AQUATOX Training Workshop

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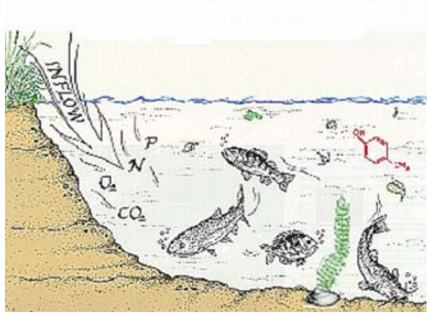
Richard A. Park, Eco Modeling, Diamondhead MS
dickpark@CableOne.net
Jonathan S. Clough, Warren Pinnacle Consulting, Warren VT
jclough@warrenpinnacle.com
Marjorie Coombs Wellman, Office of Water, US EPA, Washington DC
wellman.marjorie@epamail.epa.gov



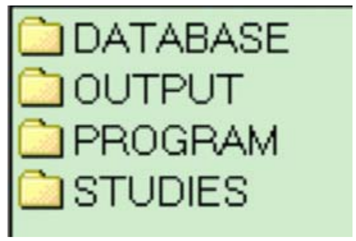
Introduction

- CD setup, installation
- Potential applications, regulatory endpoints
- Overview of AQUATOX
- Acceptance of AQUATOX
- What it does *not* do
- Structure, ecosystem primer
- State variables, processes, input requirements
- Capabilities

We will proceed from a general introduction to in-depth discussion and specific examples. Therefore, we suggest that you hold your questions until we have had a chance to present the material. There should be plenty of time in later lectures and labs to address specific questions.

CD Setup: Files, Installation

- AQUATOX Folder
  - Data Folder
  - Documents Folder
  - WinHSPF Folder
  - AQUATOX Installshield EXE
    - Which Installs to …



The **Data** folder contains all of the raw data sets that we will be using to run various simulations within AQUATOX.

The **Documents** folder contains all of the presentation materials for this short-course along with a Users Guide, Technical Documentation, and Validation Reports in PDF format.

The **WinHSPF** folder contains the WinHSPF installation program. WinHSPF is a hydrological model that can be linked to AQUATOX.

We will also discuss the AQUATOX file structure that is created when the AQUATOX Installshield is run.

Potential Applications for AQUATOX

- Many waters are impaired biologically as well as chemically
- Managers need to know:
  - Which of several stressors is causing the impairment?
  - Will proposed pollution control actions reach their goals?
    - restoration of desirable aquatic community
    - improved chemical water quality
  - Will there be any unintended consequences?
  - How long will recovery take?

Although much progress has been made in controlling water pollution in our Nation's waters since the advent of the Clean Water Act, there is still a long way to go. Under sections 303(d) and 305(b) of the CWA, States are required to identify waterbodies that don't fully support the aquatic life uses as designated in their state water quality standards.

According to the 2000 National Water Quality Inventory, 40% of river reaches and 45% of lakes that were assessed are impaired for one or more of their designated uses. Commonly reported causes of impairment included siltation, nutrients, oxygen-depleting substances, and pesticides. Many impaired waters are subjected to multiple stressors. The relative importance of each stressor to the observed biological impairment is not always evident, but the first step in corrective action is to know what stressor (or combination of stressors) is causing the impairment.

Regulatory Endpoints Modeled

- nutrient and toxicant concentrations
- biomass
  - plant, invertebrate, fish
- chlorophyll a
  - phytoplankton, periphyton, moss
- total suspended solids, Secchi depth
- dissolved oxygen
  - daily min. and max. in Rel. 3
- biochemical oxygen demand
- bioaccumulation factors
- half-lives of organic toxicants

AQUATOX has many kinds of output, many of which may be used in a regulatory context.

Potential Applications
nutrients

- Develop nutrient targets for rivers, lakes and reservoirs with nuisance algal blooms
- Determine what factor(s) is controlling algae levels
  - nutrients, suspended sediments, grazing, herbicides, flow
- Using the linkage to BASINS, evaluate effects of agricultural practices
  - Will target chlorophyll *a* concentrations be attained after BMPS are implemented?
  - Will land use changes from agriculture to residential use increase or decrease eutrophication effects?

Using a process-based model such as AQUATOX can help to provide a mechanistic link between nutrients and the algal responses. This can be used in conjunction with other efforts and approaches to establish nutrient targets. In a later module we'll explore this in greater detail.

Potential Applications of AQUATOX *toxic substances*

- Ecological risk assessment
  - Will non-target organisms be harmed?
    - Will sublethal effects cause game fish to disappear?
  - Will there be disruptions to the food web?
    - Will reduction of zooplankton reduce the food supply for beneficial fish?
    - Or will it lead to nuisance algae blooms?
- Calculate bioaccumulation factors
- Estimate time until fish are safe to eat following remediation

Potential Applications
aquatic life support

- Estimate recovery time for fish or invertebrates after reducing pollutant loads
- Evaluate potential ecosystem responses to invasive species and mitigation measures
  - Will native species disappear?
  - Will there be changes in ecosystem "services"?
  - What are the potential effects and half-life of a biocide?
- *Coordinate with biological criteria program*
  - *Estimate biological metrics*
  - *Model reference conditions where no historical, minimally altered sites exist*

The last item is in italics to reflect the fact that this is an area we are just beginning to explore.

Overview: What is AQUATOX?

- **Simulation model that links pollutants to aquatic life**
- **Integrates fate & ecological effects**
  - **nutrient & eutrophication effects**
  - **fate & bioaccumulation of organics**
  - **food web & ecotoxicological effects**
- **Predicts effects of multiple stressors**
  - **nutrients, organic toxicants**
  - **temperature, suspended sediment, flow**
- **Can be evaluative (with "canonical" or representative environments) or site-specific**
- **Peer reviewed by independent panel and in several published model reviews**
- **Distributed by US EPA**

AQUATOX is the latest in a long series of models, starting with the aquatic ecosystem model CLEAN (Park et al., 1974) and subsequently improved in consultation with numerous researchers at various European hydrobiological laboratories, resulting in the CLEANER series (Park et al., 1975, 1979, 1980; Park, 1978; Scavia and Park, 1976) and LAKETRACE (Collins and Park, 1989). The MACROPHYTE model, developed for the U.S. Army Corps of Engineers (Collins et al., 1985), provided additional capability for representing submersed aquatic vegetation. Another series started with the toxic fate model PEST, developed to complement CLEANER (Park et al., 1980, 1982), and continued with the TOXTRACE model (Park, 1984) and the spreadsheet equilibrium fugacity PART model. AQUATOX combined algorithms from these models with ecotoxicological constructs; and additional code was written as required for a truly integrative fate and effects model (Park et al., 1988; Park, 1990, 1993). The model was then restructured and linked to Microsoft Windows interfaces to provide greater flexibility, capacity for additional compartments, and user friendliness (Park et al., 1995). Release 1 from the U.S. Environmental Protection Agency (US EPA) was improved with the addition of constructs for chronic effects and uncertainty analysis, making it a powerful tool for probabilistic risk assessment (US EPA, 2000a, b, c). Release 1.1 (US EPA 2001a, b) provided a much enhanced periphyton submodel and minor enhancements for macrophytes, fish, and dissolved oxygen. Release 2, which had a number of major enhancements including the ability to model up to 20 toxic chemicals and more than twice as many biotic compartments and linkage to the BASINS system, was released in early 2004. Significant enhancements resulted in Release 2.1 in October, 2005; Release 2.2 is coming out this summer. Release 3 is in beta test at the present time; it has some powerful capabilities that will be described at the end of the workshop.

