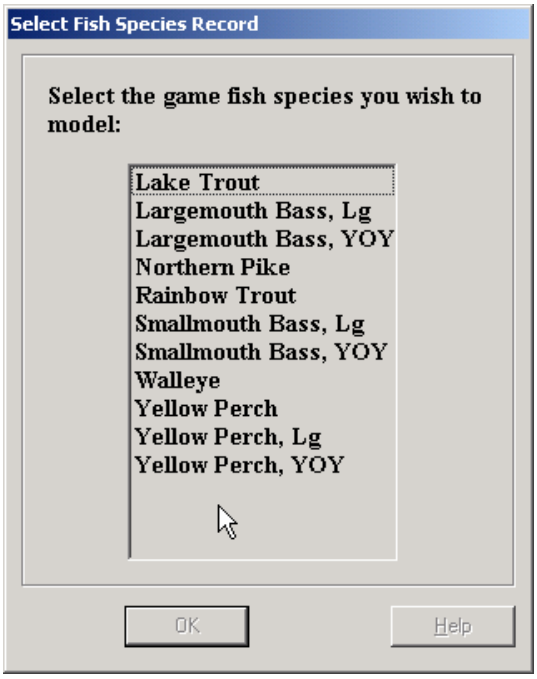


Step 7: Fish Species

Altogether, it is possible to model 13 fish species. Nominally, fish are classified as forage fish, bottom fish, and game fish, with two species for each general class. Usually two size classes are modeled for each species, but separate species can be modeled instead. Furthermore, one species can be modeled as multiple year classes. For each guild, the user can choose from a list of species in the database. The guild designations do not determine the feeding preferences–those are specified by the trophic interaction matrix, which is accessed by editing the state variable from the main screen; therefore, one could ignore the guild designations and parameterize the fish whatever way is appropriate. Initial conditions are given as g/m^2 because it is easiest to express biomass on an areal basis, and field data are usually available in that form.

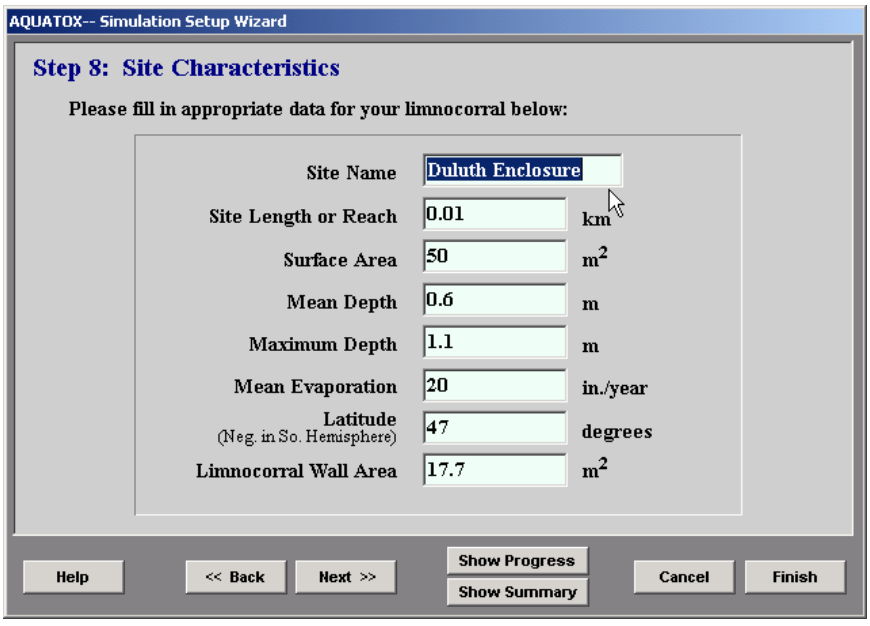

Wizard Progress
Step 1: Simulation Type
Step 2: Simulation Period
Step 3: Nutrients
Step 4: Detritus
Step 5: Plants
Step 6: Invertebrates
Step 7: Fish
Step 8: Site Characteristics
Step 9: Water Volume
Step 10: Water Temperature
Step 11: Wind Loading
Step 12: Light Loading
Step 13: Water pH
Step 14: Inorganic Solids
Step 15: Chemicals
Step 16: Inflow Loadings
Step 17: Direct Precipitation
Step 18: Point-source Loadings
Step 19: Nonpoint-source Loads
(double click on any step to jump there)
Help
Hide Progress
Notes
Edit With Wizard
Window Help Acrobat
AQUATOX-- Simulation Setup Wizard
Step 7: Fish Species
Within AQUATOX, fish are classified as forage fish, bottom fish, and game fish. Furthermore, a fish species may be simulated as a single compartment, two size-class compartments, or multiple age-class compartments.
Below is the list of fish included in the current simulation. Click the [Add] or [Remove] buttons to modify this list, or the [Next] button to move on.
Fish Species in Simulation:
Green Sunfish : forage fish, two size-class fish
Shiner: large forage fish, single-compartment fish
Add a Fish Species
Help
<< Back
Next >>
Help
Add
Wizard Summary
Simulation Name: CHLORPYRIFOS 6 ug/L
Simulation Type: Limnocorral
State Variables in Simulation:
Dissolved org. tox 1: [Chlorpyrifos]
Ammonia as N
Select Type of Fish Compartment(s)
Do you wish to add this fish species as a single compartment, two size-classes, or multiple age-classes?
Single Compartment
Size-Class
Age-Class
OK
Cancel
Help


Select Class of Fish
Which classification of fish do you wish to add to the simulation?
Small Forage Fish
Large Forage Fish
Small Bottom Fish
Large Bottom Fish
Small Game Fish
Large Game Fish
OK
Cancel
Help

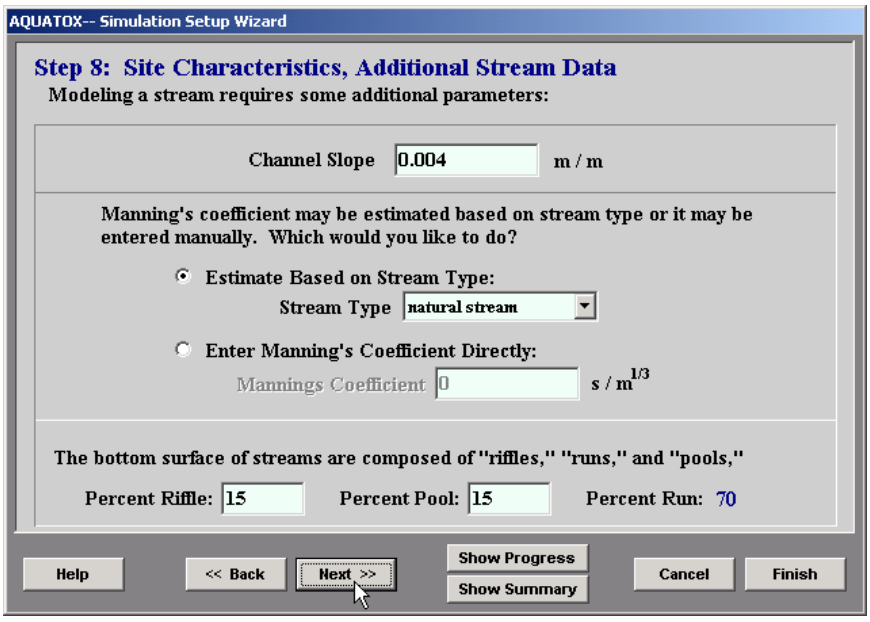


Step 8: Site Characteristics

The most important morphometric characteristic is mean depth because that controls light penetration, volatilization, and attached plant distribution. Mean annual evaporation is used for computing the water balance. Latitude is used to compute photoperiod for photosynthesis. The wall area is important for a limnocorral because it represents additional area for attachment of periphyton.

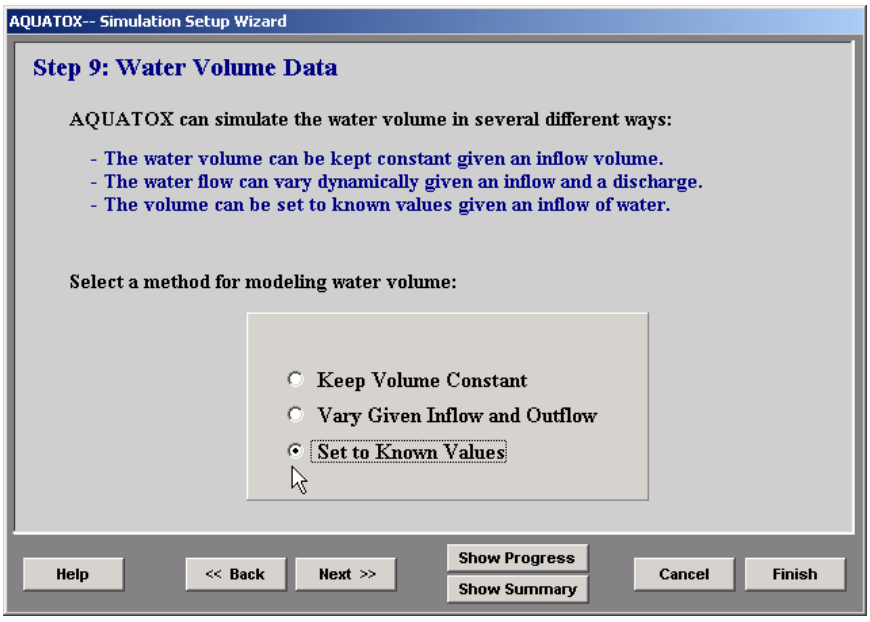


The site characteristics screen is sensitive to the type of site, so that a stream has an additional screen.

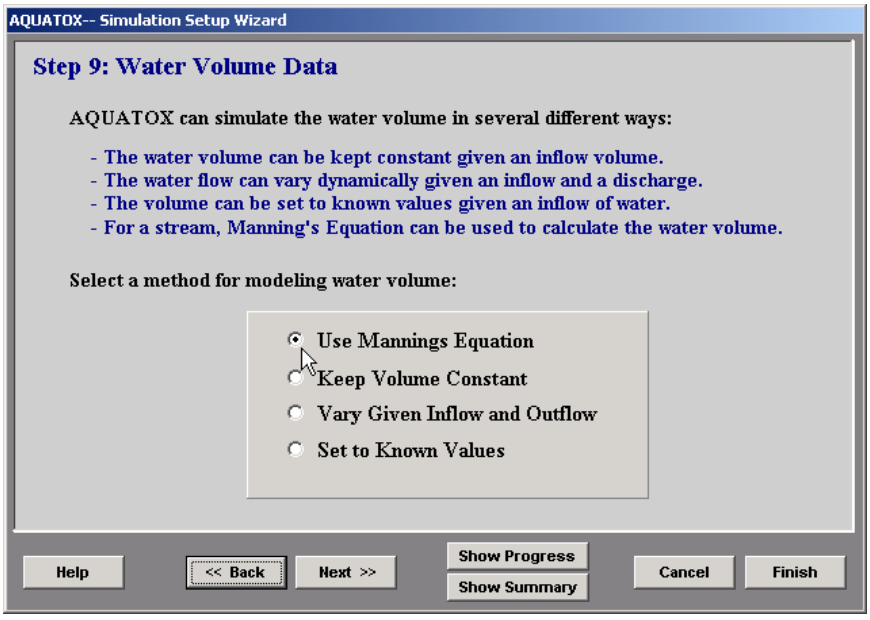


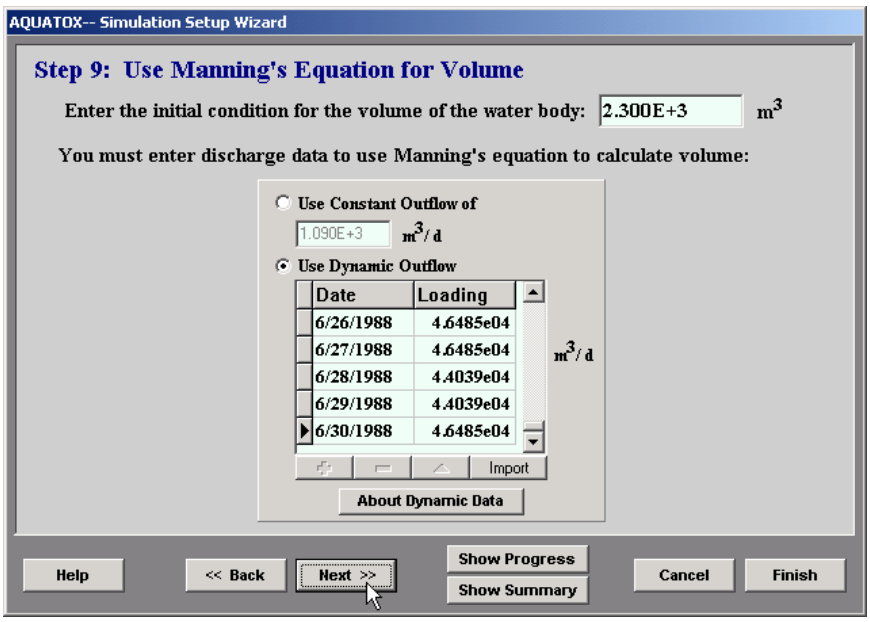
Step 9: Water Volume Data

Depending on the method chosen, inflow or discharge values may be required. The Manning's equation can be used to compute changing volumes in a stream. The simplest procedure is to hold volume constant at the initial condition. Volume can be computed dynamically, given the inflow and outflow (and factoring in evaporation). Finally, time series of known values can be entered, as was done for this closely monitored limnocorral.



If the site is a stream then there is an additional option, using the Manning's equation (see **Volume 2**) to compute the volume.

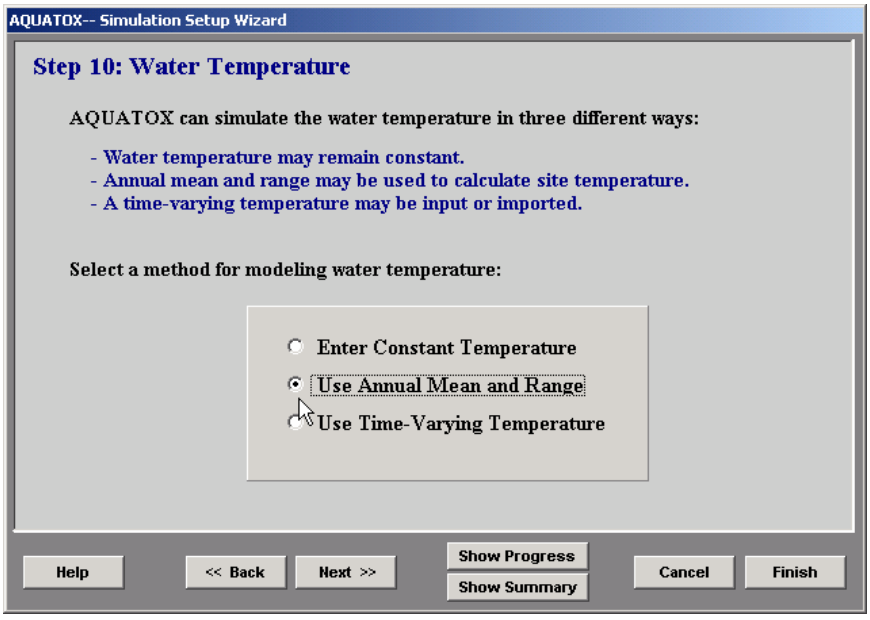


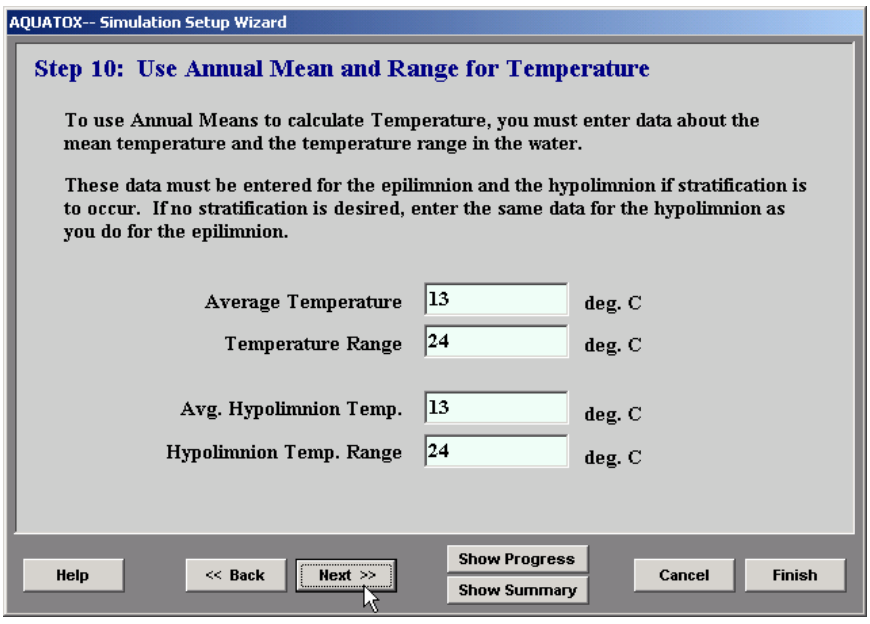


Step 10: Water Temperature

Temperature is a driving variable and is not computed as a state variable based on a heat budget. A constant temperature, annual mean and range in temperature, or time-series can be entered. Except for stratified lakes and reservoirs, the model is not very sensitive to temperature, so a sinusoidal function based on the annual mean and range is often sufficient. Even a stratified

system usually can be modeled with sinusoidal functions for the epilimnion and hypolimnion temperatures. If stratification is not desired, enter the same temperature values for "epilimnion" and "hypolimnion."

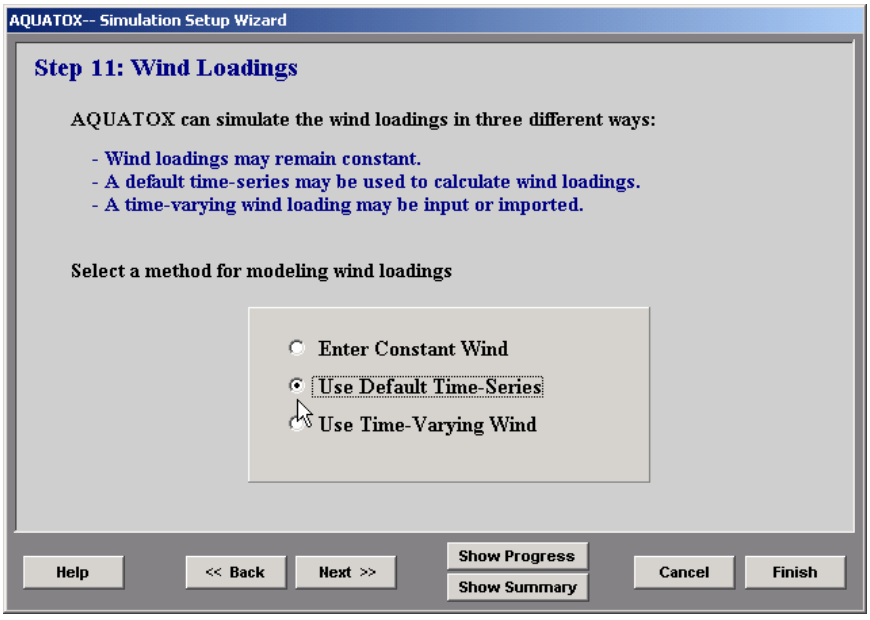




Step 11: Wind Loadings

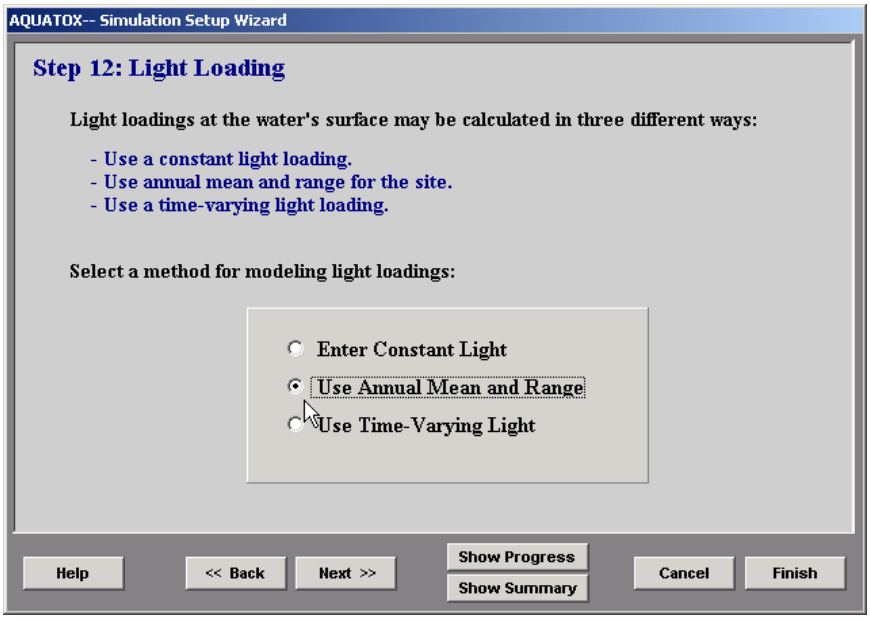
Wind loadings can be constant, a time series can be entered, or a default time series can be used. The default is a 140-day record from Columbia, Missouri, represented by a Fourier series, with a mean value that can be specified by the user (the default is 3 m/s). Near-surface

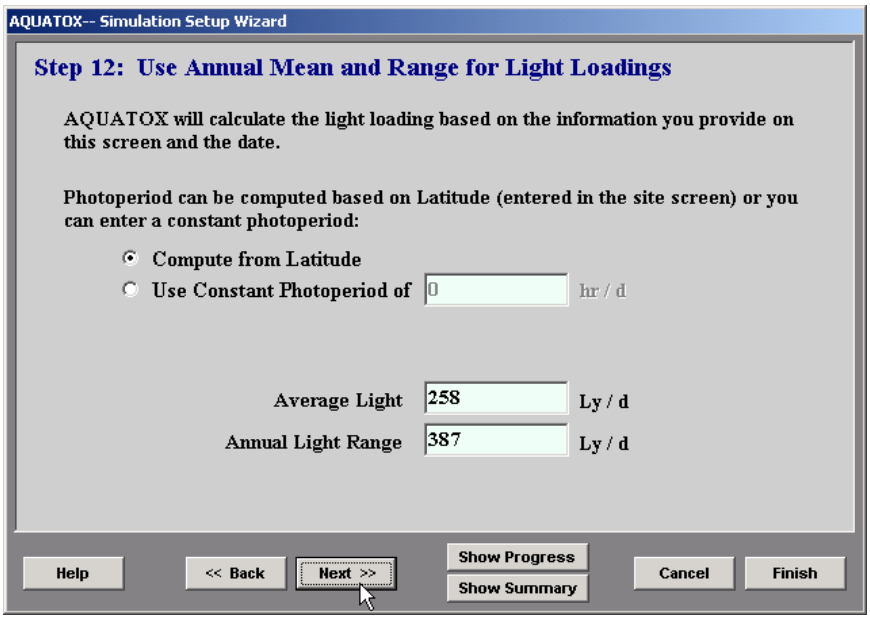
blue-green algae are represented as being sensitive to wind, so a realistically varying sequence of synthetic wind values provides a better simulation than a constant value.



Step 12: Light Loading

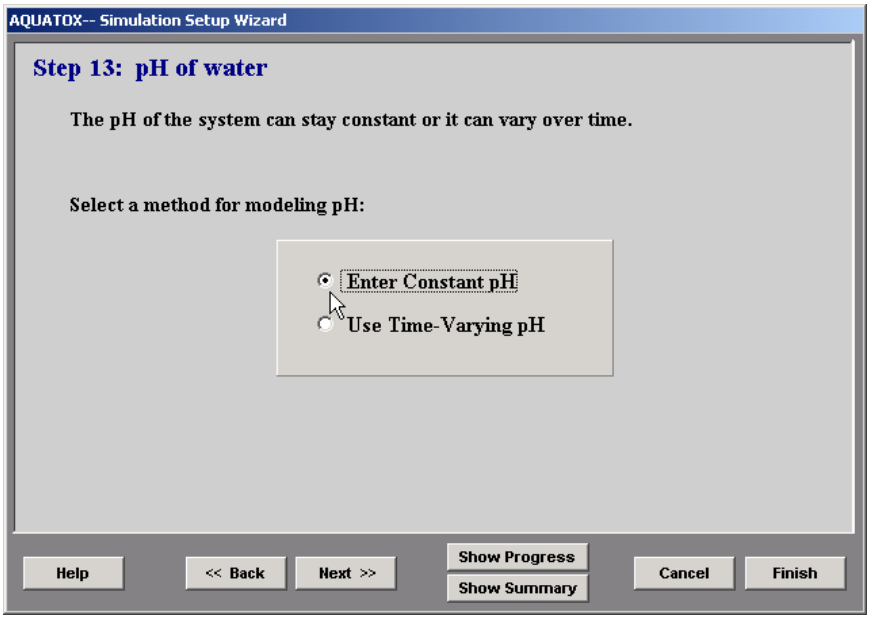
Constant, time series, and annual mean and range may be given for light in Langleys/day. The photoperiod is usually computed from the latitude, which is a site characteristic; however, the user can specify a constant photoperiod–useful in modeling some experimental facilities.





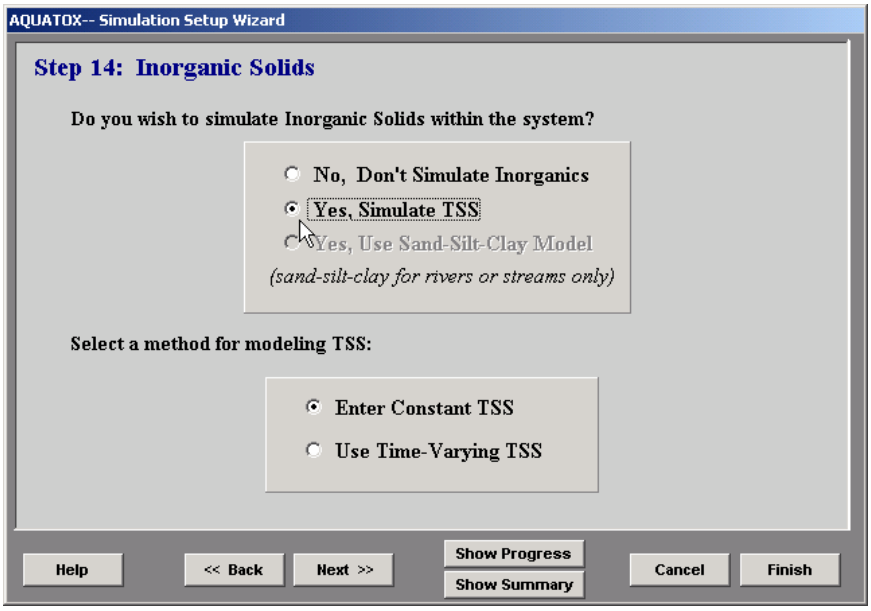
Step 13: pH of Water

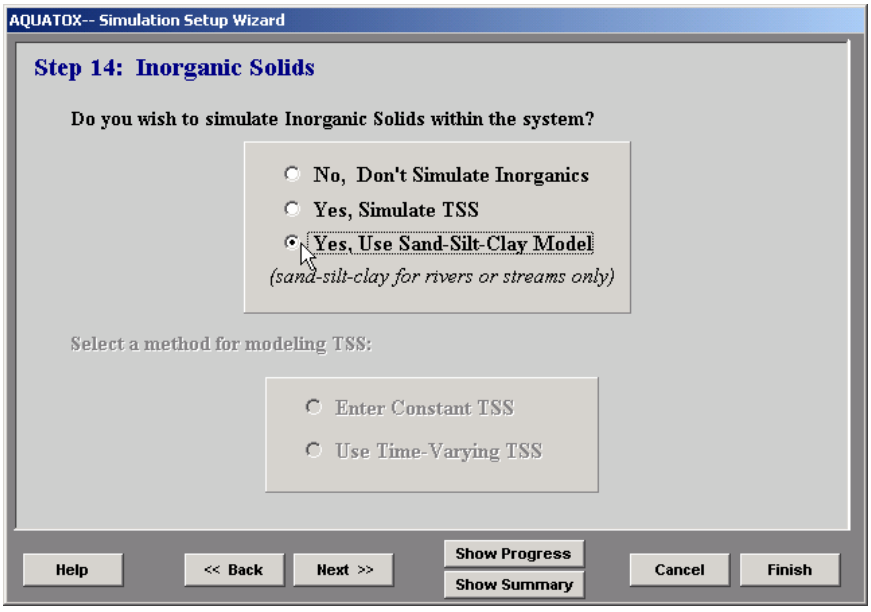
At present pH must be specified by the user, either as a constant or as a time series.

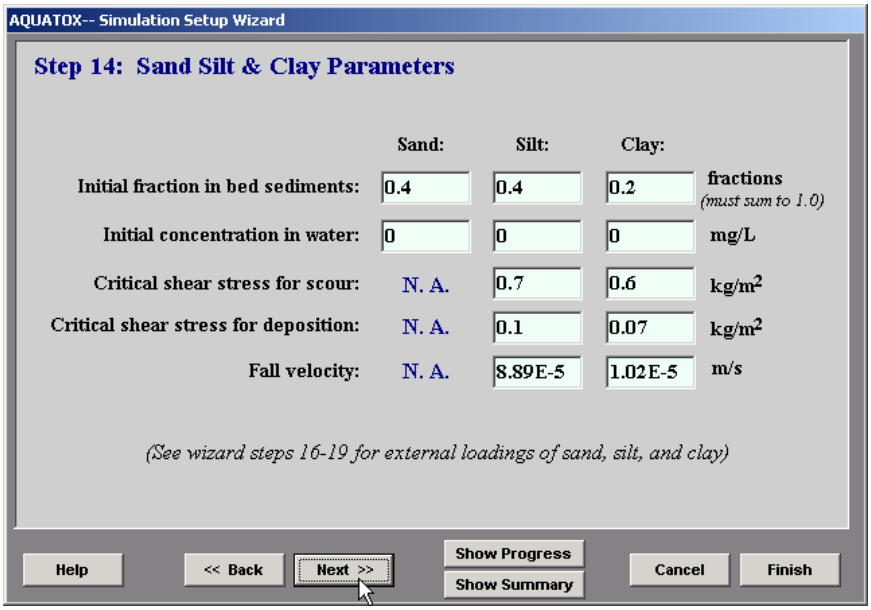


Step 14: Inorganic Solids

AQUATOX can simulate sand, silt, and clay, but only in streams. For standing water an alternative is to use total suspended solids as a measure of inorganic solids. The model subtracts phytoplankton and detritus from the TSS to estimate the inorganic solids; therefore, care should be taken to use contemporaneous TSS and nutrient time series.

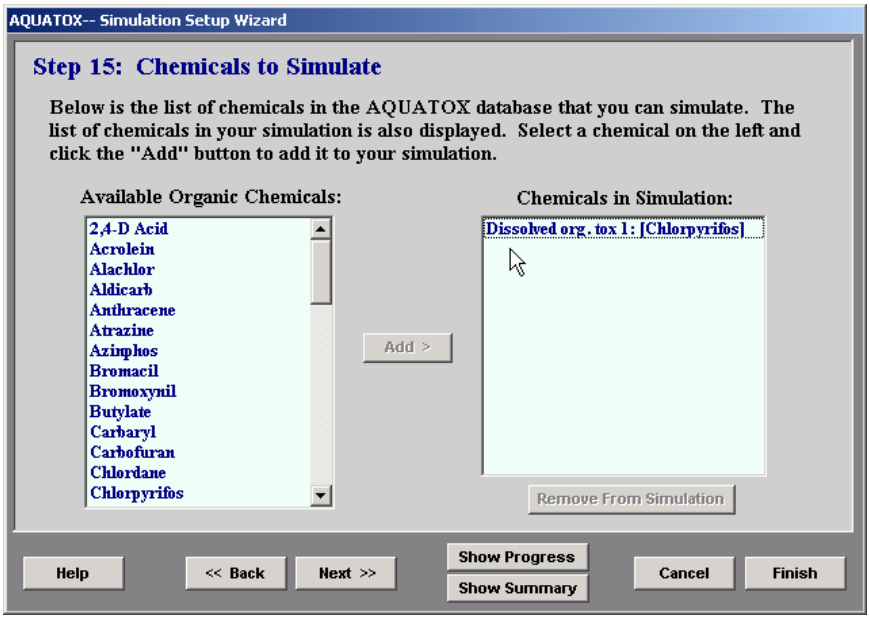


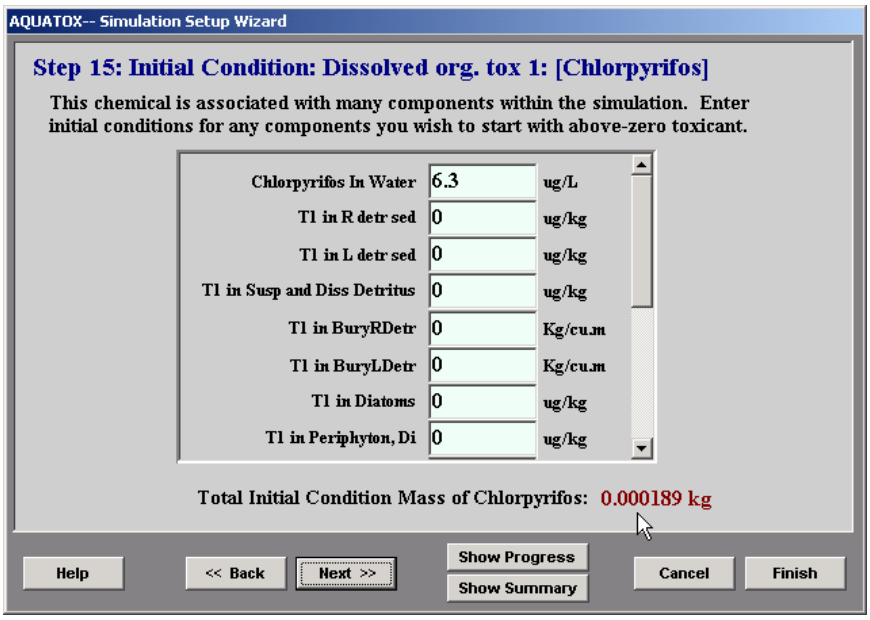




Step 15: Chemicals to Simulate

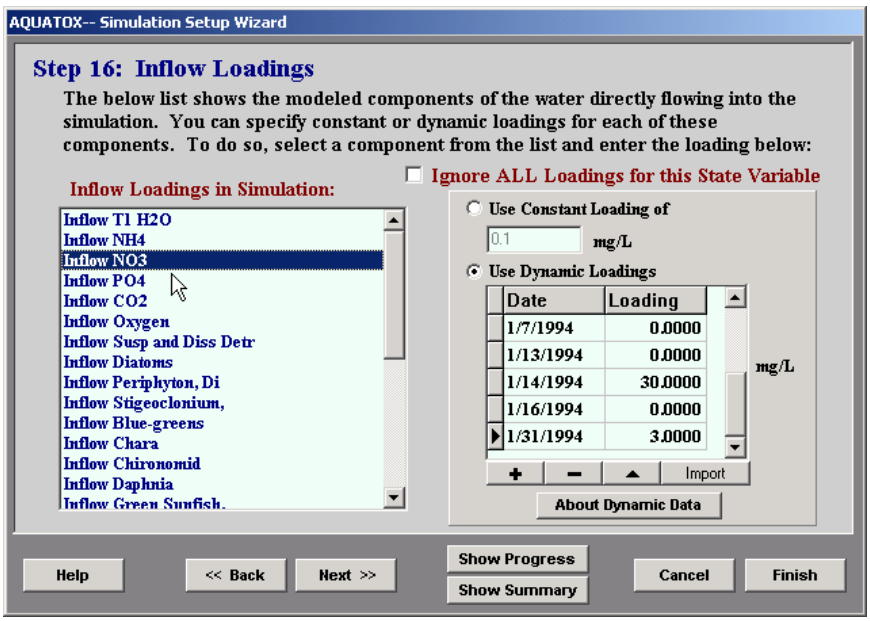
AQUATOX can simulate as many as 20 different organic chemicals simultaneously. The assumption is that the toxic effects are additive. Initial concentrations for each toxicant are required for all associated state variables; as a check, the model calculates the total mass.





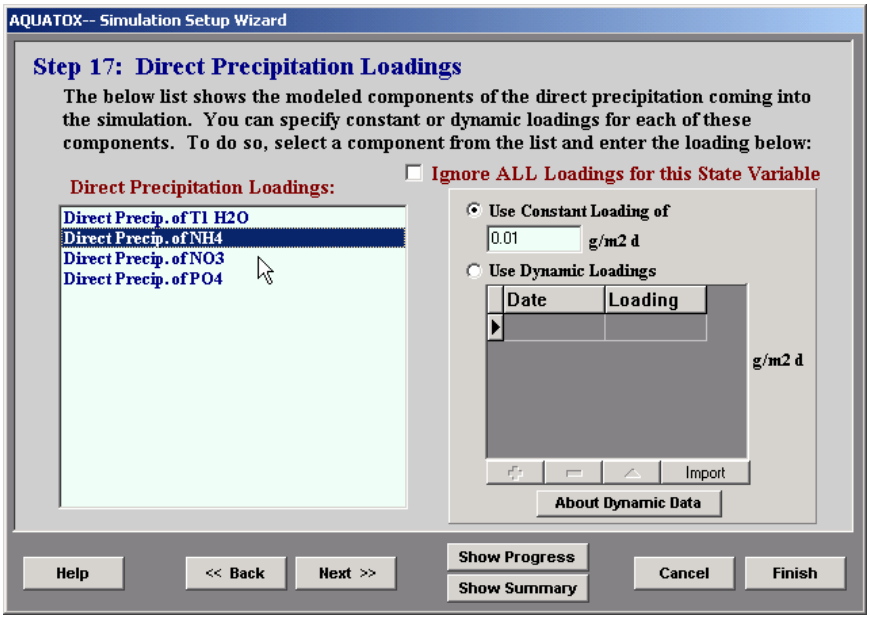
Step 16: Inflow Loadings

The Wizard compiles a list of all variables that may be loaded as concentrations in inflowing water. The units are sensitive to each given variable. Note that choosing any dynamic loading without entering at least one value will be interpreted as loadings of zero. Occasionally a user may wish to ignore all loadings for a state variable, such as when performing complex alternate simulations; this capability exists through the Wizard and each of the loading screens.



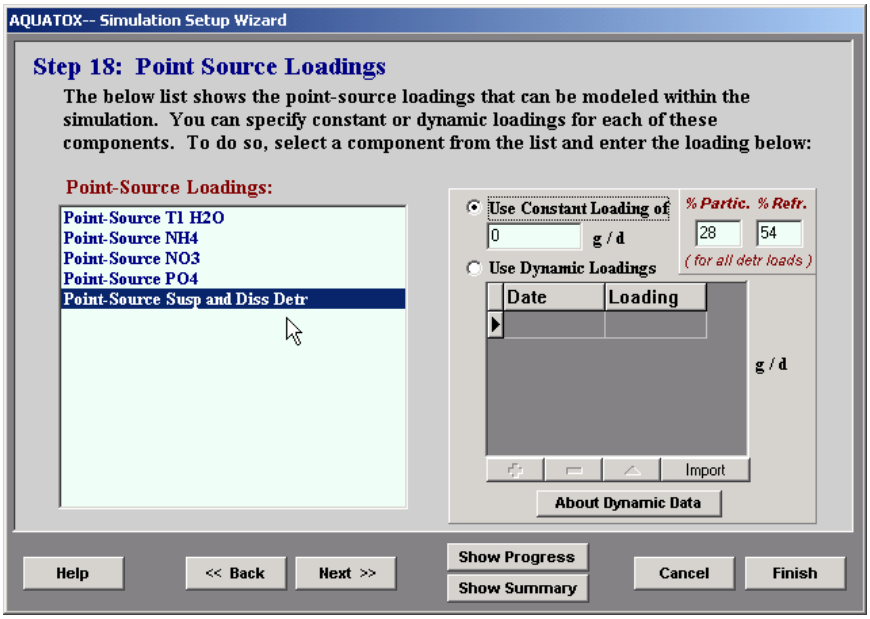
Step 17: Direct Precipitation Loadings

Another screen lists loadings from atmospheric deposition ("direct precipitation" and dry-fall). The units are on an areal basis because deposition is on the surface of the water.



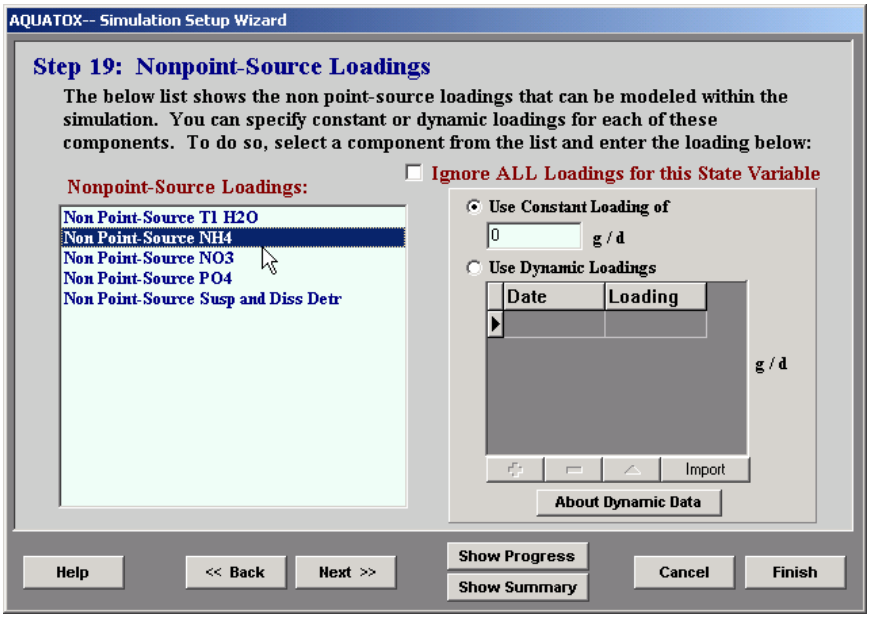
Step 18: Point-source Loadings

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



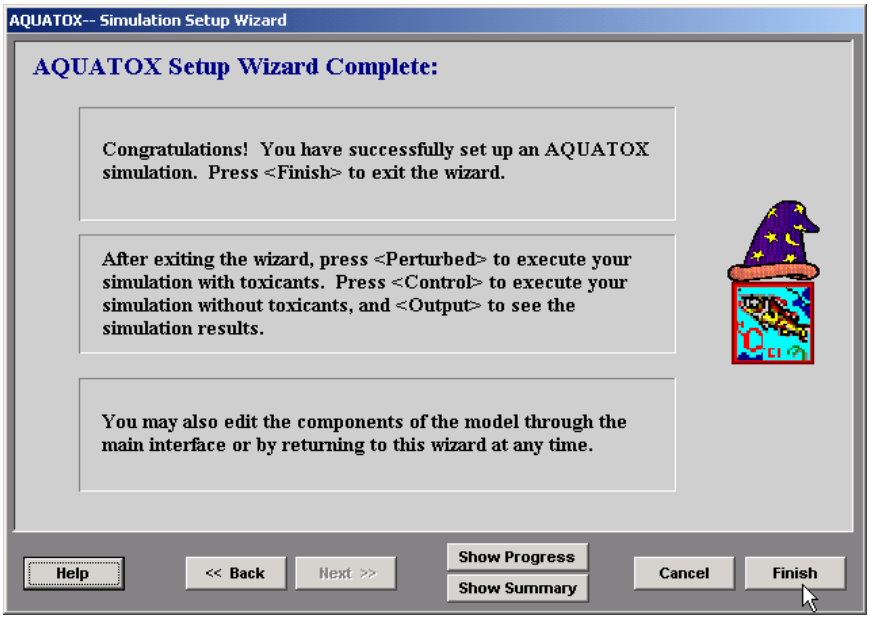
Step 19: Nonpoint-source Loadings

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



Wizard Completion

When you have completed the 19 steps in the Wizard, you should review the parameter files for the individual state variables because they are not subject to editing through the Wizard.



3 DATA CONSIDERATIONS

AQUATOX has many possible loading variables and process-level parameters. What input data are most critical for the simulations? The answer depends on the goals of the simulation and the site-specific requirements. By using the principles outlined later in **Uncertainty Analysis**, one can perform sensitivity analysis to identify the more sensitive parameters and loadings for a particular simulation. Sensitive parameters may require site-specific determination or careful calibration. Some sensitive variables have been identified in other studies and are listed below.

3.1 Toxicant

- The octanol-water partition coefficient is critical to bioaccumulation in organisms and partitioning in detritus. It often can be estimated better than it can be measured.
- Henry's law constant is important for volatilization and yet is often difficult to measure.
- Chemical and microbial degradation parameters determine the persistence in an ecosystem. If only half-lives are reported, they should be represented as uncatalyzed hydrolysis rates, which are not affected by seasonal conditions as are microbial rates.
- The thickness of the active layer, represented as the mass of sediment detritus, is important because of the simplifying conceptualization in this version that treats sediment-water interaction of contaminants as very efficient but restricted to the active layer.
- Some toxicants, such as parathion, may bind more tightly to sediments than indicated by organic partitioning. Estimation of the sediment partition coefficient may need to be overridden with observed values.

3.2 Nutrients and Remineralization

- The fraction of phosphate that is available depends on the nature of the phosphate loadings. The model distinguishes between detrital loadings, with implicit phosphorus content that is more or less available depending on whether the material is refractory or labile. Phosphate loadings may be in the dissolved phase or may be bound tightly in mineral particles; the user accounts for these by varying the fraction available: 1.0 if the phosphate is readily available and a small fraction if it is tightly bound.
- Release of phosphate from anaerobic sediments is not modeled at this time. Previously, it was a constant (during periods of anoxia) and was set in the **Remineralization** screen. It will be reinstated in the near future.
- Co-precipitation of phosphate with calcium carbonate is not modeled. In sites where that is important the best work-around is probably to decrease the loading accordingly.
- Chemical oxygen demand is not modeled explicitly because of its site-specific nature; a work-around would be to decrease oxygen loadings.
- Constant stoichiometry for nutrients in organic matter is a simplifying assumption. One can change the value of the ratio of a given nutrient to organic matter in the **Remineralization** screen. The Redfield et al. (1963) ratio is used as the default.

- The proportions of refractory and labile and dissolved and particulate organic matter in a system control the rate of remineralization. Inappropriate initial conditions will cause a transient response, but poor characterization of loadings may affect the long-term nutrient budget and bioavailability of organic contaminants. If possible, obtain seasonal values for total organic carbon (TOC), dissolved organic carbon (DOC), and biological oxygen demand (BOD, which is labile); these can be used to obtain the necessary proportions. Otherwise, consider the source of detritus loadings (forests, treatment plant, etc.) when deciding how much may be refractory and particulate.

3.3 Plants

- Half-saturation constants for nutrients control how responsive phytoplankton and periphyton are to eutrophication; parameter values may depend on trophic status.
- Maximum photosynthetic rates determine the competitiveness and resilience of algae; observed rates vary greatly and composite rates, such as for a diatom community, are most appropriate for most applications.
- The model assumes that blue-green algae float unless the wind exceeds 3 m/s; this makes the model sensitive to the mean wind loading.
- Most macrophytes are sensitive to fall dieback; cold-tolerant groups, such as charaphytes, should be so characterized with appropriately low optimal temperatures. Stream bryophytes or moss are parameterized to be tolerant of low-light, cold conditions and are subject to nutrient limitations; half-saturation constants for nutrients may require calibration.

3.4 Animals

- Consumption of refractory detrital sediments by zoobenthos increases the degradation rates of those sediments, increasing the simulated sediment oxygen demand and remineralization. The user should assume that most zoobenthos selectively feed on labile detritus, which includes freshly sedimented algae.
- The minimum biomass for feeding (*BMin*) is seldom measured, yet the model can be very sensitive to this. The *BMin* value protects prey from being totally consumed, but if it is set too high the predators may starve to death. It may require site calibration.
- Half-saturation for feeding is very seldom measured, but it can significantly reduce predicted feeding rates. Therefore, it should be set low in the absence of data.
- Consumption and respiration rates in fish are functions of body size. As a default, the model uses the allometric equations presented by Hewett and Johnson (1992). Selection of representative mean weights for use in the equations is important.
- Mortality rates may vary greatly from one site to another. This often becomes a calibration parameter, especially since fishing pressure is not modeled and death due to predation is separate in the model.
- If modeling an aquatic insect that emerges, be sure to select "Benthic Insect" in the drop-down list in the parameter screen because otherwise emergence will not be simulated.

3.5 Inorganic Sediments

- Inorganic sediments are not explicitly modeled for standing water. They can be simulated in streams, following the approach used in the HSPF model. However, if sediment transport, burial, and scour are important, the model should be coupled to a hydrodynamic model.
- Total suspended solids are used to back-calculate suspended silts and clays in the model. This loading is compared with phytoplankton biomass in the computation of Secchi depth and light extinction; therefore, it should be provided for the entire period of the simulation (most loadings can be repeated automatically if the simulation period is longer than the available data).

4 CALIBRATION FOR A CONTAMINATED STREAM

4.1 Introduction

Users often ask for guidance on the best way to calibrate such a complex model. This section is intended to provide guidance for a typical ecosystem and bioaccumulation calibration for a site given a minimum amount of data. The goal for any calibration should be to obtain a good fit to observed data by varying as few parameters as possible and only within reported ranges. The above section, **Data Considerations**, provides a list of sensitive parameters, and applicable ones are considered in the following example.