Acceptance of AQUATOX

- A truly integrated eutrophication, contaminant fate and effect model
  - "is the most complete and versatile model described in the literature" (Koelmans et al. 2001)
  - CATS-5 (Traas et al. 2001) is similar; models microcosms
  - CASM (Bartell et al. 1999) models toxic effects but not fate
- Can simulate many more types of organisms with more realism than most other water quality models
  - WASP6 models total phytoplankton and "benthic algae" (Wool et al. 2004); zooplankton are just a grazing term
  - QUAL2K models phytoplankton and "bottom algae" (Chapra and Pelletier 2003); no animals
- Very comprehensive bioaccumulation model

Bartell, Steven M., Guy Lefebvre, Gregoire Kaminski, Michel Carreau, and Kym Rouse Campbell. 1999. An Ecological Model for Assessing Ecological Risks in Quebec Rivers, Lakes, and Reservoirs. Ecological Modelling **124**:43-67.

Chapra, Steve, and Greg Pelletier. 2003. QUAL2K: A Modeling Framework for Simulating River and Stream Water Quality: Documentation and Users Manual. Medford MA: Civil and Environmental Engineering Dept., Tufts University.

Imhoff, John C., Jonathan S. Clough, Richard A. Park, and Andrew Stoddard. 2004. Evaluation Of Chemical Bioaccumulation Models of Aquatic Ecosystems: Final Report. Athens GA: U.S. Environmental Protection Agency.

Koelmans, A.A., , A. Van der Heidje, , L.M. Knijff, , and R.H. Aalderink. 2001. Integrated Modelling of Eutrophication and Organic Contaminant Fate & Effects in Aquatic Ecosystems. A Review. *Water Research* 35 (15):3517-3536.

Traas, Theo P., J.H. Janse, P.J. Van den Brink, and T. Aldenberg. 2001. A Food Web Model for Fate and Effects of Toxicants and Nutrients in Aquatic Mesocosms. Model Description. Bilthoven, The Netherlands: RIVM.

Wool, Tim A., Robert B. Ambrose, James L. Martin, and Edward A. Comer. 2004. Water Quality Analysis Simulation Program (WASP) Version 6.0 DRAFT: User's Manual. Atlanta GA: US Environmental Protection Agency – Region 4.

Comparison of Bioaccumulation Models: Biotic State Variables

Table 3.2. Comparison of Bioaccumulation State Variables

	AQUATOX Release 2	BASS v 2.1	Biotic Ligand 1.0.0	Ecofate 1.0b1, Gobas	EMCM 1.0	RAMAS Ecosystem	QEAFDCHN 1.0	TRIM.FaTE v 3.3
BIOTIC STATE VARIABLES								
Plants								
Single Generalized Water Column Algal Species	★	7		★	★			★
Multiple Generalized Water Column Algal Species	★							
Green Algae	★							
Blue-green Algae	★							
Diatoms	★							
Single Generalized Benthic Algal Species	★	7						
Multiple Generalized Benthic Algal Species	★							
Periphyton	★	7			★			
Macrophytes	★				★			★
Animals								
Generalized Compartments for Invertebrates or Fish						★	★	
Generalized Zooplankton Species	★	7		★	★		★	
Detritivorous Invertebrates	★			★	4		★	
Herbivorous Invertebrates	★		3	★			★	★
Predatory Invertebrates	★						★	
Single Generalized Fish Species	★	★		★	★		★	
Multiple Generalized Fish Species	★	★		★	★		★	
Bottom Fish	★	★		★	★		★	★
Forage Fish	★	★	3	★	★		★	★
Small Game Fish	★	★		★	★		★	★
Large Game Fish	★	★	3	★	★		★	★
Fish Organ Systems			6					
Age / Size Structured Fish Populations	★	★		★	★	5	★	
Marine Birds	★			★				★
Additional Mammals								★

Imhoff et al. 2004

AQUATOX has a very complete coverage of plants and animals with the capability to model Diatoms, Greens, Blue-greens, and Macrophytes along with a generalized “other algae” compartment. AQUATOX animal compartments are separated into shredders, sediment feeders, suspended feeders, clams, grazers, snails, predatory invertebrates, forage fish, bottom fish, and game fish.

Many models incorporate a complex animal food-web but very few have the capability to model plants with the complexity of AQUATOX.

What AQUATOX does *not* do

- It does not model metals
  - **Hg was attempted, but unsuccessful**
- It does not model bacteria or pathogens
  - **microbial processes are implicit in decomposition**
- Diel oxygen is not modeled in Rel. 2.2 (but is in Rel. 3)
- Nutrient regeneration from bottom sediments is only crudely represented in Rel. 2.2
  - **will incorporate Di Toro submodel in Rel. 3**

We have no immediate plans to add metals. Several years ago we added a mercury fate and bioaccumulation submodel. However, a test with independent data did not meet our criteria for a satisfactory fit. The problem seems to be that there is no general algorithm for methylation under varying site conditions. It has been suggested that we just use the bioaccumulation portion of the model and drive it with observed methyl mercury concentrations, and we may eventually do that.

Release 3 has the capability of modeling with a 1-hour time step, thus allowing representation of diel oxygen and time-dependent mortality due to low oxygen levels.

Nutrient release from bottom sediments is represented only to the extent that the nutrients contained in animals, plants, and detritus are released as decomposition progresses.

AQUATOX Structure

- **Time-variable**
  - **variable-step 4th-5th order Runge-Kutta**
    - **usually daily reporting time step**
    - **can use hourly time-step and reporting step in Rel. 3**
- **Spatially simple unless linked to hydrodynamic model**
  - **thermal stratification**
  - **salinity stratification (based on salt balance in Rel 3)**
- **Modular and flexible**
  - **written in object Pascal**
  - **model only what is necessary (flask to river)**
- **Control vs. perturbed simulations**

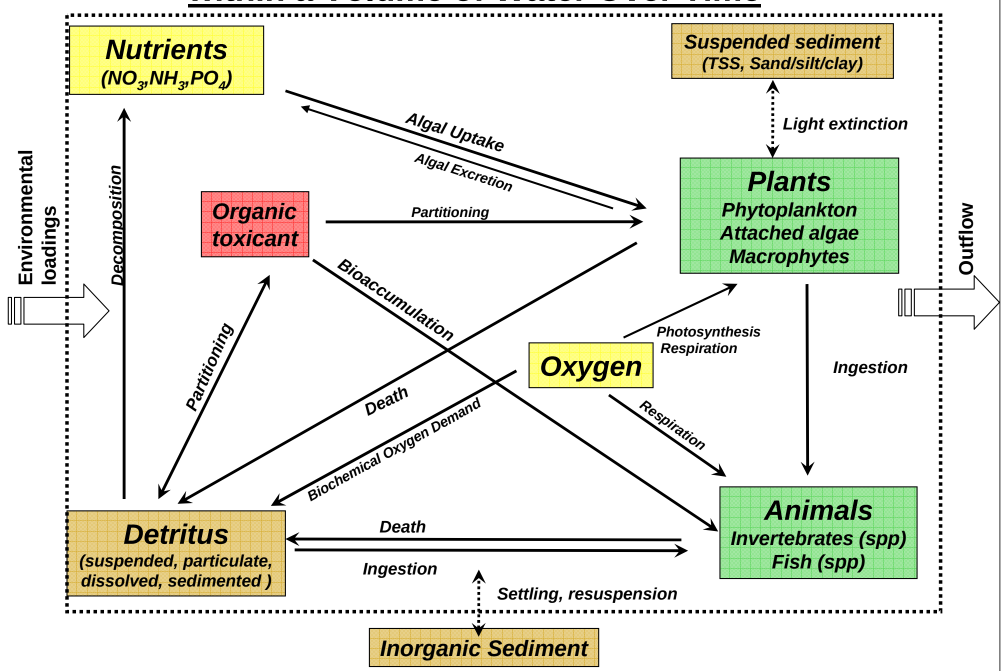
AQUATOX varies the time step of the differential equation solver in order to achieve specified accuracy. It may cut down the step to 15 minutes or less to step past a discontinuity. However, it will never increase to more than a day so that pulsed loadings can be detected. The reporting time step is usually a day, but it may be less and it can be as long as 200 days. The results are integrated over the specified time period.

Stratification with two layers can be modeled, but the stand-alone model does not represent horizontal segments unless linked to a hydrodynamic model (in one version).

State variables can be added or deleted easily because of the object-oriented Pascal. We have even modeled a flask without any biota to check the chemical fate part of the model against lab results.

The model can simulate conditions with and without a perturbation in order to distinguish impacts. This means that a simulation doesn't have to be perfectly calibrated to evaluate an impact.

AQUATOX Simulates Ecological Processes & Effects within a Volume of Water Over Time

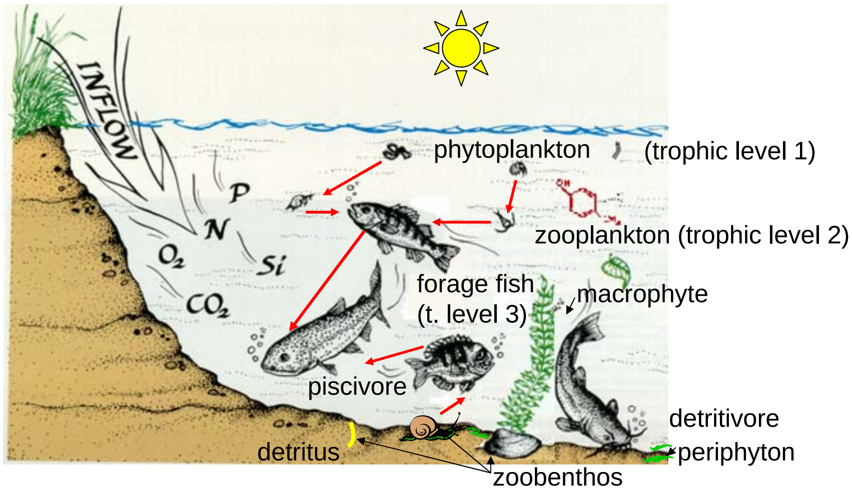


Processes Simulated

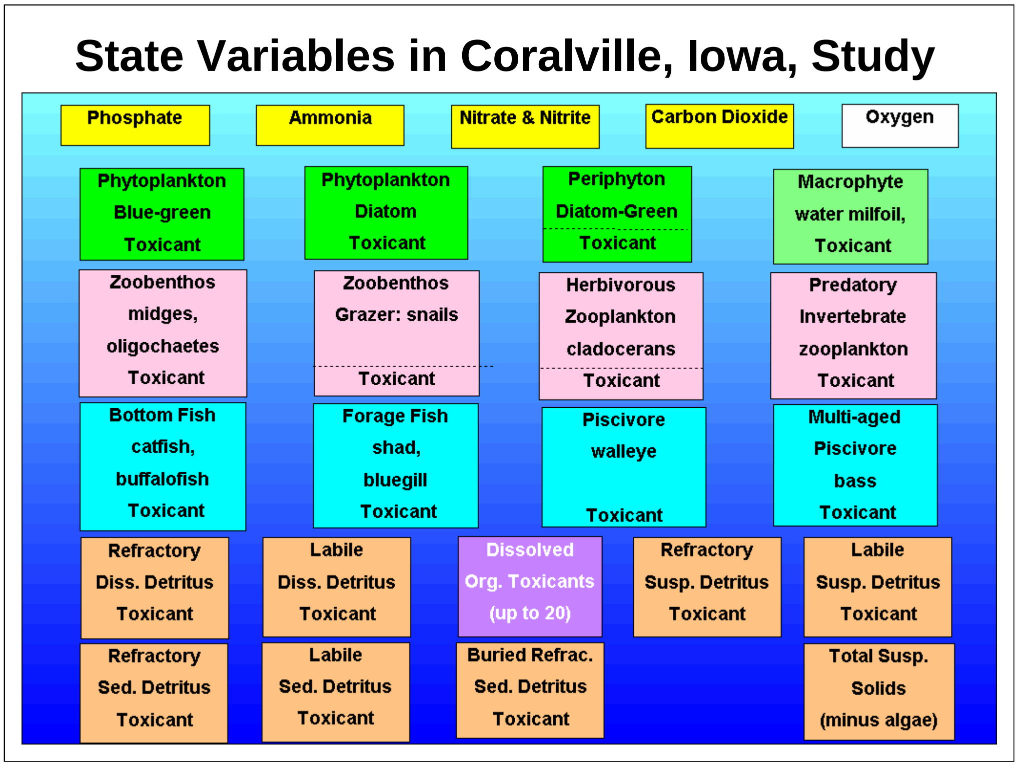
- **Bioenergetics**
  - **feeding, assimilation**
  - **growth, promotion, emergence**
  - **reproduction**
  - **mortality**
  - **trophic relations**
  - **toxicity (acute & chronic)**
- **Environmental fate**
  - **nutrient cycling**
  - **oxygen dynamics**
  - **partitioning to water, biota & sediments**
  - **bioaccumulation**
  - **chemical transformations**
  - **biotransformations**
- **Environmental effects**
  - **direct & indirect**

Both biotic and chemical processes are modeled. Because the model is a eutrophication model combined with a chemical fate model, and includes ecotoxicology, it can represent both direct and indirect effects of various pollutants. For example, it can simulate the combined effects of nutrients and pesticides in agricultural runoff, with representation of eutrophication and simultaneous removal of grazing pressure.

Ecosystem components

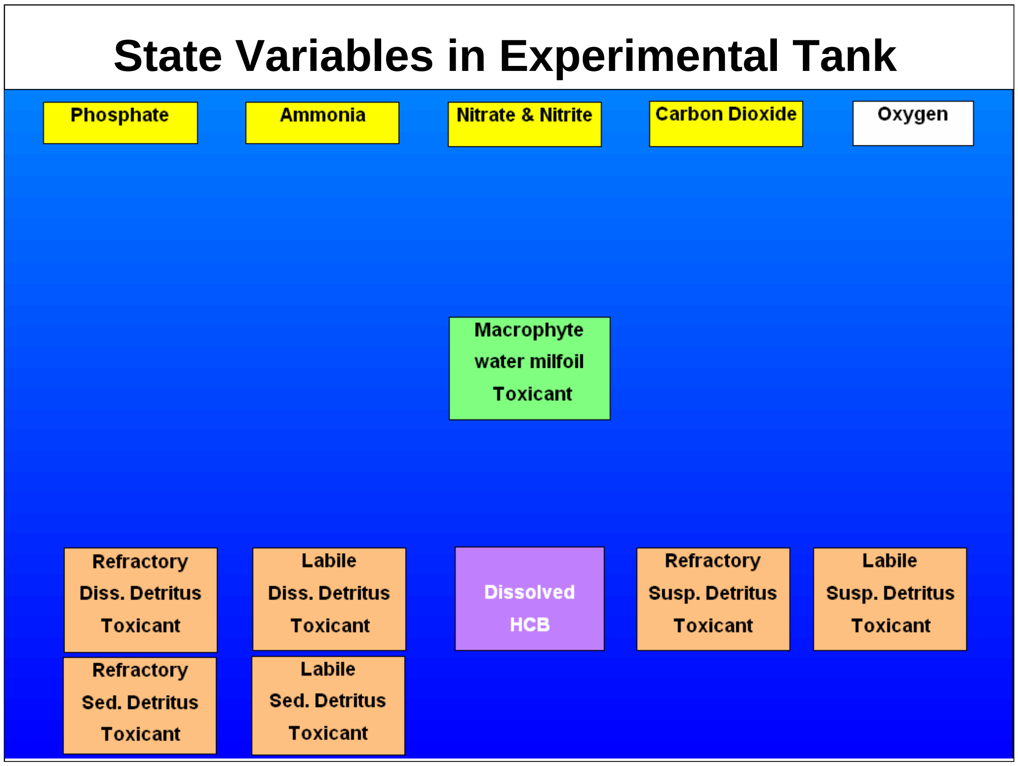


The ecosystem consists of abiotic and biotic components. Phytoplankton, periphyton, and macrophytes are the primary producers, fixing organic matter from nutrients and sunlight. As such they are the first trophic level. Zooplankton and many zoobenthos are primarily herbivores, thus they are the second trophic level. They and the higher trophic levels are consumers. However, usually there isn't a simple food chain with one trophic level feeding on another; most systems have complex food webs with organisms feeding at several trophic levels. Furthermore, animals may feed on both plants and detritus. Animals that feed on fish are termed "piscivores' and animals that feed on detritus are "detritivores." AQUATOX allows a user to specify preferences at multiple levels, thus modeling complex food webs.