Criteria for acceptance of a calibration depend in large part on the amount of available data. In general, a weight-of-evidence approach should be taken with increasingly rigorous tests. An example of calibration of AQUATOX using an extensive dataset was given by EPA (2001). With minimal or sparse data the criteria may be restricted to less rigorous tests, including:

- Observation of long-term reasonable behavior based on general experience with similar ecosystems;
- Stability of simulations of key compartments compared to observed initial conditions (does a species or group maintain roughly the observed biomass used as a starting point?);
- General concordance based on visual inspection of data points compared to plots of model results;
- Bracketing of observations by predicted bounds obtained from uncertainty analysis;
- Bracketing of predictions within ranges observed for replicated variables.

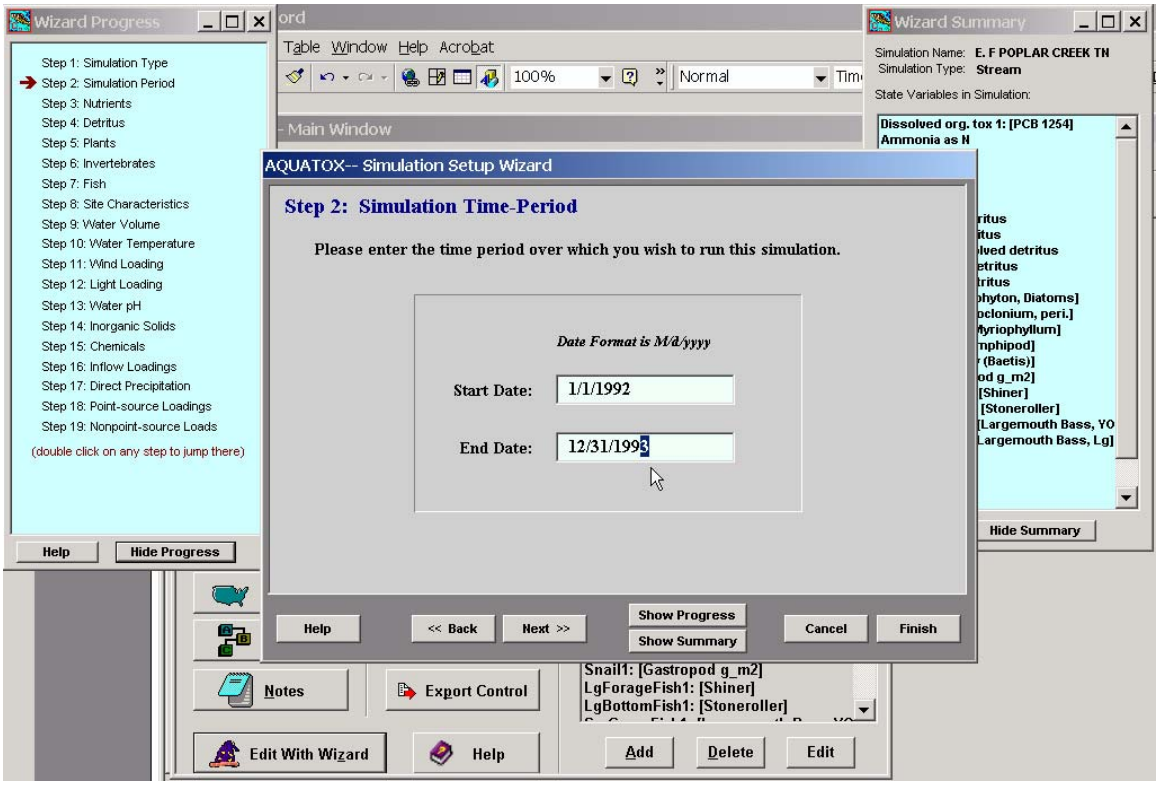
The Wizard provides a useful checklist for setting up a simulation, and it may provide the structure for reviewing and changing initial conditions and loadings. It does not provide a means for changing parameter values; and, therefore, it is not very useful for a typical calibration involving the iterative modification of parameter values.

The example given below involves both ecosystem calibration and bioaccumulation calibration for a stream contaminated with PCBs in central Tennessee. It is provided only as an example and has no regulatory implications.

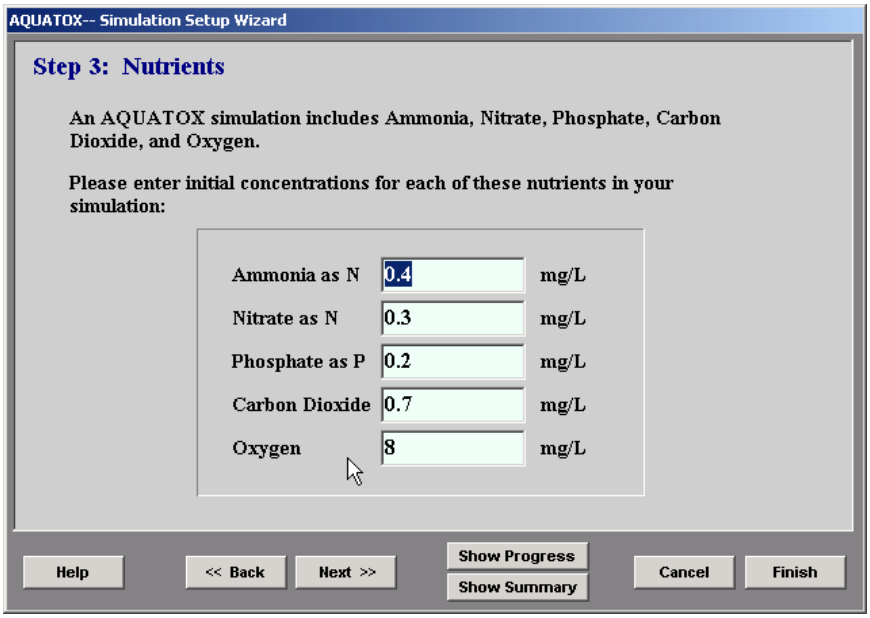
4.2 Review Initial Conditions and Driving Variable Data

Several study files with "EFPC" and "EForkPoplarCr" in their names are in the Studies directory. These are provided because you may not wish to perform all the changes described in this lengthy example. For purposes of illustration, we will begin with a prepared study labeled **EFPC3Const.aps** (East Fork Poplar Creek, station 3, constant discharge). Load the study into AQUATOX. However, before proceeding, let's save the study under a different name so that we can preserve the original study file; we'll name it **EForkPoplarCr.aps**. Now click on **Edit With Wizard**. Click on **Next** until Step 2. The two-year simulation period encompasses the period for which we have PCB data. However, stream simulations tend to be slow because of

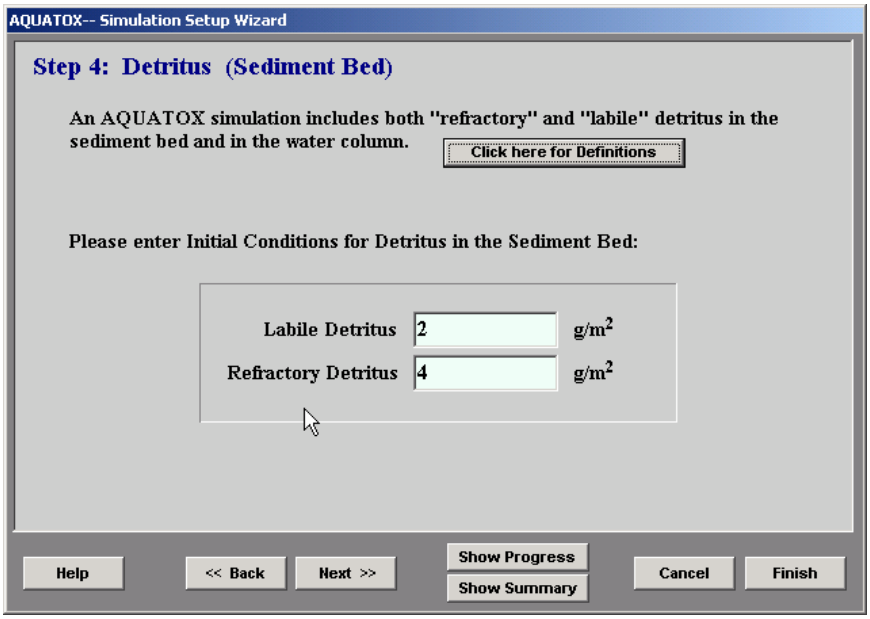
the dynamics of changing flow, and so for purposes of the tutorial we will reduce the end date from 1993 to 1992. It would be desirable to use a longer simulation period to avoid transient conditions, but we will do that only when checking the stability of the calibration and calibrating the bioaccumulation.



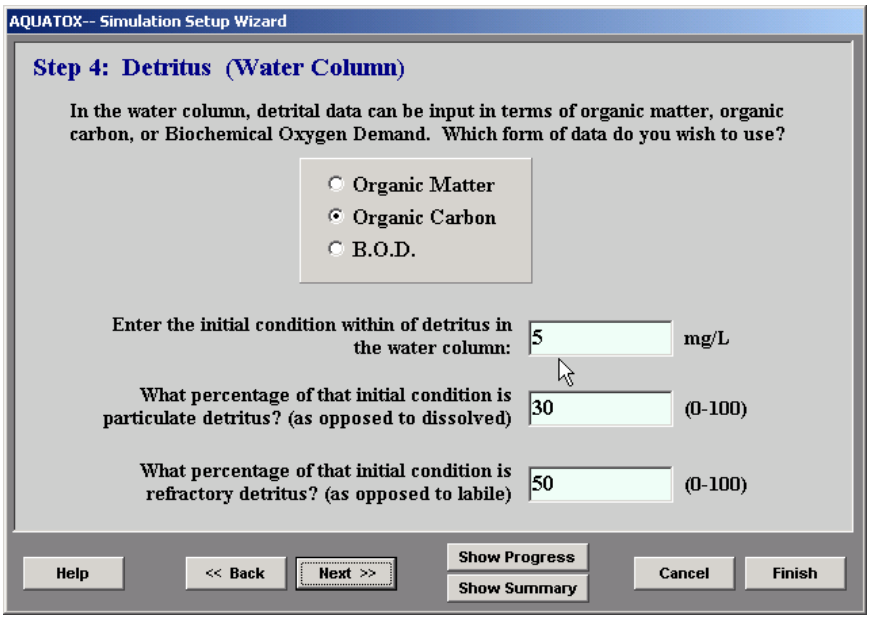
In Step 3 observed values are given for nitrogen and phosphorus initial conditions; carbon dioxide and oxygen values are based on approximate saturation levels.



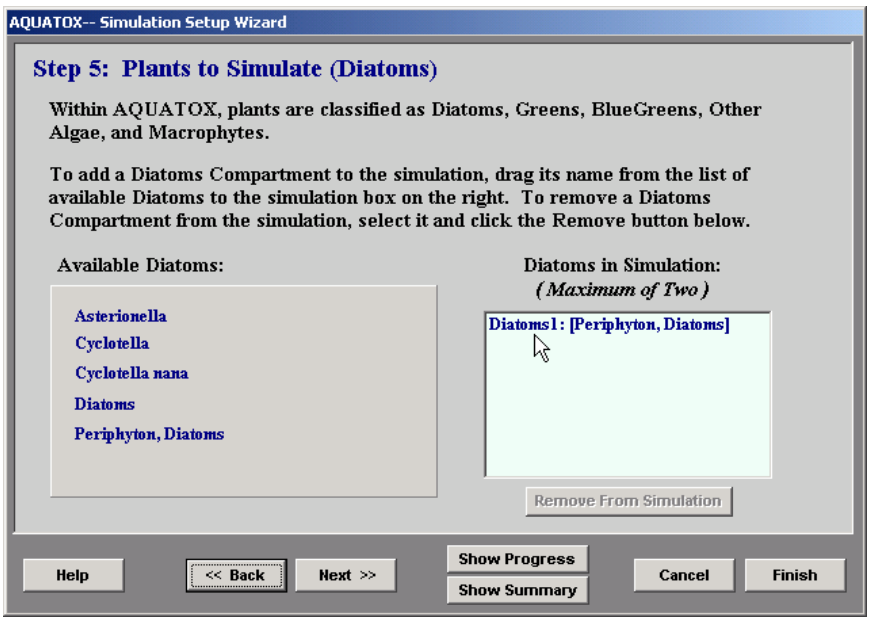
The initial condition for organic detritus in the sediment bed is important because AQUATOX assumes steady-state conditions for sediment burial. That is, as a simplifying assumption, any organic detritus in excess of the initial condition is transferred to buried detritus at the end of a year's simulation. The proportion of labile to refractory is not critical for initial conditions, so we will guess that it is 1:2.



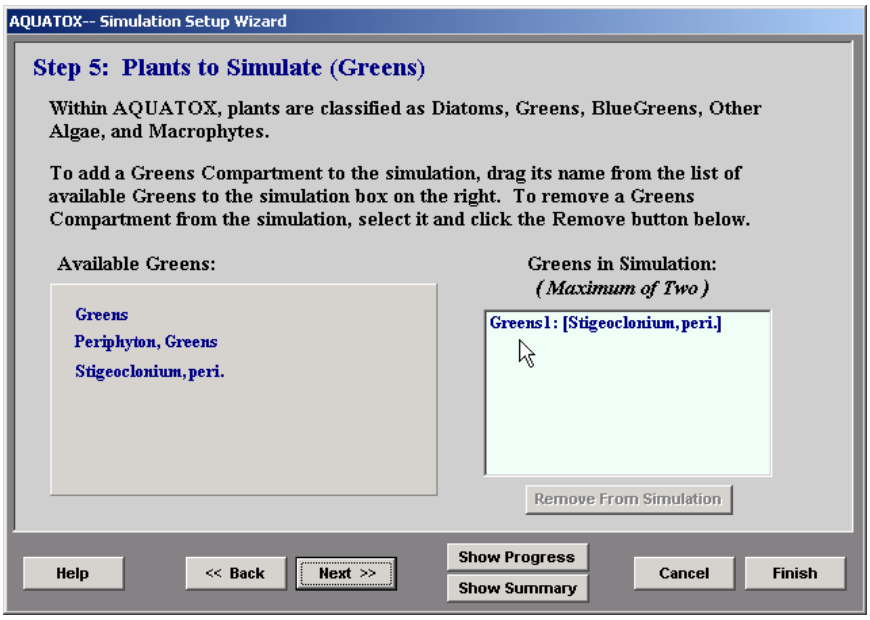
The detritus in the water column can be expressed as organic matter, organic carbon, or BOD; we have an observation of 5 mg/L organic carbon, so we will use that form and value. Seldom do we know the proportion of labile and refractory detritus. In this example, we know that the stream is fed by outflow from a holding pond with high algal biomass, so we will use our professional judgment that only 50% is refractory (it is often much higher) and that 30% is particulate (it is often only 10% in lakes and reservoirs).



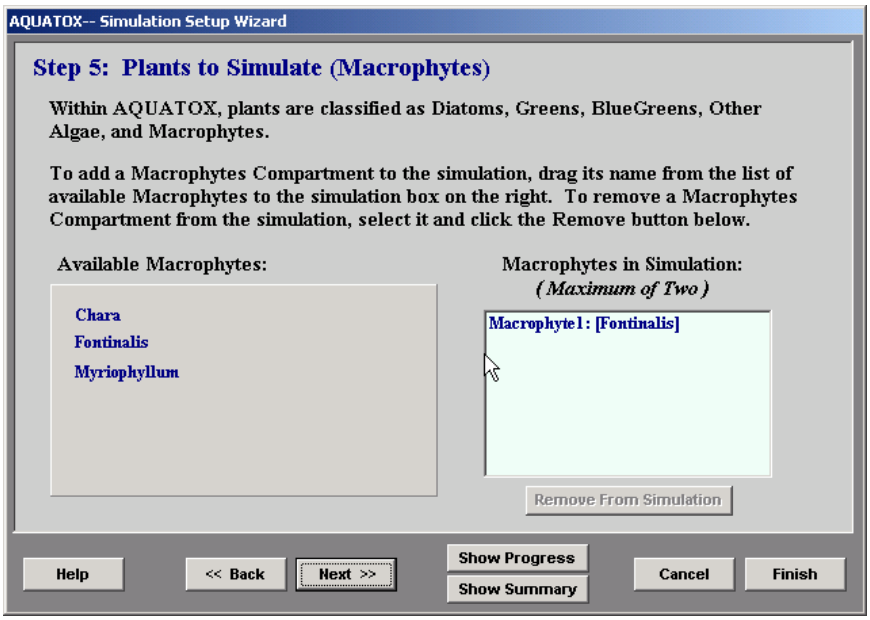
In Step 5, which spans several screens, we choose the plants to simulate. Because East Fork Poplar Creek is shallow in the reach we are simulating, we will assume that most of the algae are periphyton. Therefore, we have chosen periphytic diatoms.



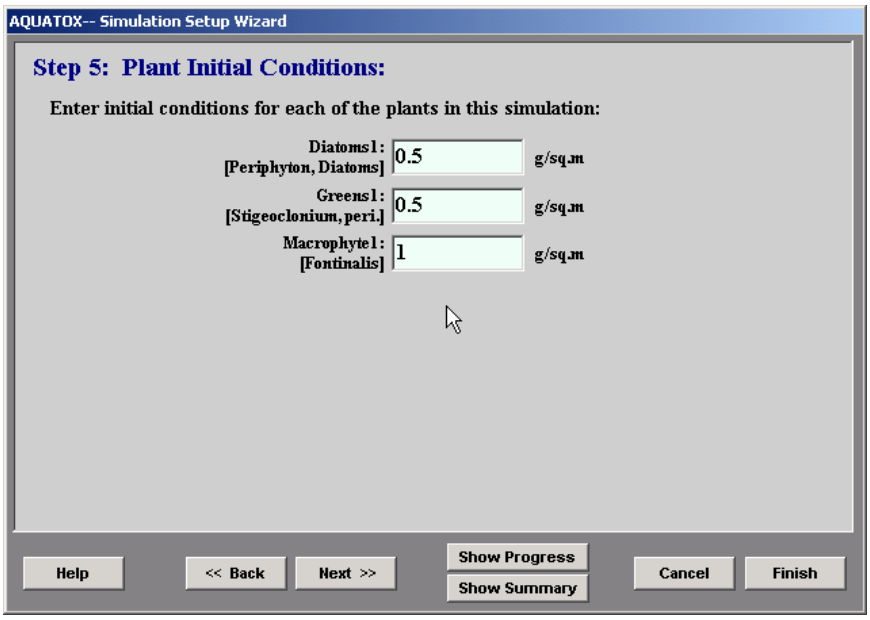
For green algae, we have a choice between periphytic greens and *Stigeoclonium*, which is a particular genus of periphytic green algae. We have chosen *Stigeoclonium* because it was calibrated and validated for a stream on the other side of the ridge (see US EPA, 2001).



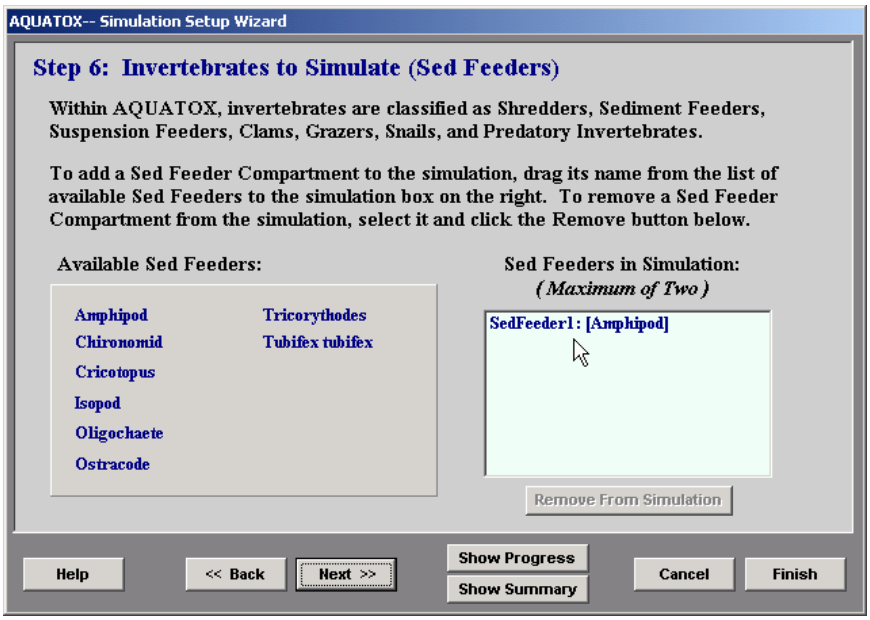
We will skip blue-green algae in the interest of using a minimal number of groups, although often we would include it because of different growth characteristics and susceptibility to grazing. For macrophytes, we will choose *Fontinalis* because this moss is well adapted to shallow streams.



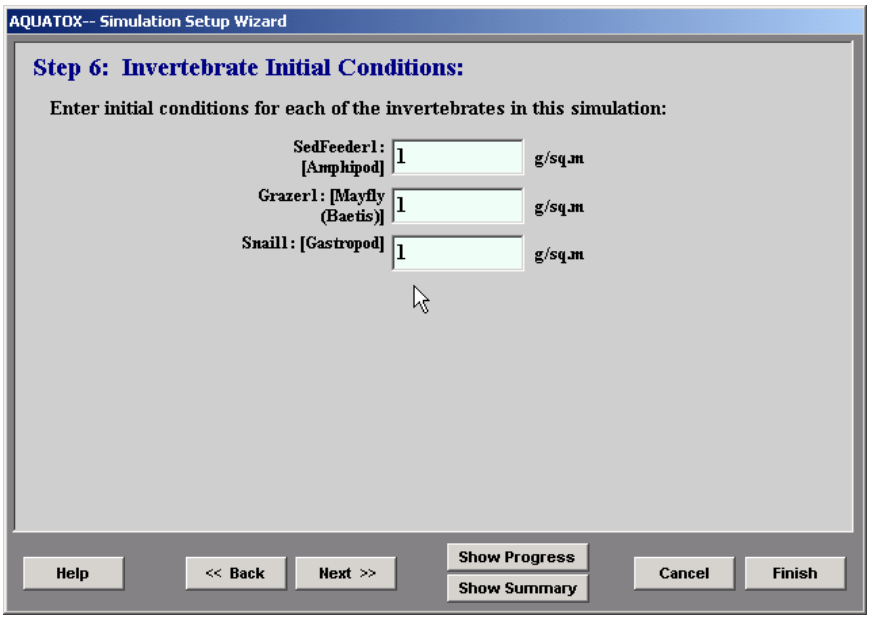
Initial conditions for plants are usually set at 0.5 or 1.0 g/m^2. These and other initial biomass values for which we have no site observations will be used as estimates, and better initial conditions will be obtained from the ending values after a "spin-up" period of one to three years to reach steady state.



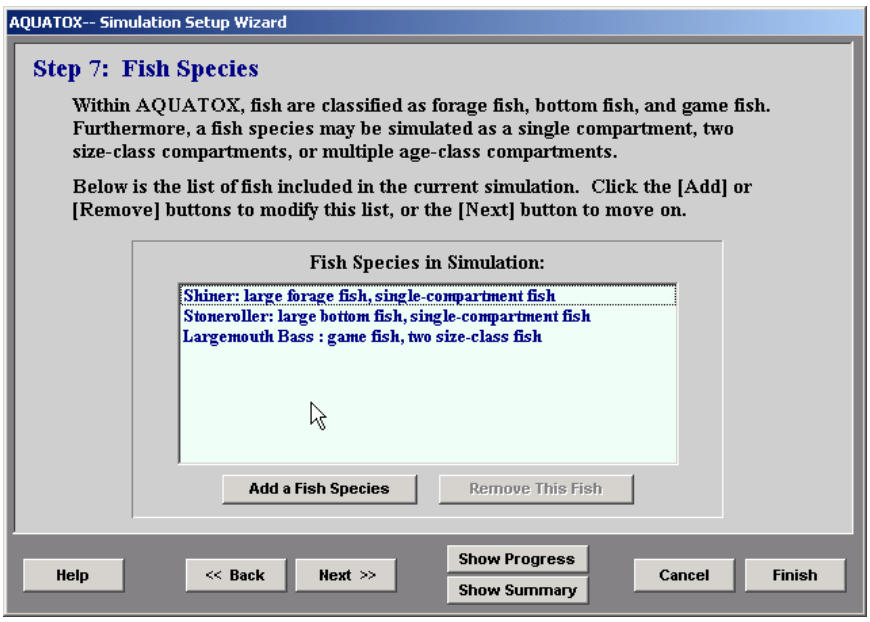
In Step 6 we have the opportunity to choose invertebrates representing several feeding guilds and taxonomic groups. We will choose amphipods to represent the invertebrates that feed on detritus in the sediments. We will choose mayfly (*Baetis*) larvae as a grazer, and we will choose gastropods as another grazer (although they are a separate taxonomic group). We could have chosen several other functional groups and we could have chosen two genera to represent each group, but our goal is to model bioaccumulation in the food web with as few groups as necessary to capture the ecosystem dynamics.



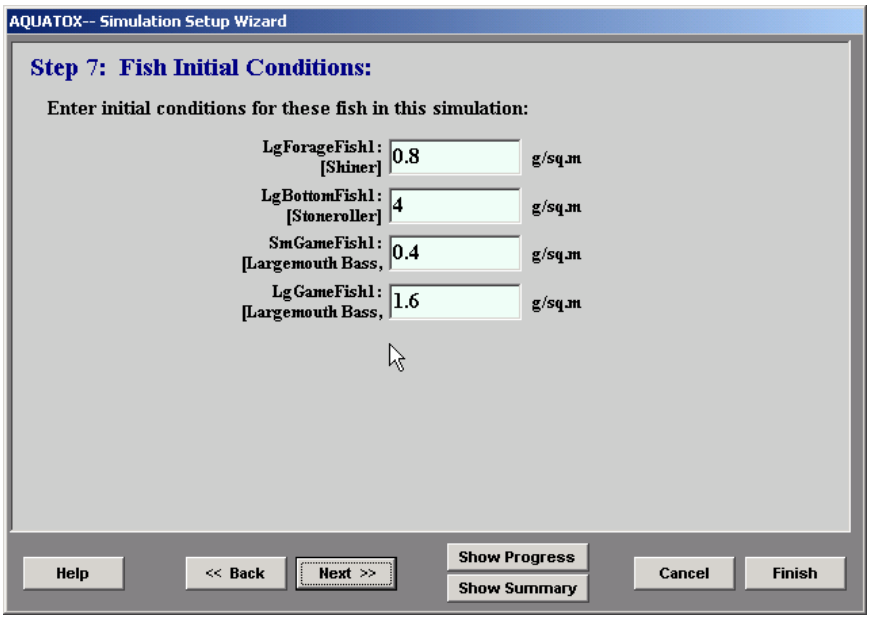
In the absence of data, we will set the initial conditions to 1.0 g/m^2 for each of the invertebrate groups.



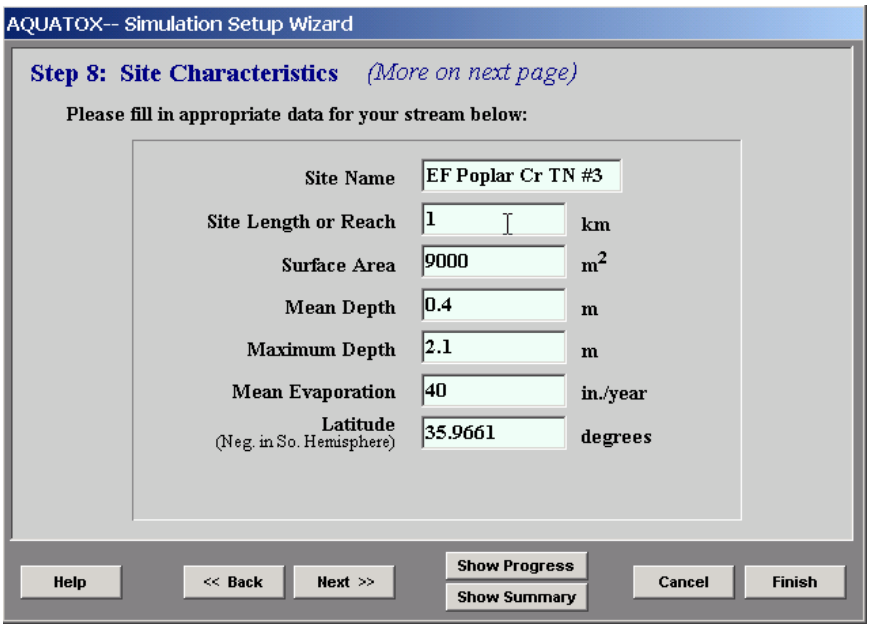
We will model three fish species, based on what we know for this reach. Other species can be added, and age classes could be simulated for bass, but we have insufficient data to support such an approach. We will use two size classes for bass.



We do have some data on abundance of fish, although upstream of this site and of unknown reliability; we convert those to biomass estimates and enter as initial conditions.

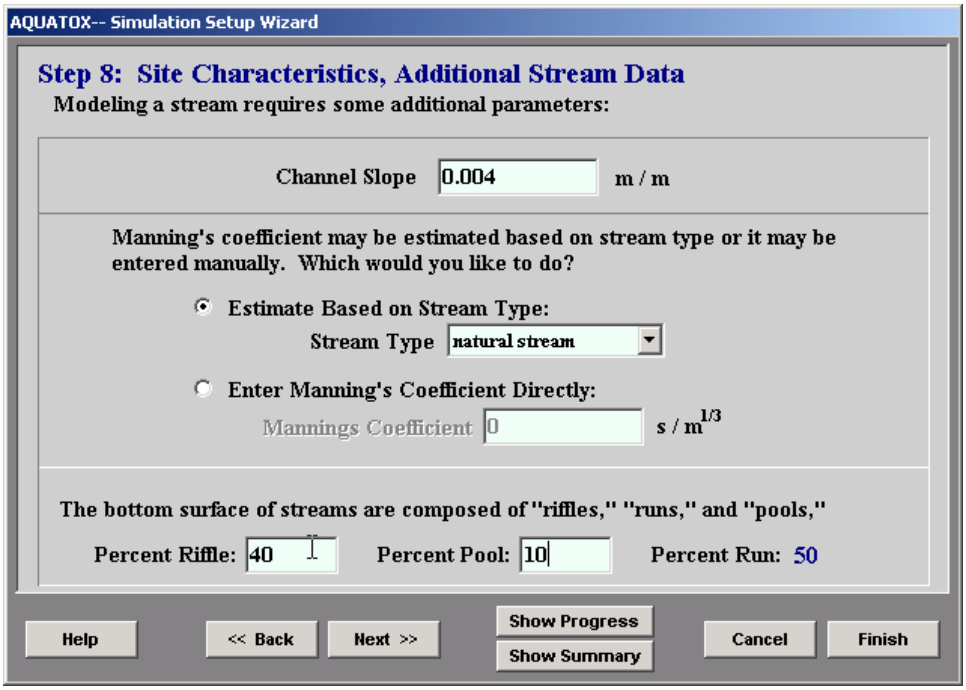


In Step 8 we can review and change site characteristics. The length is arbitrary, but the surface area is important for computing depth as a function of changing discharge; it is good practice to document the assumed channel width in the comment field for the surface area (which is available in the site screen). One consideration in specifying the reach length: the shorter the length and smaller the volume, the slower the simulation because retention time decreases, causing the solution time step to be decreased. An arbitrary length of 1.0 km is chosen so that the surface area and volume will be sufficient to avoid an unduly short retention time.

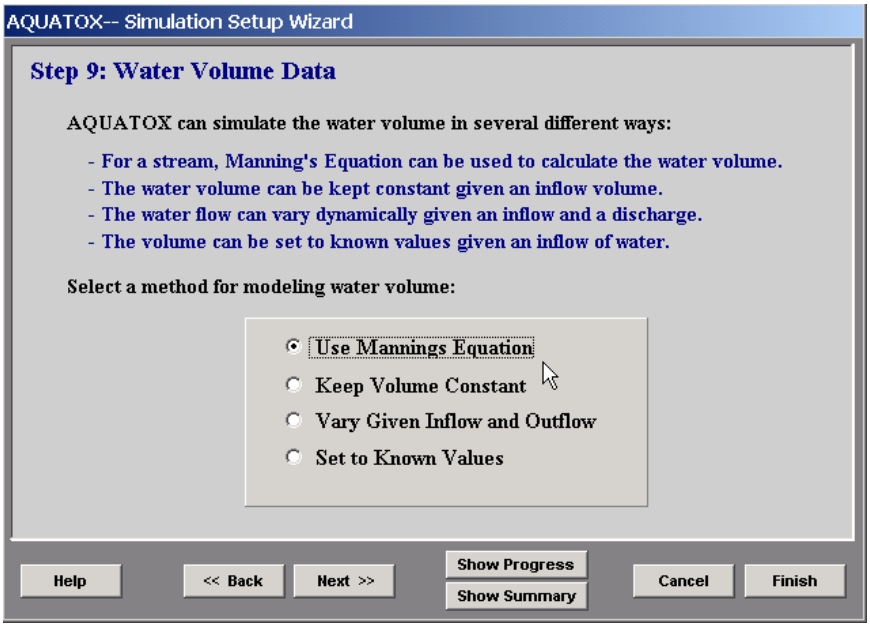


The computed velocity, which controls periphyton scour and macrophyte breakage, also is a function of channel slope, so the model is sensitive to slope. When entering a value try to represent a typical channel, not a regional slope that, for a small stream, may include rapids and

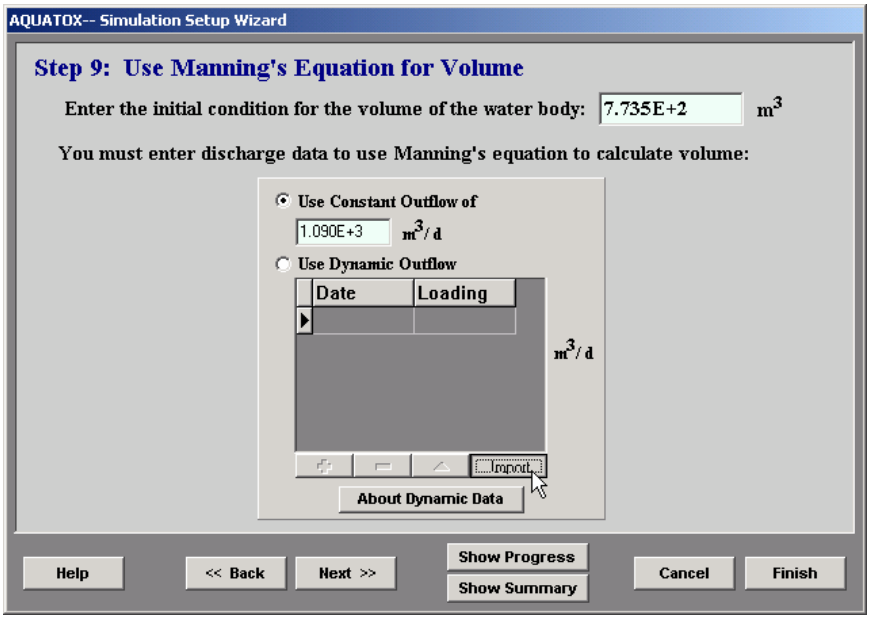
even waterfalls. Release 2 can model varying stream habitats. Rapid bioassessment data can provide percent distribution of riffle, run, and pool habitats. In the absence of such information, we will guess at a reasonable distribution for this valley and ridge stream and change it to 40% riffle and 10% pool.



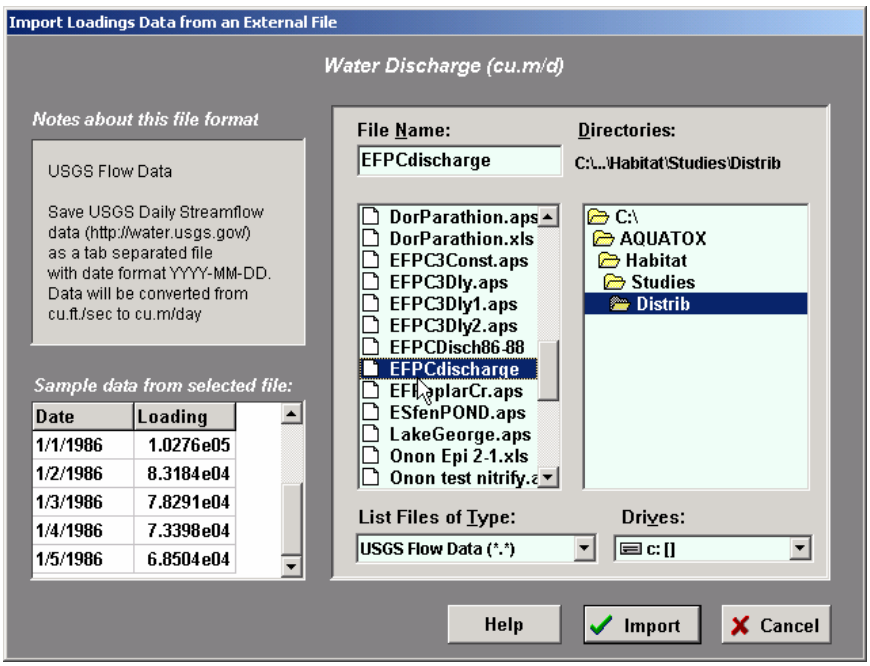
There are several ways to model water volume. If an experimental channel or pond, the volume may be held constant; computing based on inflow and outflow is also an option, but it can lead to incremental errors if the hydrodynamics are not well known. In some cases, such as managed reservoirs, the time-varying volume may be known and can be entered. Generally, for a stream with known time-varying discharge, it is preferable to use the Manning's equation to estimate the changing volume. We will change it from Keep Volume Constant to Use Mannings Equation.



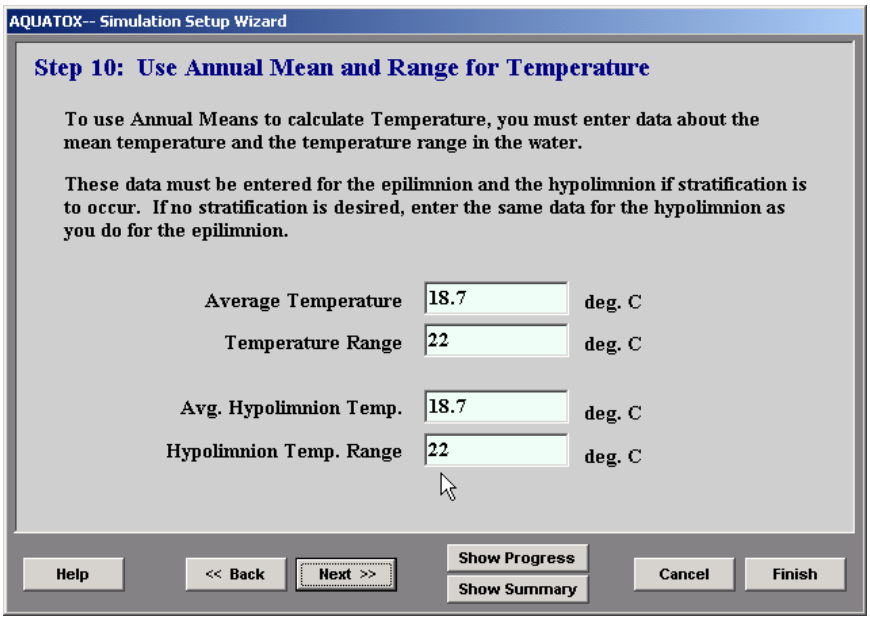
Having chosen to use the Manning's equation, it is necessary to enter dynamic outflow data. Click on the **Import** button for the **Use Dynamic Outflow** entry.



We will choose the file type as USGS Flow Data, and pick EFPCDischarge, which was downloaded earlier from the *http://waterdata.usgs.gov/nwis/discharge* site. Unfortunately, the USGS data can now be retrieved in several different formats, so you may have to copy and convert the pertinent data in a spreadsheet program rather than using the automatic conversion utility in AQUATOX. However, you should try to import it directly first. Click on **Import** to load the data and click on **Use Dynamic Outflow** to activate the dataset.

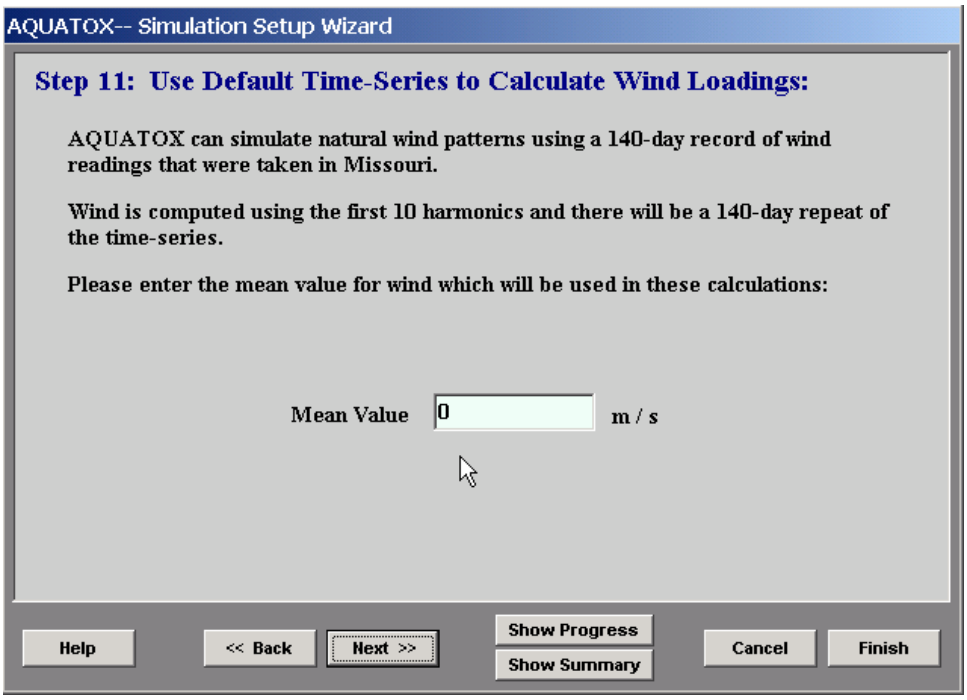


In Step 10 we have chosen to enter an average annual temperature and a range for a typical year. In order to maintain maximum flexibility, the model has separate fields for epilimnetic and hypolimnetic temperatures. Of course, these seldom apply to streams, so enter the same values in the corresponding fields.

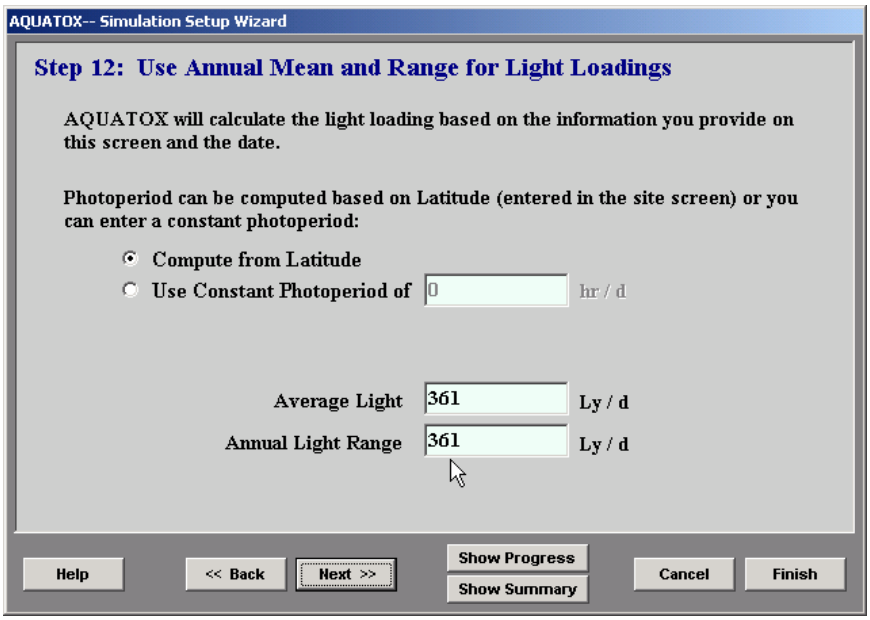


In Step 11 we can specify a constant wind, a time series of observed wind values, or a default time series. The model is insensitive to wind when simulating a small stream, although it can be important for standing water bodies. We have chosen to use a default time series. For many lakes and reservoirs a mean value of 3 m/s is appropriate, but for a sheltered stream a mean

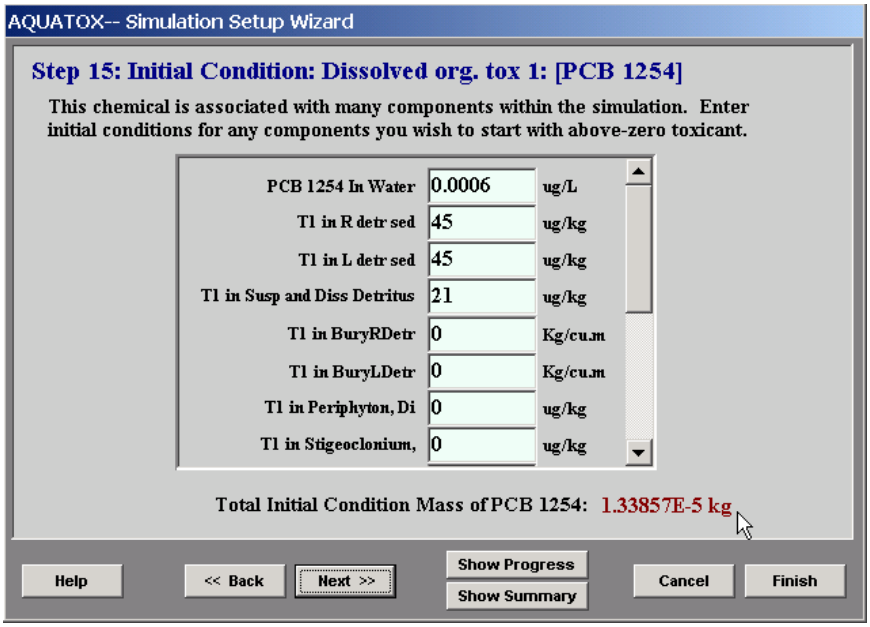
value of 0 represents the damping out of wind effects–note that with a mean of 0 there will still be wind roughly half the time.



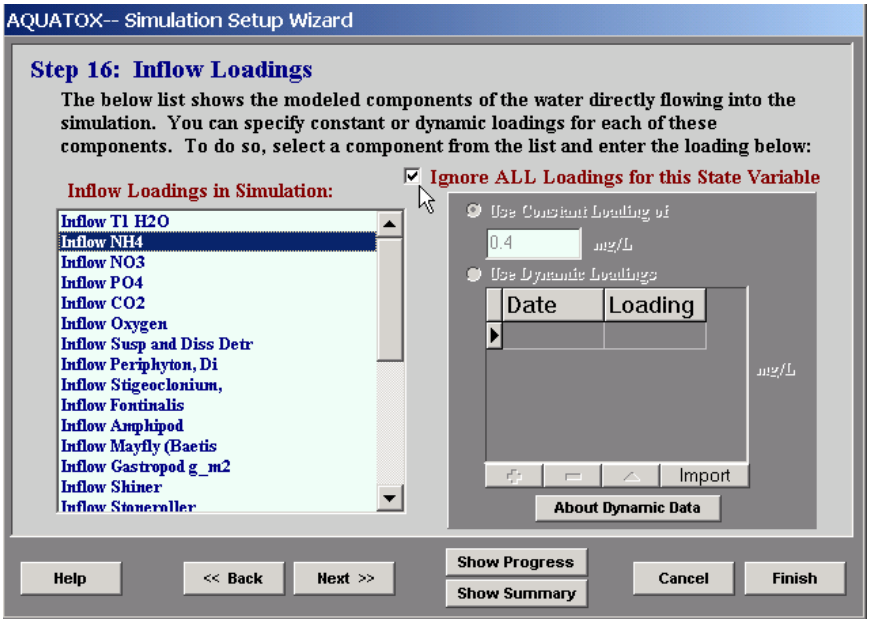
In Step 12 we will use an annual mean and range for light. These can be obtained from the Internet for any major town in the U.S. The user will have to decide if these are appropriate for the site being modeled or if they need to be adjusted, especially for shading from riparian vegetation. The adjustment can be made in the values entered here, or the user can enter a reduction factor in the light-loading screen.



The model is not sensitive to pH, so in this simulation we will use a constant pH of 8. In addition, because it is a small stream and we are lacking data, we will ignore inorganic sediments in the simulation. We have chosen to simulate PCB 1254, and observed values are entered in Step 15.

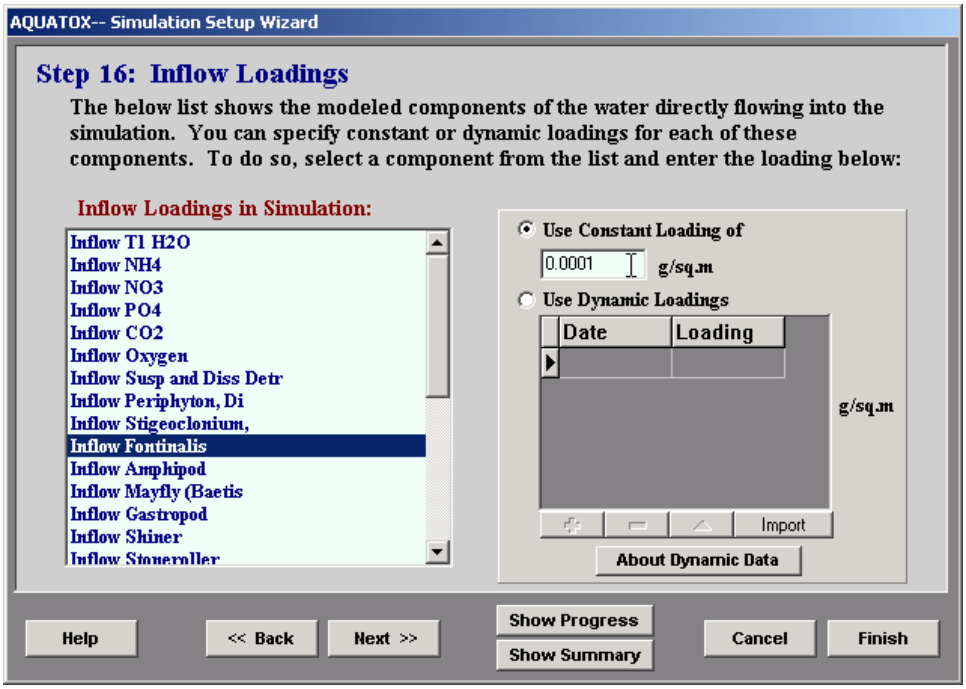


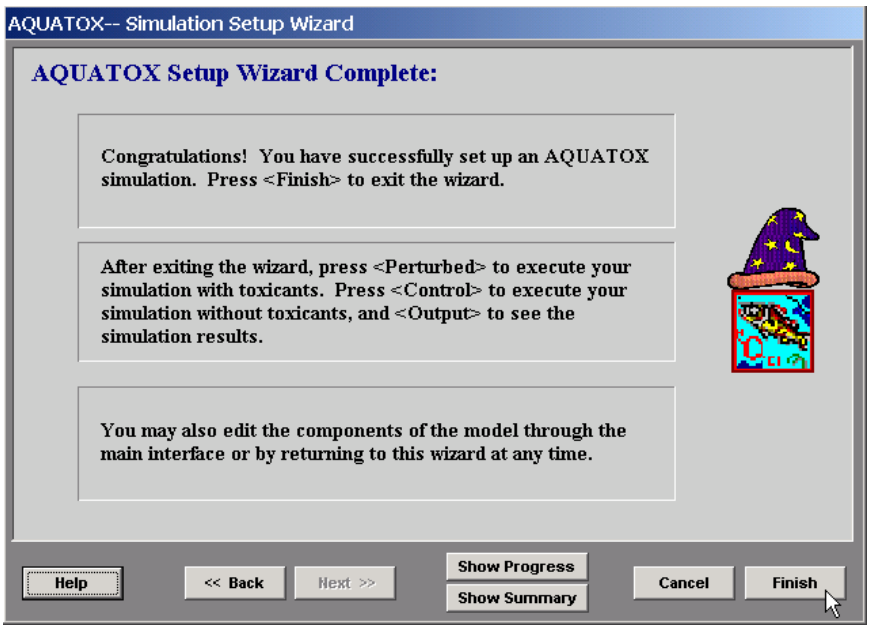
In Step 16, loadings associated with inflow can be reviewed and modified. Observed values are entered for nutrients, and constant values are used for carbon dioxide, oxygen, and detritus. For now, we'll leave the loading of the organic chemical as 0. Ammonia has **Ignore ALL Loadings for this State Variable** checked. That option is usually used for experimentation, such as sensitivity analysis, so uncheck it and check **Use Constant Loading of** (with a value of 0.4).



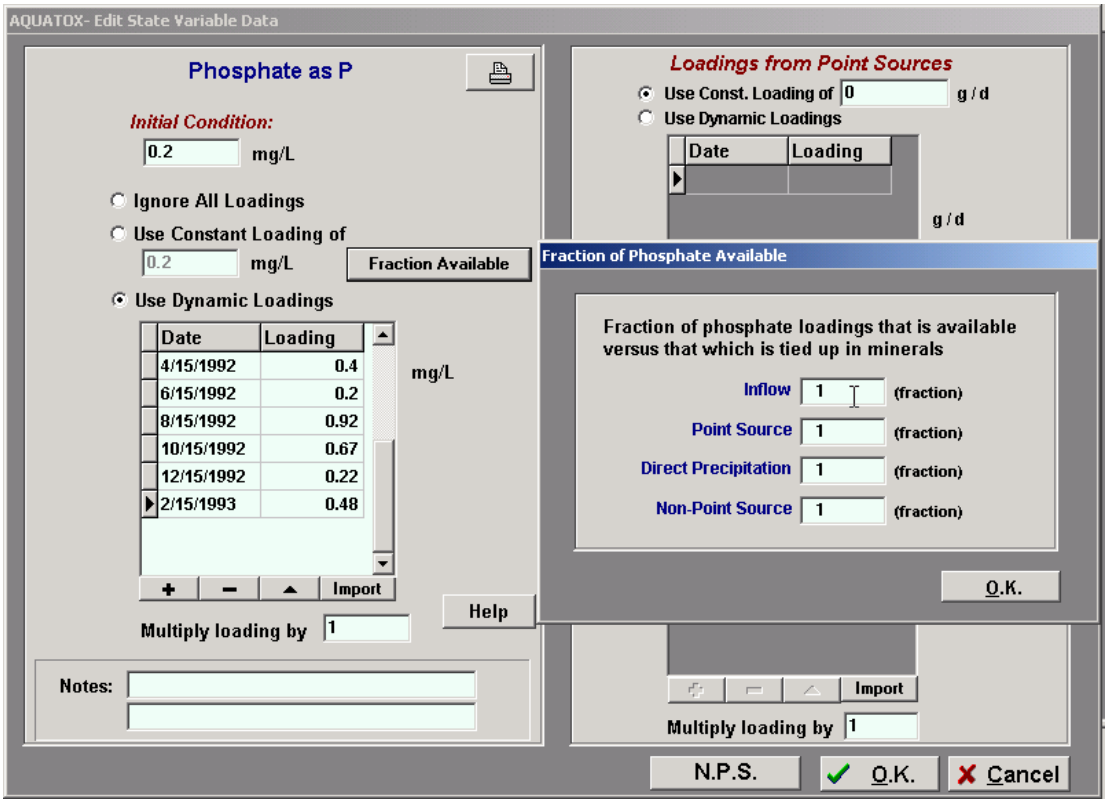
Loadings for periphyton and macrophyte groups can be considered as "seeds" to reestablish the group following scour, emergence, and toxic- and seasonal-induced mortality. The user is cautioned, though, to use a value of 0.00001 (1e-5) or less as a seed for periphyton, invertebrates, and fish; otherwise, the "loading" will dominate the rates during high-flow conditions. A value of 0.0001 is often appropriate for macrophytes because AQUATOX simulates (and most studies measure) above-ground biomass, which can be an order of magnitude greater than that of other organisms and can be replenished from rhizomes. However, this doesn't apply to moss, so we'll use a value of 0.00001 for *Fontinalis* as well.

In this example, there are no organic chemical loadings associated with any of the biota. Furthermore, there should be no loadings from direct precipitation, point- or nonpoint-sources. You should check them to make sure; and, if there are, change them to 0. (However, there are organic chemical loadings associated with detritus.) When you are finished with the review and modifications using the Wizard, click on **Finish** to save your modifications.

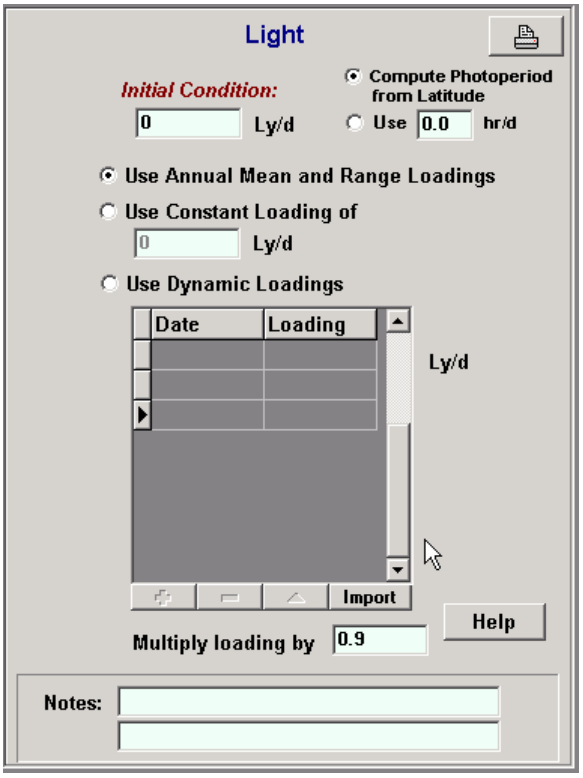




At any time, one can return to the Wizard; however, more editing functions are available by going directly to the state variables. By double-clicking on any variable listed on the right side of the main screen, a dialog screen can be pulled up. For example, one should review the loadings for phosphate and consider if the entire loading is available for utilization by algae. Click on **Fraction Available** to change the availability. In this example, we chose to accept the phosphate loadings as being entirely available.

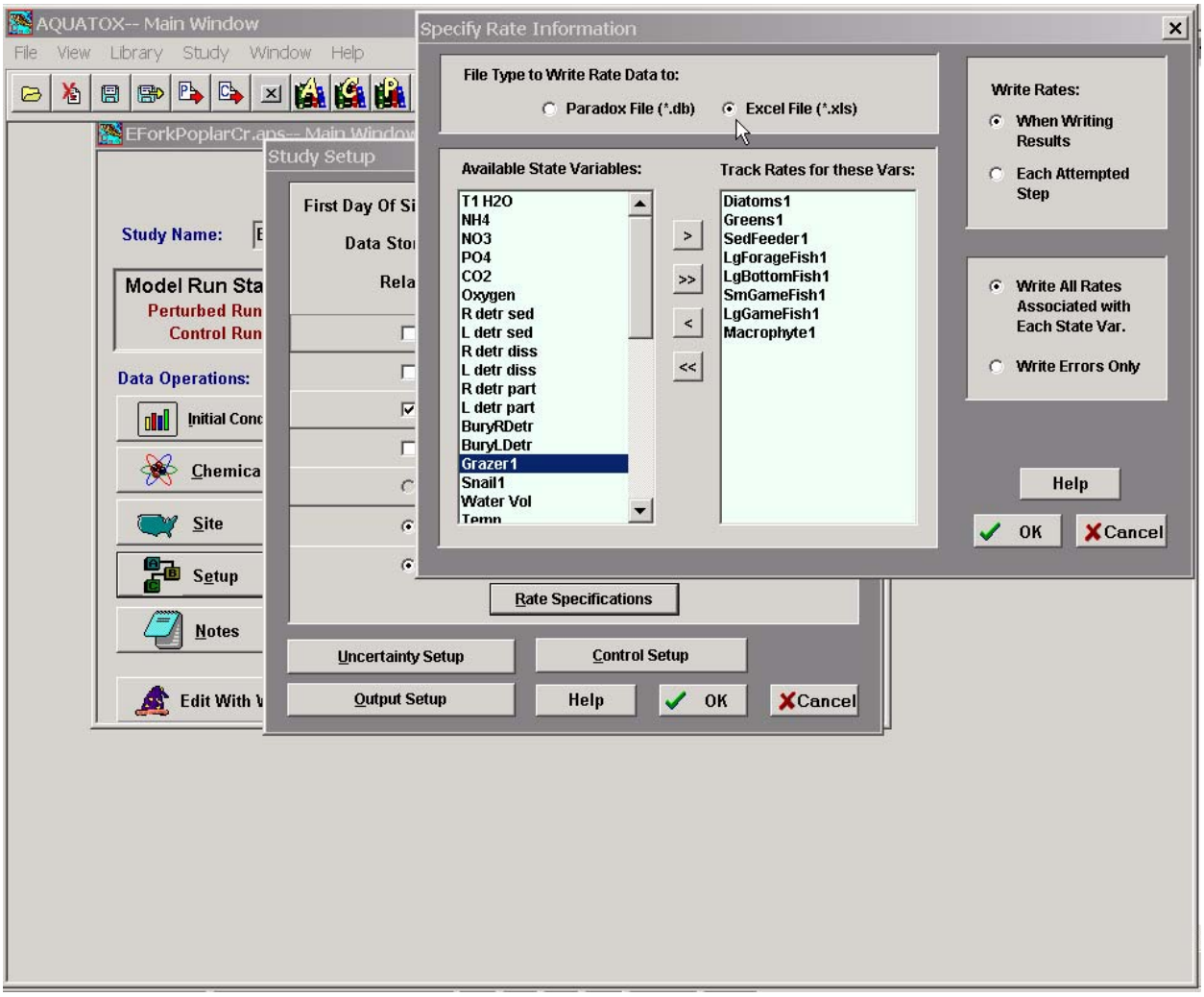


Double-clicking on **Light**, we adjust the multiplicative loading factor to 0.9 to account for nominal shading by riparian vegetation.

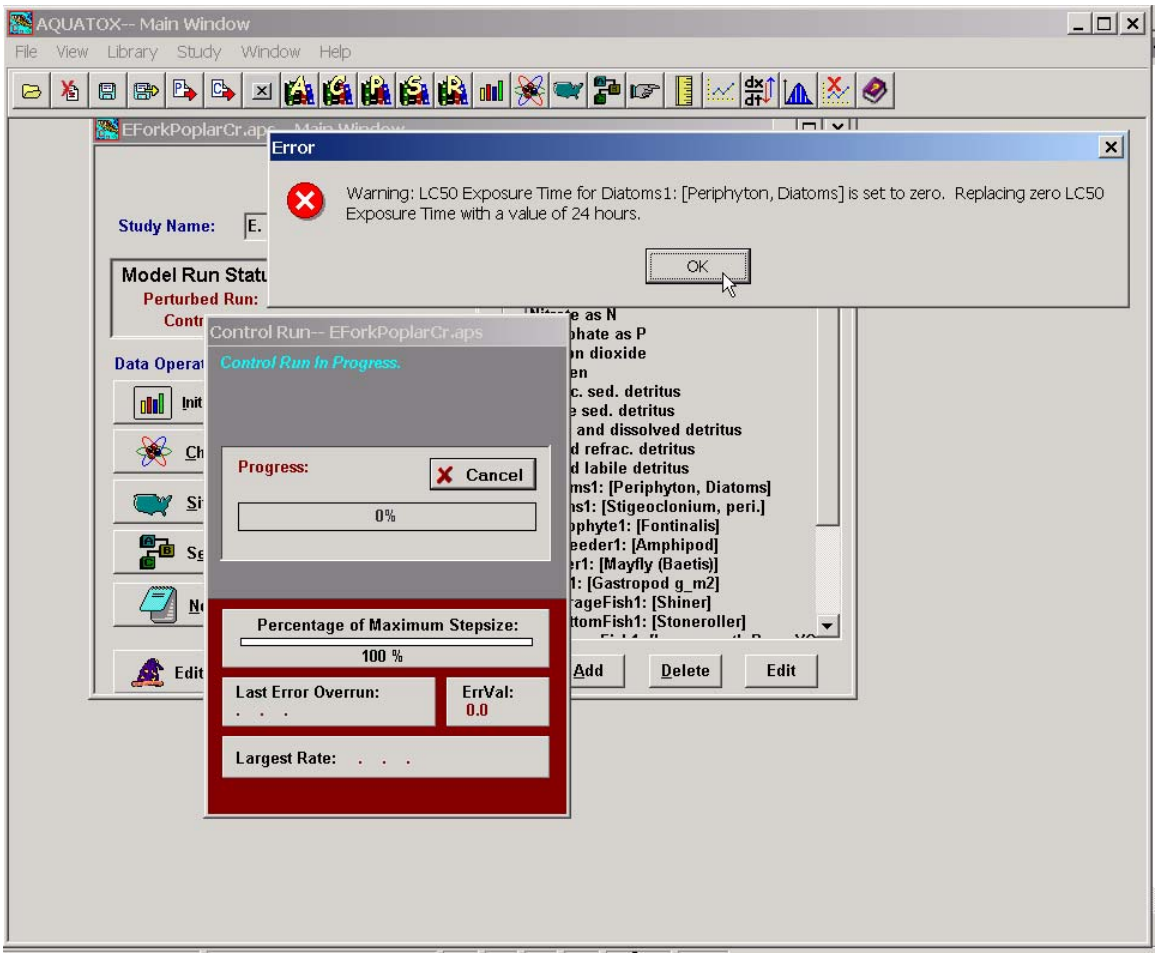


4.3 Ecosystem Calibration

Before modeling bioaccumulation, one should ensure that the ecosystem model is providing reasonable results; calibration may be necessary. (By using old parameter files, we will ensure that calibration is necessary for purposes of the tutorial.) First, let's save the study, keeping the name we gave it at the beginning: **EForkPoplarCr.aps**. Rate files are named after the study file name, so it is advisable to save the study under the desired name before running a simulation. To save the rates, click on **Setup** and **Save Biologic Rates**. Click on **Rate Specifications** to choose which variables to save (you may wish to choose all biota); also, click on **Excel File (*.xls)** unless you really want to use Paradox or Quattro.

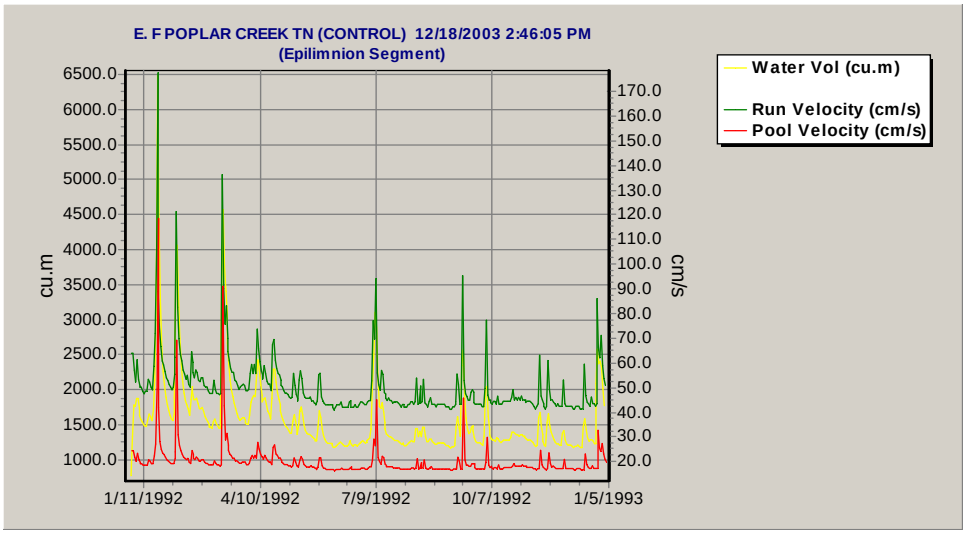


Clicking on **Control** we start the simulation. With this study, a series of warning screens will appear, cautioning that no *LC50* exposure time has been set for the algae; click on **OK** to accept a default time of 24 h. (It's a good idea, after the simulation has finished to go to the toxicity screen and specify *LC50* exposure times so the messages won't continue to appear.) Having chosen **Show Integration Info** in the **Setup** screen, we can see what process is responsible for slowing down the simulation. We also can see when periphyton sloughing is occurring.



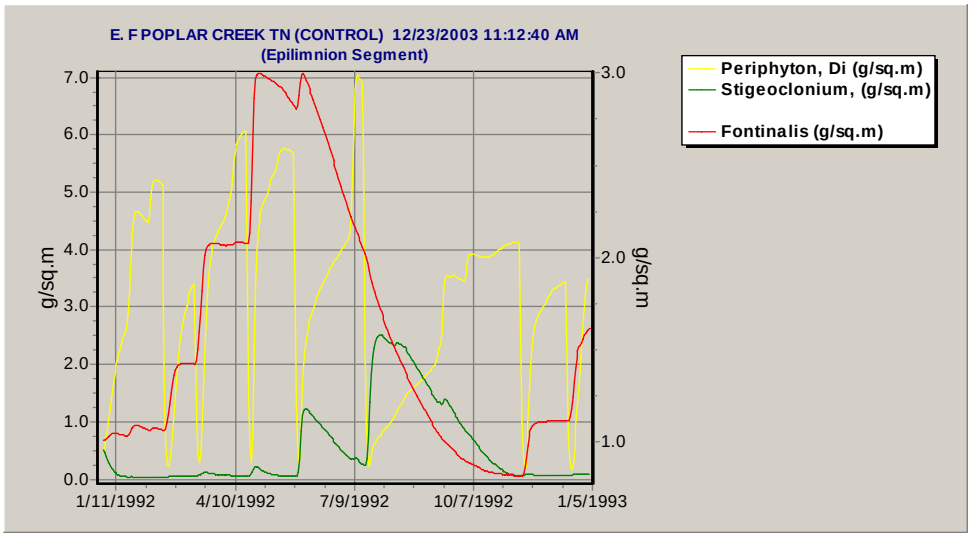
Hydrodynamics

First, the predicted volumes and velocities should be checked against known or expected values. If the values seem to be erroneous then the site characteristics and discharge driving variables should be examined. In this example, velocities range from 14 to 170 cm/s and volumes from 1000 to 6500 m^3, which are acceptable in the absence of actual site data.

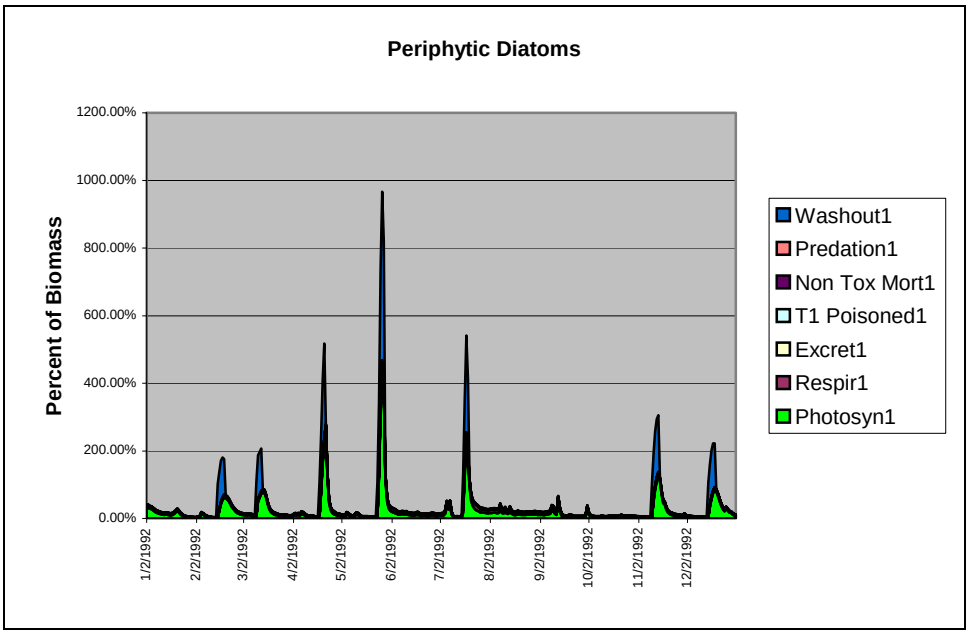


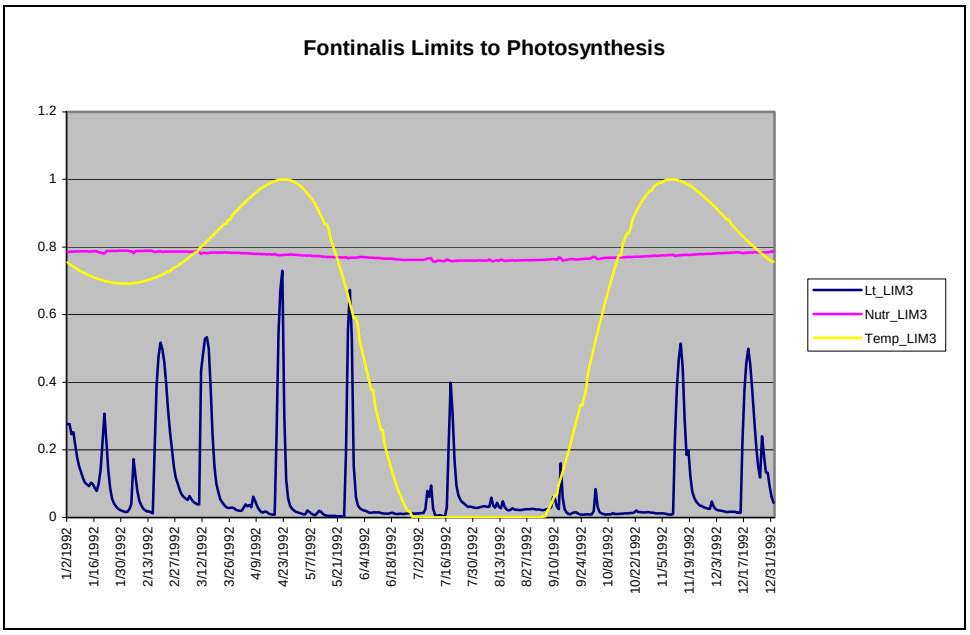
Biomass

Examining the predicted plant biomass, the combined periphyton vary between 0.1 and 6 g/m^2 and are dominated by periphytic diatoms; these values are reasonable for a shallow-water stream. The moss *Fontinalis* fluctuates from an initial condition of 1 to 3 to 0.8 g/m^2, which also is reasonable.

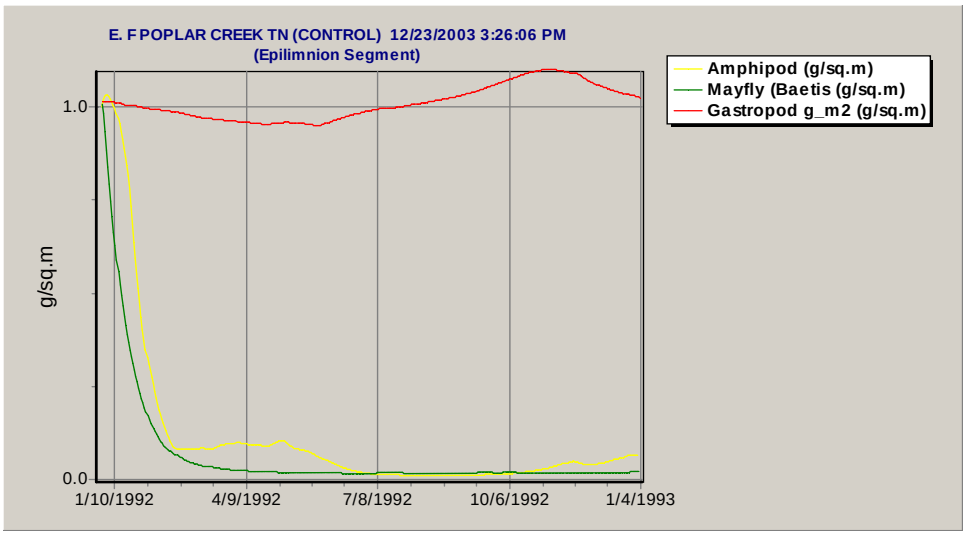


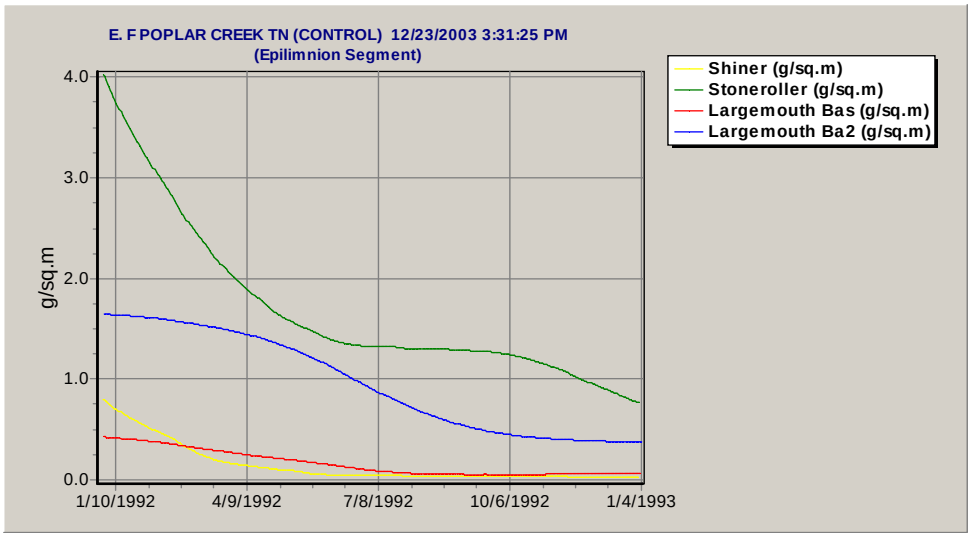
Having saved the rates, we will find the Excel file in the Output directory, and it is labeled with the study name preceded by "**C_**" because it is the control run. The rates are saved as percentages of biomass on each day, and we have chosen to plot them as areagraphs. We can see that the periphytic diatom rates indicate seven sloughing events, corresponding to the sudden drop in biomass in the previous plot. The sloughing removes the light limitation on the *Fontinalis* (shown by plotting the limitations to photosynthesis) and leads to a rapid increase in biomass of that group. The decline in *Fontinalis* in the summer is seen to be caused by the severe limitation by high temperatures.





When we plot the invertebrates and fish we find that gastropods maintain a biomass of about 1 g/m^2 while the other invertebrates decline rapidly in biomass after the initial conditions. Stonerollers, which feed on periphyton and *Fontinalis*, decline to 0.75 g/m^2. The adult bass ("Largemouth Ba2") decline to 0.3 g/m^2; and shiners decline almost to 0. Clearly, the animal initial conditions and dynamics should be calibrated, and we can expect that the periphyton dynamics will be affected. We will set the initial condition for stonerollers to 0.75 and for adult bass to 0.3 g/m^2.





Looking at the trophic interactions matrix for adult bass, we see that they have a 0 preference factor for stonerollers. This is incorrect, and should be changed to a value comparable to that for shiners (0.05). In addition, there are no sunfish in the simulation, so we will set the preference by bass for gastropods to 0.05 to account for predation pressure on gastropods. At the same time, we should set the egestion parameter for gastropods to 0.158 and correct the egestion parameters for shiners and bass to 0.05 (based on literature values). Furthermore, we will adjust the initial conditions, using the previously noted ending values, except for shiners.

Trophic Interactions of Largemouth Bass, Lg:

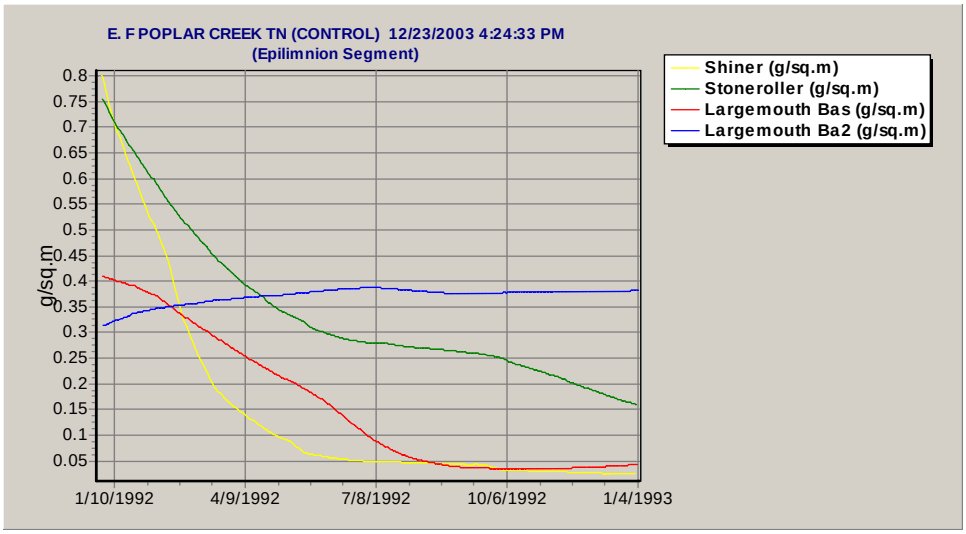
	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	0	
L detr sed	0	0	
R detr part	0	0	
L detr part	0	0	
Periphyton, Di	0	0	
Stigeoclonium,	0	0	
Fontinalis	0	0	
Amphipod	0.001	0.158	Johnson and Dropkin, 1995
Mayfly (Baetis	0.041	0.158	Johnson and Dropkin, 1995
Gastropod g_m2	0	0	
Shiner	0.05	0.158	Johnson and Dropkin, 1995
Stoneroller	0	0.05	
Largemouth Bas	0.039	0.158	Johnson and Dropkin, 1995
Largemouth Ba2	0.039	0.158	Johnson and Dropkin, 1995

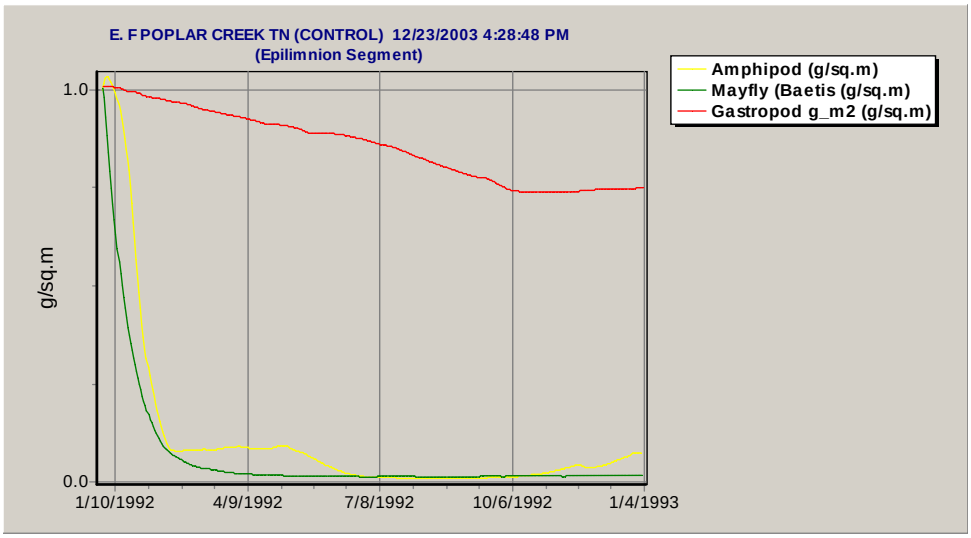
AQUATOX-- Trophic Interactions

Trophic Interactions of Largemouth Bass, Lg:

	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	0	
L detr sed	0	0	
R detr part	0	0	
L detr part	0	0	
Periphyton, Di	0	0	
Stigeoclonium,	0	0	
Fontinalis	0	0	
Amphipod	0.001	0.158	Johnson and Dropkin, 1995
Mayfly (Baetis	0.041	0.158	Johnson and Dropkin, 1995
Gastropod g_m2	0.05	0.158	
Shiner	0.05	0.05	Johnson and Dropkin, 1995
Stoneroller	0.05	0.05	
Largemouth Bas	0.039	0.05	Johnson and Dropkin, 1995
Largemouth Ba2	0.039	0.05	Johnson and Dropkin, 1995

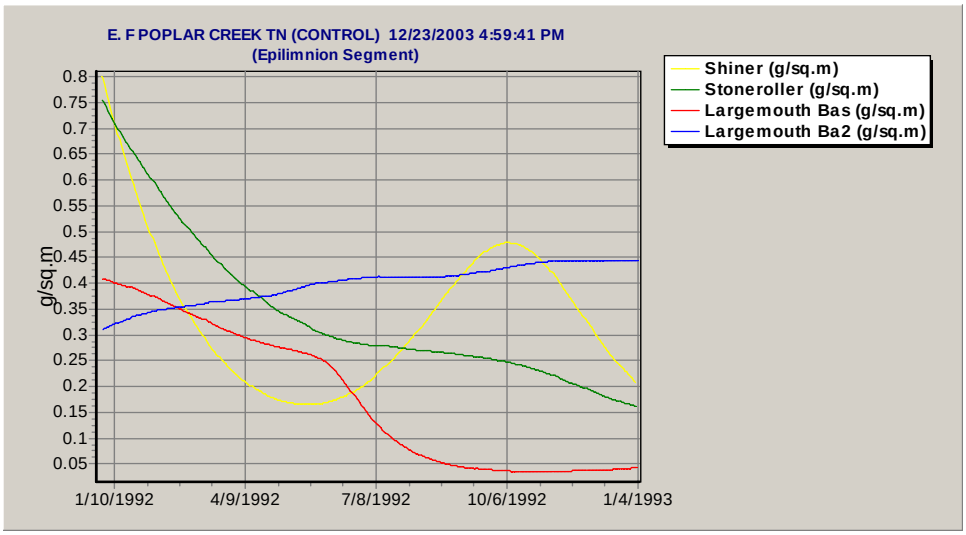
Now we find that the bass are stable at 0.35 g/m^2, with a continued decrease in other fish. Given the increased predation, gastropods decline to 0.75 g/m^2. Shiners continue to decline precipitously, although observed data indicate that they are common. Examining their preference matrix, we find that there is no preference for periphytic diatoms or labile detritus and that egestion is set at 0.6. The values are changed as pictured. The other problematic pattern is that of mayflies, which decline exponentially and do not recover; let's return to them after calibrating the fish.

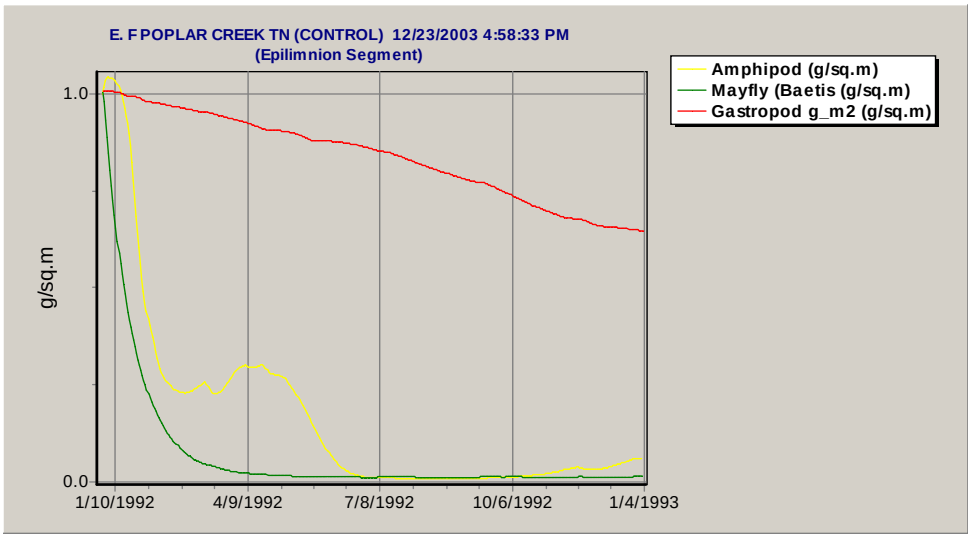


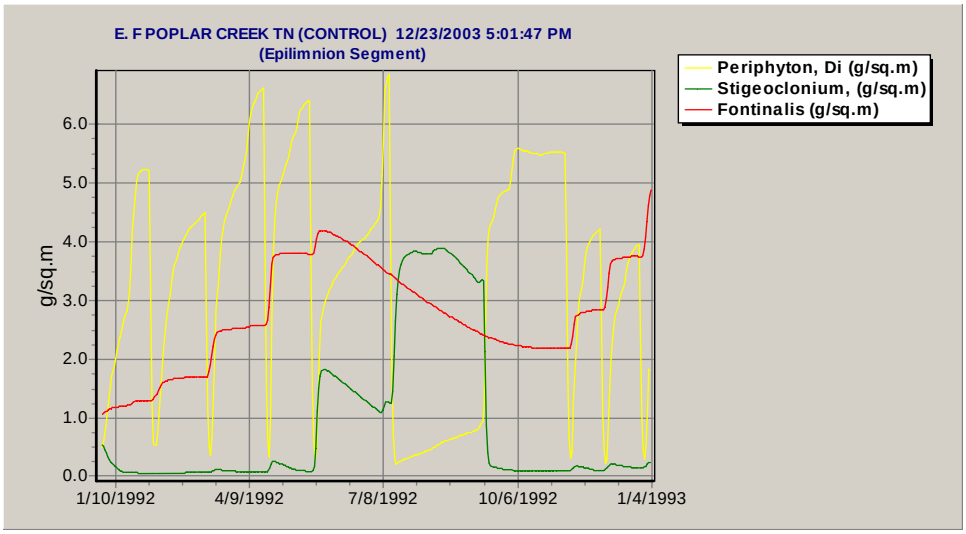


	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	1	
L detr sed	0	0	
R detr part	0	1	
L detr part	0.1	0.8	
Periphyton, Di	0.35	0.3	phyto, Hill & Napolitano, 1997, p. 451, C
Stigeoclonium,	0.35	0.3	"
Fontinalis	0	0	
Amphipod	0.1	0.158	Leidy & Jenkins 77, Kitchell et al., 1977
Mayfly (Baetis	0.1	0.158	
Gastropod	0	0	
Shiner	0	0	
Stoneroller	0	0	
Largemouth Bas	0	0	
Largemouth Ba2	0	0	

With the changes, shiners now exhibit a realistic seasonal fluctuation in biomass—in part, at the expense of the gastropods, which decline to 0.64 g/m^2. Grazing by shiners also removes competition and favors *Stigeoclonum* for part of the year. Turning our attention to mayflies, we see from a rate plot that defecation is almost equal to consumption, and drift is a continuous loss of 4%.







The bass young-of-the year (YOY) should not decline, considering that the adults are stable. Examining the trophic interaction matrix, we see that they are not parameterized to feed on mayflies and the egestion factors are too high. We change the YOY preference and egestion parameters to the values shown in the figure below.

AQUATOX-- Initial Conditions Entry Screen

Trophic Interactions of Largemouth Bass, YOY:

	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	0	
L detr sed	0	0	
R detr part	0.01	1	Leidy & Jenkins '77
L detr part	0.01	0.3	Leidy & Jenkins '77
Periphyton, Di	0	0	
Stigeoclonium,	0	0	
Fontinalis	0	0	
Amphipod	0.19	0.158	Leidy & Jenkins '77, Kitchell et al., '77
Mayfly (Baetis	0.19	0.158	
Gastropod g_m2	0	0	
Shiner	0	0.05	YOY
Stoneroller	0	0.05	YOY
Largemouth Bas	0	0.05	no cannabalism in YOY
Largemouth Ba2	0	0	

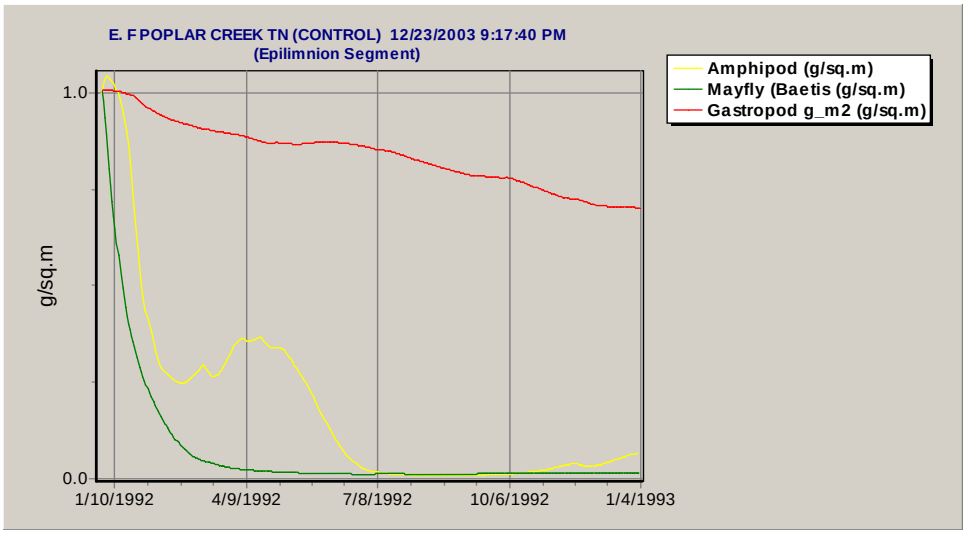
Turning our attention to mayflies, we suspect that, here again, the preference matrix is responsible for the poor simulation. The preference of mayflies for periphytic diatoms should be the same as for *Stigeoclonum*, there should be no preference for refractory detritus, and the egestion factor for periphyton should be set to 0.3 as in the other consumers.

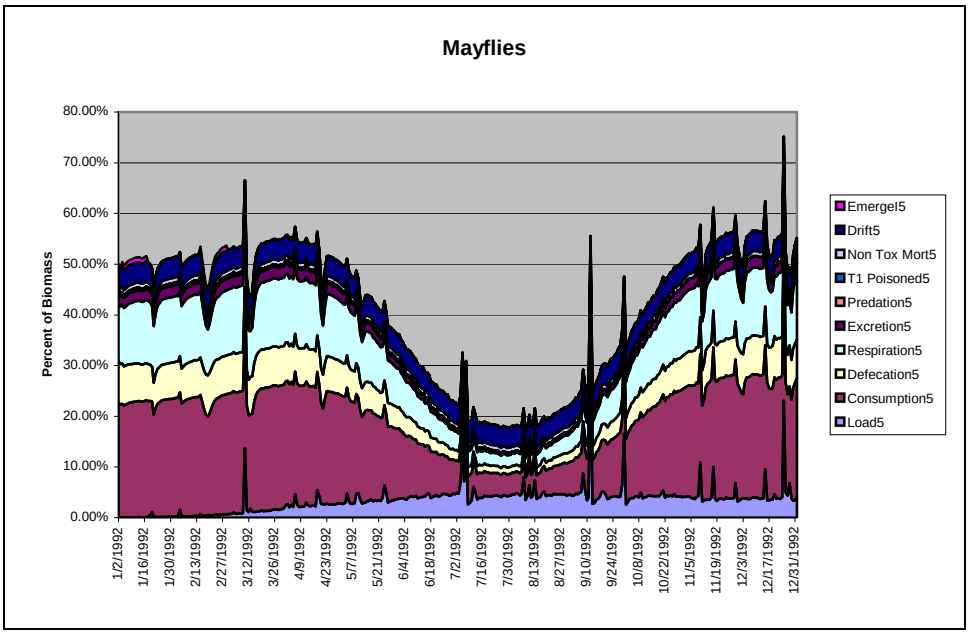
AQUATOX-- Initial Conditions Entry Screen

Trophic Interactions of Mayfly (Baetis):

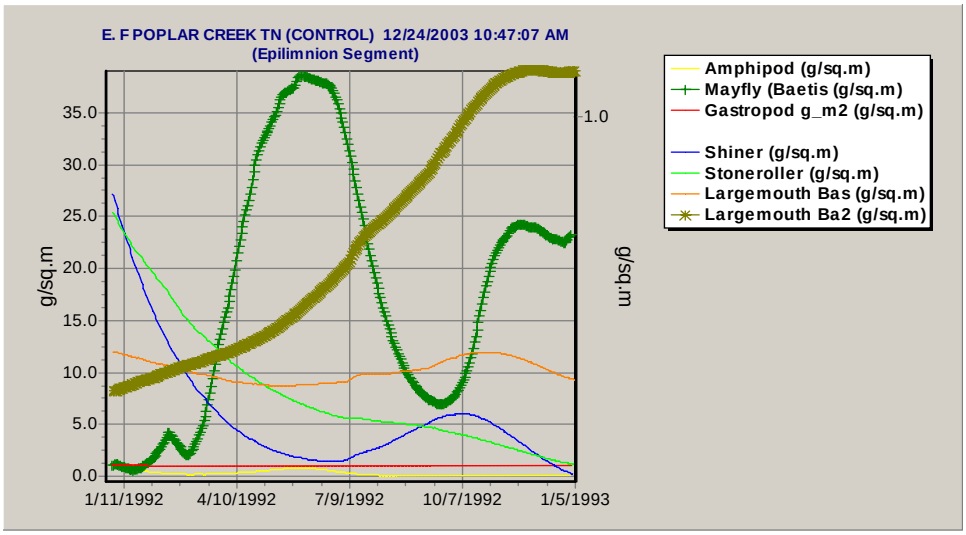
	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	1	
L detr sed	0.1	0.5	
R detr part	0	0	
L detr part	0	0	
Periphyton, Di	0.4	0.3	
Stigeoclonium,	0.4	0.3	pref. generally accepted, assim: L&P C
Fontinalis	0	0	
Amphipod	0	0	
Mayfly (Baetis	0	0	
Gastropod g_m2	0	0	
Shiner	0	0	
Stoneroller	0	0	
Largemouth Bas	0	0	
Largemouth Ba2	0	0	

Interestingly, the mayflies still decline to almost to 0. When we plot the rates, we find that respiration accounts for much of the loss. (The rates have spikes during storm events because the loading or "seed" is set too high.) Examination of the parameter file reveals that specific dynamic action (which is a fraction of the consumed food) is set at 0.8, although the literature value is 0.15. We set it to the proper value and re-run the simulation.