Here is an example of a typical set of compartments used in simulating a eutrophic reservoir. The model can represent complex food webs with ease. Up to 20 organic toxicants can be simulated; however, a toxicant is associated with each compartment, so the total number of state variables may be quite large, slowing down the simulation.

Several detrital compartments are modeled, providing more realistic dynamics for detrital feeding and for decomposition and oxygen demand. Labile detritus is nutritious and decomposes rapidly; refractory detritus is not assimilated and decomposes slowly. Detrital compartments also differ in their sorptive capacity for organic chemicals.



You can simulate as few state variables as you wish. These are the state variables used in Lab 10, which simulates an experimental tank (aquarium) with a toxicant and a macrophyte. The absolute minimal simulation consists of detritus, nutrients, and oxygen; AQUATOX will not let you delete those.

Global vs. Site-Specific Input Requirements

Many model inputs are required on a site-by-site basis:

- nutrient loadings
- organics, sediment loadings
- water volume setup
- site characteristics
- chemical loadings
- temperature, pH
- animal, plant initial conditions (often defaults with "spin-up")

Many parameters may be assumed to be global parameters, i.e. no adjustment is required from site-to-site:

- most animal, plant parameters
- "remineralization" parameters
- chemical parameters
- chemical toxicity parameters

AQUATOX Capabilities

(Release 3 in red)

- **Ponds, lakes, reservoirs, streams, rivers, estuaries**
- **Riffle, run, and pool habitats for streams**
- **Completely mixed, thermal stratification, or salinity stratification**
- **Linked segments & multiple sediment layers with pore waters**
- **Diel oxygen and low oxygen effects, ammonia toxicity**
- **Variable stoichiometry, nutrient mass balance, TN & TP**
- **Dynamic pH**
- **Biota represented by guilds, key species**
- **Constant or variable loads**
- **Latin hypercube uncertainty analysis (all parameters)**
- **Wizard & help files, multiple windows, task bar**
- **Links to HSPF and SWAT in BASINS**
- **Can be linked to hydrodynamic model**

Because you may have been using an earlier version of the model, it is instructive to highlight the capabilities of successive versions. Release 2 was issued by the US EPA in April 2004. Release 2.1 was issued in October, 2005. Release 2.2 will be issued momentarily. Release 3 is a much more powerful version, which can model linked segments, layered sediments, and estuaries, and is currently in beta test.

Lab 1: A Tour Through the AQUATOX Screens

- ❑ Main Screen
- ❑ Toolbar
- ❑ Simulation Window
- ❑ Initial Conditions
- ❑ Chemical Screen
- ❑ Site Screen
- ❑ Stream Data
- ❑ Remineralization Data
- ❑ Setup Screen
- ❑ Rates Screen
- ❑ Libraries
- ❑ Uncertainty Screen
- ❑ Output Setup
- ❑ Control Setup Screen
- ❑ Help File
- ❑ Wizard
- ❑ Run Buttons
- ❑ Export of Results
- ❑ State Variable List (Chemicals, Nutrients, Organics, Plants, Animals, etc.)

This lab is not intended to describe the functionality of any of these screens in particular, but rather to get you used to navigating through AQUATOX and provide an overview of model and interface design. We will start by loading **FarmPond MO Esfenvalerate.aps** into AQUATOX as a basis for exploring these screens. In the next few pages we will run a few experiments with this simulation.

Questions to answer on your own as you explore the screens:

•What period is simulated?

•What rates are being saved?

•What is the mean temperature for the site?

•What is the mean light?

•What is the pH?

•What is the ammonia loading?

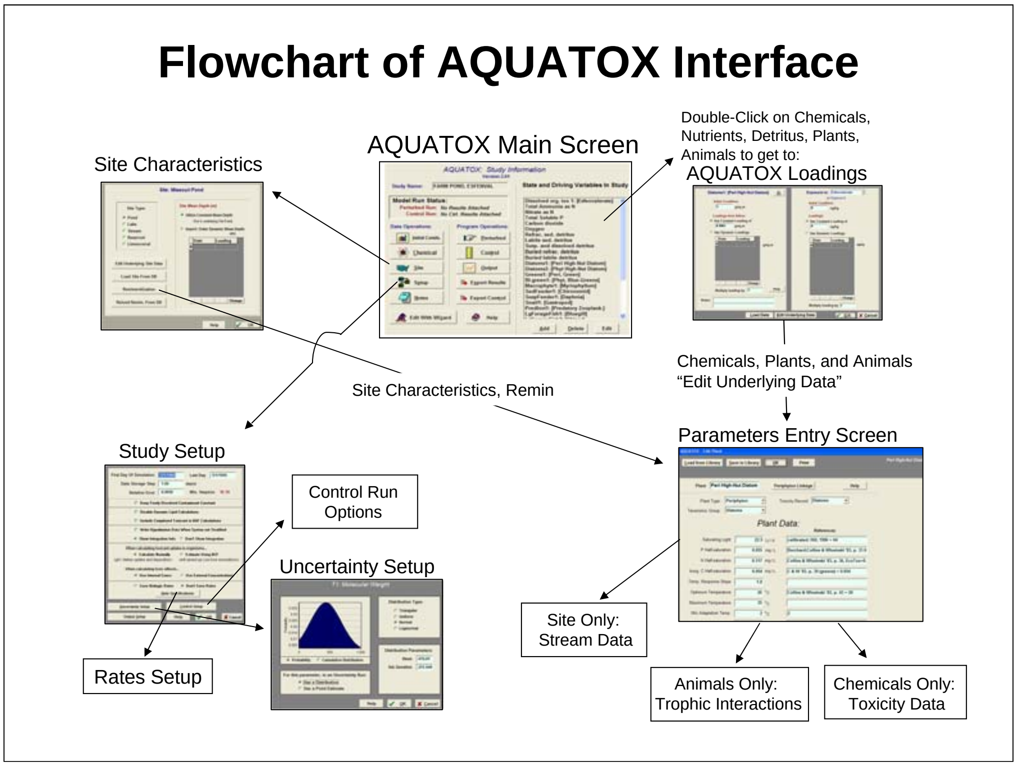
•What is the nitrate loading? Source?

•Does water volume vary?

•What is mean wind speed?

•What is the source of the esfenvalerate loadings?

•How long would it take for esfenvalerate to reach equilibrium (in fish)?

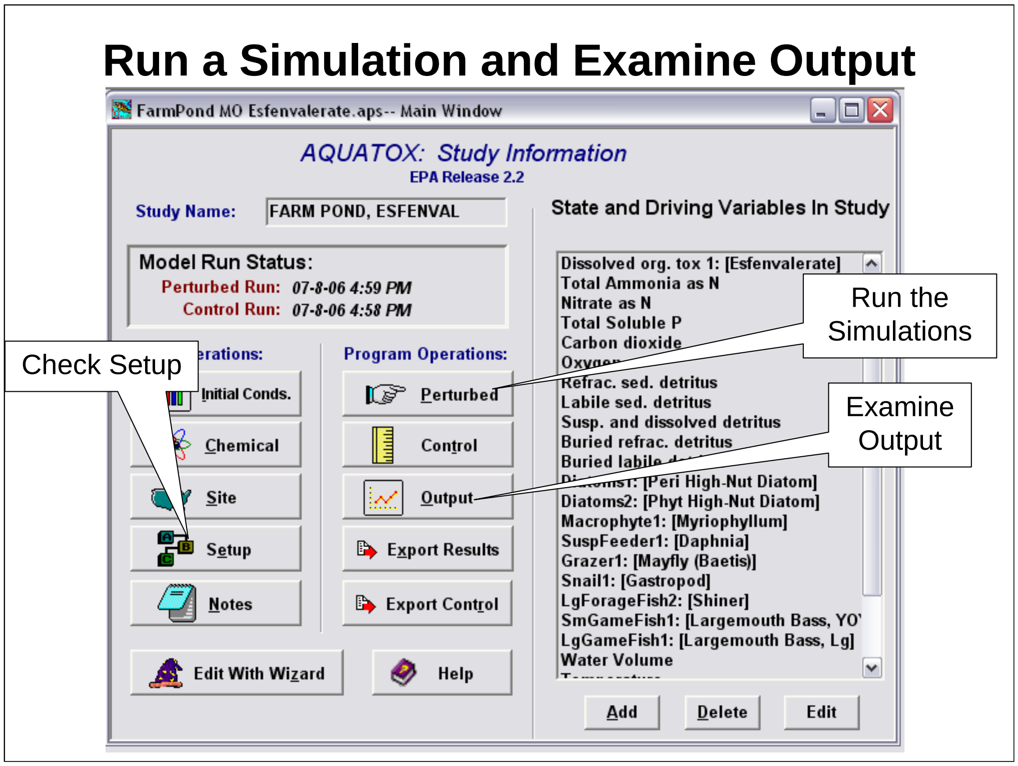


This page provides a general overview of the navigation through the AQUATOX Interface.

Double-click on the state variable list to bring up initial conditions and loadings for each state variable. For animals, chemicals, and plants, you can move from the loadings screen down into the "underlying data" which is a list of parameters that describe the organisms.

Other important buttons on the main interface include the "Site" button which brings you to site type and characteristics. From here you can move down into "site underlying data" or site parameters and characteristics and "Remineralization" which are parameters pertaining to the organic matter.

Finally, the "Setup" button is important to note as it allows the user to change the characteristics of a study run (e.g. time-period and differential equations solver options). The study setup screen is also where settings for control runs, uncertainty setup, and the saving of differential equation rates may be specified.



We spent a few minutes going through each of the AQUATOX screens that show all of the model input that comprise this particular simulation. The next thing to do is to run the simulation and examine results.

The Many Types of AQUATOX Output

(in order of output list)

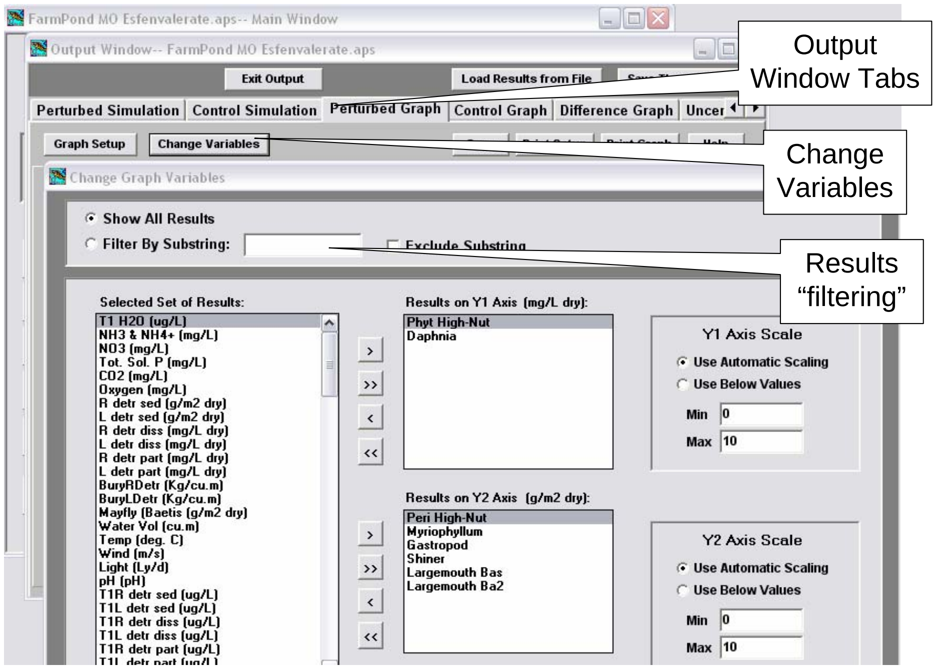
- Concentrations of State Variables
  - toxicants in water
  - nutrients and gasses
  - organic matter, plants, invertebrates, fish
- Physical Characteristic State Variables
  - water volume, temperature, wind, light, pH
- Mass of Toxicants within State Variables (normalized to water vol.)
  - T1-T20 in organic matter, plants, invertebrates, and fish
- Additional Model Calculations
  - Secchi depth, chlorophyll *a*, velocity, TN, TP
- Toxicant PPB
  - T1-T20 (PPB) in organic matter, plants, invertebrates, and fish
- Nitrogen and Phosphate Mass Tracking Variables
- Bioaccumulation Factors

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

When a toxicant is included in a simulation, the amount of output in a simulation more than triples. Additional chemical output includes the toxicant dissolved in water, the mass of toxicants in state variables normalized to the water volume (units of μg/L), the concentration of toxicants in state variables (PPB), and bioaccumulation factors for organisms.

Because there are so many types of AQUATOX output you may use the “filter” option whenever looking through this list to reduce the amount of output. Try filtering on units (“mg/L” or “g/m2”) or on partial state variable names (“peri” “phyto”). Only state variables that include your sub-string will be displayed making it far easier to find the output you wish to graph.

Output Screen: Tabular and Graphic Output



We will work together and look at the tabular output then produce a simple graph that shows the toxicant concentration in the water column.

After that, please spend 5-10 minutes working with the output screens to familiarize yourself with the interface. Please be sure to ask us if you have any questions. Some exercises you can work on:

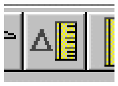
•Can you produce an output table with parts per billion output for Esfenvalerate throughout the food-chain? Is there evidence of biomagnification through the food-chain?

•Can you produce a graph that displays parts per billion output for Esfenvalerate in all animals (*Chironomid* through Largemouth Bass 2)?

•To help answer “why are the parts per billion output for Shiner and Gastropod falling to zero” graph the Gastropod and Shiner state variables as shown above.

•If time permits, explore graphs containing other output categories (i.e. detrital state variables, bioaccumulation factors).

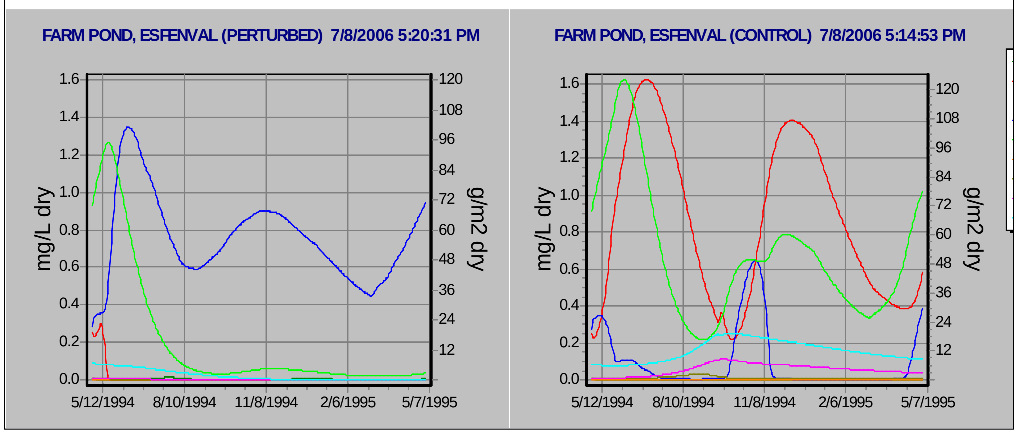
Comparing Scenarios: Execute a Control Run



Use the Control Setup toolbutton to examine control run options

Use the Control button to execute the simulation

Perturbed | Control



AQUATOX allows you to have results from two scenarios in memory at any given time and to compare those results. These simulations are named “Control” and “Perturbed,” although there is considerable flexibility as to how you can modify the two simulations.