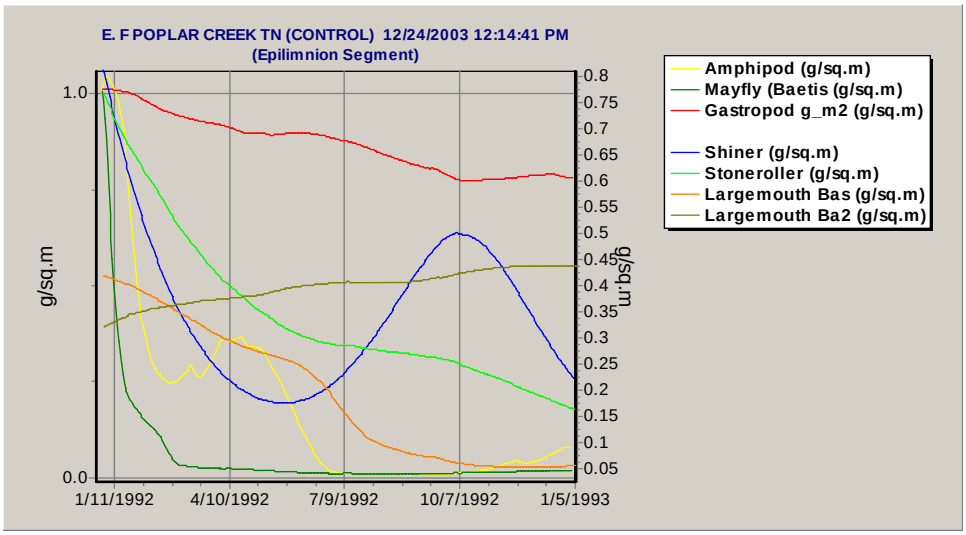


Mayflies are now an important component in the simulation—perhaps too important. Furthermore, bass increase significantly, probably because of the increased secondary productivity through the mayflies.



With shiners parameterized to eat mayflies, we would expect mayflies to decline and shiners to increase, but that is not the case. Examining the mayfly parameter file, we will cut the maximum consumption rate from 0.5 to 0.25 g/g d, set the minimum prey for feeding to 0.1 g/m^2, set respiration rate to 0.05 /d, change the mortality coefficient from 0.01 to 0.05 /d, and specify that there is a 75% preference for riffles. (These were obtained by calibration at another site, so we will use them here to speed up the process.) We will ignore the steep decline in the stonerollers because it may reflect competition from the mayflies. The decline in shiners is puzzling, but we will wait to address it further.

Plotting the results, we see that mayflies now slowly decline and disappear. On the other hand, shiners exhibit a stable fluctuation and stonerollers do not decline as much as previously, indicating that, indeed, competition from mayflies is important. However, we know that mayflies are important at the site, so we will set the maximum consumption rate for mayflies back to 0.5 g/g d.



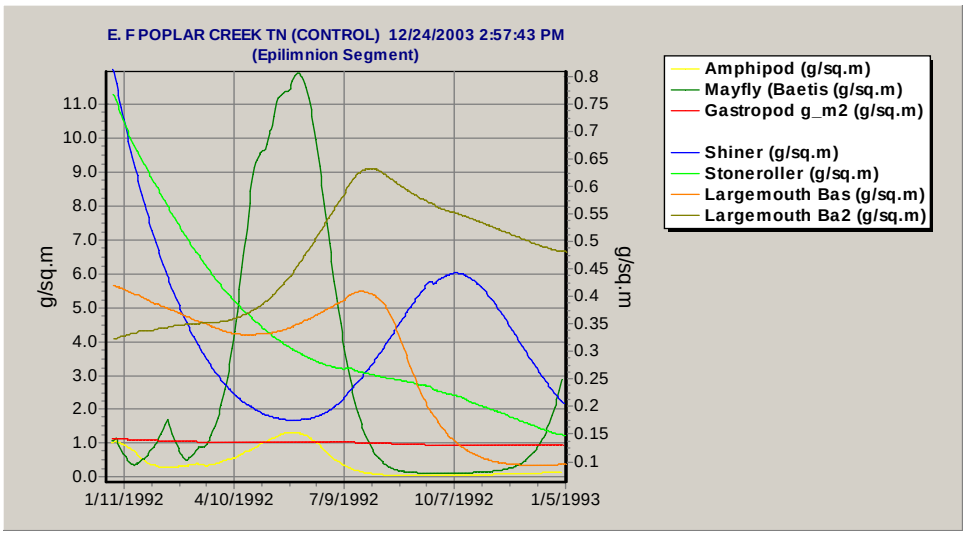
With the change in the maximum consumption rate (*CMax*), mayflies reach a predicted maximum biomass of 15 g/m^2, and the shiners reach a slightly lower equilibrium. Obviously, *CMax* is a sensitive parameter. We could run sensitivity analysis to suggest an optimal value that would constrain the mayflies and permit the other grazers to coexist. However, in the interest of time, we will split the difference in the values, changing *CMax* for mayflies from 0.5 to 0.45 g/g d. Bass reach an end value of 0.54 g/m^2, which seems high. Intrinsic mortality often is site-specific because of factors that are not simulated adequately, such as fishing pressure. To hold the bass at approximately the initial condition, we calculate that we need to increase the mortality rate by 1.6e-3 /d; we will increase the mortality factor by that amount (from 0.0004 to 0.002 /d).

Calculating Rate of Change

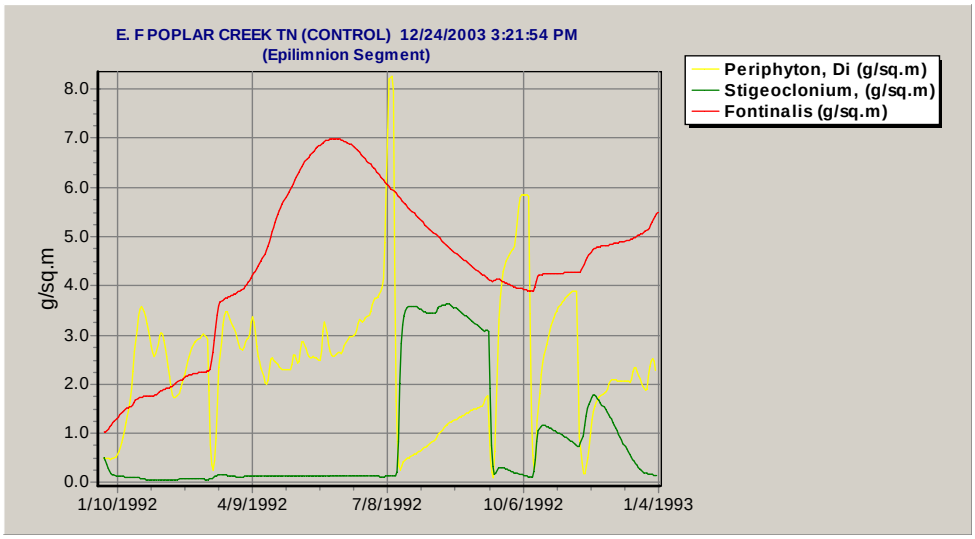
To calculate the increased mortality required to offset the increase in biomass of bass, we observe that the initial biomass is 0.3 g/m^2 and the end value is 0.54 365 days later:

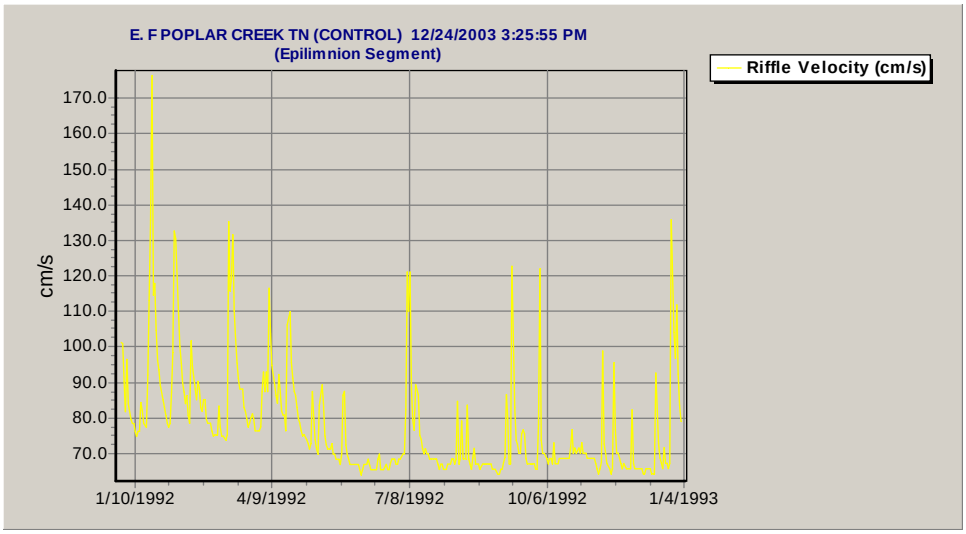
$$rate\ of\ increase \quad = \quad \ln\left(\frac{0.54}{0.3}\right)/365 \quad = \quad 1.6e-3/d$$

With the change in maximum consumption in mayflies, the animals now exhibit a reasonable pattern, except for stonerollers, which decline to 0.13 g/m^2. However, stonerollers are usually not an important component of stream ecosystems, so we will reserve judgment until obtaining a longer simulation.



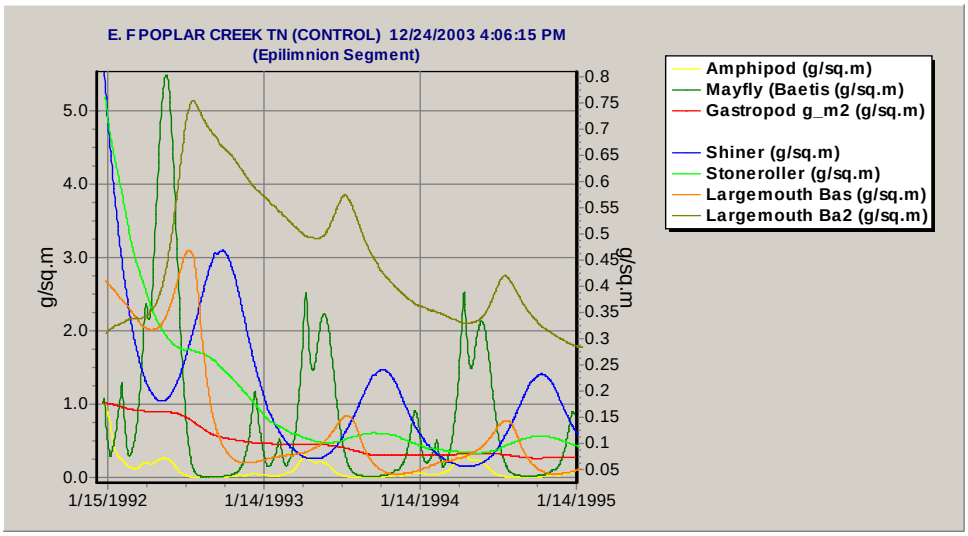
A plot of the plants shows that they are still providing a reasonable predicted pattern of algal succession although the moss is increasing because of increased grazing on periphyton and removal of light limitation. The problem with *Fontinalis* is that the biomass will continue to build from one year to the next. There is predicted mortality during the summer months when the temperature is too high, but the moss is not being set back to some nominal level. One way to reset the biomass is to parameterize breakage to occur during the maximum discharge event each year. Plotting velocity, we see that the maximum riffle velocity is about 176 cm/s, so we will use 170 as the *VelMax* value instead of 500 cm/s. This is a site-specific solution, but both breakage and scour can be expected to vary from one site to another.

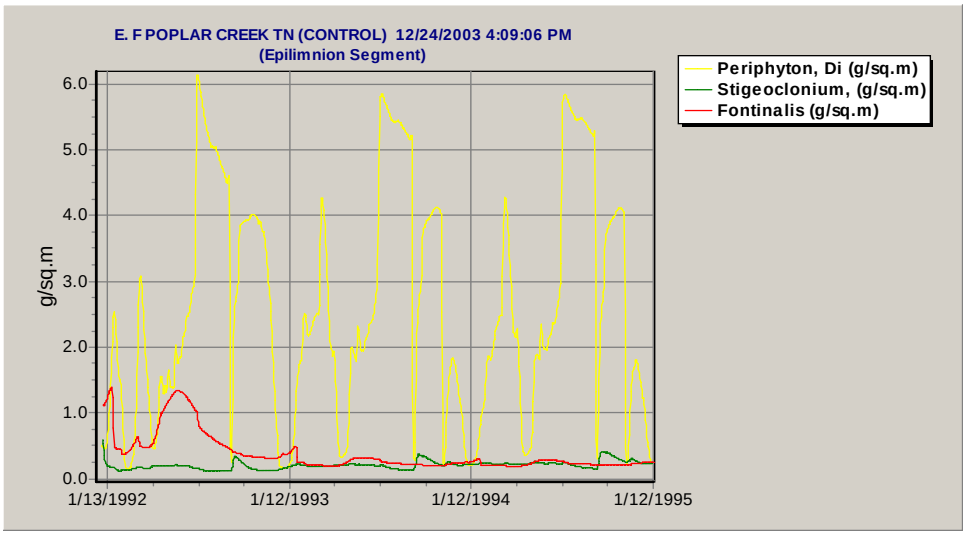




At this time, we need to run the simulation for a longer period to confirm that there is a stable, repeating pattern of biomass for the various groups. We will want to run the model for at least three years to simulate PCB accumulation, so let's use that period for the control as well. We enter **Setup** and change the end date to 12/31/1994.

A three-year simulation indicates that we have an issue with transient conditions for both animals and plants in the first year. That is almost certainly because the initial conditions are inappropriate. The remedy is to set the initial conditions to the end conditions predicted after three years. The best way to obtain the end conditions is to click on the **Control Simulation** tab in Output, click on **Change Variables**, and select the biotic state variables. Then you can scroll to the bottom of the table to see the end values. The quickest way to enter initial conditions is through the Wizard. Double-click on **Step 5** and click on **Next** until the initial condition screen for plants appears. Change the values and then click on **Next** again until you get the initial condition screen for invertebrates. Repeat the process for fish. Finally, click on **Finish** to leave the Wizard and save the changes. As a check, you can click on the **Initial Conds.** button to display all the initial conditions.



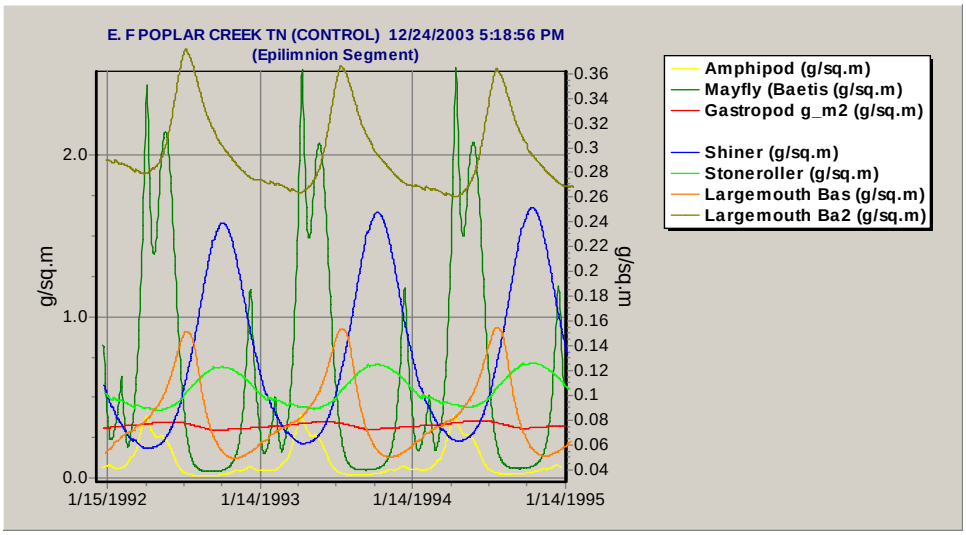


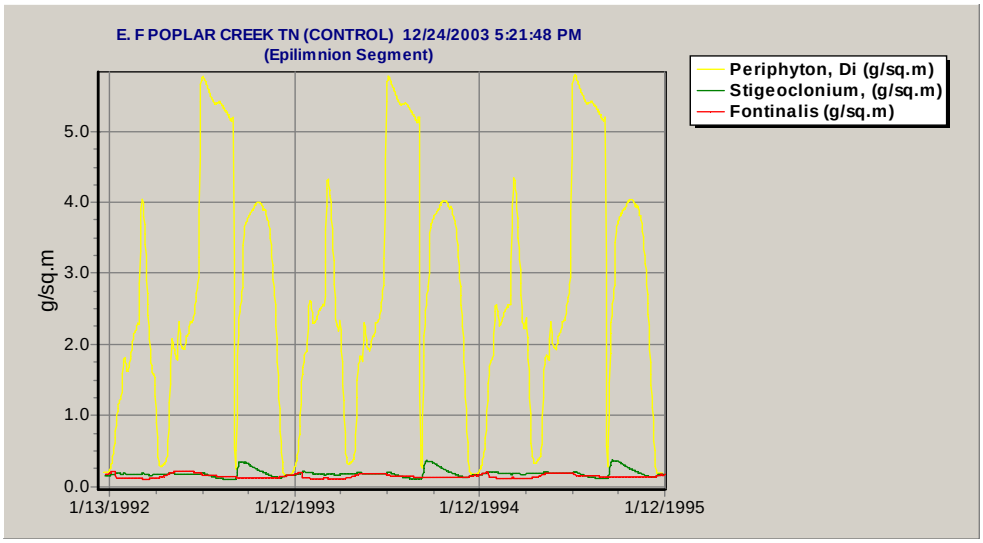
AQUATOX-- Initial Conditions Entry Screen

State Variables' Initial Conditions:

	Init. Cond.	Units	Tox1 I. C.	Tox1 Units
T1 H2O	0.0006	ug/L		
NH4	0.4	mg/L		
NO3	0.3	mg/L		
PO4	0.2	mg/L		
CO2	0.7	mg/L		
Oxygen	8	mg/L		
R detr sed	4	g/sq.m	45	ug/kg
L detr sed	2	g/sq.m	45	ug/kg
R detr diss	3.325	mg/L	21	ug/kg
L detr diss	3.325	mg/L	21	ug/kg
R detr part	1.425	mg/L	21	ug/kg
L detr part	1.425	mg/L	21	ug/kg
BuryRDetr	2	Kg/cu.m	0	Kg/cu.m
BuryLDetr	2	Kg/cu.m	0	Kg/cu.m
Periphyton, Di	0.2	g/sq.m	0	ug/kg
Stigeoclonium,	0.1	g/sq.m	0	ug/kg
Fontinalis	0.1	g/sq.m	0	ug/kg
Amphipod	0.06	g/sq.m	0	ug/kg
Mayfly (Baetis	0.8	g/sq.m	0	ug/kg
Gastropod g_m2	0.26	g/sq.m	0	ug/kg
Shiner	0.1	g/sq.m	0	ug/kg
Stoneroller	0.09	g/sq.m	0	ug/kg
Largemouth Bas	0.04	g/sq.m	0	ug/kg
Largemouth Ba2	0.27	g/sq.m	0	ug/kg
Water Vol	773.5	cu.m		
Temp	0	deg. C		
Wind	0	m/s		
Light	0	Ly/d		
pH	8	pH		

With the changes in initial conditions, we have a reasonably stable simulation with seasonal fluctuations of all state variables over the course of three years. The biomass patterns are repeated because constant loadings of nutrients and only 1½ years of discharge data are used. We will consider that to be a calibrated ecosystem simulation, and save it as **EForkPoplarCr3.aps**. (You may wish to use the file provided instead--your results may differ.)





4.4 PCB Calibration

Now we need to run the perturbed simulation to represent the bioaccumulation of PCBs at Station 3 on East Fork Poplar Creek (**EForkPoplarCr3.aps**). Unfortunately, we have sparse data for comparison to the simulations. Based on conversions of data given in Moore et al. (1999), we expect the concentration of PCBs in periphyton to be about 40 ug/kg (wet). Unpublished data of SAIC (1998) indicate that the concentrations of PCB 1254 in fish are 66 +/- 36 ug/kg (wet); if those are based on fillets, as Moore et al. (1999) suggest, then those convert to about 150 +/- 84 ug/kg (wet). The concentrations of PCB 1254 in whole sediments are based on observed data (SAIC, 1998, unpublished data), but there is no information on what fraction was organic matter, so the data are not useful. The concentrations in dissolved phase in the water are below detection limits (1 to 1.3 ug/L). We will use the value of 0.0006 ug/L estimated by Moore et al. (1999) as a starting point; make sure that value is entered as both an initial condition and as an inflow loading.

Given the available data, our objective is to calibrate the water concentration of PCB 1254 so that the simulations are consistent with the observed concentrations in biota. If we can obtain consistent results, then we could decrease the loadings to predict long-term recovery.

Looking at the toxicity records, we find that there are no toxicity values for PCB Aroclor 1254.

Plant Toxicity Data | Add a Plant Toxicity Record | Print

Plant name	EC50 photo (ug/L)	EC50 exp. time (h)	EC50 dislodge (ug/L)	EC50 comment
Greens	0	0	0	Hill & Napolitano, 1997, p. 451
Diatoms	0	0	0	Hill & Napolitano, 1997, p. 451
Bluegreens	0	0	0	
Macrophytes	0	0	0	

A quick check of US EPA's ECOTOX database shows that there are *EC50* values for algal mats. We will use an *EC50* of 50 ug/L for the two groups of periphytic algal.

Search Results - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Your Report for Aquatic Data is Ready! Click Here!

Record Count : 4

ECOTOX:Ecotoxicology Database
USEPA/ORD/NHEERL
Mid-Continent Ecology Division

Contact: T:218-529-5225 F:218-529-5003
E-mail: ecotox.support@epa.gov
It is recommended that users consult the original scientific paper to ensure an understanding of the context of the data retrieved from the ECOTOX database.

Report Generated: Wed Dec 24 17:09:56 2003

Aquatic records found: 4

Page 1 of 3

1 2 3 Next >>

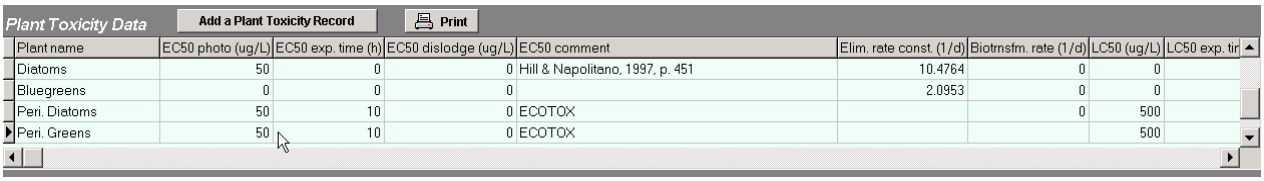
Laboratory Data Field Study Data References

NR = Not Reported

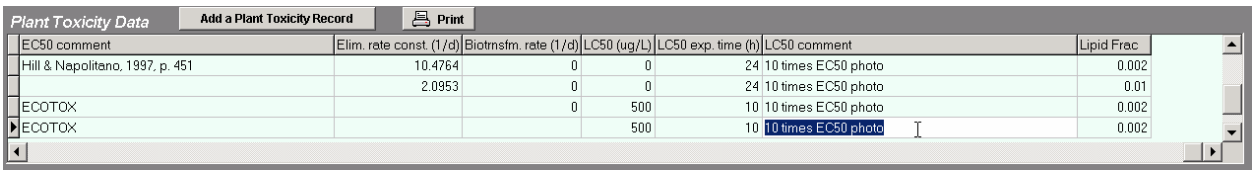
Scientific name, Common name	Endpoint	Effect	Effect Measurement	Trend --- Effect %	Media Type	Duration --- Exp Typ	Conc (ug/L)	Signif --- Level	Response Site --- BCF	Ref #
Test Loc: LAB										
CAS #/Chemical: 11097691, Aroclor 1254										
Algae Algae, algal mat	EC50	PHY	PSYN	---	SW	8 - 10 h --- S	F 65		---	8926
Algae Algae, algal mat	EC50	PHY	PSYN	---	SW	8 - 10 h --- S	F 50		---	8926
Algae Algae, algal mat	NR-LETH	MOR	MORT	--- 100	SW	6 d --- F	F 10		---	2227

Page 1 of 3

In the toxicity screen click on **Add a Plant Toxicity Record** and enter the two algal groups as shown below, keeping in mind that you probably added an LC50 exposure time earlier for the other groups to avoid the repetitive warning message. You have to provide the EC50, an estimate of the LC50, and the lipid fraction; leave the elimination constants blank: the program will provide estimates for them.

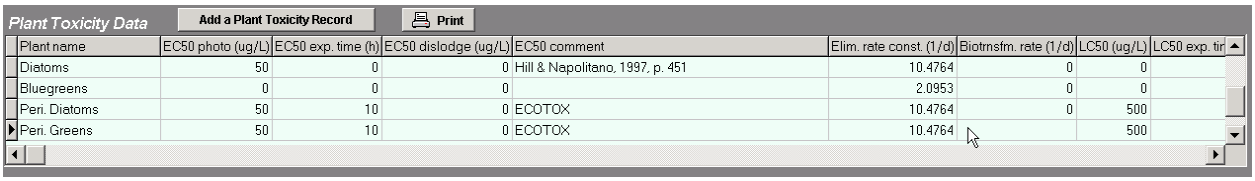


Plant name	EC50 photo (ug/L)	EC50 exp. time (h)	EC50 dislodge (ug/L)	EC50 comment	Elim. rate const. (1/d)	Biotrnsfm. rate (1/d)	LC50 (ug/L)	LC50 exp. tir
Diatoms	50	0	0	Hill & Napolitano, 1997, p. 451	10.4764	0	0	
Bluegreens	0	0	0		2.0953	0	0	
Peri. Diatoms	50	10	0	ECOTOX		0	500	
Peri. Greens	50	10	0	ECOTOX			500	

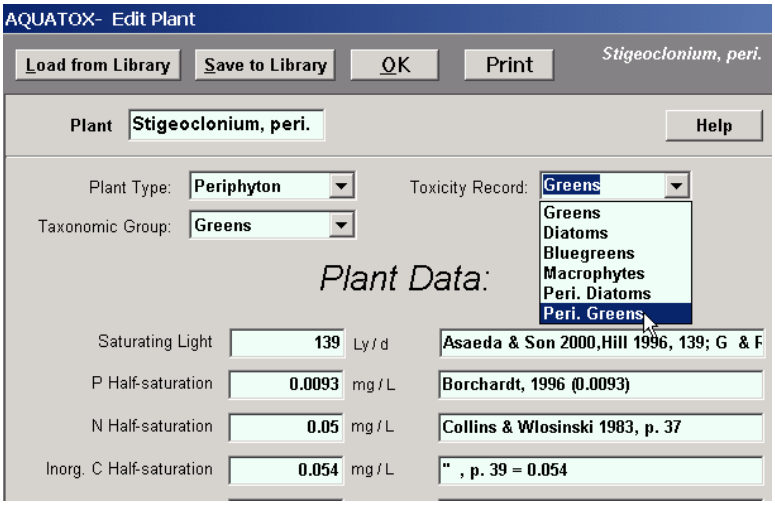


EC50 comment	Elim. rate const. (1/d)	Biotrnsfm. rate (1/d)	LC50 (ug/L)	LC50 exp. time (h)	LC50 comment	Lipid Frac
Hill & Napolitano, 1997, p. 451	10.4764	0	0	24	10 times EC50 photo	0.002
	2.0953	0	0	24	10 times EC50 photo	0.01
ECOTOX		0	500	10	10 times EC50 photo	0.002
ECOTOX			500	10	10 times EC50 photo	0.002

Now click on **Estimate elimination rate constants ….** The rate coefficients will be estimated using the octanol water partition coefficient and the plant's lipid content, which is why it is important to completely fill in each record. After saving the toxicity and chemical screens, double-click on each of the plant state variables, open the parameter screen, and associate the plant with the appropriate toxicity record. Save the study (as **EForkPoplarCr3 PCB**), so that your changes will not be lost in the event of a problem—although we have not mentioned it before, it's a good practice to save the study periodically. (If you are just following along in the text, a copy of the file is provided in the InstallShield and will be installed on your system.)

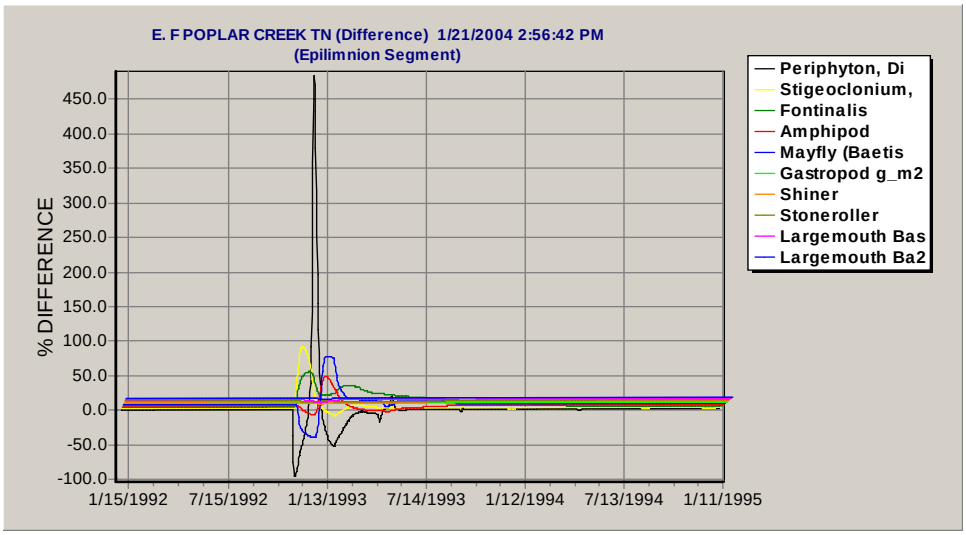


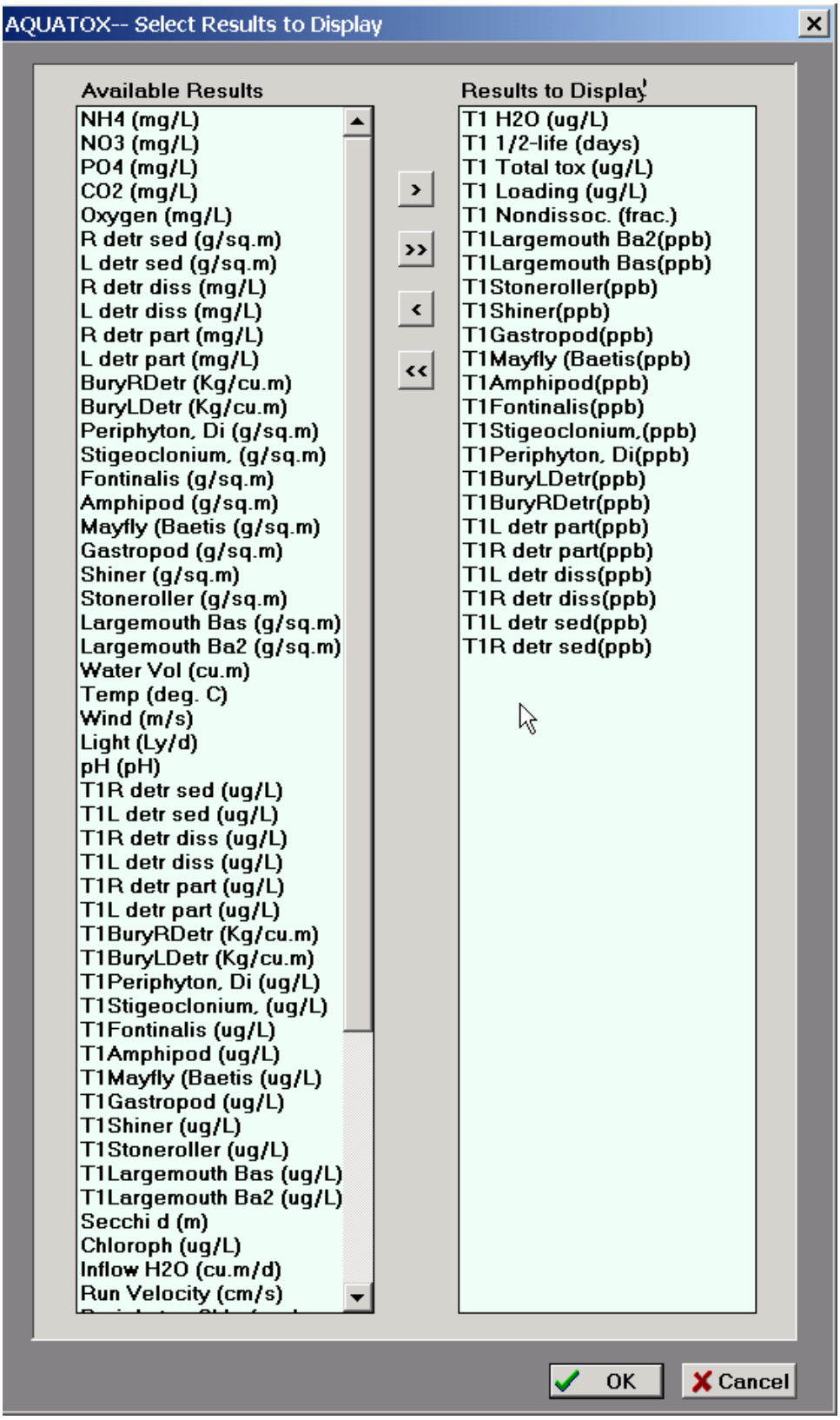
Plant name	EC50 photo (ug/L)	EC50 exp. time (h)	EC50 dislodge (ug/L)	EC50 comment	Elim. rate const. (1/d)	Biotrnsfm. rate (1/d)	LC50 (ug/L)	LC50 exp. tir
Diatoms	50	0	0	Hill & Napolitano, 1997, p. 451	10.4764	0	0	
Bluegreens	0	0	0		2.0953	0	0	
Peri. Diatoms	50	10	0	ECOTOX	10.4764	0	500	
Peri. Greens	50	10	0	ECOTOX	10.4764		500	

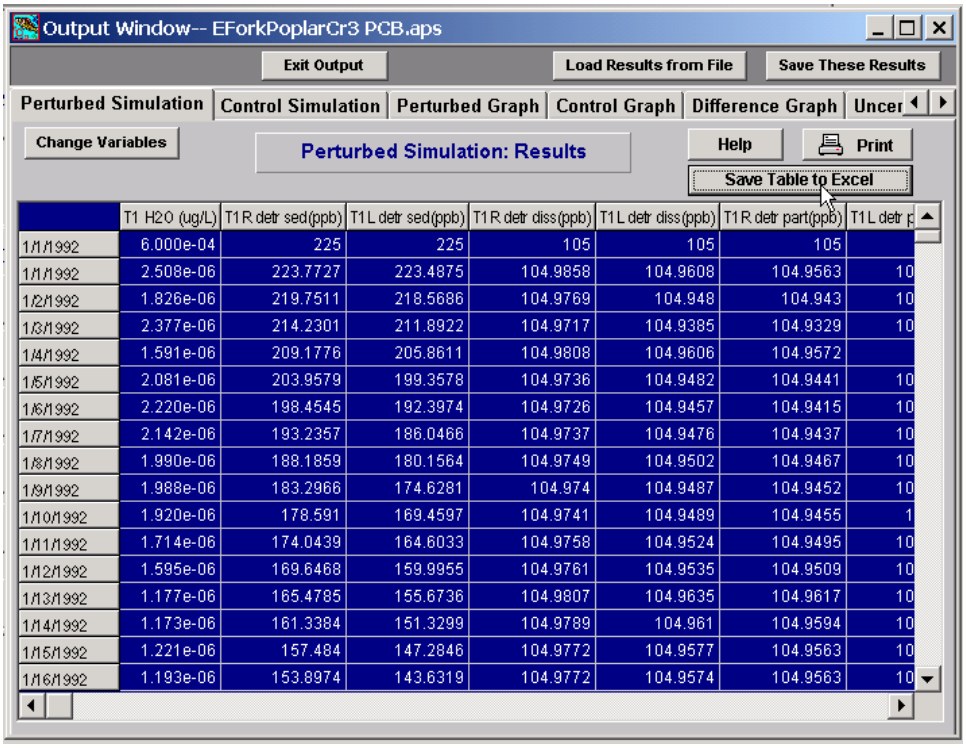


Having run the perturbed simulation, we should first examine the difference graph to see if there were any predicted toxic effects of PCBs at the concentrations used. In one run there was less than a 4% difference for any variable, well within the integration differences for the two simulations. However, another run exhibited a peculiar set of spikes, initiated by the diatoms. Switching back and forth between the control and perturbed simulations (not shown), it eventually becomes clear that a minor sloughing event for the diatoms occurred in the control simulation and not in the perturbed simulation. The fact that it wasn't consistent suggests it could be just a numerical glitch (although the relative error is set quite low), or it may indicate a very small toxic effect on photosynthesis that kept the diatom biomass from reaching a threshold value at which sloughing would occur. The effect is short-lived so we will ignore it.

We then plot the concentrations in the biota, and compare them with the observed data. An easy way to do this is to set up a spreadsheet as a template with the observed data and a default graph. Click on the **Perturbed Simulation** tab for Output, then click on **Change Variables** and choose the T1 H2O (ug/L) and ppb output. These will be displayed in tabular form and can be saved to an Excel file. We'll label the file "**1-EFPC3 PCB**" so that it will appear near the top of the list of files in the Output directory. We also prepared a template with the observed data and labeled it "**2-EFPC3 PCB**." We then cut and paste the predicted data from **1-EFPC3 PCB.xls** into **2-EFPC3 PCB.xls** and inspect the fit between the observed and predicted concentrations.

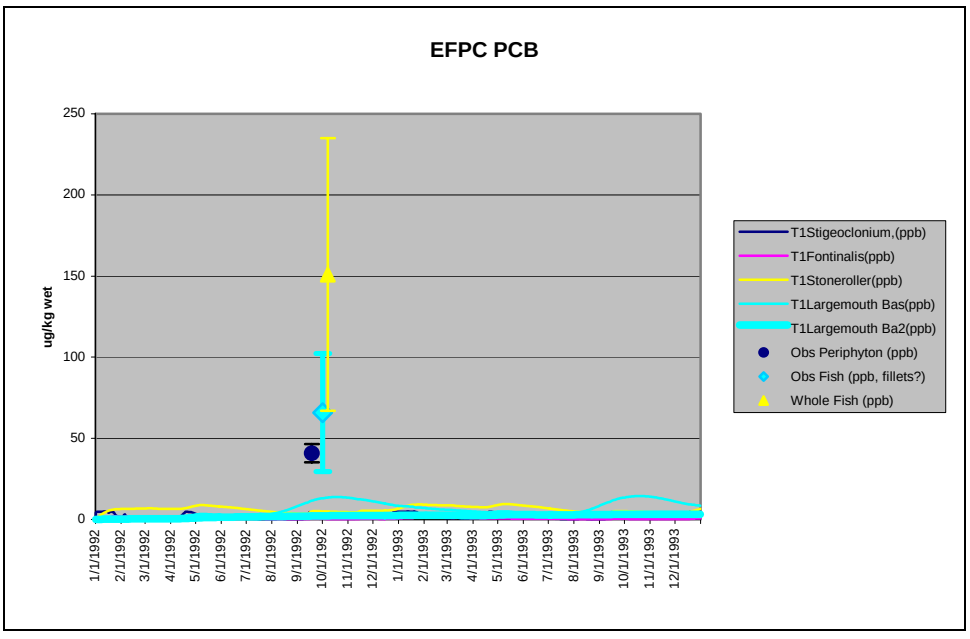



AQUATOX-- Select Results to Display
Available Results
NH4 (mg/L)
NO3 (mg/L)
PO4 (mg/L)
CO2 (mg/L)
Oxygen (mg/L)
R detr sed (g/sq.m)
L detr sed (g/sq.m)
R detr diss (mg/L)
L detr diss (mg/L)
R detr part (mg/L)
L detr part (mg/L)
BuryRDetr (Kg/cu.m)
BuryLDetr (Kg/cu.m)
Periphyton, Di (g/sq.m)
Stigeoclonium, (g/sq.m)
Fontinalis (g/sq.m)
Amphipod (g/sq.m)
Mayfly (Baetis (g/sq.m)
Gastropod (g/sq.m)
Shiner (g/sq.m)
Stoneroller (g/sq.m)
Largemouth Bas (g/sq.m)
Largemouth Ba2 (g/sq.m)
Water Vol (cu.m)
Temp (deg. C)
Wind (m/s)
Light (Ly/d)
pH (pH)
T1R detr sed (ug/L)
T1L detr sed (ug/L)
T1R detr diss (ug/L)
T1L detr diss (ug/L)
T1R detr part (ug/L)
T1L detr part (ug/L)
T1BuryRDetr (Kg/cu.m)
T1BuryLDetr (Kg/cu.m)
T1Periphyton, Di (ug/L)
T1Stigeoclonium, (ug/L)
T1Fontinalis (ug/L)
T1Amphipod (ug/L)
T1Mayfly (Baetis (ug/L)
T1Gastropod (ug/L)
T1Shiner (ug/L)
T1Stoneroller (ug/L)
T1Largemouth Bas (ug/L)
T1Largemouth Ba2 (ug/L)
Secchi d (m)
Chloroph (ug/L)
Inflow H2O (cu.m/d)
Run Velocity (cm/s)
>
>>
<
<<
Results to Display
T1 H2O (ug/L)
T1 1/2-life (days)
T1 Total tox (ug/L)
T1 Loading (ug/L)
T1 Nondissoc. (frac.)
T1Largemouth Ba2(ppb)
T1Largemouth Bas(ppb)
T1Stoneroller(ppb)
T1Shiner(ppb)
T1Gastropod(ppb)
T1Mayfly (Baetis(ppb)
T1Amphipod(ppb)
T1Fontinalis(ppb)
T1Stigeoclonium,(ppb)
T1Periphyton, Di(ppb)
T1BuryLDetr(ppb)
T1BuryRDetr(ppb)
T1L detr part(ppb)
T1R detr part(ppb)
T1L detr diss(ppb)
T1R detr diss(ppb)
T1L detr sed(ppb)
T1R detr sed(ppb)
OK
Cancel



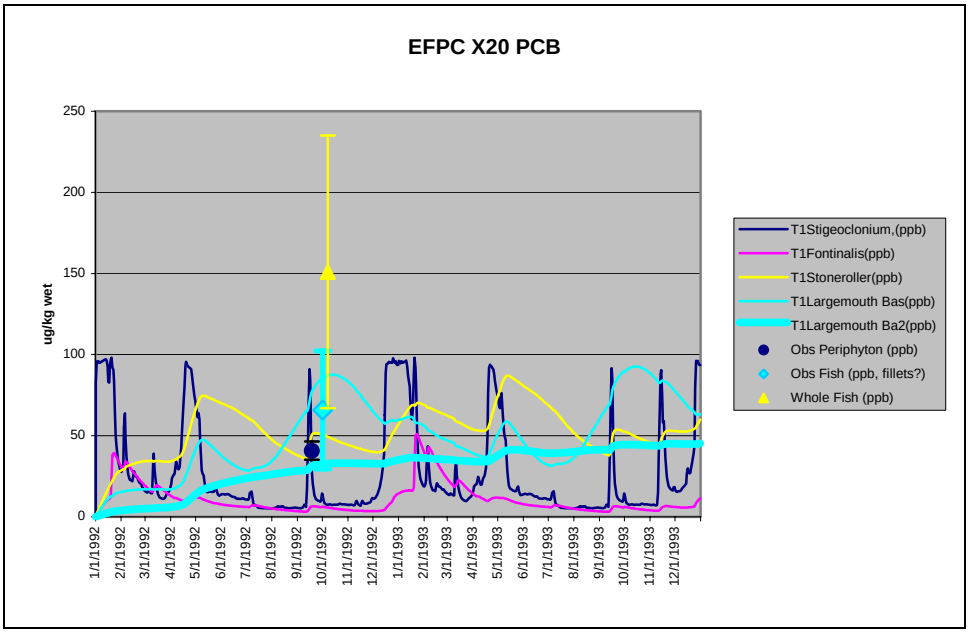
	T1 H2O (ug/L)	T1 R detr sed(ppb)	T1 L detr sed(ppb)	T1 R detr diss(ppb)	T1 L detr diss(ppb)	T1 R detr part(ppb)	T1 L detr p
1/1/1992	6.000e-04	225	225	105	105	105	
1/1/1992	2.508e-06	223.7727	223.4875	104.9858	104.9608	104.9563	10
1/2/1992	1.826e-06	219.7511	218.5686	104.9769	104.948	104.943	10
1/3/1992	2.377e-06	214.2301	211.8922	104.9717	104.9385	104.9329	10
1/4/1992	1.591e-06	209.1776	205.8611	104.9808	104.9606	104.9572	
1/5/1992	2.081e-06	203.9579	199.3578	104.9736	104.9482	104.9441	10
1/6/1992	2.220e-06	198.4545	192.3974	104.9726	104.9457	104.9415	10
1/7/1992	2.142e-06	193.2357	186.0466	104.9737	104.9476	104.9437	10
1/8/1992	1.990e-06	188.1859	180.1564	104.9749	104.9502	104.9467	10
1/9/1992	1.988e-06	183.2966	174.6281	104.974	104.9487	104.9452	10
1/10/1992	1.920e-06	178.591	169.4597	104.9741	104.9489	104.9455	1
1/11/1992	1.714e-06	174.0439	164.6033	104.9758	104.9524	104.9495	10
1/12/1992	1.595e-06	169.6468	159.9955	104.9761	104.9535	104.9509	10
1/13/1992	1.177e-06	165.4785	155.6736	104.9807	104.9635	104.9617	10
1/14/1992	1.173e-06	161.3384	151.3299	104.9789	104.961	104.9594	10
1/15/1992	1.221e-06	157.484	147.2846	104.9772	104.9577	104.9563	10
1/16/1992	1.193e-06	153.8974	143.6319	104.9772	104.9574	104.9563	10

As seen in the following graph, the results are off by a factor of at least 20.

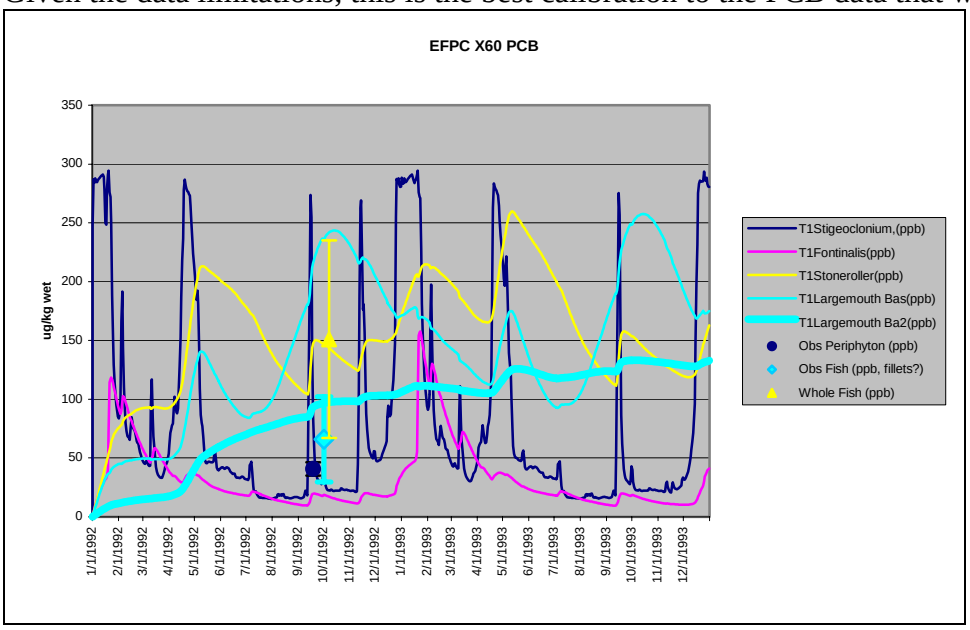


The concentration 0f 0.0006 ug/L estimated by Moore et al. (1999) was based on the assumption of equilibrium between periphyton and the water column using a single observed BCF for PCBs and *Anabaena*. This was sufficient for their risk assessment, but AQUATOX is more sensitive to the dissolved concentrations and, with its nonlinear representation of bioavailability and fate, can be used to obtain a more robust estimate through calibration.

Therefore, we will increase the concentration in water by a factor of 20 to 0.012. The study will be saved as "**EForkPoplarCr3 X20 PCB.aps**." The results are closer to what we would expect, although they are still too low.



Next, we will increase the dissolved concentration by a factor of 60 to 0.036 ug/L, and save the study as "**EForkPoplarCr3 X60 PCB.aps**." The results look good: the observed periphyton concentration is on the predicted periphyton line, and the observed range of fish concentrations encompasses both the predicted stoneroller and adult bass concentrations. The young-of-the-year bass are predicted to bioconcentrate more PCB 1254 because of their small size and high respiratory rates; however, they are not an important component of the fish community, probably were not sampled, and were virtually ignored in our ecosystem calibration. Given the data limitations, this is the best calibration to the PCB data that we can expect.