In this case we will first go to the Control Setup screen and note that all sources of Esfenvalerate are set to zero in the control simulation. Use the toolbar or go through the Setup button to get to the Control Setup screen.

Then run a “control simulation” to see how the ecosystem reacts when there are no toxicants in the system.

Compare plant-biomass by setting up a perturbed graph with Periphyton and Myriophyllum (macrophytes) on the Y1 axis and phytoplankton on the Y2 axis. Set the Y1 axis maximum scale to 150 and the Y2 axis maximum to 0.1. Then go to the control simulation and select “Copy graph setup from perturbed.”

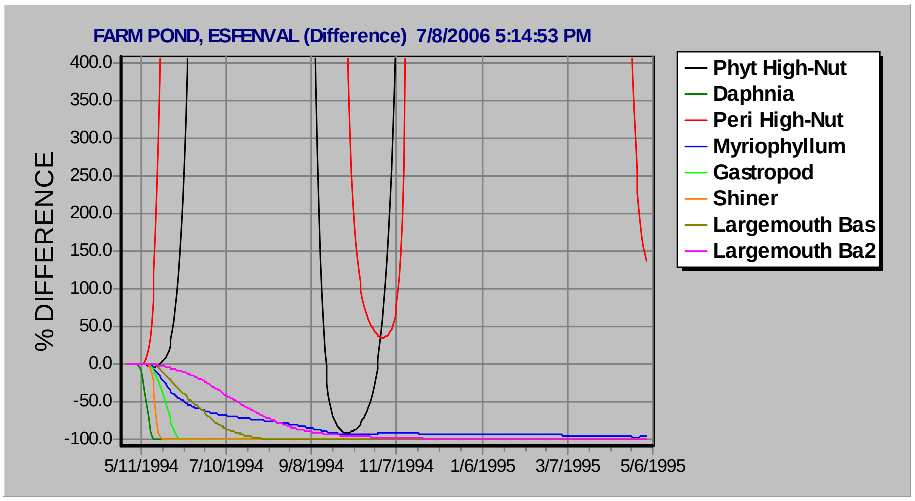
Note that the biomass of plants is affected by the application of Esfenvalerate but in some cases plant biomass increases due to application.

Exercise on your own: Look at the effects on animals using the same technique shown above. Are the effects more or less pronounced than they were for plants?

Comparing Scenarios: the "Difference" Graph

Difference graph designed to capture the percent change in results due to perturbation:

$$\%\ Difference = \left(\frac{Result_{Perturbed} - Result_{Control}}{Result_{Control}} \right) \cdot 100$$



The equation shown calculates the percent difference that the perturbation causes from the control simulation. By this formulation a 100% difference means that the perturbation caused the state variable to double. A negative 50% difference means that the perturbation caused the state variable to halve.

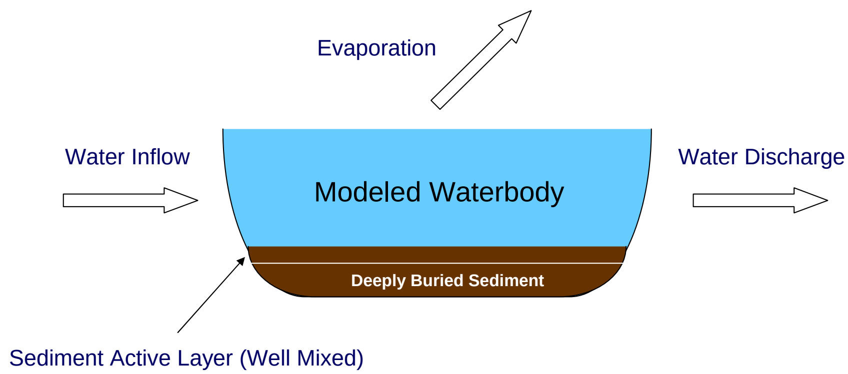
We will first examine a difference graph of all of the macrophytes, the invertebrates, and fish in the simulation (graph above). Note that the animals go extinct. Why do you suppose the macrophyte *Myriophyllum* declines?

The difference graph is especially useful when comparing differences in fairly stable sets of results such as fish biomass. As an example of a different type of difference graph, graph the difference in periphyton biomass between control and perturbed.

Care should be taken when interpreting spikes of short duration in a difference graph, this could simply be the result of a short (and potentially unimportant) difference in the timing of events. Also note that when biomass values fall to very low values in both simulations, large differences could be unimportant.

Physical Characteristics of a Site

Water Balance and Sediment Structure



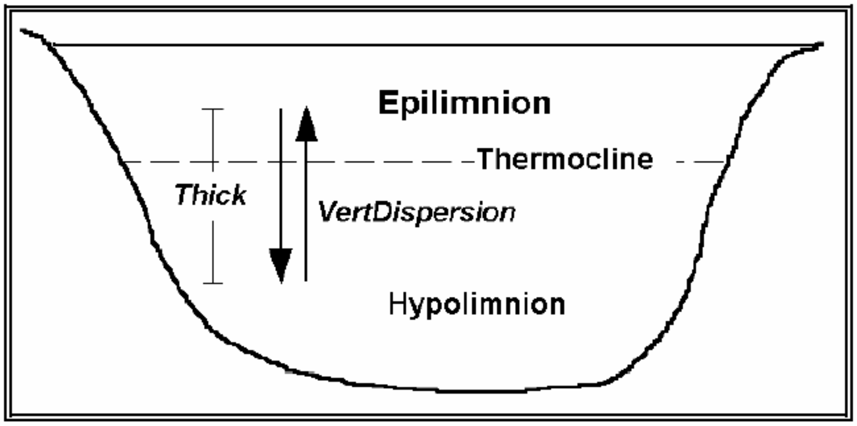
Water balance is defined as a function of inflow, evaporation, and discharge. We will discuss the various mechanisms for modeling water balance in a future slide. The modeled waterbody or river segment is assumed to be well mixed. Evaporation is a function of the site's surface area and the mean annual evaporation at the site.

Nutrients, plankton, and organics wash in and out of the system along with the flow of water.

The bottom sediment includes an active layer and a deeply buried sediment layer that is not reactive with the overlying water unless scour reduces the active layer and the deeply buried sediment is exposed.

This information covered in Section 3 of the **Technical Documentation**.

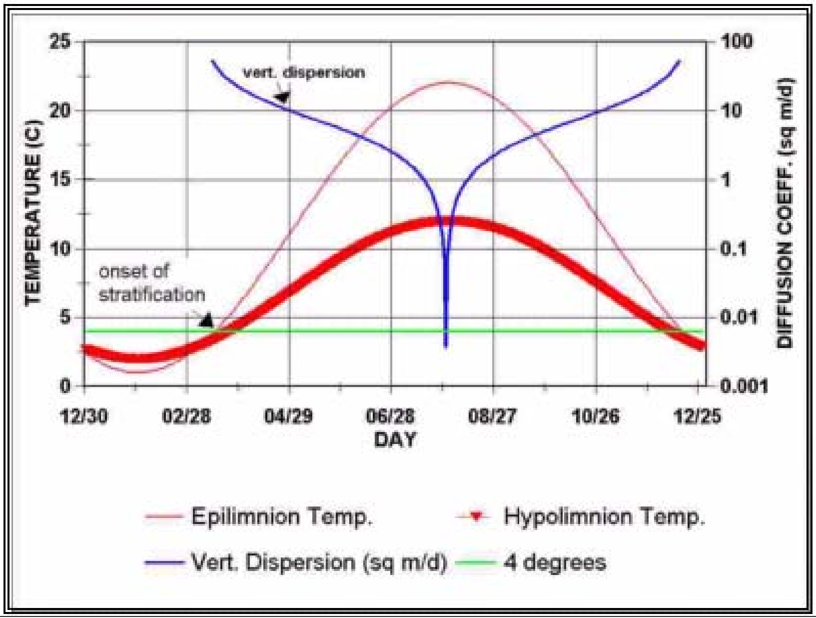
Thermal Stratification in a Lake



Thermal stratification is handled in the simplest form consistent with the goals of forecasting the effects of nutrients and toxicants. Lakes and reservoirs are considered in the model to have two vertical zones: epilimnion and hypolimnion; the metalimnion zone that separates these is ignored. Instead, the thermocline, or plane of maximum temperature change, is taken as the separator; this is also known as the mixing depth (Hanna, 1990).