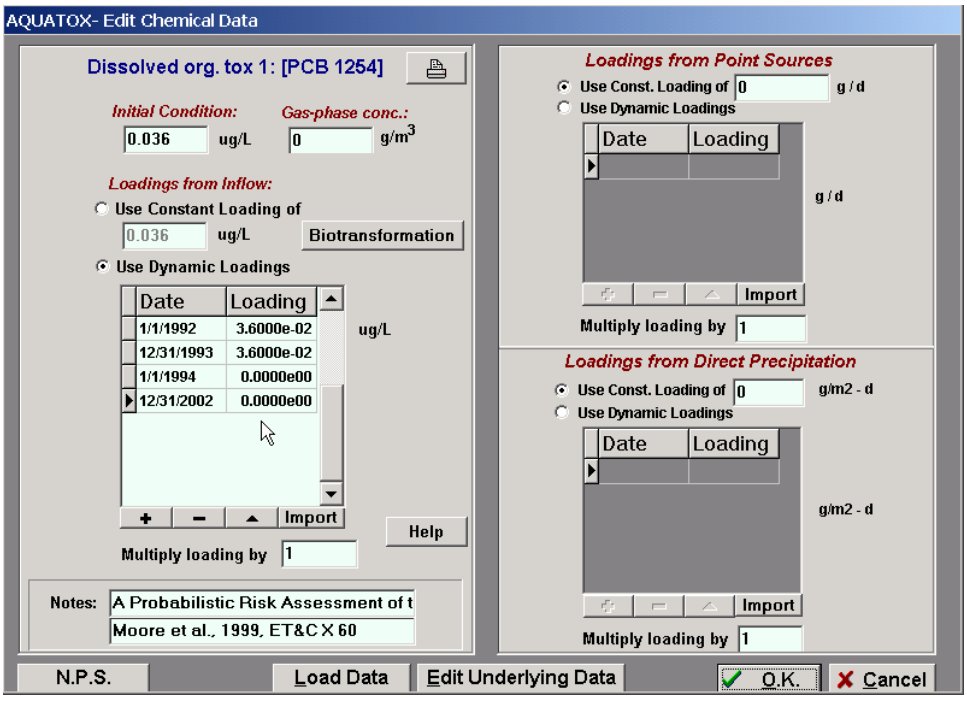
5 APPLICATIONS

The following examples are intended as illustrations of potential applications. AQUATOX has been validated with several data sets from diverse sites and applications; however, like any complex model, it should be evaluated for the intended use. More detailed reports on model validation, including analysis of model predictions as compared to observed data, are found in (U.S. Environmental Protection Agency 2000). No warranty, either expressed or implied, is made.

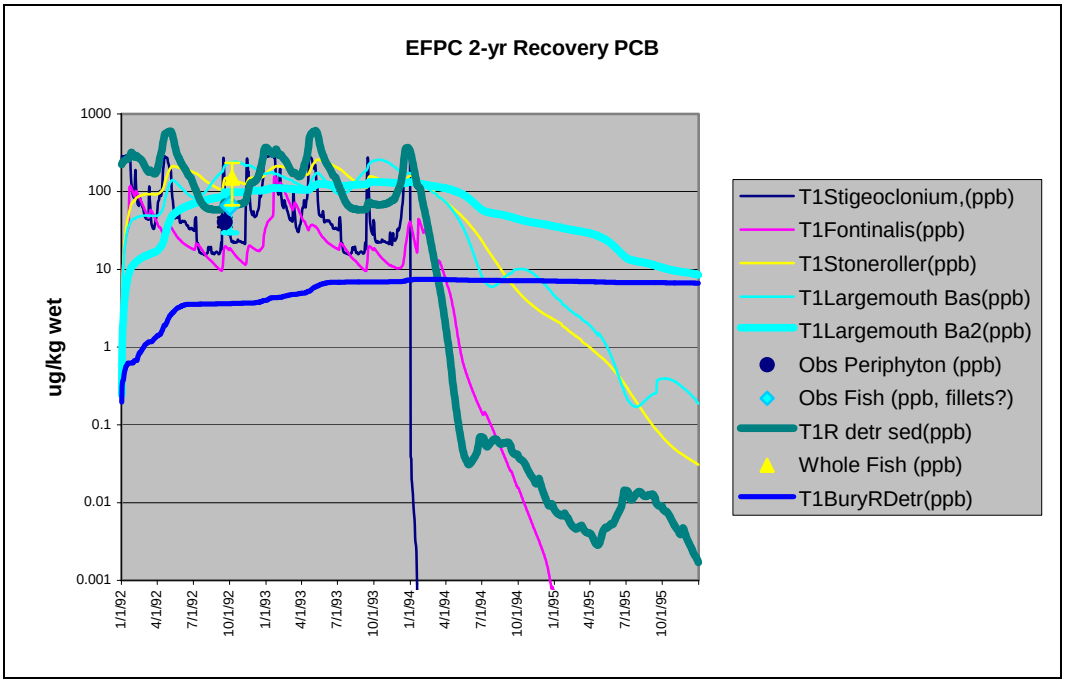
5.1 Recovery Following PCB Remediation

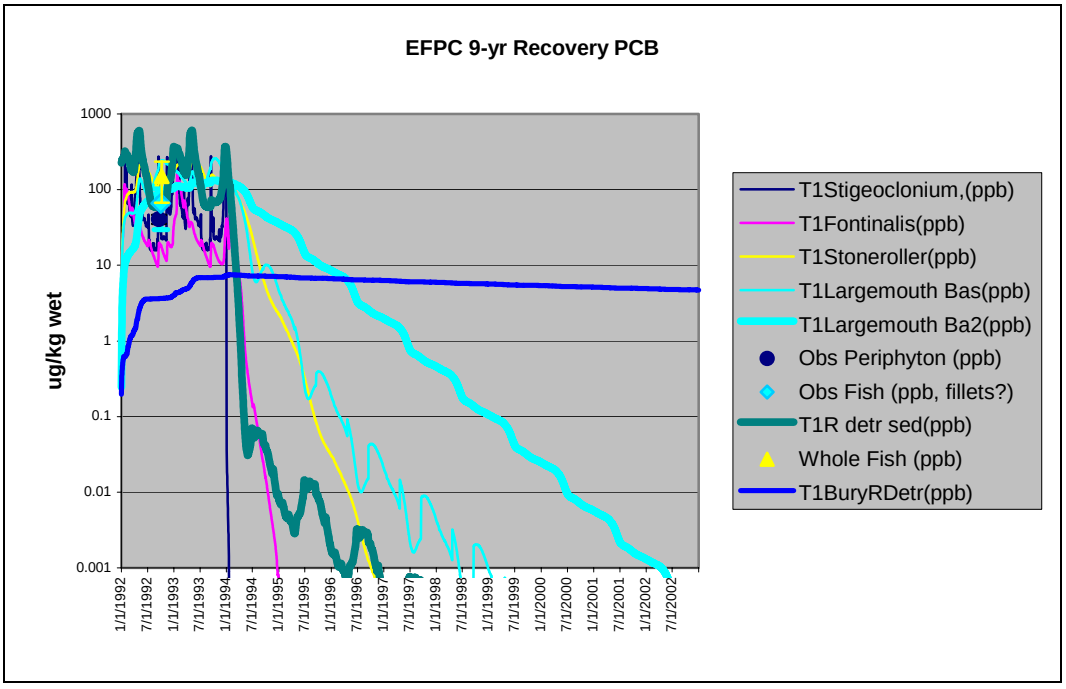
With a calibrated model of East Fork Poplar Creek, we can now forecast the consequences of planned and unplanned modifications to the stream. Two examples are given, this and the one following. Recently, PCBs were removed from East Fork Poplar Creek. As part of a remedial investigation, it is prudent to estimate the time to recovery once the contaminants are removed. That can be done by running the model for a sufficiently long period and noting when pollutants drop below the level of concern. We will take a concentration of 1 ppb PCB 1254 in bass as our endpoint.

Let's start with **EForkPoplarCr3 X60 PCB.aps**. We will keep the loadings for the first two years as a spin-up for the recovery simulation, then drop the loadings of dissolved and detrital PCBs to 0 on 1/1/1994. In our initial simulation, we set the end date to 12/31/2002; however, for purposes of the tutorial and if you have a slow computer, you may wish to set the end date to 12/31/1994. We'll save it as "**EForkPoplarCr3 PCB recovery.aps**."



At the end of the 4-year simulation, and two years after the "cleanup," the predicted concentration in bass was 8.5, in stonerollers was 0.03, and in buried refractory detritus was 6.7 ppb. The target value of 1 ppb in bass was predicted to be reached on 6/19/1997, three and a half years after the PCB loadings were removed. Unfortunately, we don't know what the actual recovery time was after cleanup. According to the longer simulation, buried detritus still had 4.7 ppb nine years after the simulated cleanup; however, the model was not run with the more realistic scour and deposition algorithms of the inorganic sediment submodel.

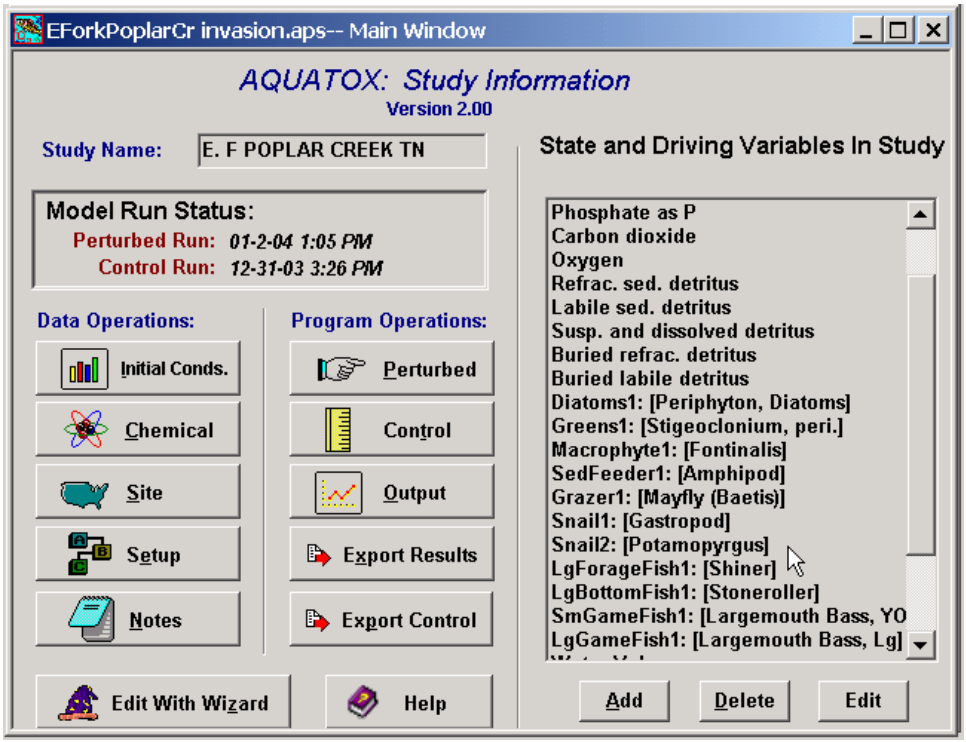




5.2 Possible Response to Invasive Snail Species

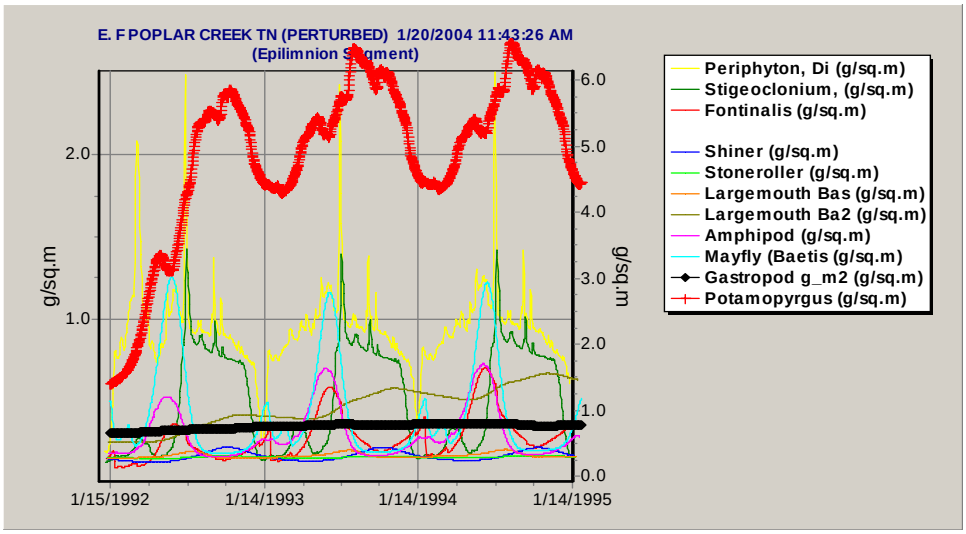
Another possible impact on the stream ecosystem could come from invasion by the New Zealand mud snail *Potamopyrgus antipodarum*. This exotic species has invaded the rivers in Yellowstone National Park (Hall et al. 2003) and is spreading through the Missouri River watershed. Based on data presented by (Hall et al. 2003), the species was added to the AQUATOX animal library.

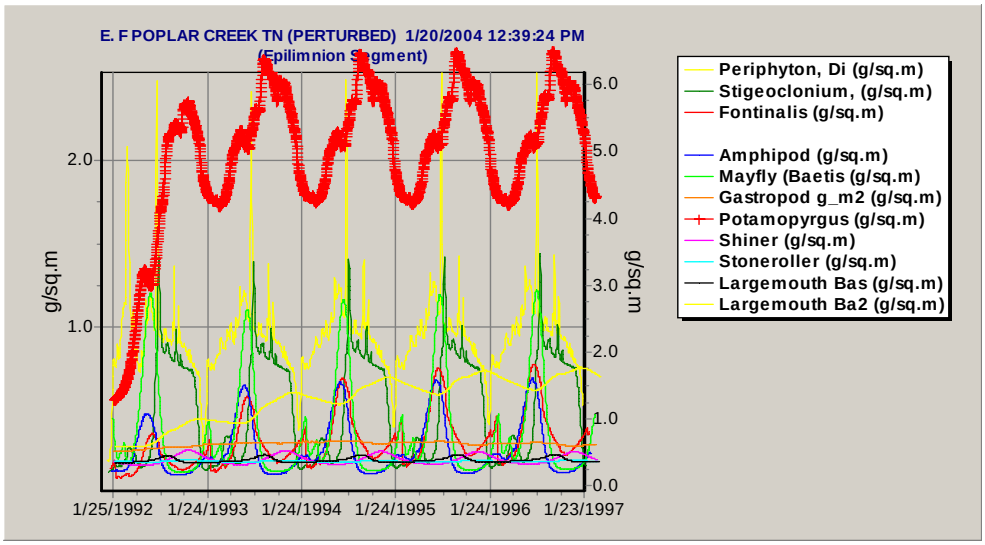
Let's add the species to the baseline East Fork Poplar Creek study (**EForkPoplarCr3.aps**) and rename that file "**EForkPoplarCr invasion.aps**." Click on **Add** below the list of state variables, and then choose **Snail** and **Potamopyrgus**. Double-click **Snail2** to open the initial condition and loading window. We will set the initial condition to 1 g/m^2. Next, double-click on **LgGamefish1**, then **Trophic Interactions** and set the preference and egestion for Potamopyrgus to the same values as Gastropod so that bass will serve as a predator (we have no reason to believe that bass, as a surrogate for sunfish, would treat the two types of gastropods differently). Finally, select **Dissolved org. tox 1:[PCB 1254]** in the state variable list and click on **Delete**. Since we are not interested in bioaccumulation in this application, simulating PCB fate would only slow down the simulation.



The results are striking. Within two years, *Potamopyrgus* goes from 1 to 6 g/m^2. A 5-year simulation (**EForkPoplarCr 5yr invasion.aps**) shows that a seasonal maximum of 6 g/m^2 is maintained. At the same time, the native gastropod increases slightly in biomass, perhaps because competition for food is offset by decreased predation pressure due to an alternate food source for predators. Inspection of the parameter files for these two gastropods shows that the

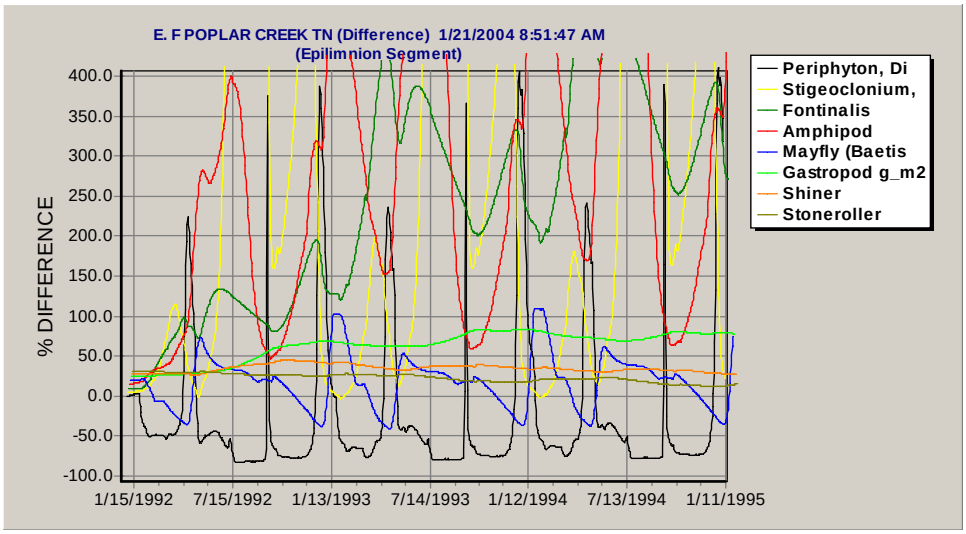
consumption rate for *Potamopyrgus* is three times that of the native gastropod and the egestion coefficient is half again as great.

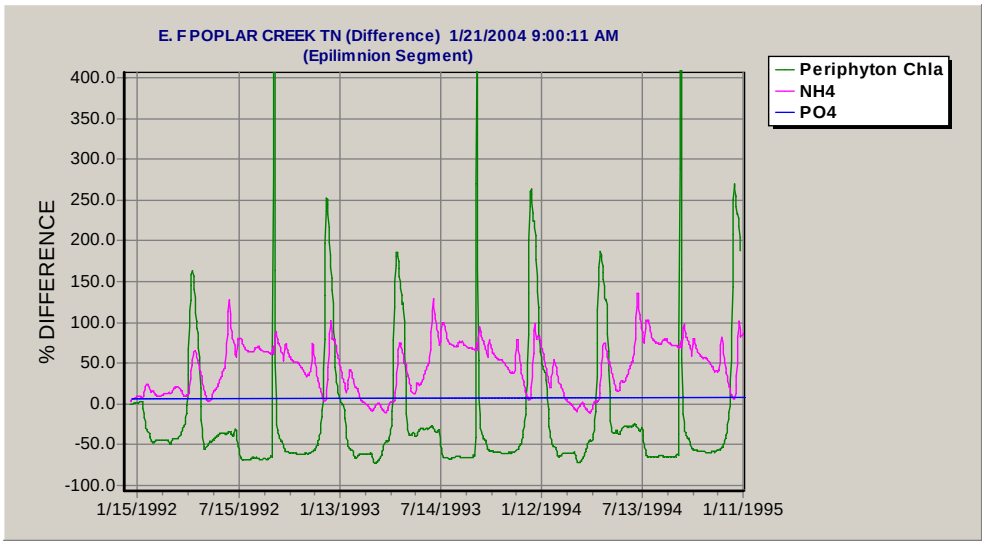


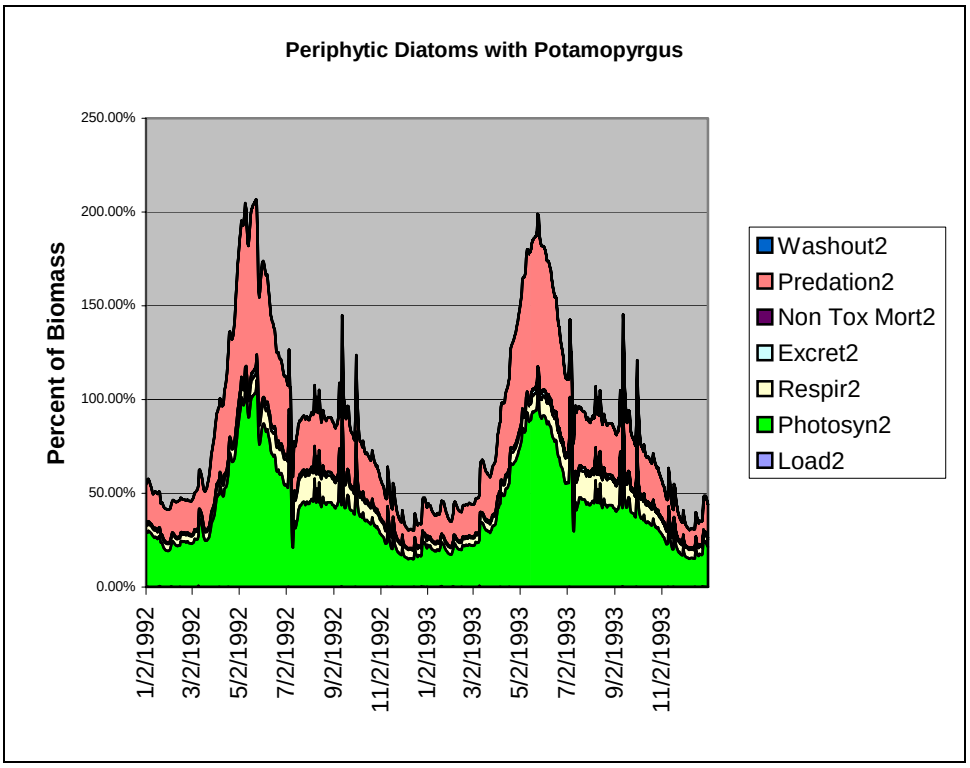


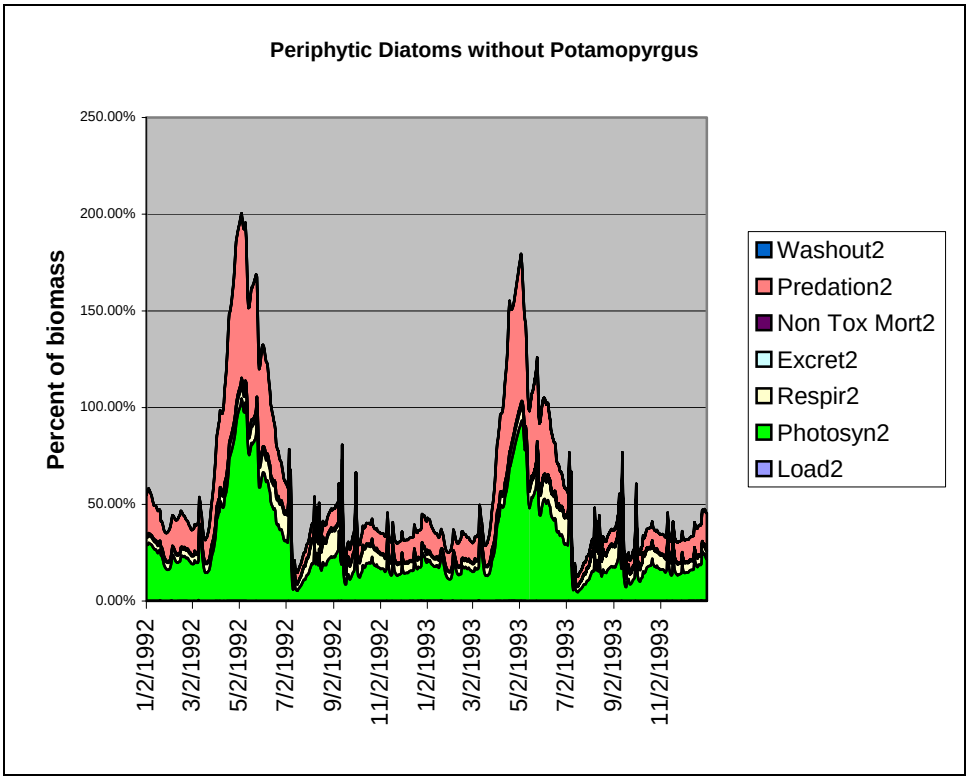
The other changes are subtler and are best depicted with the difference graph, which shows that mayflies and stonerollers also decline. Amphipods increase, probably through increased production of detritus by *Potamopyrgus* due to their high defecation rate. Shiners, which feed on amphipods, increase even more—demonstrating an interesting cascade of productivity. Surprisingly, the periphytic greens (*Stigeoclonum*) actually increase, although at the expense of the diatoms. *Fontinalis* also increases significantly due to decreased shading by periphyton. A difference graph shows that periphytic chlorophyll is about 50% less except for brief periods of accelerated growth of diatoms. Thirty percent more ammonia is predicted during the growing season with *Potamopyrgus*. This is quite similar to what was found in the field study by (Hall et al. 2003). A detailed comparison of plant rates and limitations for the simulations, with and without *Potamopyrgus,* shows that diatoms have a higher overall productivity, which is offset by the higher grazing rates of *Potamopyrgus*. The higher

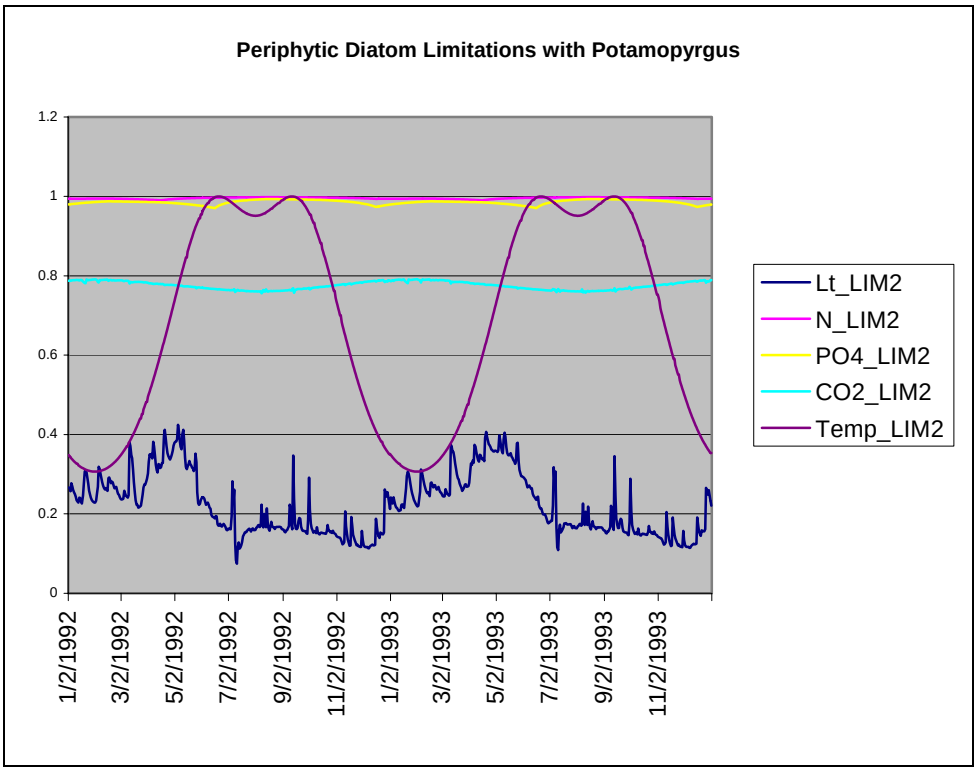
productivity with *Potamopyrgus* is seen in the limitation plots to be a result of less light limitation; nutrient limitation is unchanged.

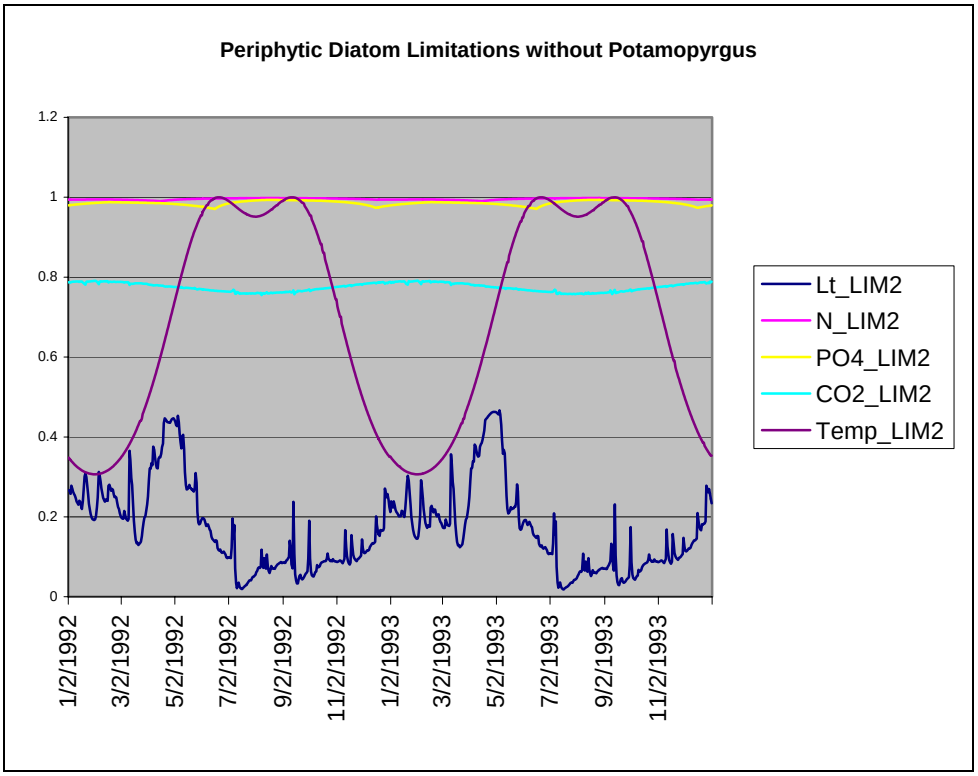





Periphytic Diatoms with Potamopyrgus
Percent of Biomass
250.00%
200.00%
150.00%
100.00%
50.00%
0.00%
1/2/1992
3/2/1992
5/2/1992
7/2/1992
9/2/1992
11/2/1992
1/2/1993
3/2/1993
5/2/1993
7/2/1993
9/2/1993
11/2/1993
Washout2
Predation2
Non Tox Mort2
Excret2
Respir2
Photosyn2
Load2


Periphytic Diatoms without Potamopyrgus
Percent of biomass
250.00%
200.00%
150.00%
100.00%
50.00%
0.00%
1/2/1992
3/2/1992
5/2/1992
7/2/1992
9/2/1992
11/2/1992
1/2/1993
3/2/1993
5/2/1993
7/2/1993
9/2/1993
11/2/1993
Washout2
Predation2
Non Tox Mort2
Excret2
Respir2
Photosyn2
Load2


Periphytic Diatom Limitations with Potamopyrgus
1.2
1
0.8
0.6
0.4
0.2
0
1/2/1992
3/2/1992
5/2/1992
7/2/1992
9/2/1992
11/2/1992
1/2/1993
3/2/1993
5/2/1993
7/2/1993
9/2/1993
11/2/1993
Lt_LIM2
N_LIM2
PO4_LIM2
CO2_LIM2
Temp_LIM2


Periphytic Diatom Limitations without Potamopyrgus
1.2
1
0.8
0.6
0.4
0.2
0
1/2/1992
3/2/1992
5/2/1992
7/2/1992
9/2/1992
11/2/1992
1/2/1993
3/2/1993
5/2/1993
7/2/1993
9/2/1993
11/2/1993
Lt_LIM2
N_LIM2
PO4_LIM2
CO2_LIM2
Temp_LIM2

5.3 Nutrient Enrichment

AQUATOX has its roots in what was basically a eutrophication model, and it provides a reasonable representation of the effects of nutrient enrichment. It can be configured to depict a complex food web that is both phytoplankton- and detritus-based, with both game fish and bottom fish—often considered regulatory endpoints. It also reports phytoplankton both as biomass and as chlorophyll *a*, which is an important index of water quality. Dissolved oxygen is another important index that is computed. The Secchi depth, an indicator of clarity, also is estimated.

For this example, we will use data from Onondaga Lake, New York (**Onondaga.aps**). The lake has been described very well in a book edited by Effler (1996). It has received municipal and industrial wastes for many years, and effluent from the municipal wastewater treatment plant accounts for nearly 20% of the annual inflow to the lake (Effler et al. 1996). Of particular concern are the combined sewer overflows (CSOs) that carry storm water and raw sewage into tributary creeks about 50 times a year. In 1991 there were 45 CSOs discharging into Onondaga Creek, 19 into Harbor Brook, and 2 into Ley Creek. In a separate report, Park (U.S. Environmental Protection Agency 2000) described three levels of analyses in validating Version 1.66 with Onondaga Lake data. For purposes of this example, we will use the third-level implementation with detailed loadings for nutrients, a site-specific mixing depth, and compartments parameterized for cryptomonads and rotifers.

Discharge data from the four gauged streams in the watershed (Onondaga Creek, Ninemile Creek, Ley Creek, and Harbor Brook, listed in order of importance) were downloaded from the U.S. Geological Survey Web site (see Table 1). Discharge from four ungauged streams was estimated, assuming that they had an aggregate flow rate that was 94% of the discharge of Ley Creek and Harbor Brook based on data in Effler (1996, p. 102).

Table 9-1. Input Data for Onondaga Lake Simulation

Variable	Source	Format
Inflow	www.waterdata.usgs.gov (note: URLs may change)	daily values for 4 gauged streams; extrapolated to ungauged streams
Phosphorus, NPS	Effler 1996, calc. from p. 162 Effler 1996, calc. from p. 159	mean annual conc., 7 tributaries, 1989-1990; mult. by respective inflow
METRO	Effler 1996, p. 162	mean loads, April-September, 1990
NO_x & NH_3, NPS	Effler 1996, calc. from p. 138 Effler 1996, calc. from p. 128	mean annual concentrations for 1989 for 4 tributaries
METRO	Effler 1996, calc. from p. 138	mean annual loads for 1989
Org. matter, NPS	Effler 1996, calc. from p. 138 Effler 1996, calc. from p. 128	back-calculated from organic-N
METRO	Effler 1996, calc. from p. 138	mean annual loads for 1989
Epilimnion temperature	Effler 1996, p. 207	monthly interpolation from figure
Hypolimnion temperature	Effler 1996, p. 247	monthly interpolation from figure
Wind	Effler 1996, p. 248	mean value est. from figure for 30 years
Solar radiation	unpub. data, Lake George, N.Y.	observed annual mean and range
Initial conditions	Effler 1996	obs. data and professional judgment

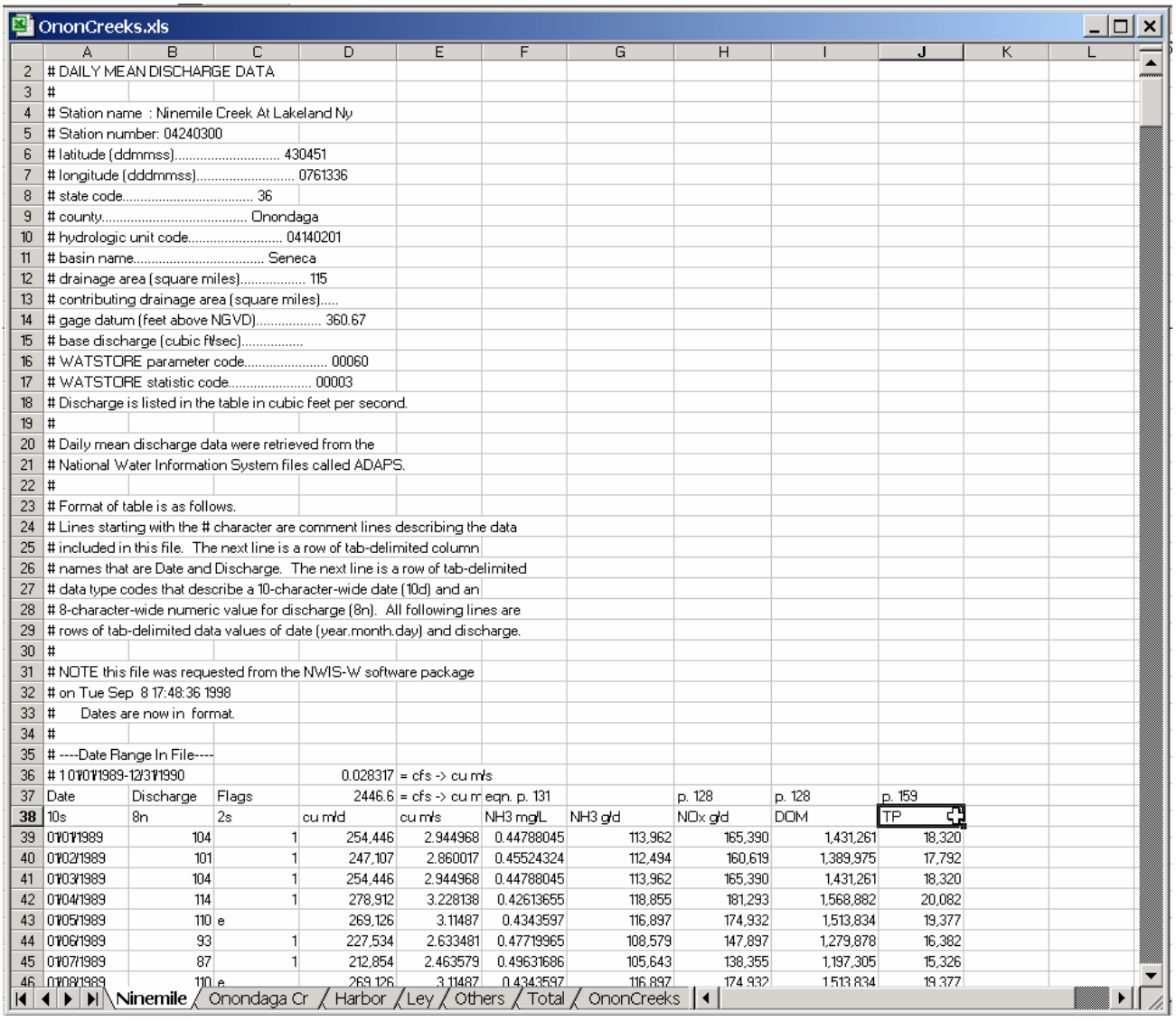
The loadings were then computed using average concentrations for the respective streams, assuming a constant relationship between concentration and discharge. Different average phosphate values were used for 1989 and 1990 for Onondaga and Ninemile Creeks, which varied considerably between the two years due to combined sewer overflows. Also, the concentration of ammonia in Ninemile Creek, which flows through soda ash waste beds, exhibits an inverse relationship to flow rate according to Effler (1996, p. 131); therefore, his Equation 3.12 was used to compute the ammonia concentrations:

$$[T - NH_3] = 0.20 + \frac{0.73}{Flow}$$

where:

$[T\text{-}NH_3]$ = concentration of total ammonia (mgN/L),
Flow = flow rate (m^3/s).

The computations were performed in a spreadsheet by first converting the discharge data from cfs to m^3/d and m^3/s then, for the nutrients, multiplying by the given concentrations to obtain mass per day (g/d) in successive columns. The loadings were imported into AQUATOX by clicking on **Import** in the Edit State Variable screen and choosing the appropriate comma-delimited (csv) or database file.

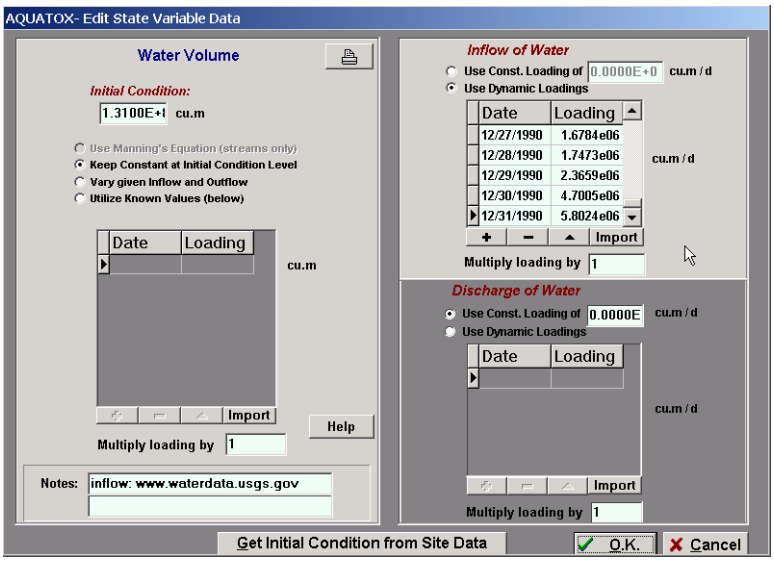


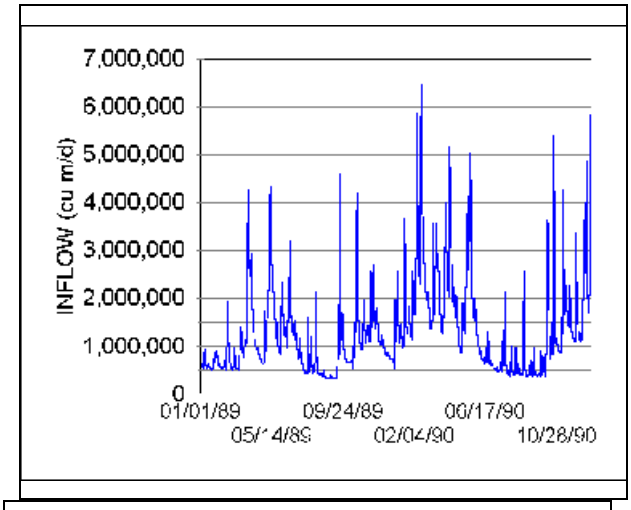
OnonCreeks.xls

	A	B	C	D	E	F	G	H	I	J	K	L
2	# DAILY MEAN DISCHARGE DATA											
3	#											
4	# Station name : Ninemile Creek At Lakeland Ny											
5	# Station number: 04240300											
6	# latitude (ddmmss)..... 430451											
7	# longitude (dddmmss)..... 0761336											
8	# state code..... 36											
9	# county..... Onondaga											
10	# hydrologic unit code..... 04140201											
11	# basin name..... Seneca											
12	# drainage area (square miles)..... 115											
13	# contributing drainage area (square miles).....											
14	# gage datum (feet above NGVD)..... 360.67											
15	# base discharge (cubic ft/sec).....											
16	# WATSTORE parameter code..... 00060											
17	# WATSTORE statistic code..... 00003											
18	# Discharge is listed in the table in cubic feet per second.											
19	#											
20	# Daily mean discharge data were retrieved from the											
21	# National Water Information System files called ADAPS.											
22	#											
23	# Format of table is as follows.											
24	# Lines starting with the # character are comment lines describing the data											
25	# included in this file. The next line is a row of tab-delimited column											
26	# names that are Date and Discharge. The next line is a row of tab-delimited											
27	# data type codes that describe a 10-character-wide date (10d) and an											
28	# 8-character-wide numeric value for discharge (8n). All following lines are											
29	# rows of tab-delimited data values of date (year.month.day) and discharge.											
30	#											
31	# NOTE this file was requested from the NWIS-W software package											
32	# on Tue Sep 8 17:48:36 1998											
33	# Dates are now in format.											
34	#											
35	# ----Date Range In File----											
36	# 1 01\01\1989-12\31\1990			0.028317	= cfs -> cu m/s							
37	Date	Discharge	Flags	2446.6	= cfs -> cu m	eqn. p. 131		p. 128	p. 128	p. 159		
38	10s	8n	2s	cu m/d	cu m/s	NH3 mg/L	NH3 g/d	NOx g/d	DOM	TP		
39	01\01\1989	104	1	254,446	2.944968	0.44788045	113,962	165,390	1,431,261	18,320		
40	01\02\1989	101	1	247,107	2.860017	0.45524324	112,494	160,619	1,389,975	17,792		
41	01\03\1989	104	1	254,446	2.944968	0.44788045	113,962	165,390	1,431,261	18,320		
42	01\04\1989	114	1	278,912	3.228138	0.42613655	118,855	181,293	1,568,882	20,082		
43	01\05\1989	110	e	269,126	3.11487	0.4343597	116,897	174,932	1,513,834	19,377		
44	01\06\1989	93	1	227,534	2.633481	0.47719965	108,579	147,897	1,279,878	16,382		
45	01\07\1989	87	1	212,854	2.463579	0.49631686	105,643	138,355	1,197,305	15,326		
46	01\08\1989	110	e	269,126	3.11487	0.4343597	116,897	174,932	1,513,834	19,377		

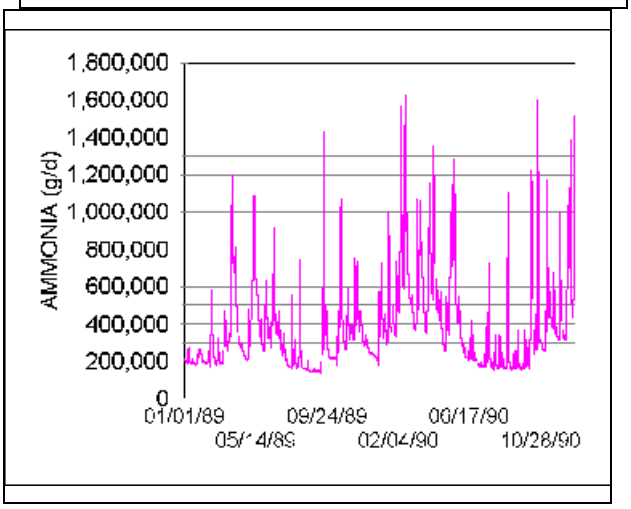
Ninemile | Onondaga Cr | Harbor | Ley | Others | Total | OnonCreeks

Given the readily available hydrologic data, both 1989 and 1990 were simulated with daily loadings. Examination of the loading plots confirms that the streams draining into Onondaga Lake are indeed "flashy" or subject to fast runoff with distinct peaks; the nutrient and organic matter loadings vary accordingly, except the ammonia loadings, which vary slightly from the other loadings due to the inverse flow relationship cited above. The data files and plots were prepared using Quattro Pro and Excel.





Onondaga Lake inflow



Onondaga Lake ammonia loadings

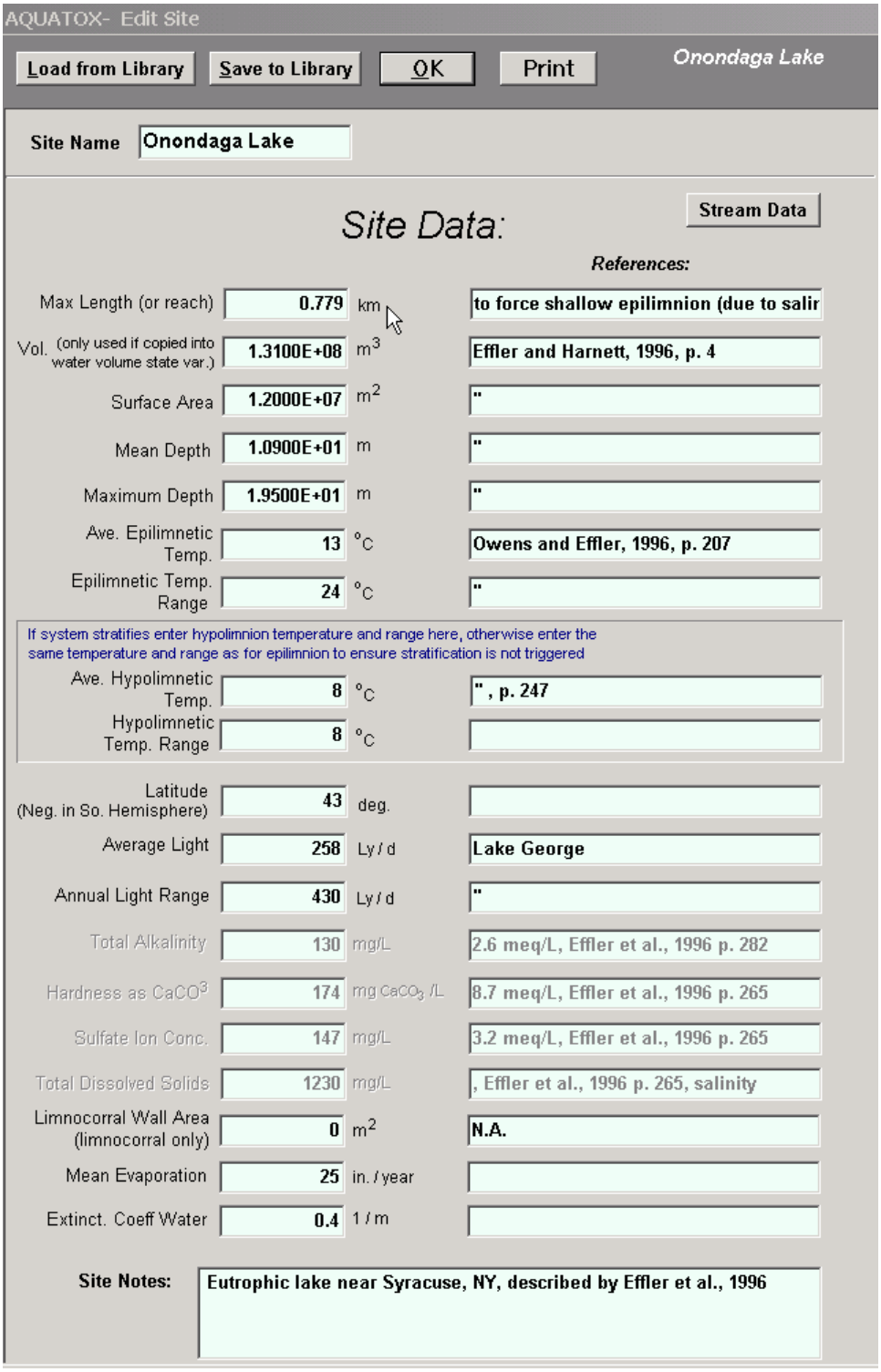
Results from preliminary model runs indicated that some of the model assumptions and defaults were inappropriate for this application, and therefore needed to be modified. For instance, the model computes the depth of the well-mixed layer (epilimnion) using a robust regression equation with the fetch (distance across which the wind can blow) as the independent variable; this equation is based on a dataset for 167 lakes. In Onondaga Lake the computed mixing depth of 15 m is twice as deep as observed (Effler, 1996). It appears that salinity from industrial pollution in the lake is restricting the mixing depth. By back-calculating from the regression equation, a fetch (*Length*) of 0.779 km was found to give the observed well mixed depth (*MaxZMix*) of 7.75 m:

$$MaxZMix = Length^{0.336} \cdot 0.569$$

$$\log(Length) = \frac{\log(7.75)}{0.336} + 0.245$$

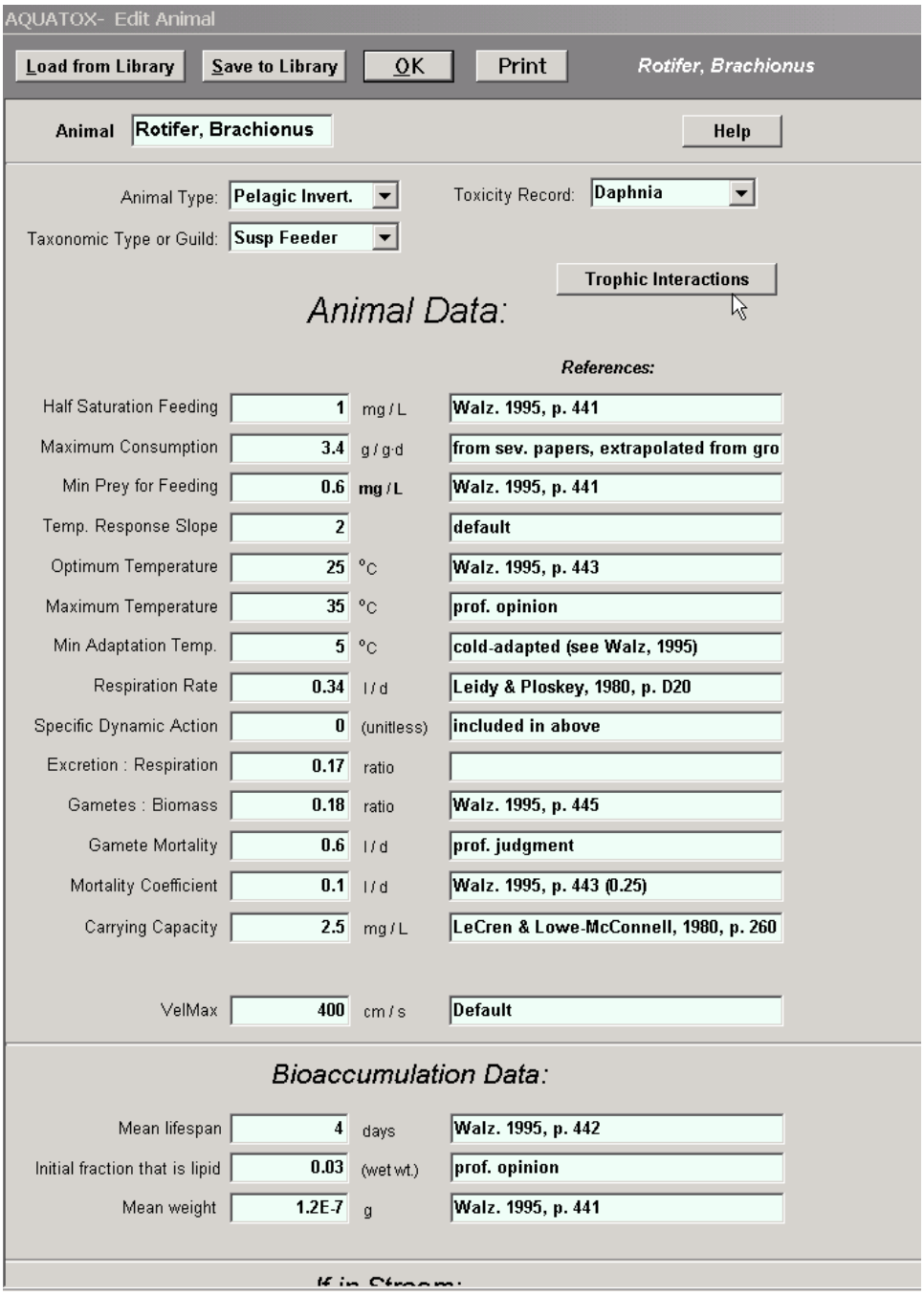
$$Length = 779\ m$$

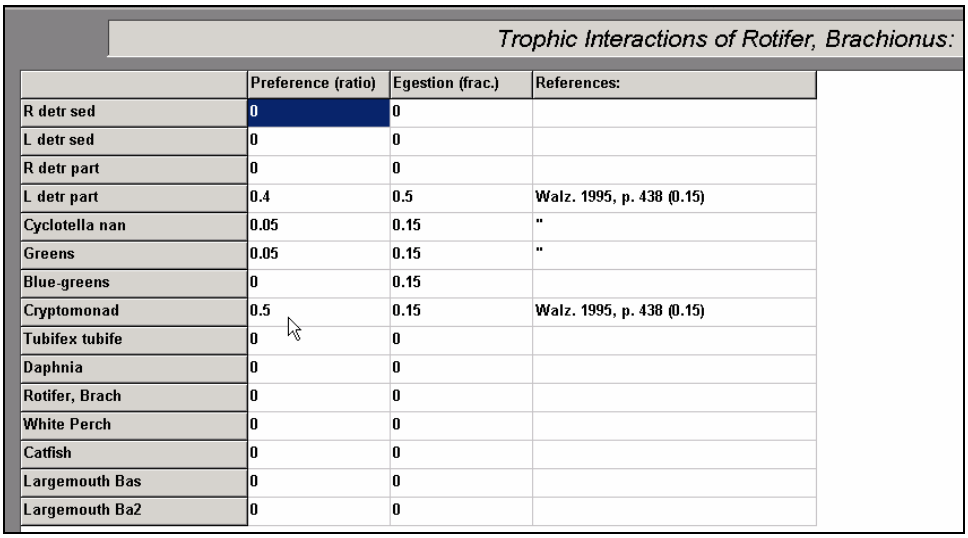
The maximum length was then changed in the Site Characteristics screen.



A second modification was necessary because the observed spring algal bloom was not predicted in initial runs. The spring bloom was reported to be due to cryptomonads, a flagellated algal group that was not in the default data set. Using values from Collins and Wlosinski (1983), a cryptomonad compartment was parameterized. The present version of AQUATOX can simulate four algal groups: diatoms, green algae, blue-greens, and "others." Cryptomonads were

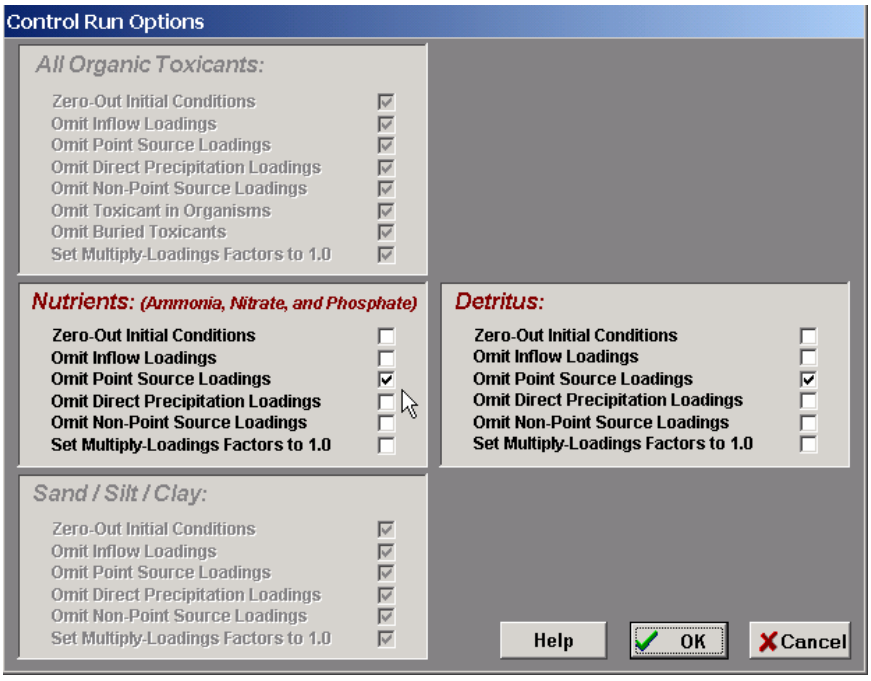
classified as "others." Rotifers are important grazers on cryptomonads, so they were parameterized based on the literature, especially one paper (Walz 1995).





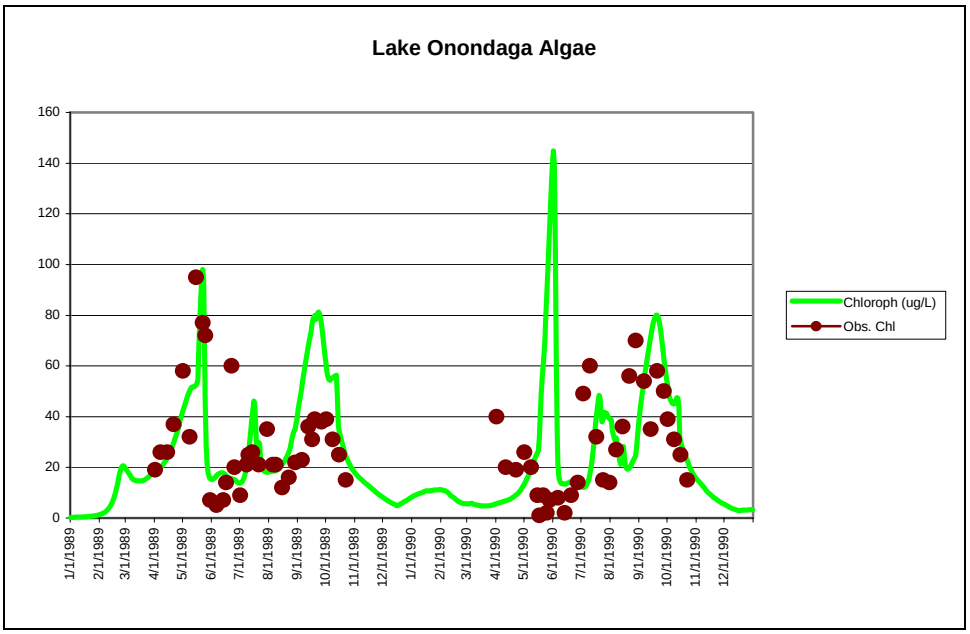
	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	0	
L detr sed	0	0	
R detr part	0	0	
L detr part	0.4	0.5	Walz. 1995, p. 438 (0.15)
Cyclotella nan	0.05	0.15	"
Greens	0.05	0.15	"
Blue-greens	0	0.15	
Cryptomonad	0.5	0.15	Walz. 1995, p. 438 (0.15)
Tubifex tubife	0	0	
Daphnia	0	0	
Rotifer, Brach	0	0	
White Perch	0	0	
Catfish	0	0	
Largemouth Bas	0	0	
Largemouth Ba2	0	0	

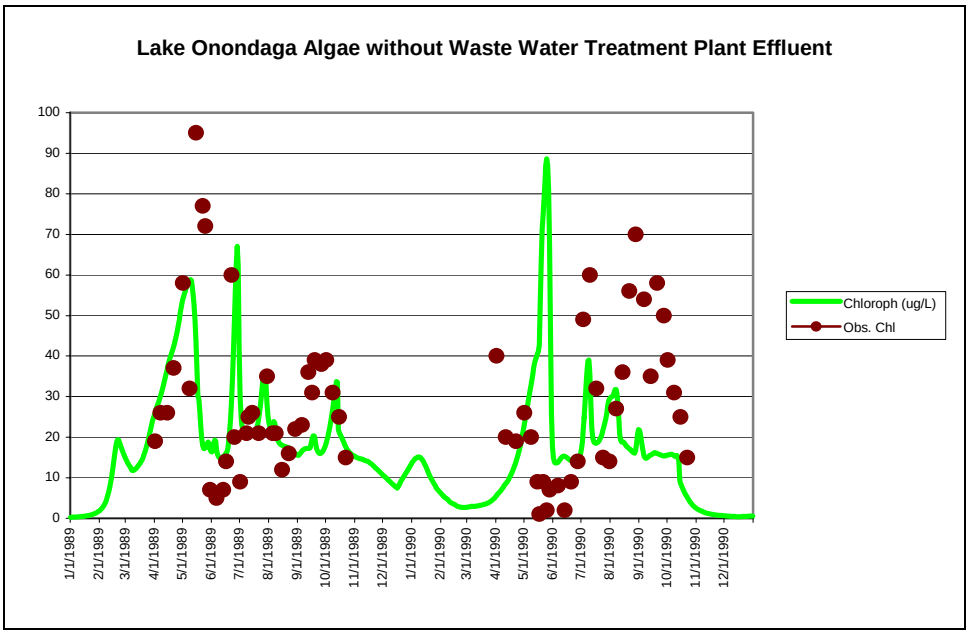
In order to conduct "what if" exercises with the model, we will set the control options to remove point source loadings for nutrients and detritus (click on **Setup** then **Control Setup**). This effectively turns off the contributions of the metropolitan sewage treatment plant. (Another option would be to turn off the non-point source loadings.) Save the study as "**Onondaga no effluent.aps**."



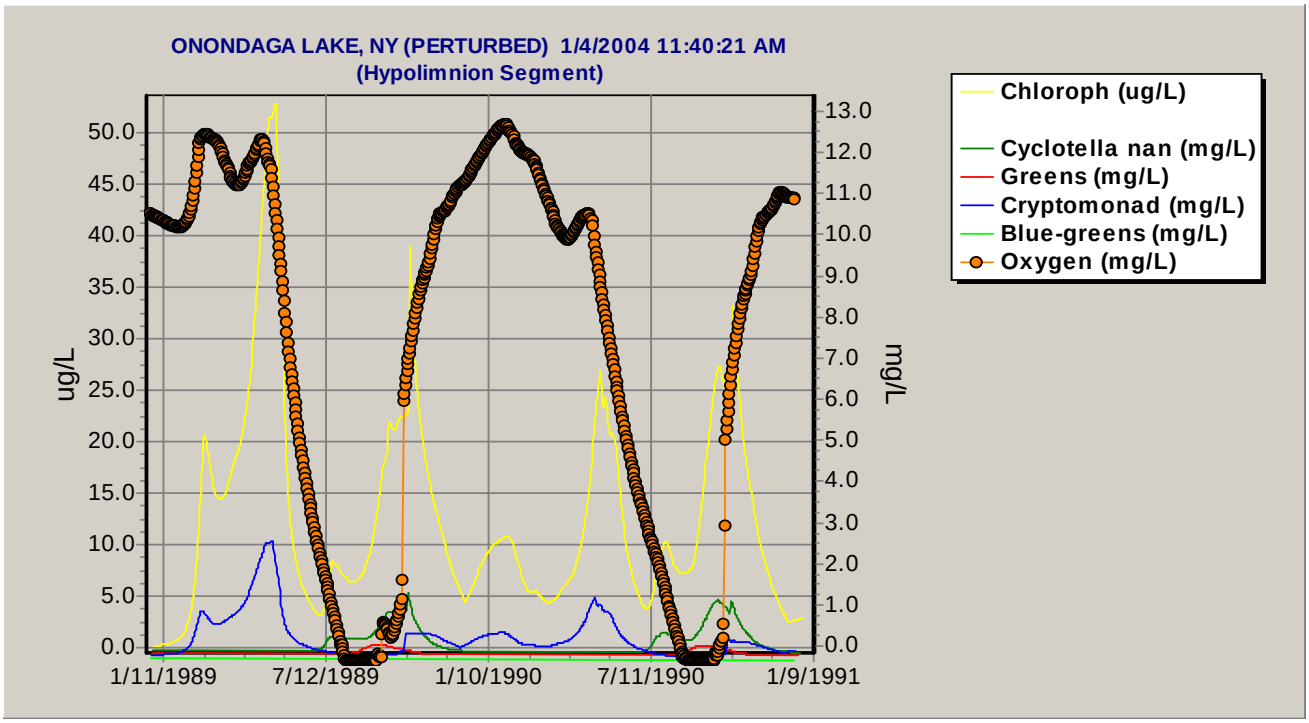
Using chlorophyll *a* as an indication of water quality, and plotting the **Export**ed results with observed values, we can see the normal predicted responses and those predicted if sewage effluent were diverted. A cryptomonad bloom in spring of 1990 is not supported by the observed

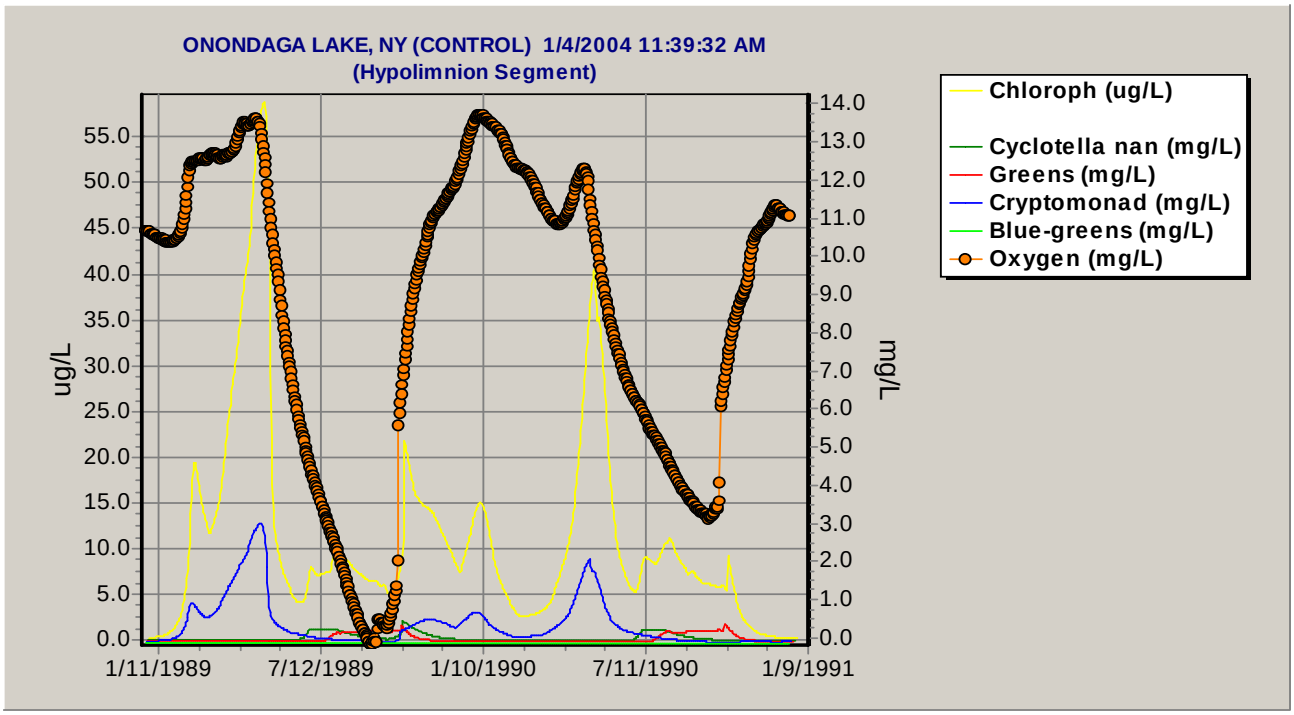
data. As expected, diversion is predicted to result in substantially lower chlorophyll and thus better water quality, especially after the first year.





Other water quality parameters related to eutrophication and nutrients are also computed, such as dissolved oxygen, Secchi depth, nitrate, ammonia, and phosphate. The user could perform similar analyses with these parameters as was just shown with chlorophyll *a*. This would give a more complete picture of the lake's responses to proposed nutrient control scenarios, and whether water quality standards would be met. For example, the anoxia that occurs in the hypolimnion is predicted to go away with diversion of effluent. See an earlier validation document (U.S. Environmental Protection Agency 2000) for a more detailed discussion of the application to this highly eutrophied lake.

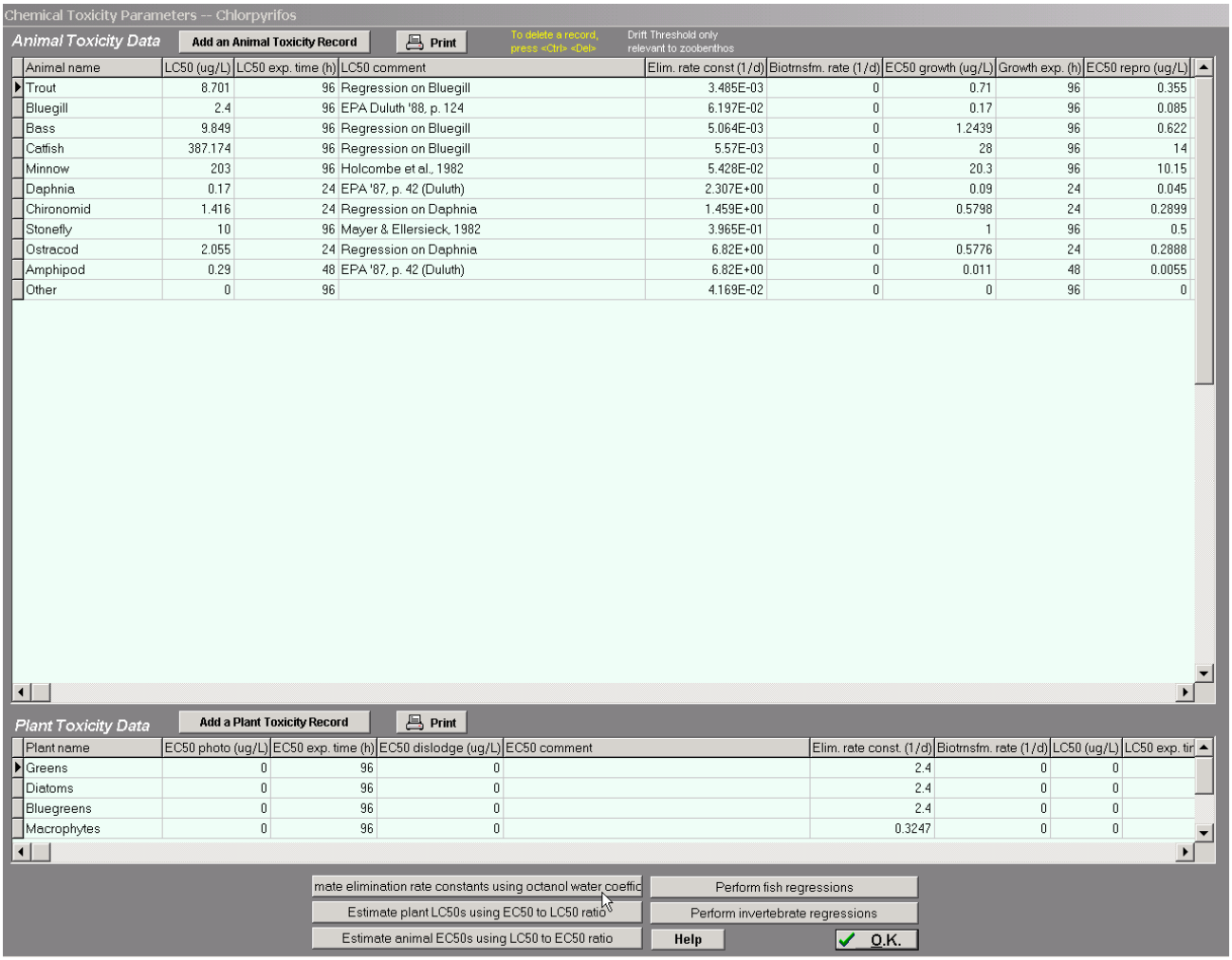




5.4 Pesticides in a Pond Mesocosm

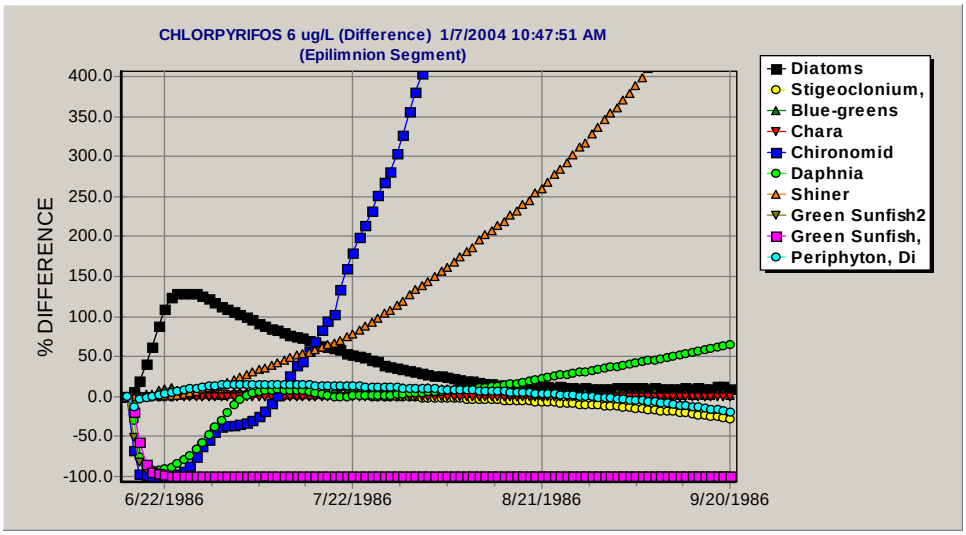
As the only general fate and effects model of potentially toxic chemicals in aquatic ecosystems, AQUATOX is well suited for risk assessment of organic toxicants. An earlier

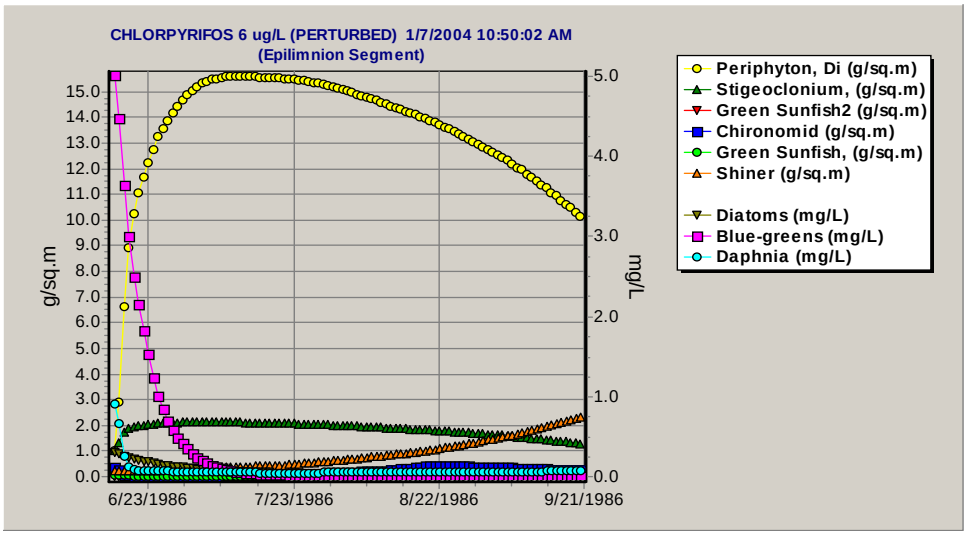
version was used in a comparative risk assessment of twenty-five pesticides. As an example, let's consider the ecological risk assessment of the pesticide chlorpyrifos in an experimental pond enclosure. Load the study **ChlorMed.aps** and click on **Chemical**. You will see the **Edit State Variable** window. First, check to be sure that **Gas-phase conc**. is set to 0 and that the initial condition is 6.3 **:**g/L (we will start the simulation with an initial concentration and no loadings). Then click on **Edit Underlying Data** to get the chemical parameters. Click on **Toxicity Data** or page down to see the ecotoxicology parameters. Click on **Estimate Elimination Rate Constants** to be sure that estimates are up to date. See **Volume 2: Technical Documentation** for a discussion of elimination rate constants (*K2*s). Then save and go back to main menu to run the perturbed and control simulations. If you wish to evaluate biologic rates, that should be specified in the **Setup** screen prior to running the simulations.

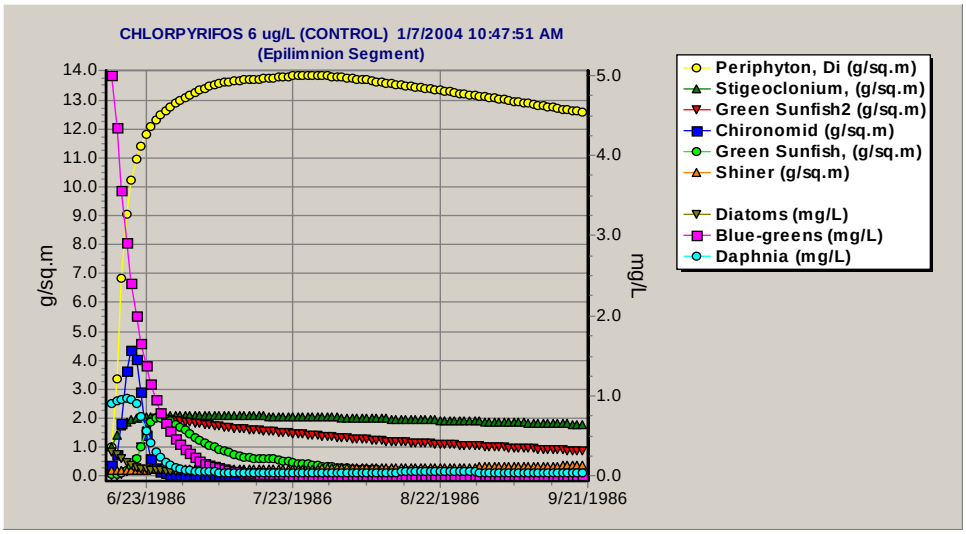


The impacts are substantial when the Perturbed simulation is contrasted with the Control simulation. The difference graph shows the direct and indirect effects of the chlorpyrifos. It is obvious that a significant fraction of the invertebrates are killed immediately, only to recover later. Algae benefit immediately from decreased grazing pressure. Some of the effects are subtler, and interpretation requires additional information. Examination of the plots suggests that

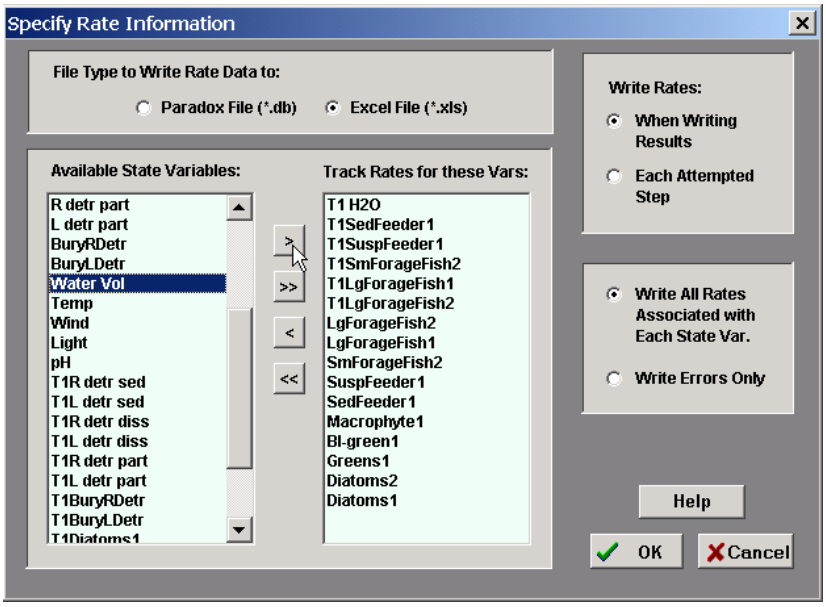
the study is not well calibrated; for example, there are transient conditions in the Control simulation, such as the rapid buildup and decline of chironomids and its effect on the sunfish, that may reflect a poor choice of initial conditions. However, the comparison of Perturbed and Control results is still valid, and the user is able to isolate the effects of the pesticide because of the use of the baseline simulation.



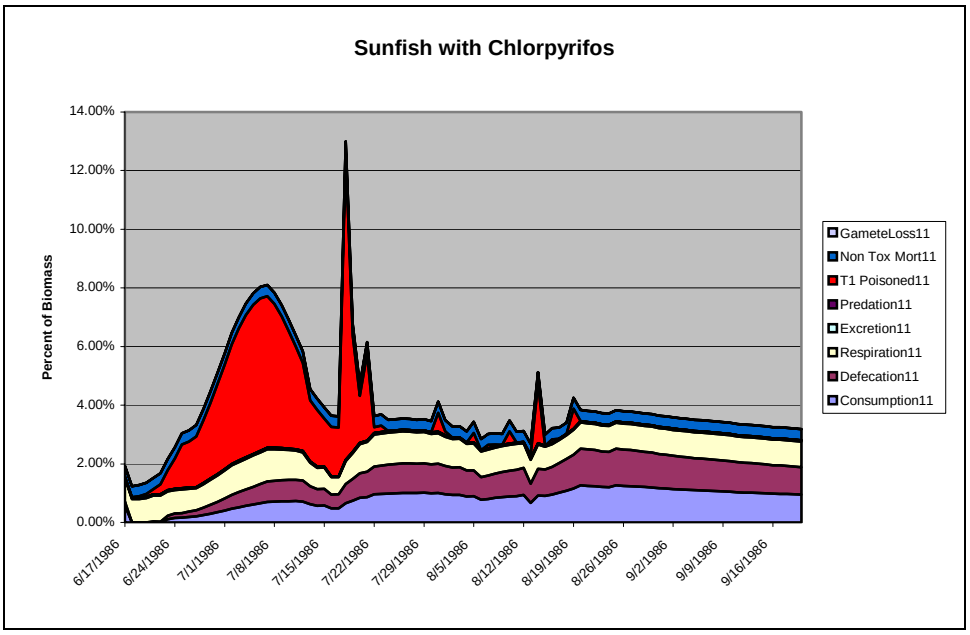


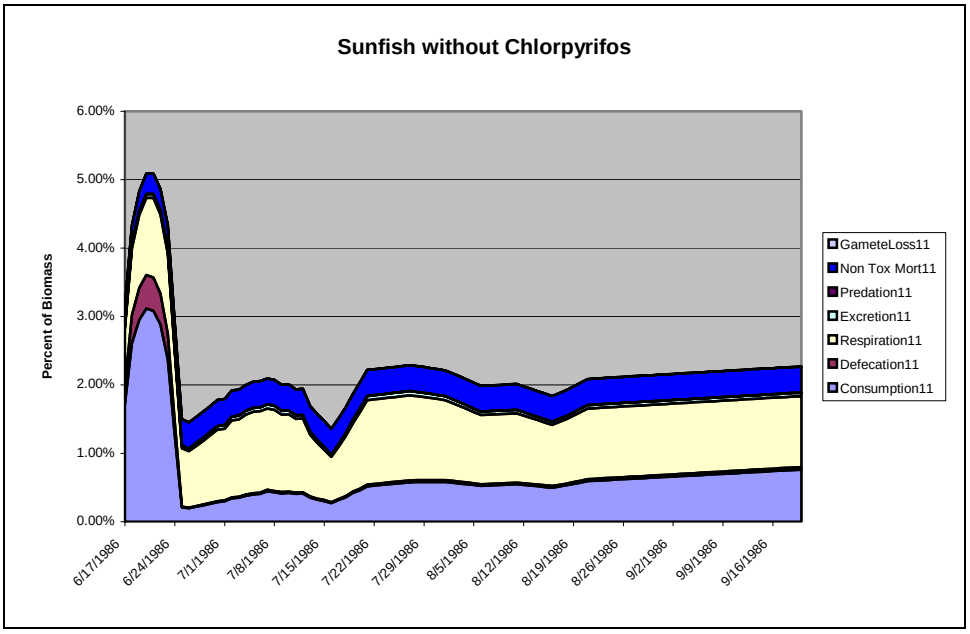


The rates were saved by choosing **Setup** from the main screen, **Save Biologic Rates**, and then **Rate Specifications**. The state variables and file type were chosen in the following screen. The plots were produced using Excel, but any spreadsheet or graphing program could be used.

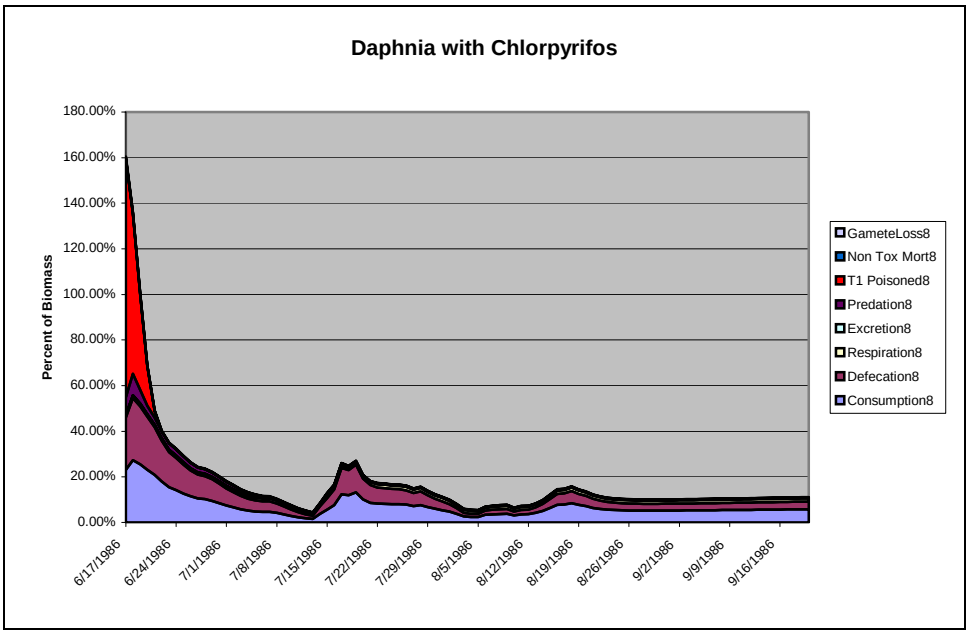


With chlorpyrifos, the sunfish immediately suffer loss of food base; there is a slight increase in defecation that is paralleled by decreased consumption in the simulation, indicating initial chronic toxicity; but, more important, there is acute toxicity as the fish bioaccumulate more chlorpyrifos. Examination of the chemical record shows that sunfish (bluegill) have a laboratory *LC50* of 2.4 **:**g/L As the bluegill begin to recover, they are still affected by chronic and acute toxicity. In particular, compare the percent defecation in the perturbed graph with the percent in the control graph that follows.

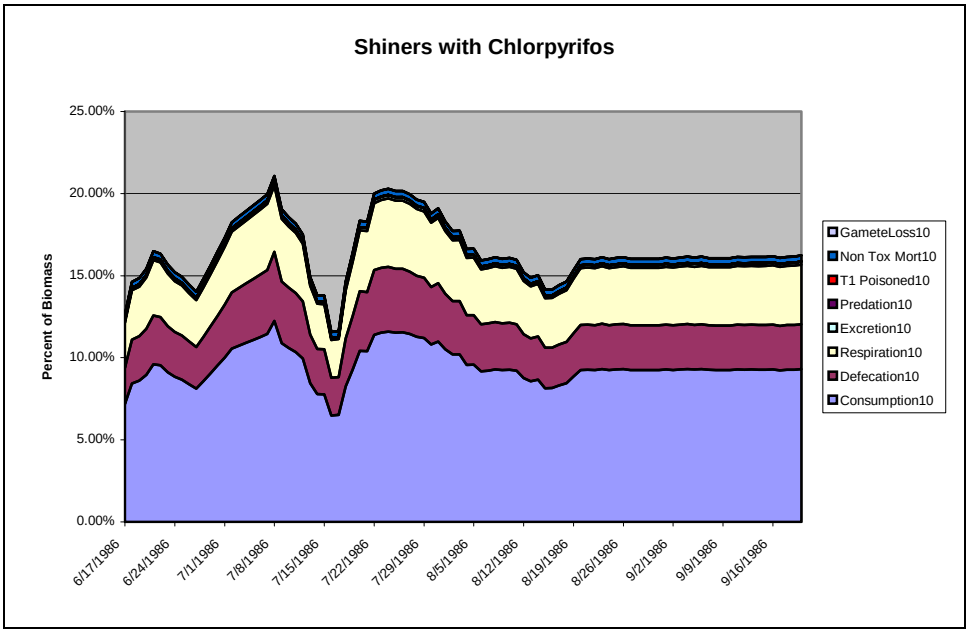




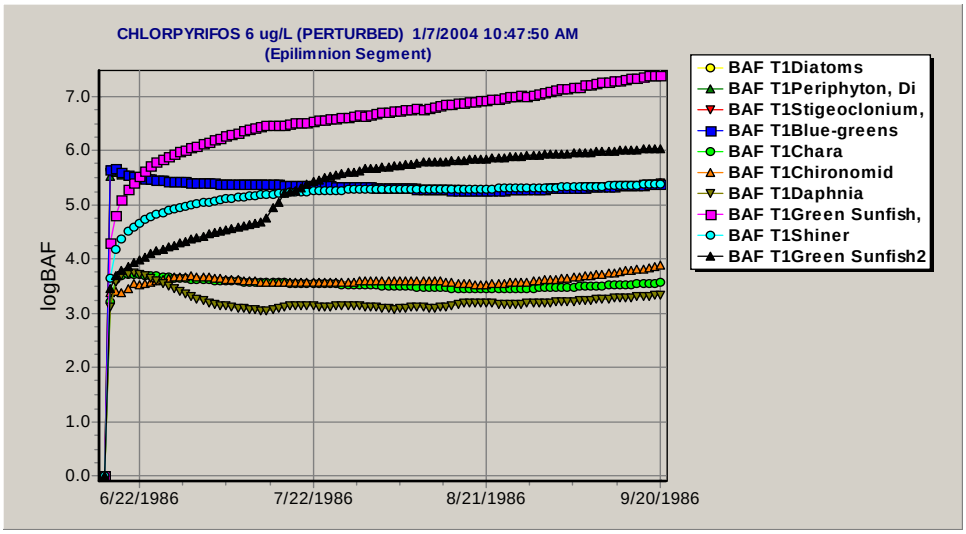
Daphnia exhibit a similar response with almost complete and immediate mortality. Their *LC50* is very low (0.17); however, there is not complete mortality, so they rebound with decreased predation pressure.



The shiners suffer a short-lived loss of food base and low-level chronic effects, but there is no acute toxicity (the minnow *LC50* is 203 ug/L), and they increase in the absence of predation pressure.



Chlorpyrifos is a bioaccumulative chemical. A plot of bioaccumulation factors indicates that there is biomagnification up the food chain, from *Daphnia* to sunfish, and that steady state has not been achieved for the fish in the three-month simulation.



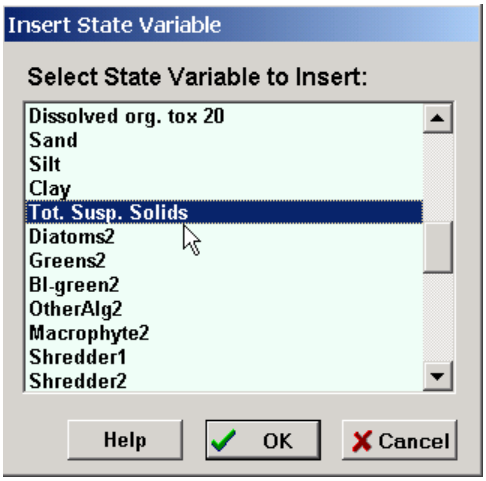
5.5 Multiple Stressors Due To Agricultural Runoff

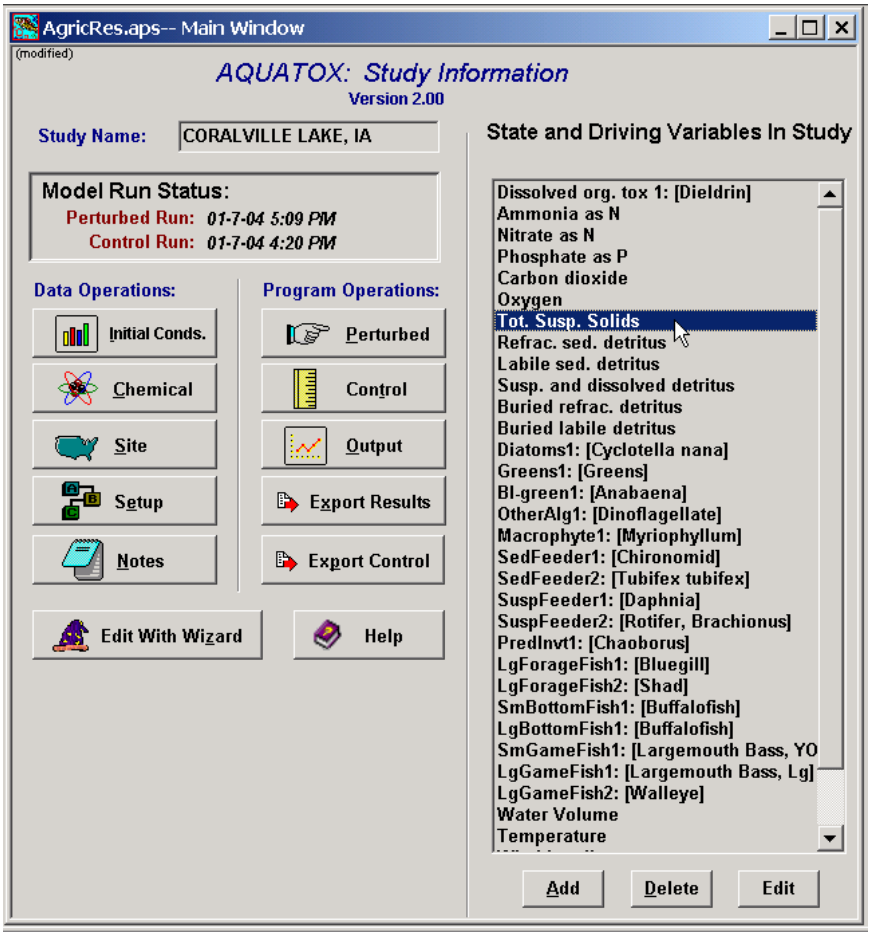
In our example, we will model a run-of-the-river reservoir receiving extensive agricultural runoff and minimal municipal and industrial effluents (Park, 1999a). In the 1970s approximately 90% of the watershed of Coralville Lake, Iowa, was in agricultural land (MacDonald and MacDonald, 1976). Water quality was so poor that the lake was referred to locally as the "Dead Sea." We will use the reservoir study ***Coralville.aps*** as a starting point. Open the file, then click on **File** and **Save As**, and name it ***AgricRes.aps*** so we don't write over the default reservoir study by mistake. Also, change the Study Name to "CORALVILLE LAKE, IA" (this will be the heading for the graphs).

Controlling Nutrients and Sediments

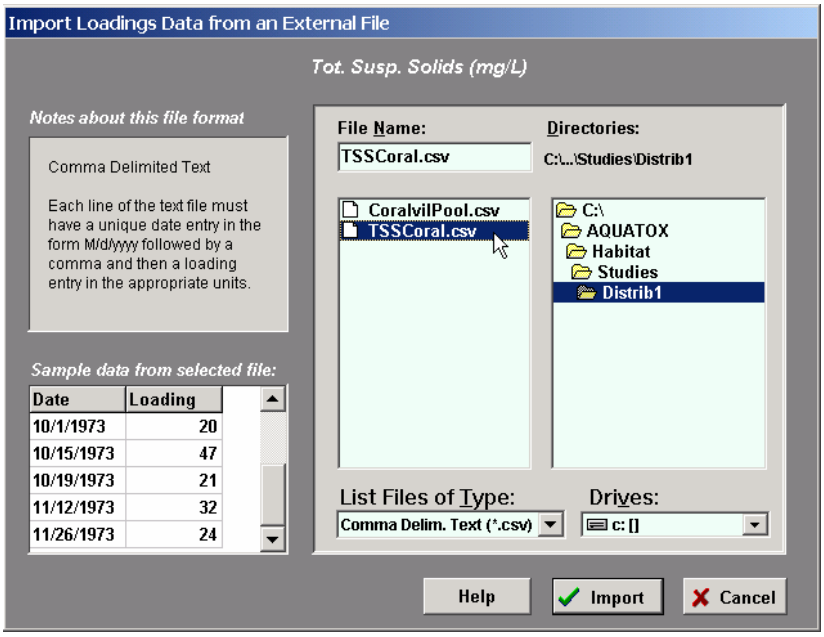
Because this reservoir receives a large quantity of suspended sediments, we need to load observed total suspended solids (TSS). Clay, silt, and sand are only available if the site is a stream. Suspended algae and detritus are subtracted from the observed TSS and the difference is considered suspended inorganic sediments. These are used in calculating the extinction coefficient and the Secchi depth.

Click on **Add** at the bottom of the state variable list and choose **Tot. Susp. Solids**. In the main screen we then see this as an additional state variable.

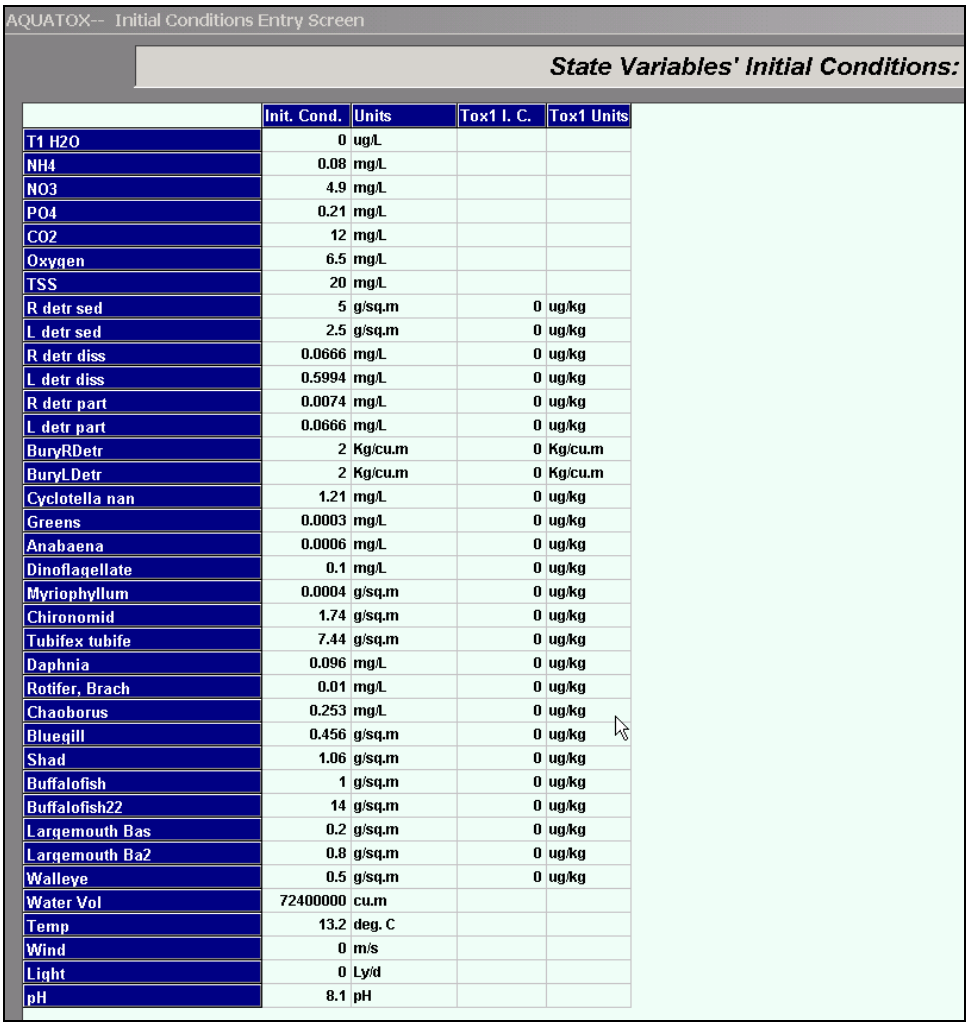




Double-click on Tot. Susp. Solids obtain the loadings screen. Then click on **Use Dynamic Valuation** and **Import** to load the file **TSSCoral.csv**. Change the initial condition of TSS to 20. **Save** the file (under the same name, **AgricRes.aps**).



Click on **Initial Conditions** to see the initial values for all the state variables. Dieldrin is 0 because we will let the model compute the concentration in the reservoir.

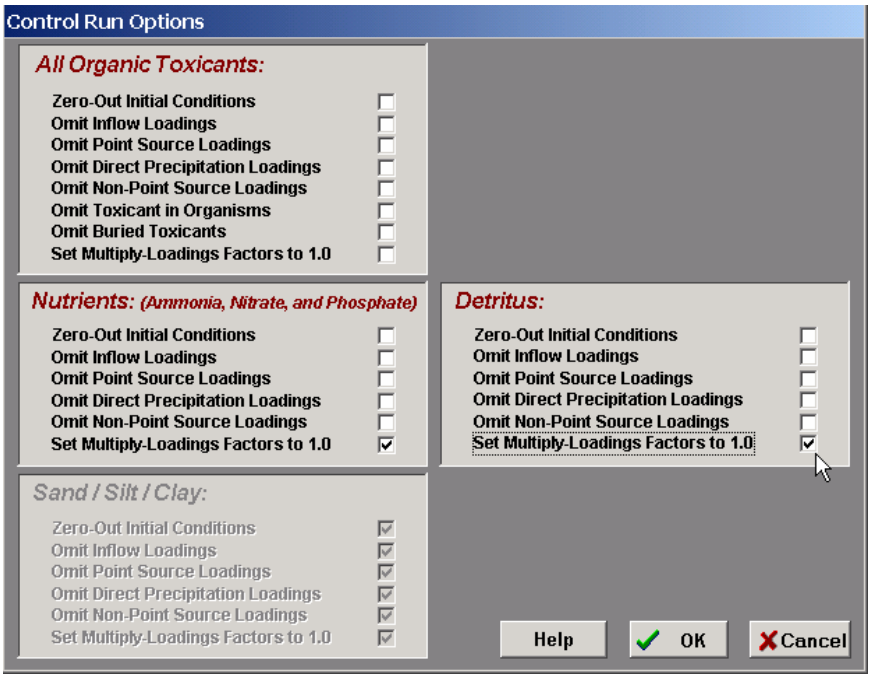


	Init. Cond.	Units	Tox1 I. C.	Tox1 Units
T1 H2O	0	ug/L		
NH4	0.08	mg/L		
NO3	4.9	mg/L		
PO4	0.21	mg/L		
CO2	12	mg/L		
Oxygen	6.5	mg/L		
TSS	20	mg/L		
R detr sed	5	g/sq.m	0	ug/kg
L detr sed	2.5	g/sq.m	0	ug/kg
R detr diss	0.0666	mg/L	0	ug/kg
L detr diss	0.5994	mg/L	0	ug/kg
R detr part	0.0074	mg/L	0	ug/kg
L detr part	0.0666	mg/L	0	ug/kg
BuryRDetr	2	Kg/cu.m	0	Kg/cu.m
BuryLDetr	2	Kg/cu.m	0	Kg/cu.m
Cyclotella nan	1.21	mg/L	0	ug/kg
Greens	0.0003	mg/L	0	ug/kg
Anabaena	0.0006	mg/L	0	ug/kg
Dinoflagellate	0.1	mg/L	0	ug/kg
Myriophyllum	0.0004	g/sq.m	0	ug/kg
Chironomid	1.74	g/sq.m	0	ug/kg
Tubifex tubife	7.44	g/sq.m	0	ug/kg
Daphnia	0.096	mg/L	0	ug/kg
Rotifer, Brach	0.01	mg/L	0	ug/kg
Chaoborus	0.253	mg/L	0	ug/kg
Bluegill	0.456	g/sq.m	0	ug/kg
Shad	1.06	g/sq.m	0	ug/kg
Buffalofish	1	g/sq.m	0	ug/kg
Buffalofish22	14	g/sq.m	0	ug/kg
Largemouth Bas	0.2	g/sq.m	0	ug/kg
Largemouth Ba2	0.8	g/sq.m	0	ug/kg
Walleye	0.5	g/sq.m	0	ug/kg
Water Vol	72400000	cu.m		
Temp	13.2	deg. C		
Wind	0	m/s		
Light	0	Ly/d		
pH	8.1	pH		

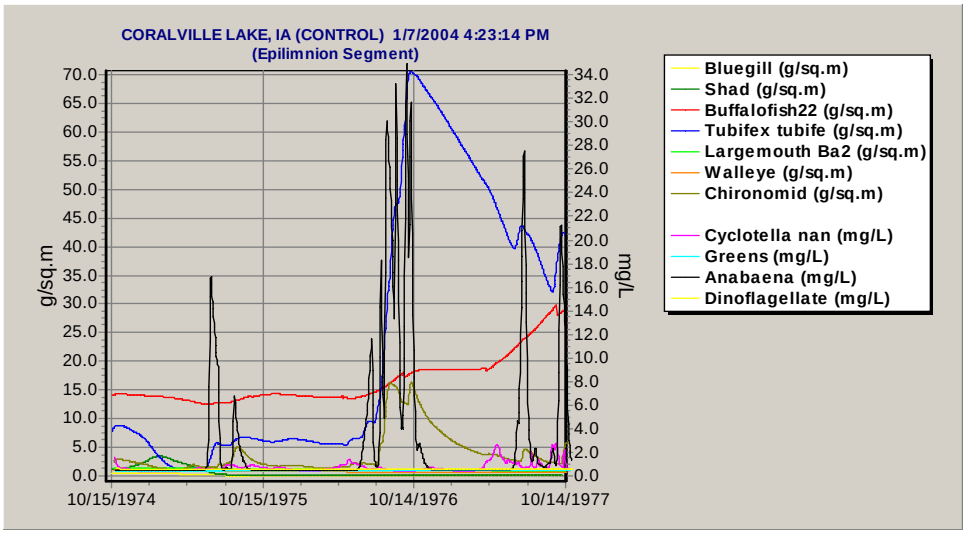
Click on **Setup** and make sure that the simulation dates correspond to, or are less than, the range of dates for TSS, 10/1/1973 to 9/30/1978. Be careful, if you enter "10/1/73" it will be interpreted as "10/01/2073." Because observed TSS values are being used in lieu of dynamically simulated inorganic sediments, the capability of the model to repeat a time-series loading should not be used for TSS unless all other loadings, particularly inflow, are restricted to the same range. Otherwise, the model will extrapolate the TSS beyond the observed dates and obtain unacceptable estimates of suspended sediments. Note that the 5-year simulation may be quite lengthy on a slow machine; you may wish to decrease the period.

First, we will investigate the impact of nutrient reduction, most likely through best management practices, without any change in loadings of dieldrin or inorganic sediments. Click on **Control Setup** and uncheck all the **Organic Toxicant** controls, and check **Set Multiply Loadings Factors to 1.0** for **Nutrients** and **Detritus**. Then, going back to the main screen, double-click on ammonia, nitrate, phosphate, and suspended and dissolved detritus and enter a multiplicative loading of 0.5 on the **Edit State Variable Data** screen for each. In doing so, we have set the model so that nutrients and detritus will be halved in the perturbed run and kept unchanged for the control run. Dieldrin will be present in both simulations. This demonstrates

the power of the control settings to set up various pollution control scenarios. Save as "**AgricRes less nutr detr.aps."**

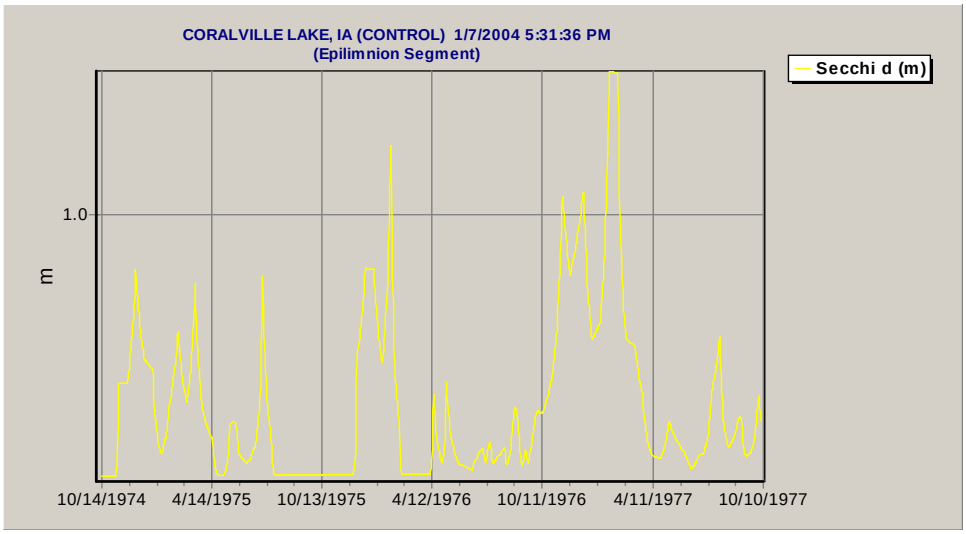


Run the simulation without any additional changes, clicking on **Perturbed** and **Control**. Select **Output,** and view the **Control** graph. Note that detritivorous invertebrates, especially *Tubifex*, have a high biomass, reflecting the large influx of detritus from upstream. Algal blooms occur periodically, with maximum biomass of about 35 mg/L.

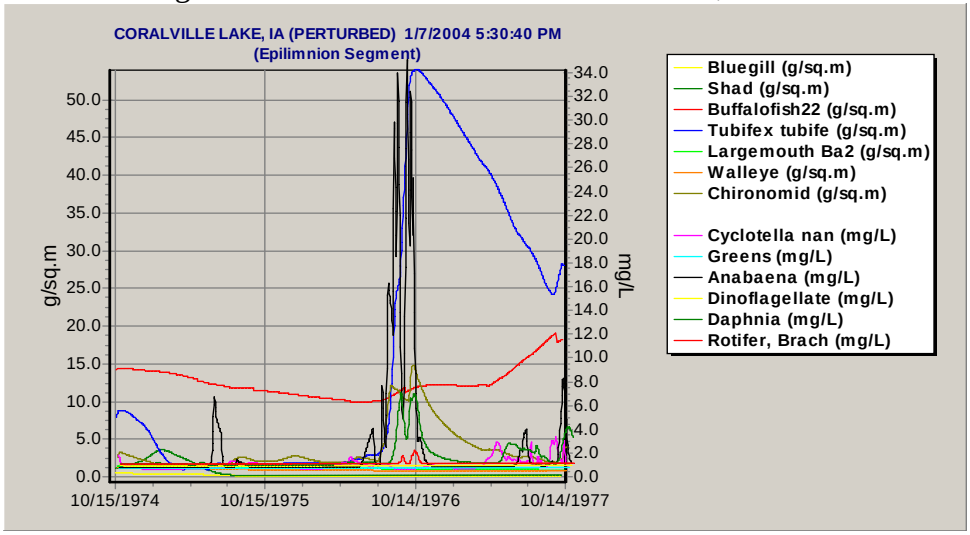


If we plot Secchi depth, we see that it varies considerably. By tabulating and exporting to Excel (click on the **Control Simulation** tab in **Output**, display Secchi d, then **Save Table to**

Excel) we can obtain statistics. In the simulation, Secchi depth has a maximum of 1.5, minimum of 0.08, and mean of 0.32 m.

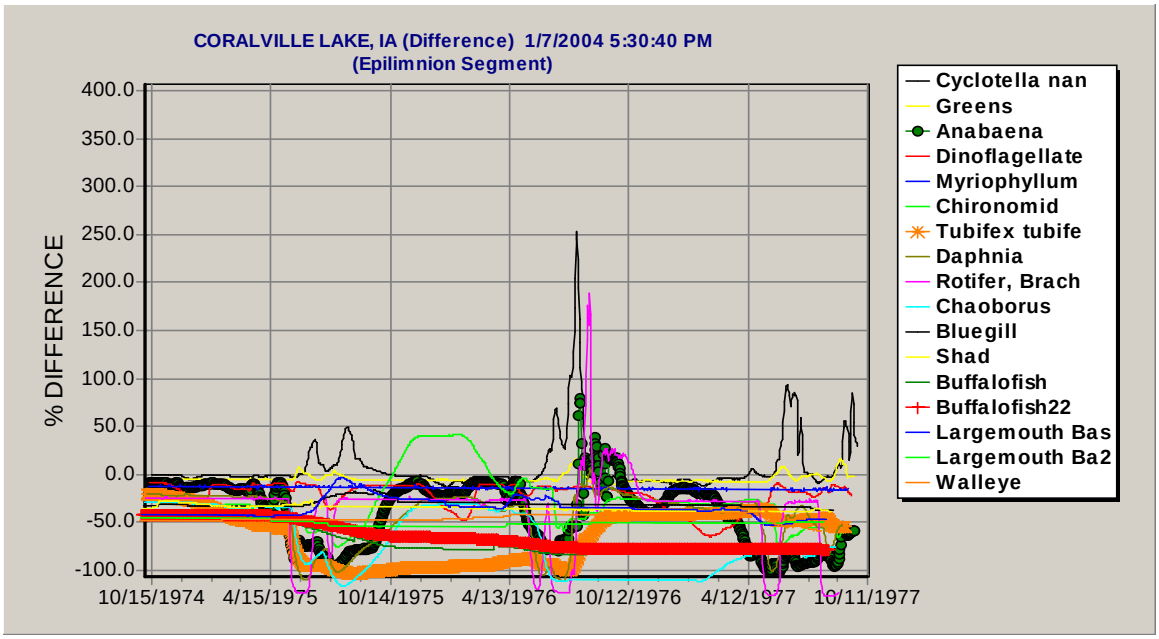


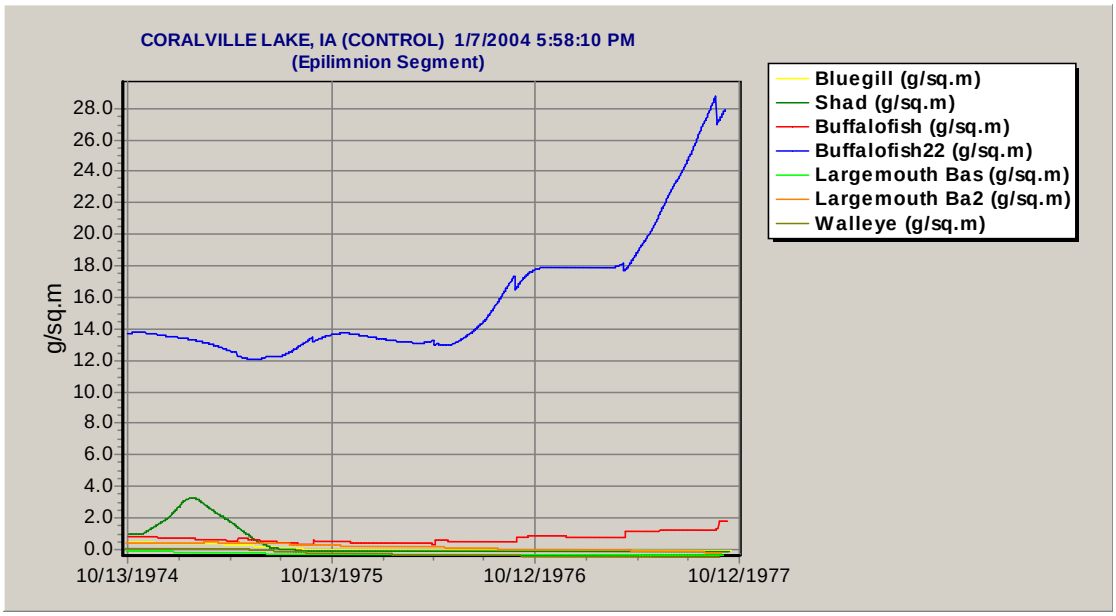
Now view the **Perturbed** graph. There is an overall similarity with the Control graph, but several algal blooms are do not occur. Furthermore, there is a decline in detritivore biomass.



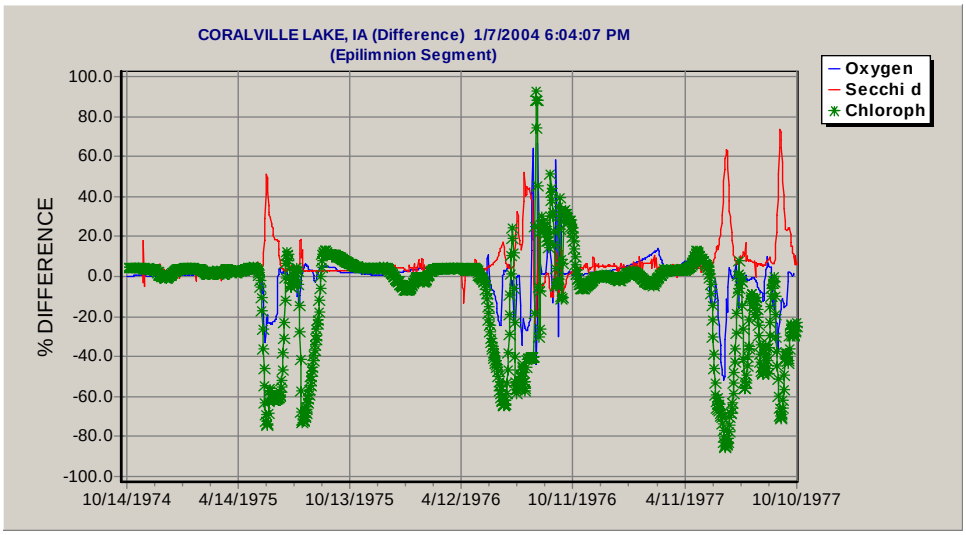
A better way to portray the changes is by plotting a **Difference** graph. Because we have set the nutrient and organic loadings in the perturbed simulation to half the normal values, a positive percent difference means an increase in biomass with decreasing nutrient and organic loadings. (Remember that the **Difference** graph plots the percent difference of **Perturbed** minus **Control.**) We also will plot bottom fish (buffalofish), which were so abundant in Coralville Reservoir that they supported a commercial fishery in the early 1970s. Based on this graph and examination of predicted rates for the invertebrates and fish, which were saved and plotted in Excel (not shown), we observe that invertebrate detritivores (*Tubifex*) declined due to decreased detritus loadings; this caused a decline in buffalofish. The blue-green *Anabaena*, another indicator of poor water quality, also declined. Caution should be exercised in interpreting difference graphs; these are plotted as percent changes, and small absolute differences are

magnified. For example, due to the toxicity of dieldrin, bass exhibit very low biomass values (<0.1 g/m^2), even in the control. This can be seen by plotting just the fish in the control simulation.



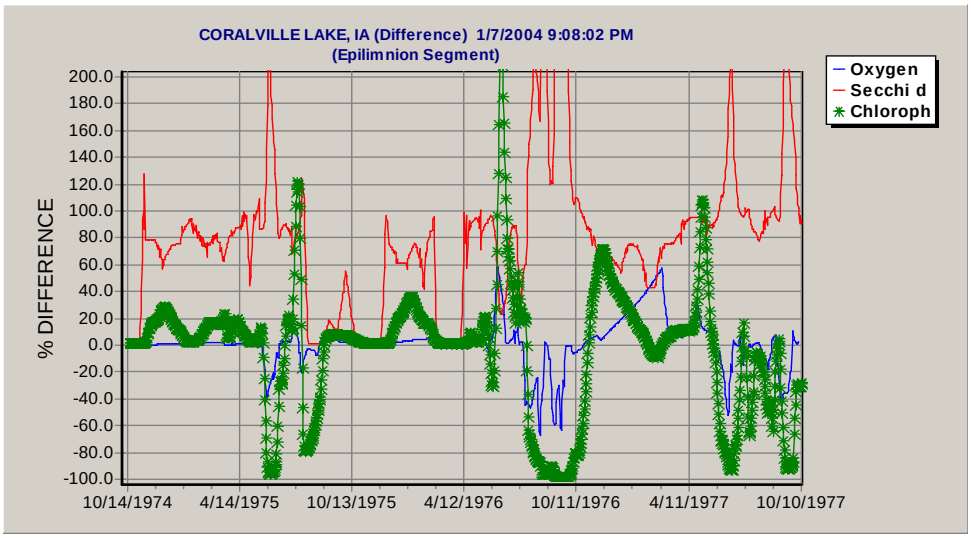


If we plot the difference graph for the key environmental indicators, oxygen, Secchi depth, and chlorophyll, we see that halving the nutrient and detrital loadings improves the water quality as indicated by decreased chlorophyll levels and increased Secchi depths during times of algal blooms. Because the reservoir is shallow and seldom stratified, oxygen levels are not good indicators of water quality in this system; actually, supersaturation of oxygen is predicted during blooms.

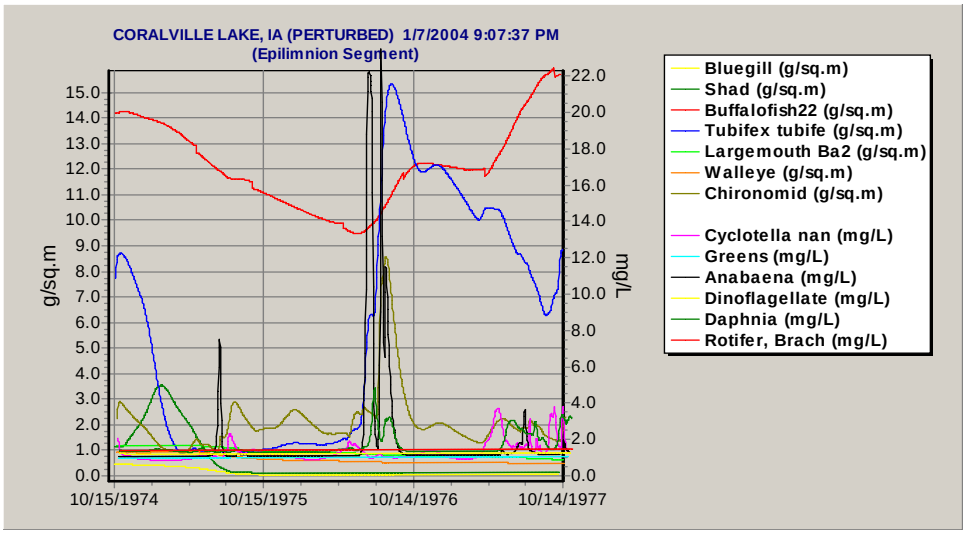


We have seen the effects of halving the nutrient and detritus loadings; let us now investigate the effects of suspended sediments. In this run-of-the-river reservoir, most of the suspended solids are silt and clay, and most are from upstream. In the event that best management practices (BMPs) were to halve the TSS as well as the other pollutants, what would be the impacts on the Coralville ecosystem? This is easily analyzed with AQUATOX. In the main window, double-click on **Tot. Susp. Solids** and set the **Multiply loading** to 0.5. Save the modified study as "**AgricRes less nutr detr TSS.aps**." Then click **Perturbed** (but do not run **Control**) to obtain a simulation in which all the loadings are halved.

Click **Output** and plot Secchi depth, chlorophyll *a*, and oxygen in the **Difference** graph. By decreasing TSS, and hence inorganic sediments, turbidity decreases, and Secchi depth increases considerably. Baseline chlorophyll *a* increases marginally; blooms appear to be short-lived, followed by even greater declines in chlorophyll. Phytoplankton are not as severely light limited in the simulation. In turn, during blooms phosphate is quickly depleted—almost certainly becoming limiting for the phytoplankton.

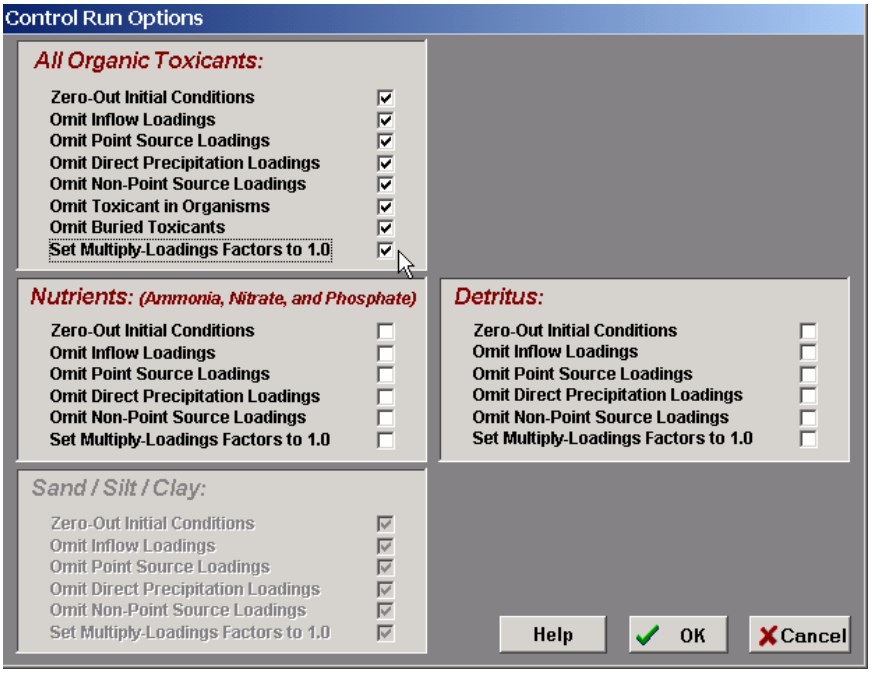


The perturbed graph demonstrates the changes in biomass; *Tubifex* reaches a maximum of 14 g/m^2, and *Anabaena* reaches a maximum of 17 g/m^2. Compare those with values of 34 and 70 g/m^2 in the control.

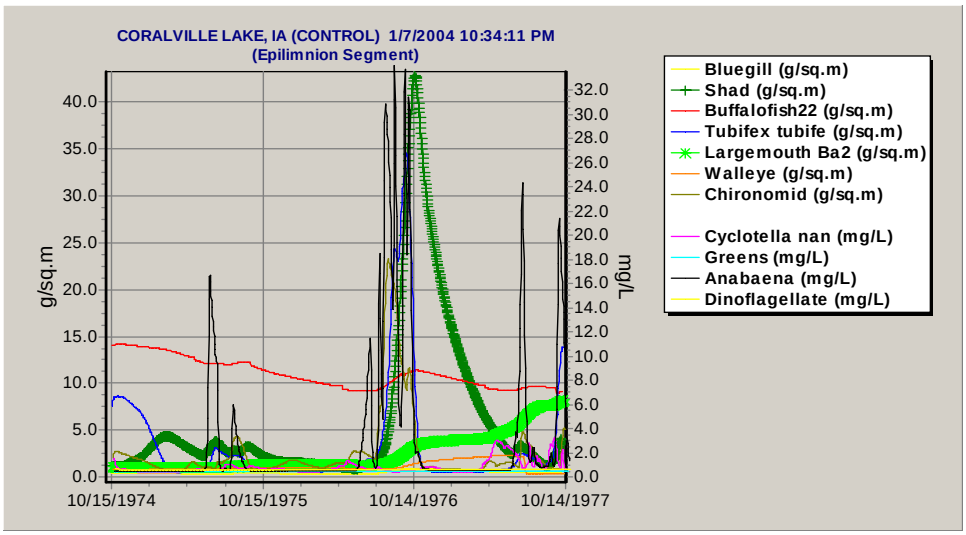


Controlling Pesticides

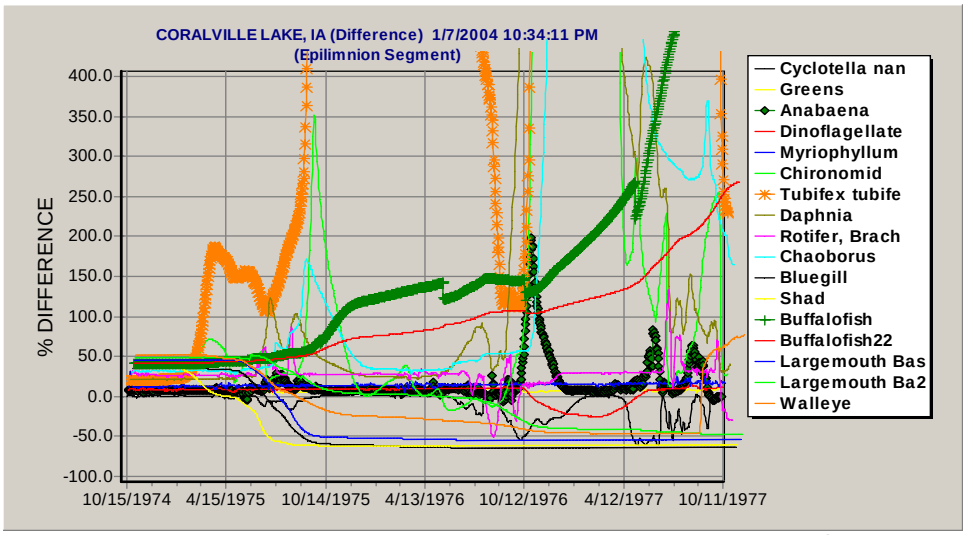
Next, we will examine the effects of the dieldrin independent of the nutrients, detritus, and TSS. Similar to the example of esfenvalerate in the pond, we will use the perturbed run to simulate the toxicant and the control run without the toxicant. Therefore, open **AgricRes.aps**, open the **Setup** window, and choose **Control Setup**. Now set the remaining options back to their original state, with all the **Organic Toxicant** choices checked, and the **Nutrient** and **Detritus** choices unchecked.



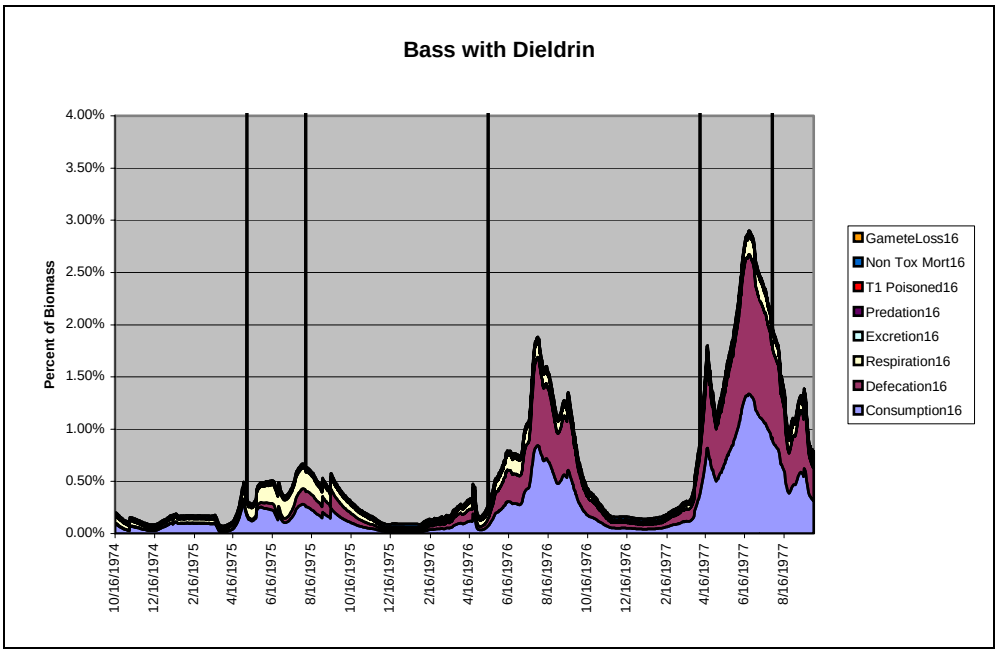
Click **Perturbed** and **Control** to run the simulations. The perturbed graph is the equivalent of the control graph seen earlier with the effects of dieldrin on selected state variables. The control graph shows the seasonal patterns in biomass in this highly productive reservoir without dieldrin. Note that forage fish (shad) reach a maximum of 42 g/m^2, and bass slowly increase to a maximum of 7.8 g/m^2, while buffalofish gradually decline.

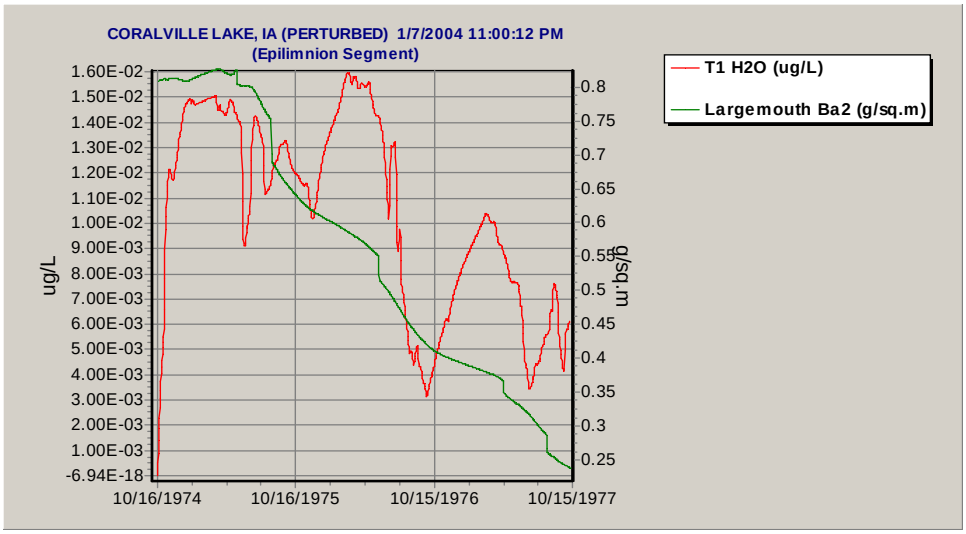


The differences between the perturbed and control graphs are emphasized in the difference graph. Negative values indicate relatively low biomass values in the perturbed simulation (in other words, in the presence of dieldrin). The decline of all fish except the hardy buffalofish is easily seen; first shad, then YOY bass, walleye, and adult bass decline in that order. The tolerant chironomids and tubificids benefit from the decreased predation and exhibit positive values.



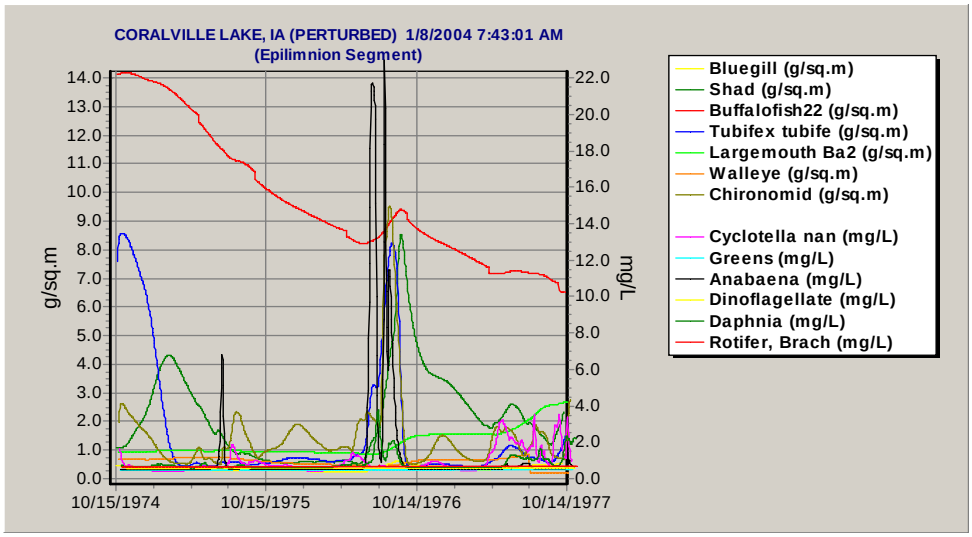
From these results, we postulate that the decline in fish is a combination of direct and indirect effects of dieldrin. We can examine the rates for largemouth bass by clicking on **Setup** in the main screen and **Save Biologic Rates** and **Rate Specifications**, then choosing **Lg g fish** prior to running the model. The rates will be saved, with Excel format as the default, in the Output subdirectory. The rates then can be plotted. In this example, consumption is very low due to chronic toxicity and loss of forage base. Acute toxicity does not seem to be a factor; the *LC50* for bass is 3.5 ug/L, and the maximum concentration of dieldrin in the dissolved phase is 0.016 ug/L during the period of the simulation. Defecation increases due to the modeled effect of chronic toxicity on assimilation. This illustrates the use of biologic rates for analyzing cause and effect relationships.



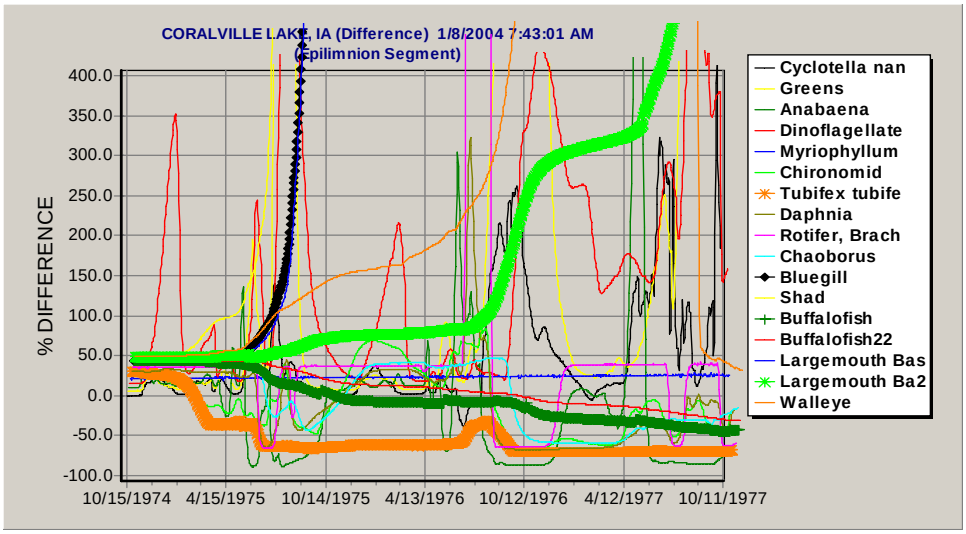


Controlling All Pollutants

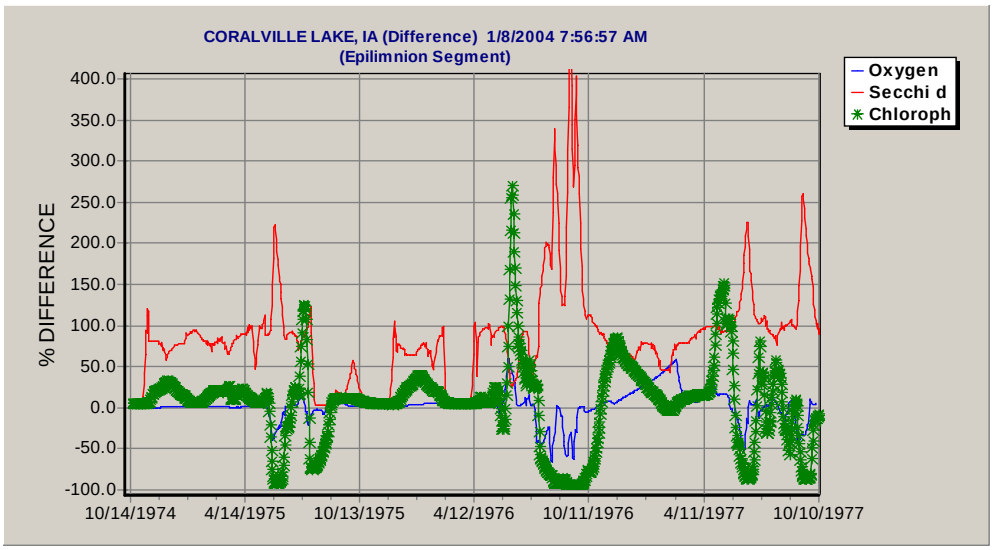
Finally, we can examine the effects of decreasing all pollutants from agricultural runoff simultaneously in the perturbed simulation. Dieldrin was set to a minimal value (loading multiplier of 0.001), and the nutrient, organic matter, and TSS multiplicative loading factors were set to one-half. As we have seen from the above applications, there are many complex interactions, and comparing the perturbed and control graphs is difficult.



However, the difference graph provides a direct comparison. Bluegill (diamonds) and bass (heavy light-green line) increase significantly in the absence of dieldrin. Tubificids (heavy orange line) and chironomids decline due to increased predation pressure. The buffalofish (heavy dark-green line) exhibit a long-term decline due to loss of forage because of increased competition.



To better determine the effects of decreasing all pollutants on water quality, we will again plot several environmental indices in a difference graph. We see that chlorophyll a is generally lower, oxygen does not supersaturate during blooms, and Secchi depth is improved.



We could have performed a full factorial analysis to isolate the effects of individual pollutants. For example, we could have decreased phosphate loadings while holding all other pollutant loadings at the observed levels. However, that is beyond the scope of this tutorial.

In conclusion, AQUATOX can be used to analyze complex relationships in impaired ecosystems and to suggest the relative importance of various causes of impairment. In this example, dieldrin was shown to be a very important stressor, completely changing the fish community, even at sub-acute concentrations. The simulations suggest that external loadings of nutrients and organic matter are also important; and, based on the model, halving the loadings could improve water quality significantly. Therefore, this ecosystem model has the potential not only to help identify stressors, but to assess possible environmental management scenarios as well.

6 UNCERTAINTY ANALYSIS

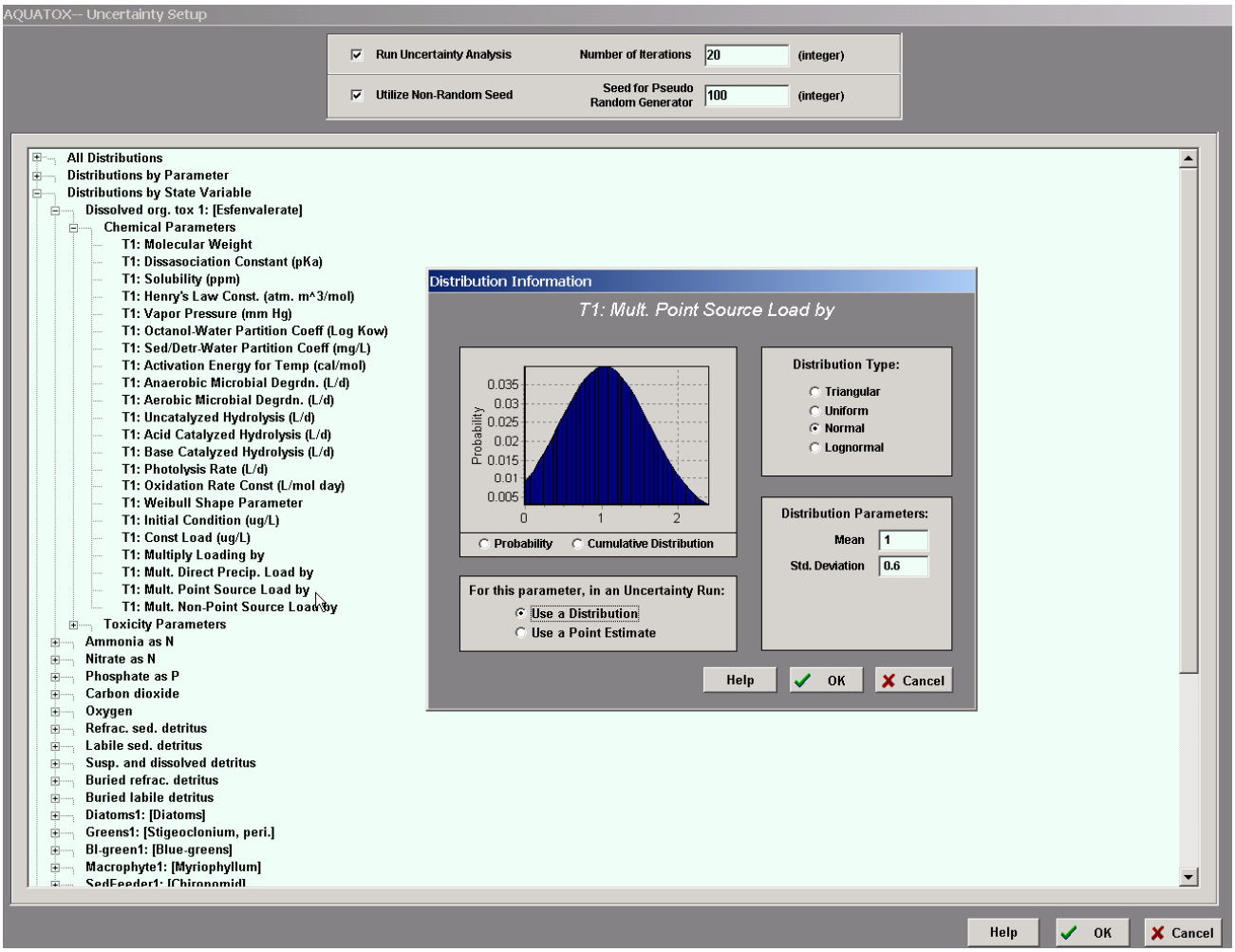
Until now we have dealt with deterministic simulations. However, there are numerous sources of uncertainty and variability in natural and polluted aquatic systems. These can be represented easily in AQUATOX (see **Technical Documentation**), although access to the additional analytical power is not obvious to the casual user. We will go back to **ESFenPond.aps** for this example. Open and rename the study "**ESFenPond U.aps."** Click on the **Setup** button and choose **Uncertainty Setup**.

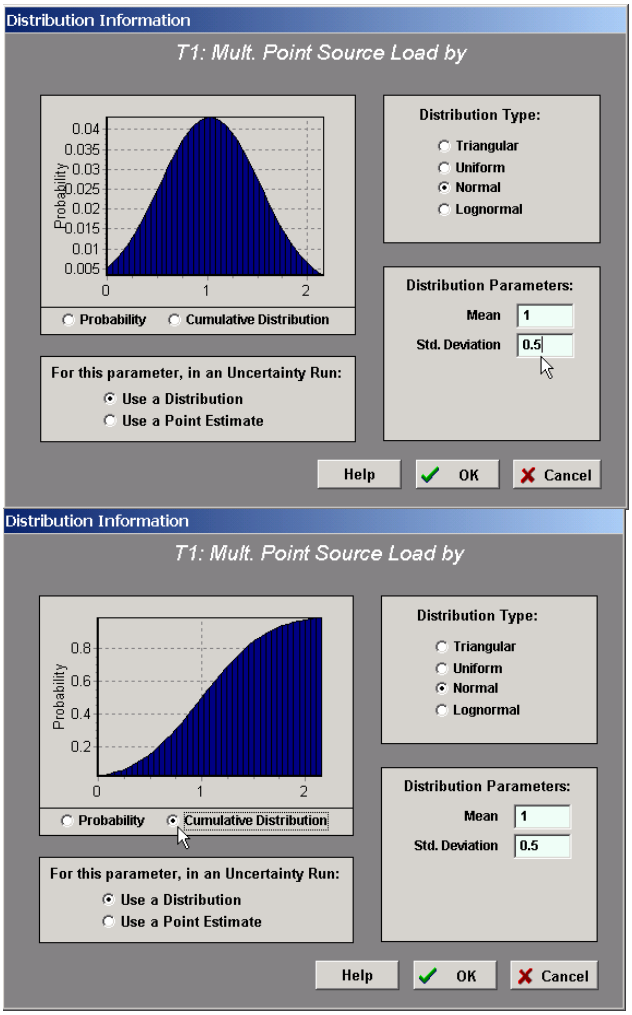
That will open a large window with several choices at the top. Because AQUATOX uses a Latin hypercube sampling algorithm, it requires far fewer iterations than brute-force Monte Carlo sampling. Therefore, the default number of iterations is 20. This is probably adequate for an analysis involving a single variable; however, it should be increased as more variables are chosen for analysis (and could be decreased if you just wish to become familiar with the procedure). To replicate the sampled values in successive analyses, you should choose a non-random seed for the number generator and keep it the same.

A tree structure allows the user to navigate easily through all variables subject to uncertainty analysis and to list those variables already chosen for analysis. We will choose **Distributions by State Variable**, **Dissolved org. tox 1:[Esfenvalerate]**, **Chemical Parameters**, and **T1: Mult. Point Source Load by**. The latter will open a separate interactive window to aid in picking a distribution and choosing the parameters. Choose **"Use a Distribution**" to activate the window.

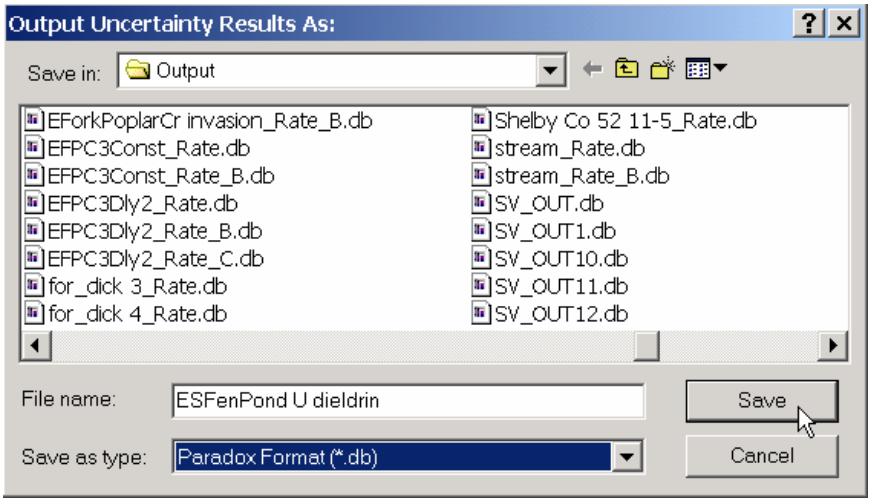
A normal distribution is the default, with a standard deviation of 60% of the mean. The user can accept the default distribution parameters or change them. The graph will show the results of any changes. The mean values are derived from the underlying parameter sets, but altering them in the uncertainty screen will not change them in the database and the deterministic simulation. We will keep the normal distribution, but change the standard deviation to 0.5 to avoid significant truncation at 0 (which has the effect of biasing the distribution toward higher values). We can also plot the approximate cumulative distribution that is used in the Latin hypercube sampling. Let's use that distribution to vary the multiplicative factor for point-source loadings of esfenvalerate in water. For each iterative simulation, the model will sample one value from the distribution and use it as a multiplicative factor for all dynamic point-source loading values.

Click on **OK**, which will take you back to the tree structure. You should collapse the tree structure and choose **Selected Distributions for Uncertainty Run** to make sure that you are using only the distributions that you intend to use. Also, be sure that the button in the upper left is checked to **Run Uncertainty Analysis** (that button is a convenient way to toggle between the deterministic and uncertainty options without disturbing the individual distributions). Back on the main screen, we see that there is now a message in red in the upper right indicating the number of iterations chosen. That message only appears when the uncertainty analysis is enabled.

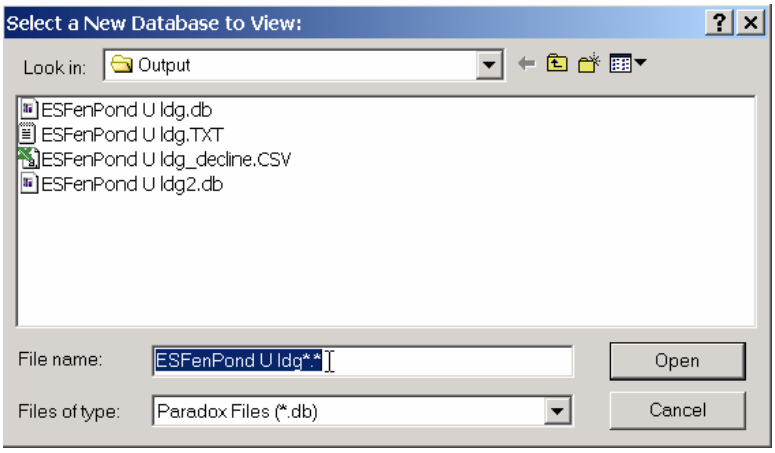

AQUATOX-- Uncertainty Setup
Run Uncertainty Analysis
Number of Iterations
20
(integer)
Utilize Non-Random Seed
Seed for Pseudo Random Generator
100
(integer)
All Distributions
Distributions by Parameter
Distributions by State Variable
Dissolved org. tox 1: [Esfenvalerate]
Chemical Parameters
T1: Molecular Weight
T1: Dissasociation Constant (pKa)
T1: Solubility (ppm)
T1: Henry's Law Const. (atm. m^3/mol)
T1: Vapor Pressure (mm Hg)
T1: Octanol-Water Partition Coeff (Log Kow)
T1: Sed/Detr-Water Partition Coeff (mg/L)
T1: Activation Energy for Temp (cal/mol)
T1: Anaerobic Microbial Degrdn. (L/d)
T1: Aerobic Microbial Degrdn. (L/d)
T1: Uncatalyzed Hydrolysis (L/d)
T1: Acid Catalyzed Hydrolysis (L/d)
T1: Base Catalyzed Hydrolysis (L/d)
T1: Photolysis Rate (L/d)
T1: Oxidation Rate Const (L/mol day)
T1: Weibull Shape Parameter
T1: Initial Condition (ug/L)
T1: Const Load (ug/L)
T1: Multiply Loading by
T1: Mult. Direct Precip. Load by
T1: Mult. Point Source Load by
T1: Mult. Non-Point Source Load by
Toxicity Parameters
Ammonia as N
Nitrate as N
Phosphate as P
Carbon dioxide
Oxygen
Refrac. sed. detritus
Labile sed. detritus
Susp. and dissolved detritus
Buried refrac. detritus
Buried labile detritus
Diatoms1: [Diatoms]
Greens1: [Stigeoclonium, peri.]
Bl-green1: [Blue-greens]
Macrophyte1: [Myriophyllum]
SedFeeder1: [Chironomid]
Distribution Information
T1: Mult. Point Source Load by
Probability
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
1
2
Probability
Cumulative Distribution
Distribution Type:
Triangular
Uniform
Normal
Lognormal
Distribution Parameters:
Mean
1
Std. Deviation
0.6
For this parameter, in an Uncertainty Run:
Use a Distribution
Use a Point Estimate
Help
OK
Cancel
Help
OK
Cancel



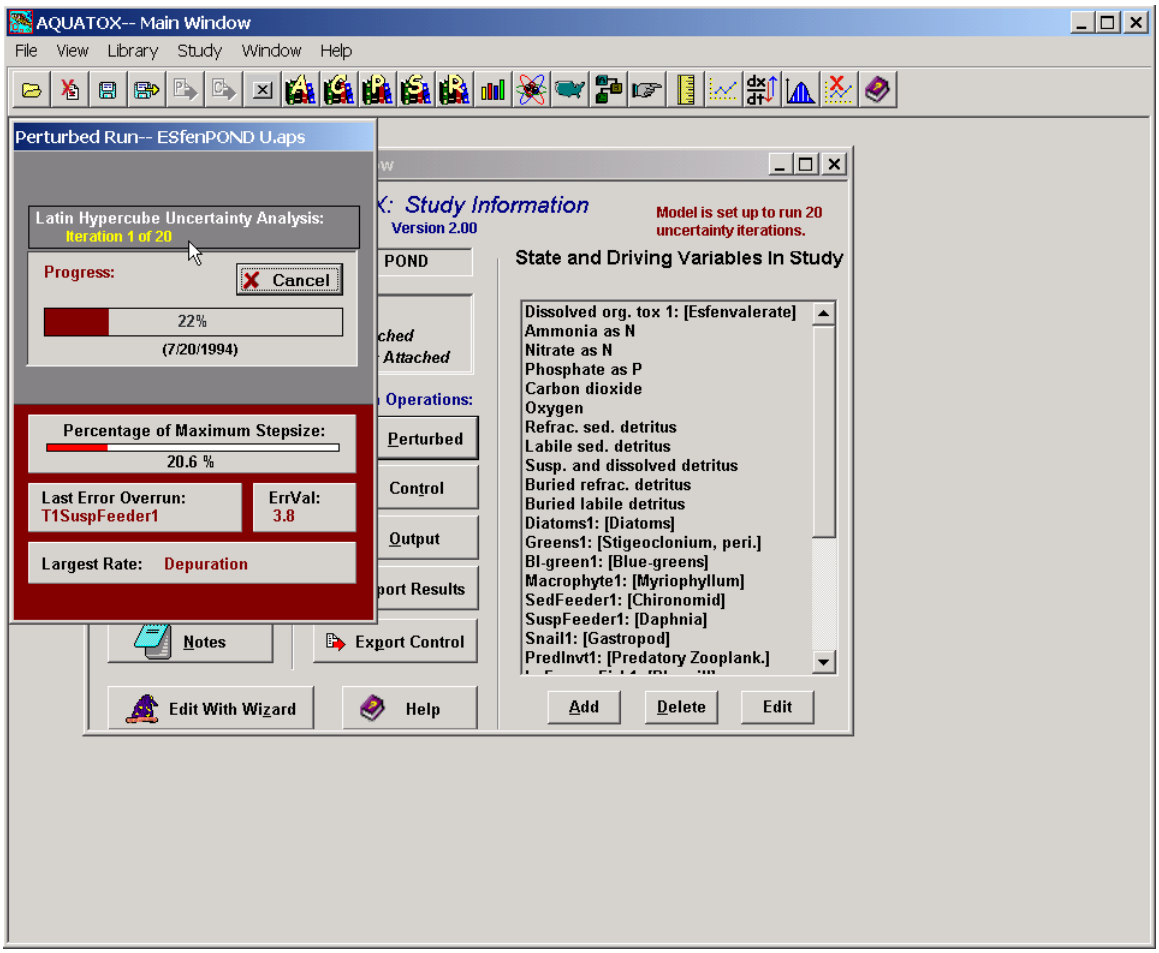
When you click on **Perturbed** or **Control** you will be asked to give the output file name and location. The folder to **Save** in will be given as the Output folder, which is the default; you might wish to change that to the Studies folder or some other special folder.

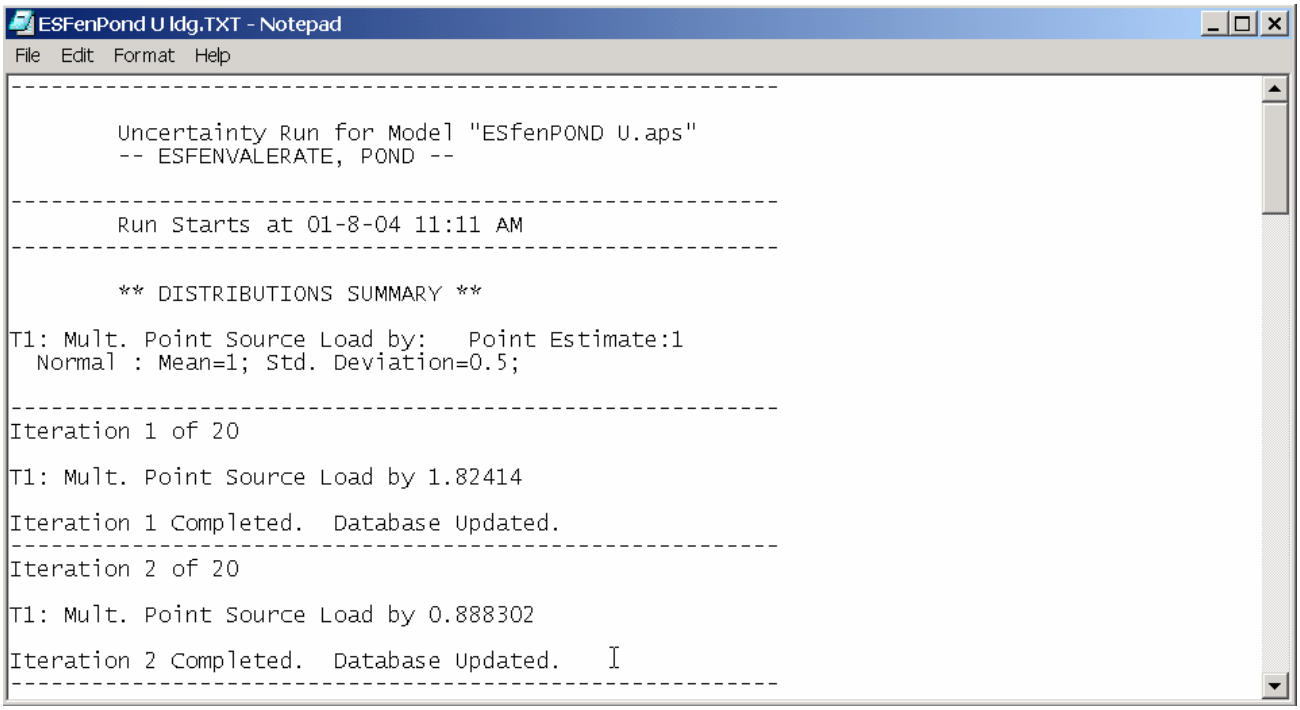


Because of the voluminous output, it will be split into two or more separate files using the root name that you provide. Ordinarily, you will not have to concern yourself with the supplemental files, which will be listed in subsequent Save operations. However, you can load a different database file to view a previous uncertainty analysis.

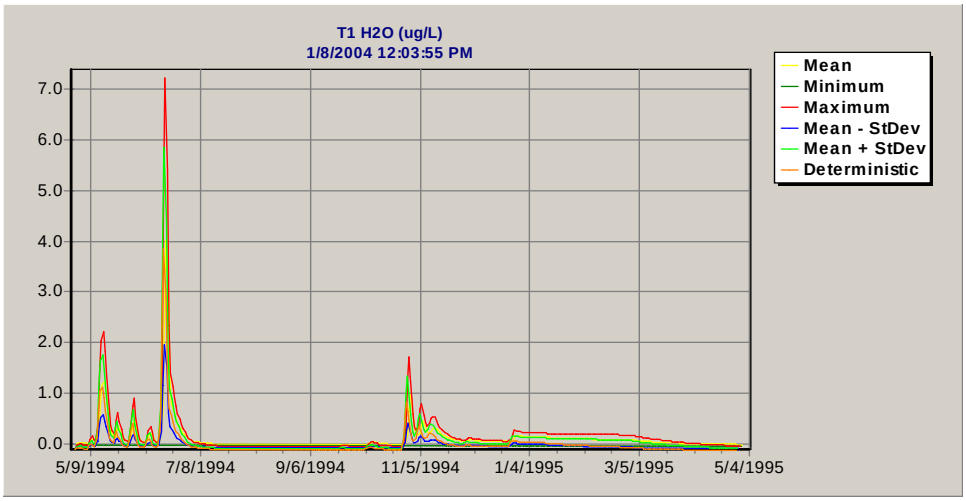


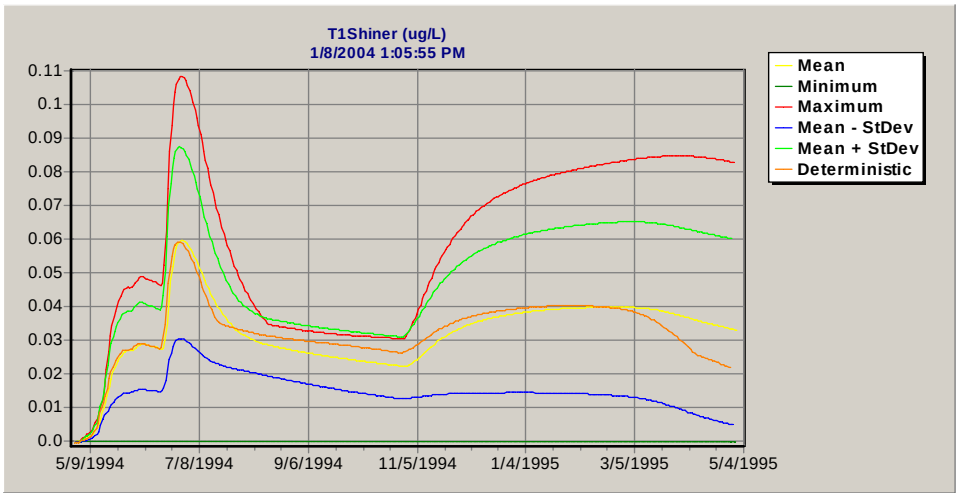
The model will perform a deterministic simulation first to provide a baseline. Then it will cycle through the uncertainty iterations, with a window to keep you informed of the progress. The specifications for each successive simulation are saved in a text file so that one can determine exactly what parameter values were used. A file labeled with a suffix of "_decline.CSV" saves the results for the biomass risk graph, discussed below.

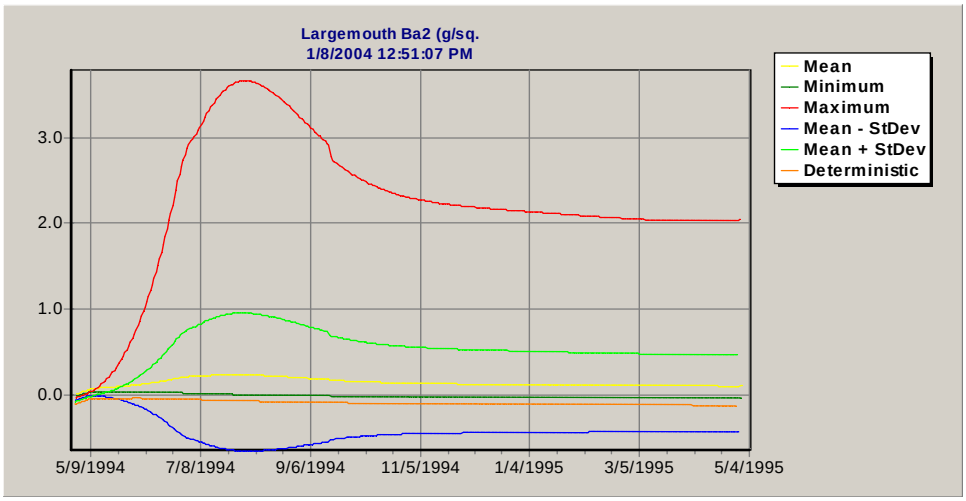

AQUATOX-- Main Window
File View Library Study Window Help
Perturbed Run-- ESfenPOND U.aps
Latin Hypercube Uncertainty Analysis:
Iteration 1 of 20
Progress:
Cancel
22%
(7/20/1994)
Percentage of Maximum Stepsize:
20.6 %
Last Error Overrun:
T1SuspFeeder1
ErrVal:
3.8
Largest Rate: Depuration
Study Information
Version 2.00
Model is set up to run 20 uncertainty iterations.
POND
State and Driving Variables In Study
Operations:
Perturbed
Control
Output
Notes
Export Control
Edit With Wizard
Help
Add
Delete
Edit
Dissolved org. tox 1: [Esfenvalerate]
Ammonia as N
Nitrate as N
Phosphate as P
Carbon dioxide
Oxygen
Refrac. sed. detritus
Labile sed. detritus
Susp. and dissolved detritus
Buried refrac. detritus
Buried labile detritus
Diatoms1: [Diatoms]
Greens1: [Stigeoclonium, peri.]
Bl-green1: [Blue-greens]
Macrophyte1: [Myriophyllum]
SedFeeder1: [Chironomid]
SuspFeeder1: [Daphnia]
Snail1: [Gastropod]
PredInvt1: [Predatory Zooplank.]

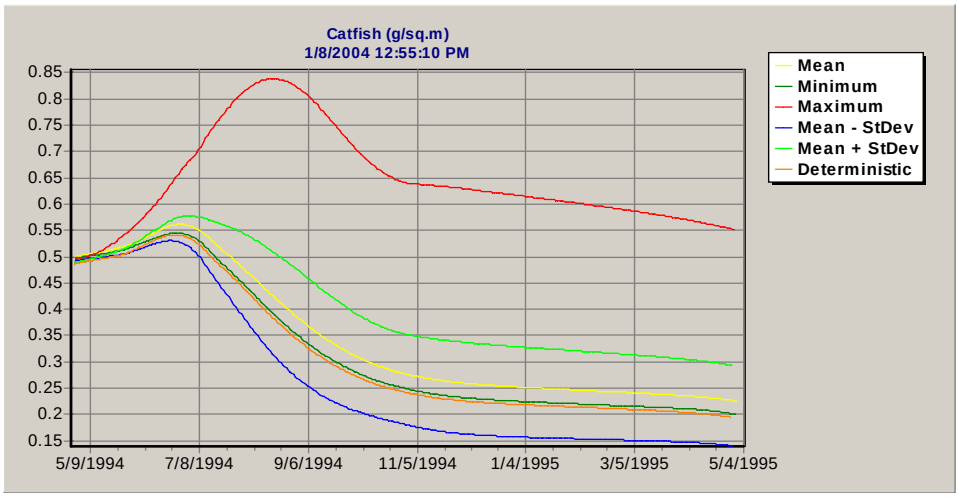

ESFenPond U ldg.TXT - Notepad
File Edit Format Help
Uncertainty Run for Model "ESfenPOND U.aps"
-- ESFENVALERATE, POND --
Run Starts at 01-8-04 11:11 AM
** DISTRIBUTIONS SUMMARY **
T1: Mult. Point Source Load by: Point Estimate:1
Normal : Mean=1; Std. Deviation=0.5;
Iteration 1 of 20
T1: Mult. Point Source Load by 1.82414
Iteration 1 Completed. Database Updated.
Iteration 2 of 20
T1: Mult. Point Source Load by 0.888302
Iteration 2 Completed. Database Updated.

The results of the uncertainty analysis can be viewed by scrolling to the far right tab in the **Output**, and clicking on **Uncertainty Graph**. If you have not run a simulation or if you wish to see the results of a different simulation, you may choose to **View a Different Database**; furthermore, with a large number of state variables in a study, you may have to load a different database (it will have the same name you gave the uncertainty output followed by "2"). Only one state variable is plotted at a time, with separate curves for mean, minimum, maximum, mean - one standard deviation, mean + one standard deviation, and deterministic results. The deterministic simulation will use the value(s) entered for the uncertainty simulations. In this example, the concentration of esfenvalerate in the water is the default plot. You may choose to **View a Different Variable**, such as the mass of toxicant associated with shiners or the biomass of bass. These are the distributions of the results for a particular state variable and are not necessarily a reflection of the distribution of the sampled input variable. For example, the maximum loading of esfenvalerate would almost certainly result in the minimum biomass of the bass (the mean – standard deviation is negative in this example, and the minimum is 0). Plotting catfish, we see that they are much more tolerant of esfenvalerate, although their biomass in the pond declines under all scenarios. Unless you specify a seed value for the random number generator and use the same number of iterations, you will get different results for these probabilistic simulations.

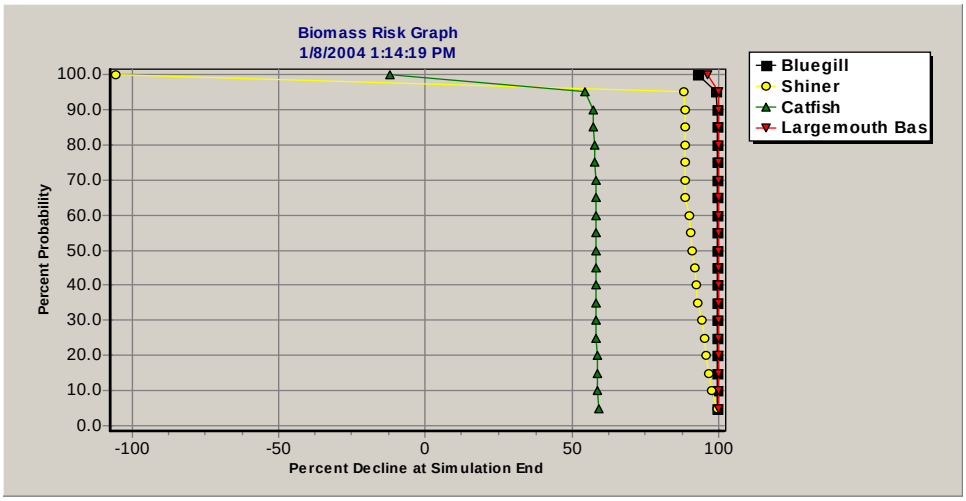




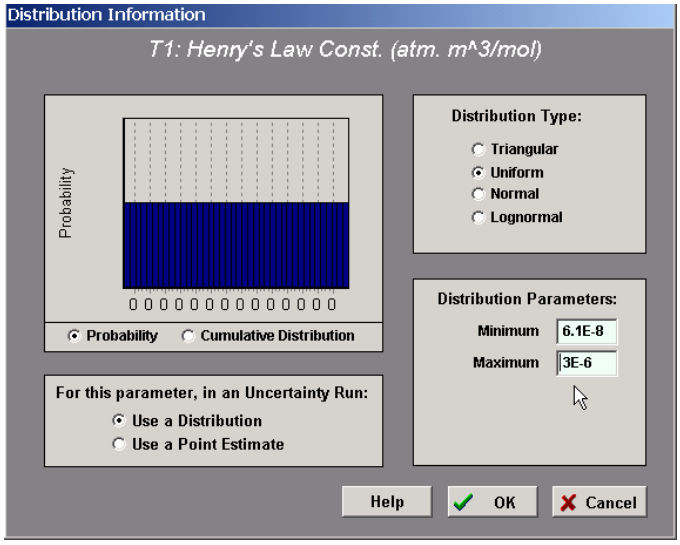




A better way to compare the relative responses of organisms is to **View Biomass Risk Graph** and designate the organisms you wish to compare. In this example, catfish and shiners are the most tolerant to esfenvalerate; and, under at least one exposure scenario, they actually increase (a "negative decline"). Note that each point on the graph corresponds to an iteration; if the curves are not smooth, you may wish to increase the number of iterations to provide more control. See **Volume 2: Technical Documentation** for additional information.

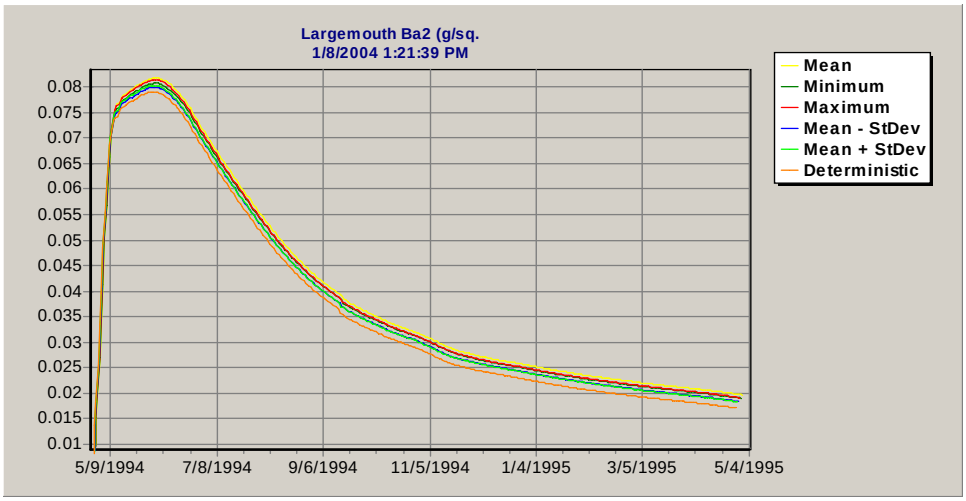


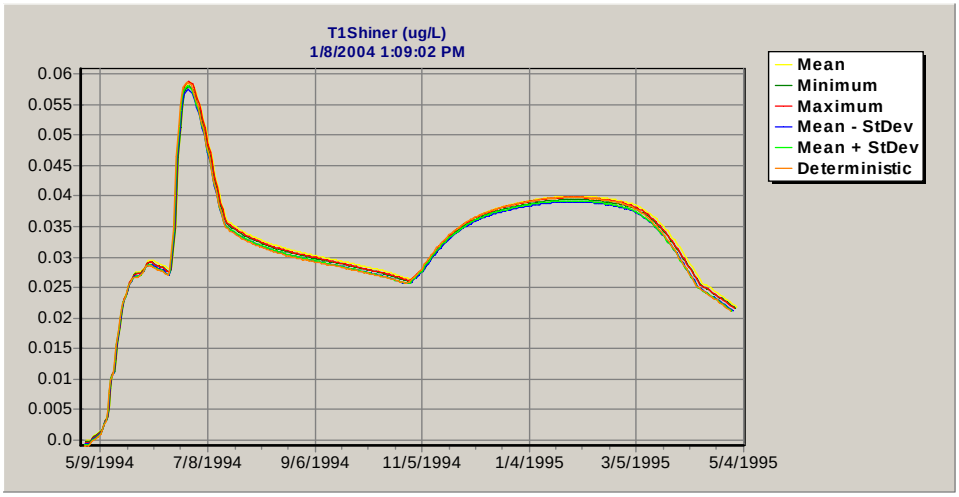
Similarly, we can vary the input values for other variables by sampling from the appropriate distributions. For example, we have two values for the Henry's Law constant for esfenvalerate: a measured value of 6.1E-8 and a calculated value of 3.0E-6 (ARS Pesticide Property Database). Why not just use the measured value? Unfortunately, the constant is not easily measured, so the calculated value may have as much validity as the measured value. Therefore, we can use a uniform distribution defined by the two values, with equal probability of any value over that range being chosen. Henry's Law constant helps control the bioavailability of organic toxicants, so the sensitivity to a range of possible values is of interest. Before running the simulation, though, let's change the multiplicative loading for point sources back to 0.2, and click on **Use a Point Estimate** to remove that variable from the uncertainty analysis. Furthermore, it is not necessary to use 20 iterations for a single uniform distribution, so change it to 10.



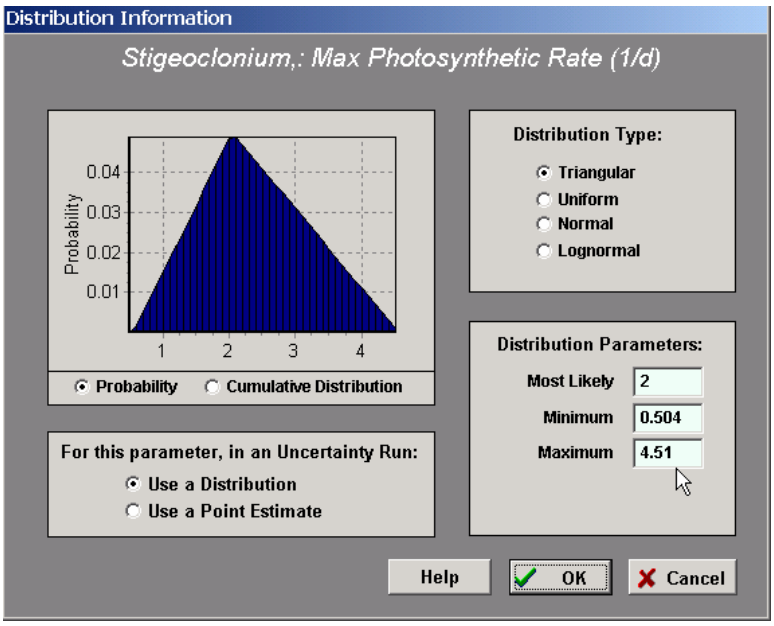
The results of varying just the Henry's Law constant for esfenvalerate are shown in the Uncertainty Graph for bass. The spread of values, although very small, is due to the differences in bioavailability and therefore differences in amount of toxicity. Likewise, the spread of

predicted esfenvalerate mass associated with shiners is small, suggesting that the model is not sensitive to the uncertain Henry's Law constant values.

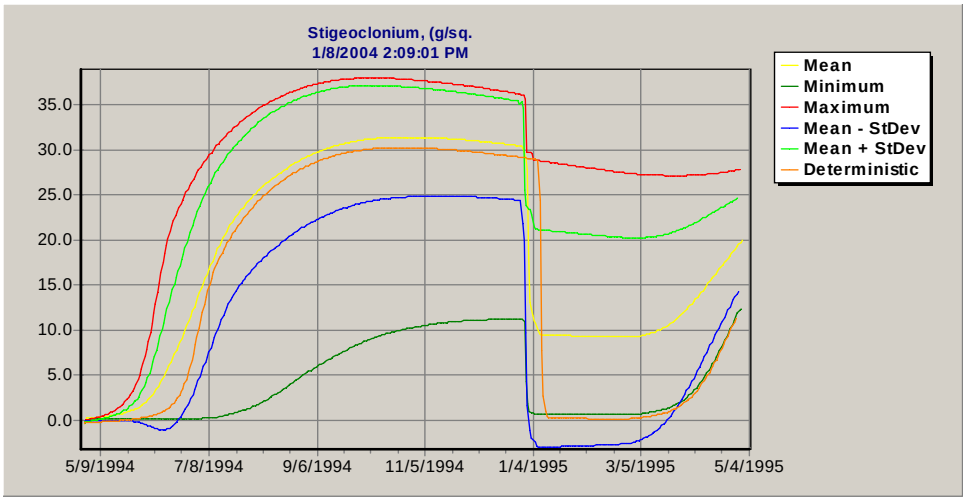


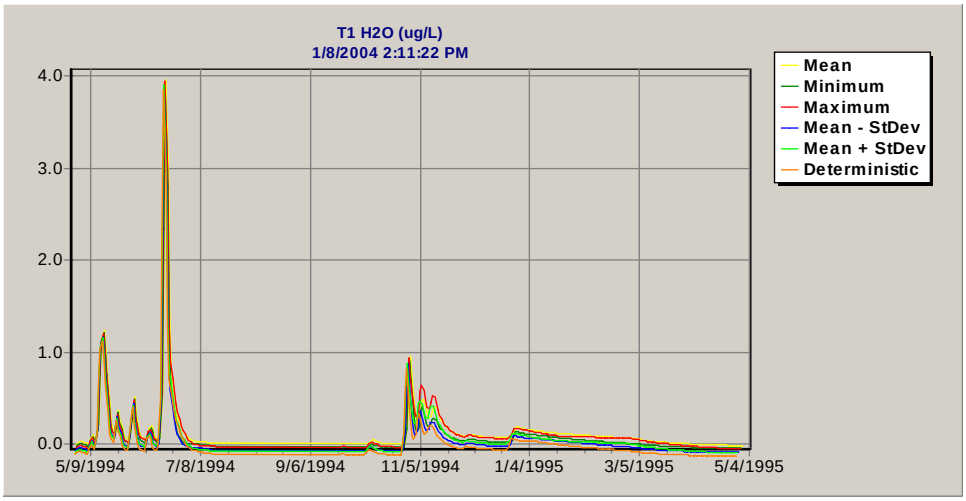


In another example, we will vary a critical parameter for the periphytic greens (nominally *Stigeoclonum*) to see how it affects the response of this group. The most likely maximum photosynthetic rate is set at 2 g/g-d; however, there is considerable variation reported in the literature (Collins and Wlosinski 1983). The extreme values reported are 0.56 and 4.1. We could take these as the constraints for a triangular distribution, but that would mean throwing out the lowest and highest observed values because the constraints have zero probability. Therefore, we will extend the constraints by 10% of the observed values.



The results of varying this one photosynthetic parameter indicate that the model is sensitive to it. It has a large effect on the biomass of the dominant periphyton; and, evidently, that in turn affects the fate of esfenvalerate to some small extent in the latter part of the simulation.

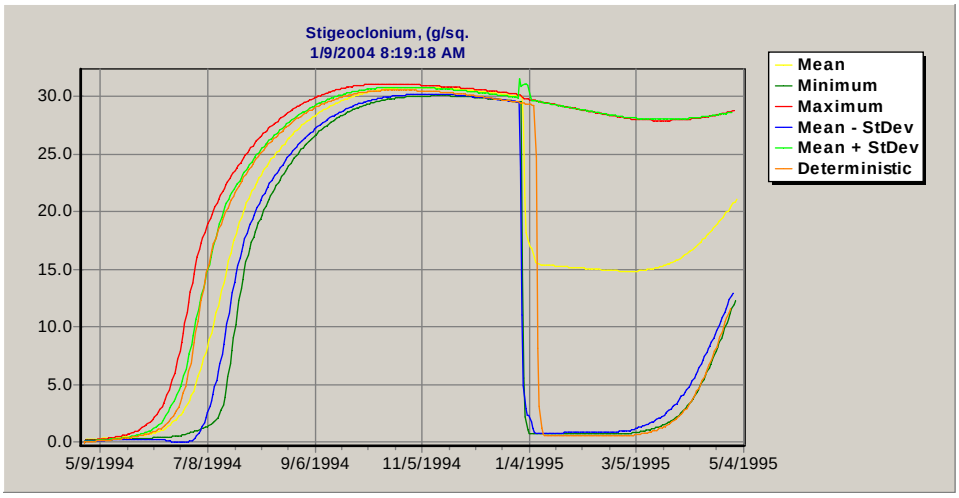


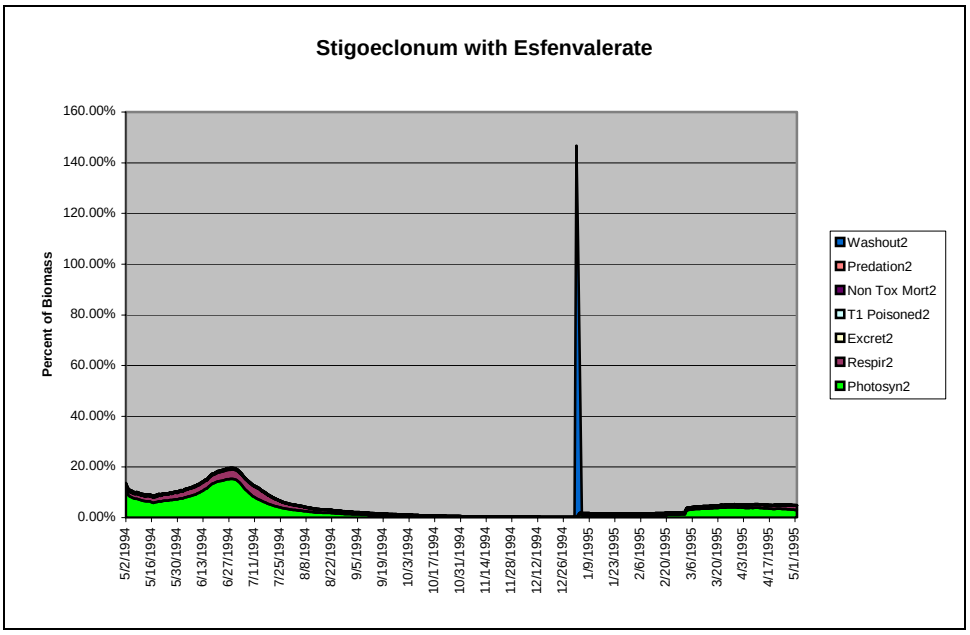


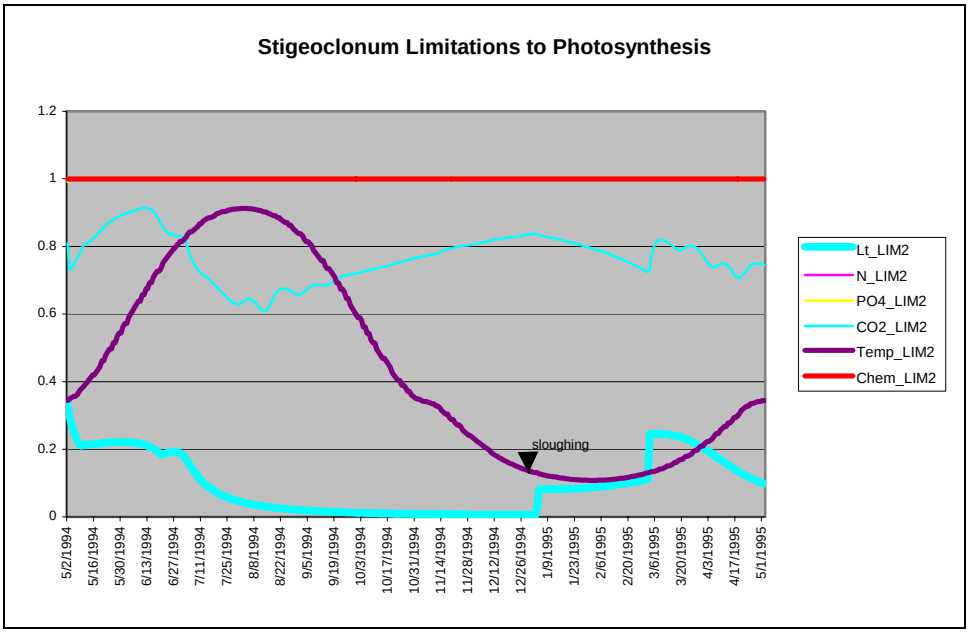
In the final analysis, we will examine the effects of varying mean depth of water in the pond. A normal distribution is used with a mean of 1.2 m and a standard deviation of 0.4. Based on the log of the uncertainty analysis (ESFenPond U Depth.TXT), the minimum depth simulated was 0.018 m, and the maximum depth was 1.859 m.

The periphyton biomass is sensitive to water depth. Periphyton are well adapted to shallow water; the maximum biomass is at the minimum depth. However, they are light-limited at the greater depths simulated in this turbid pond.

Because there is an abrupt decline in *Stigeoclonum* biomass that affects the deterministic simulation and one tail of the distribution but not the other, we should examine the saved rates to determine the cause of the decline. We see that on 1/1/1995 there was a sloughing event. A plot of the limitations to photosynthesis suggests that there wasn't any sudden change in conditions that caused the sloughing; rather, it was probably the combination of changing temperature limitation coupled with severe light limitation (predicted ice-on occurred on 1/1/).




Stigoeclonum with Esfenvalerate
Percent of Biomass
160.00%
140.00%
120.00%
100.00%
80.00%
60.00%
40.00%
20.00%
0.00%
5/2/1994
5/16/1994
5/30/1994
6/13/1994
6/27/1994
7/11/1994
7/25/1994
8/8/1994
8/22/1994
9/5/1994
9/19/1994
10/3/1994
10/17/1994
10/31/1994
11/14/1994
11/28/1994
12/12/1994
12/26/1994
1/9/1995
1/23/1995
2/6/1995
2/20/1995
3/6/1995
3/20/1995
4/3/1995
4/17/1995
5/1/1995
Washout2
Predation2
Non Tox Mort2
T1 Poisoned2
Excret2
Respir2
Photosyn2

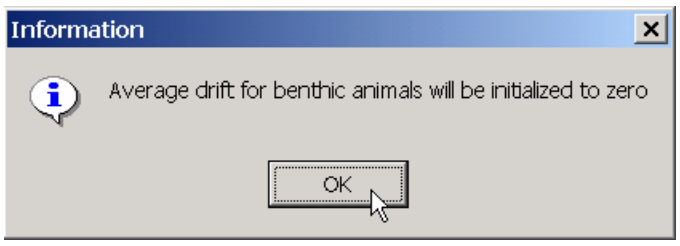

Stigeoclonum Limitations to Photosynthesis
1.2
1
0.8
0.6
0.4
0.2
0
sloughing
5/2/1994
5/16/1994
5/30/1994
6/13/1994
6/27/1994
7/11/1994
7/25/1994
8/8/1994
8/22/1994
9/5/1994
9/19/1994
10/3/1994
10/17/1994
10/31/1994
11/14/1994
11/28/1994
12/12/1994
12/26/1994
1/9/1995
1/23/1995
2/6/1995
2/20/1995
3/6/1995
3/20/1995
4/3/1995
4/17/1995
5/1/1995
Lt_LIM2
N_LIM2
PO4_LIM2
CO2_LIM2
Temp_LIM2
Chem_LIM2

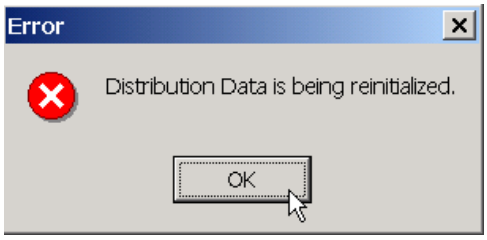
7 QUALITY ASSURANCE

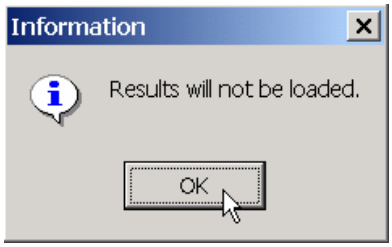
AQUATOX is designed to facilitate documentation of assumptions and data sources for specific applications and to archive results. Note fields are provided for the study and for each of the state-variable loading screens. These are intended to provide the user with a way to record an overview of the study and to describe sources and salient features of the loading data. Furthermore, almost every parameter has an associated comment field to document the source of the value used. These fields are not fully utilized in the example sets; but, as additional data are incorporated, comments should be used liberally.

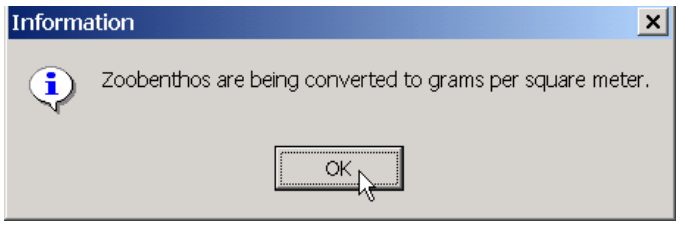
A study, with all associated data and output, can be archived in a study file. ***Good practice dictates that the version of AQUATOX used for the application should be saved as well.*** In that way the study can be opened and results examined at any time; and, if necessary, the model can be re-run. The main screen indicates the dates and times that the perturbed and control simulations were run. If you make a change to a study, you may choose not to save the changed file. To minimize file size, do not save the output; this can be done by clicking on **Study** on the menu bar in the main screen and choosing **Clear Results**. The file will usually be much smaller, but you will have to re-run the simulation to see the results.

AQUATOX versions are upwardly compatible within reason—but not necessarily years later—so if you open an old study with a newer version of the model, the data structure will be updated. Usually this is automatic, but often the user will be informed of critical steps in the upgrade, as shown in the sequence of information windows below, which take a study from Release 1 (File Version 1.69) to Release 2. Some of these steps may indicate changes that should be examined and perhaps changed in the updated study, such as initializing the fractions available for phosphate loadings.

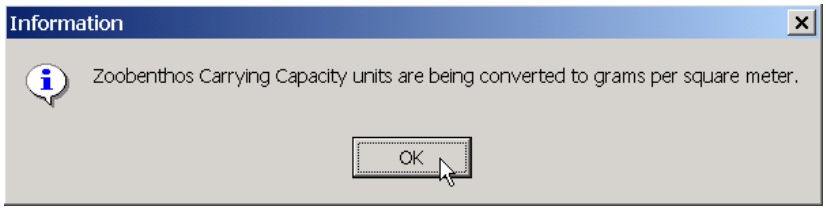


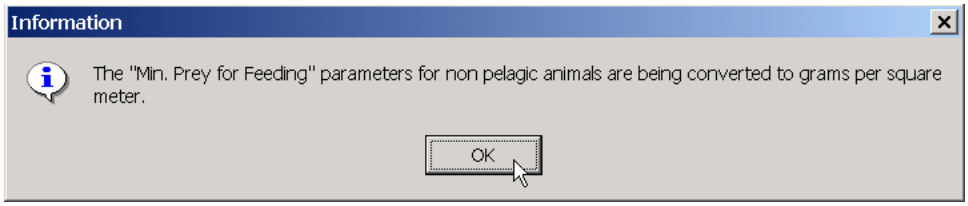

Error
Distribution Data is being reinitialized.
OK


Information
Results will not be loaded.
OK

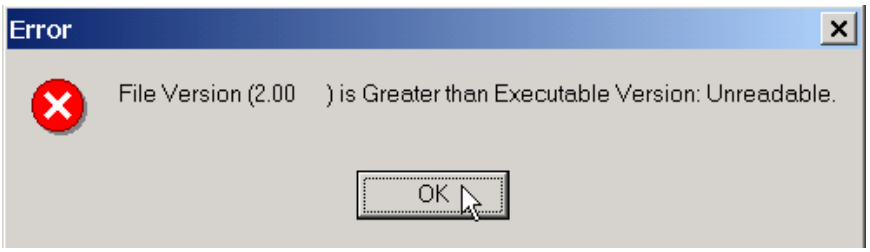

Information
Zoobenthos are being converted to grams per square meter.
OK


Information
Fish units are being converted to grams per square meter.
OK


Information
Zoobenthos Carrying Capacity units are being converted to grams per square meter.
OK


Information
The "Min. Prey for Feeding" parameters for non pelagic animals are being converted to grams per square meter.
OK

Of course, studies are ***not*** backward compatible. If an earlier version of the program attempts to access a later version of a study, an error message will be displayed and the study will not be loaded.



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