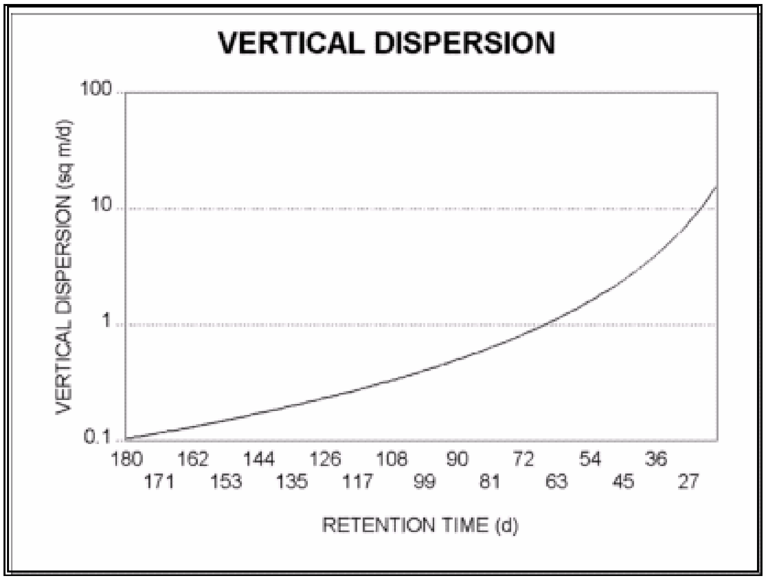
Dividing the lake into two vertical zones follows the treatment of Imboden (1973), Park et al. (1974), and Straškraba and Gnauck (1983). The onset of stratification is considered to occur when the mean water temperature exceeds 4° and the difference in temperature between the epilimnion and hypolimnion exceeds 3°; overturn occurs when this temperature difference is less than 3°, usually in the fall. Winter stratification is not modeled. For simplicity, the thermocline is assumed to occur at a constant depth.

Stratification is a Function of Temperature Differences



Diffusion between the epilimnion and hypolimnion is a function of the temperature differential. The user specifies the temperatures (or mean and range) for each layer and the model computes when stratification occurs and how much turbulent diffusion occurs.

Stratification Also is a Function of Discharge



In reservoirs, stratification can be broken down by high discharge using an empirical relationship determined by Straškraba for Czech reservoirs.

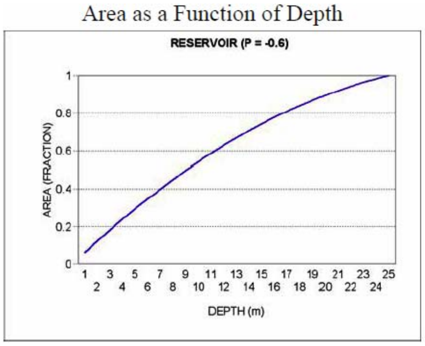
Bathymetric Approximations

The P parameter, differentiating different elliptic shapes, is calculated as a function of mean and maximum depth:

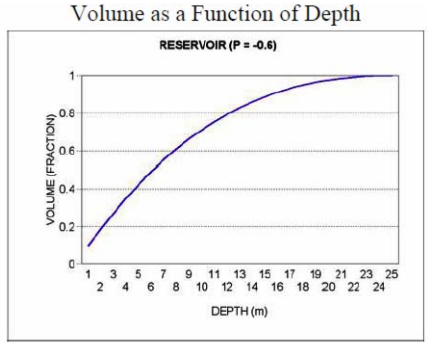
$$P = 6.0 \cdot \frac{ZMean}{ZMax} - 3.0$$

Based on these relationships, fractions of volumes and areas can be determined for any given depth:

Area as a Function of Depth



Volume as a Function of Depth



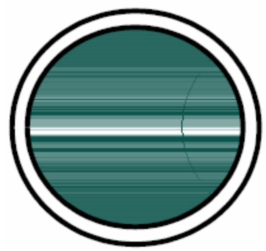
The depth distribution of a water body is important because it determines the areas and volumes subject to mixing and light penetration. The shapes of ponds, lakes, reservoirs, and streams are represented in the model by idealized geometrical approximations, following the topological treatment of Junge (1966; see also Straškraba and Gnauck, 1985). Shallow constructed ponds and ditches may be approximated by an ellipsoid. Reservoirs and rivers generally are extreme elliptic sinusoids. Lakes may be either elliptic sinusoids or elliptic hyperboloids. The distinguishing parameter is based on the mean and maximum depth. Not all water bodies fit the elliptic shapes, but the model generally is not sensitive to the deviations. Based on these relationships, fractions of volumes and areas can be determined for any given depth. For example, by setting depth to the depth of the euphotic zone, the fraction of the area available for colonization by macrophytes and periphyton can be computed.

Littoral Fraction

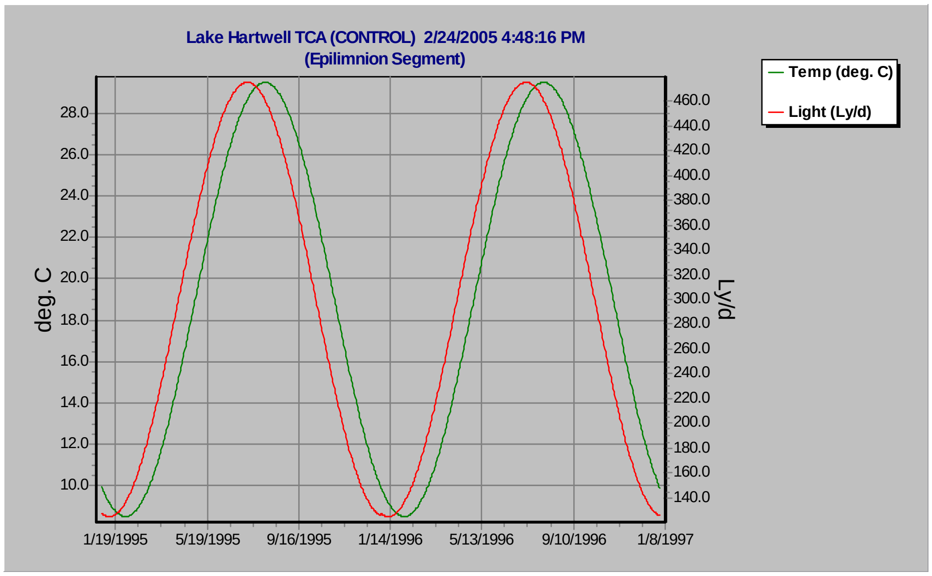
By setting Z to the depth of the euphotic zone, the fraction of the area available for colonization by macrophytes and periphyton can be computed:

$$FracLit = (1 - P) \cdot \frac{ZEuphotic}{ZMax} + P \cdot \left(\frac{ZEuphotic}{ZMax} \right)^2$$

A relatively deep, flat-bottomed basin would have a small littoral area and a large sublittoral area:

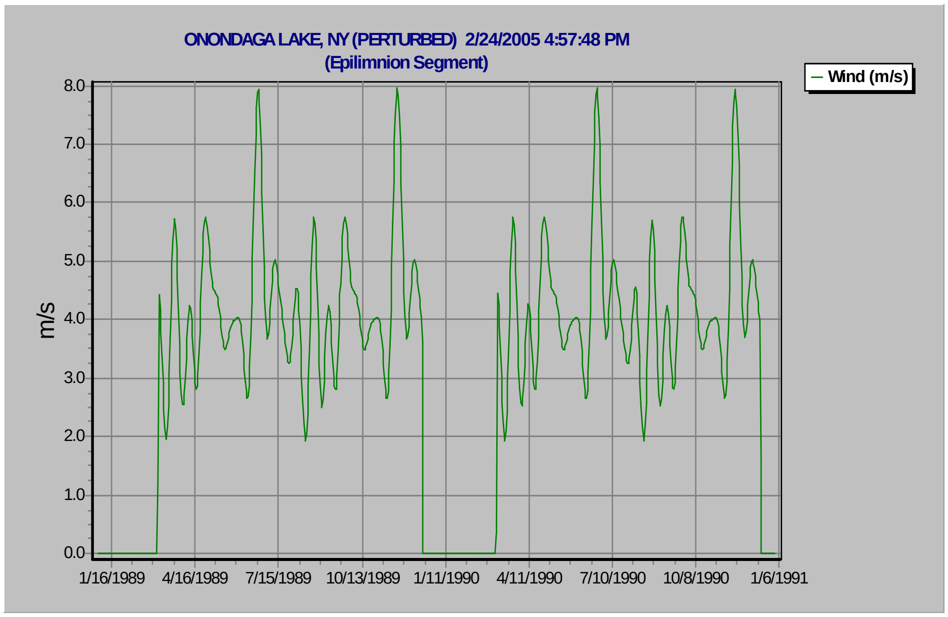


Temperature and Light



The user can enter means and annual ranges for temperature and light and the model will compute sinusoidal values over time. Alternatively, observed values or values predicted by a hydrologic model can be entered for temperature and observed values can be entered for light.

Wind



Variable wind can have an important effect on standing water, affecting volatilization and breaking up floating blue-green algal blooms. A default 144-day sequence from Missouri is provided as a default; the user can specify the mean wind (4.17 m/s in this example). The model accounts for ice cover. Alternatively, the user can specify a time series.

Lab 2: Setup of a New Study

- Rum River, MN, as template
- Rum River Background
- Use of the Wizard
- Site Characteristics
- Importing Loadings

Photo: MN Pollution Control Agency

In Lab 1 we worked with an existing simulation to give you a preview of the types of analyses that can be performed with AQUATOX.

In Lab 2 we will start the process of setting up an AQUATOX simulation for a new site. In this case we will be applying the AQUATOX model to “your site” assuming “your site” is the Boise River in Idaho.

When you are applying AQUATOX to a new site it is usually most efficient to find a surrogate site that best matches the characteristics of the site you are modeling. You will then take that site and modify its characteristics so that it matches your site with respect to Nutrients, Organic Matter, Turbidity, Biota, and Organic Chemicals (if relevant).

In this laboratory we will start this process by taking the following steps

- Find a surrogate site (Rum River, MN)
- Modify the physical characteristics of the surrogate site to match “your site” (Boise River, ID).
- Modify the nutrients, organics loadings, and turbidity using data from “your site.”

Rum River Background

- Located in south central Minnesota
- Tributary to the Upper Miss. River
- Watershed Area is about 1,325 sq.miles
- Land use is 17% ag, 23% range (dairy farms), 31% forest
- Shallow with cobbles, gravel, & sand
- Nutrient concentrations moderate, turbidity low
- Abundant periphyton

The Rum River study file provides a useful template for this simulation. We will be modifying the site and biotic characteristics to match the Lower Boise River, Glenwood Bridge, Boise, Idaho, which is somewhat similar to the Rum River.

Boise River Background

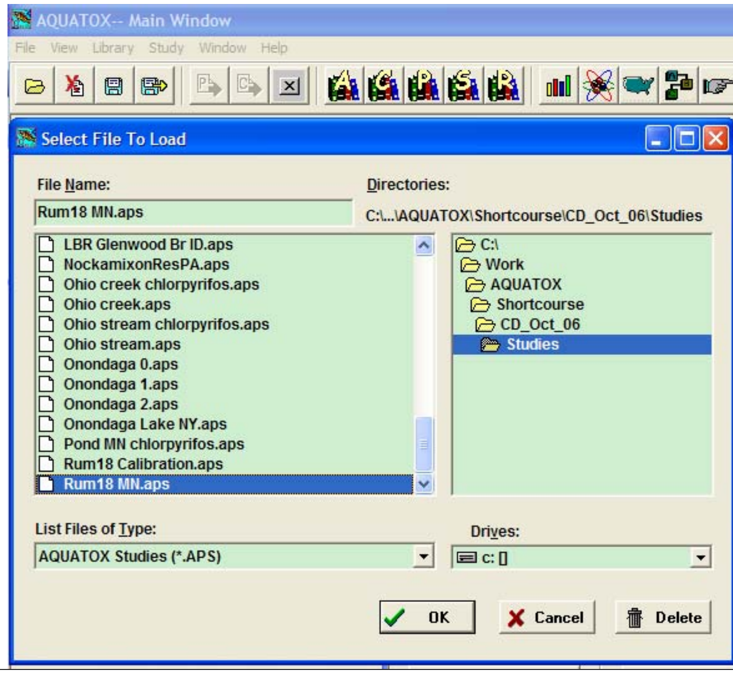
- Located in southern Idaho
- Typical of rivers in arid West
- Controlled releases upstream and diversions for irrigation
  - hydrology is opposite of normal seasonal
- Shallow with cobbles, gravel, & sand
- Nutrient concentrations moderate, turbidity low
- Abundant periphyton

The Lower Boise River, Glenwood Bridge, Boise, Idaho, is somewhat similar to the Rum River. However. it is heavily managed for irrigation purposes. As USGS states in their Web site:

REMARKS.--Flow regulated by Anderson Ranch Reservoir, Arrowrock Reservoir and Lucky Peak Lake (sta 13201500). The New York, Ridenbaugh and eight small canals (sta 13205995) divert between station "near Boise" (see sta 13202000) and this station.

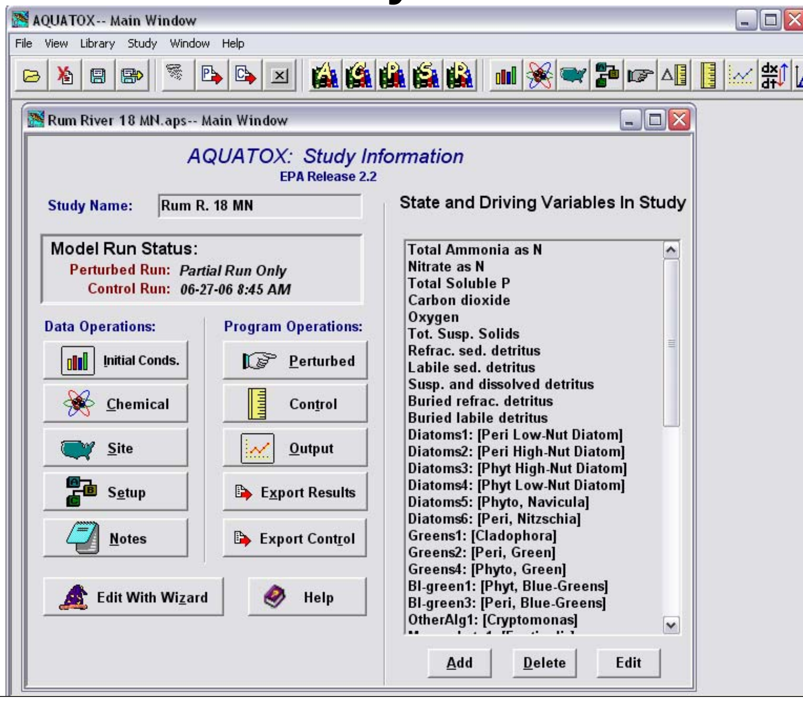
High flow is in the summer and low flow is in the winter, starting about October 15.

Load Rum18 MN.aps



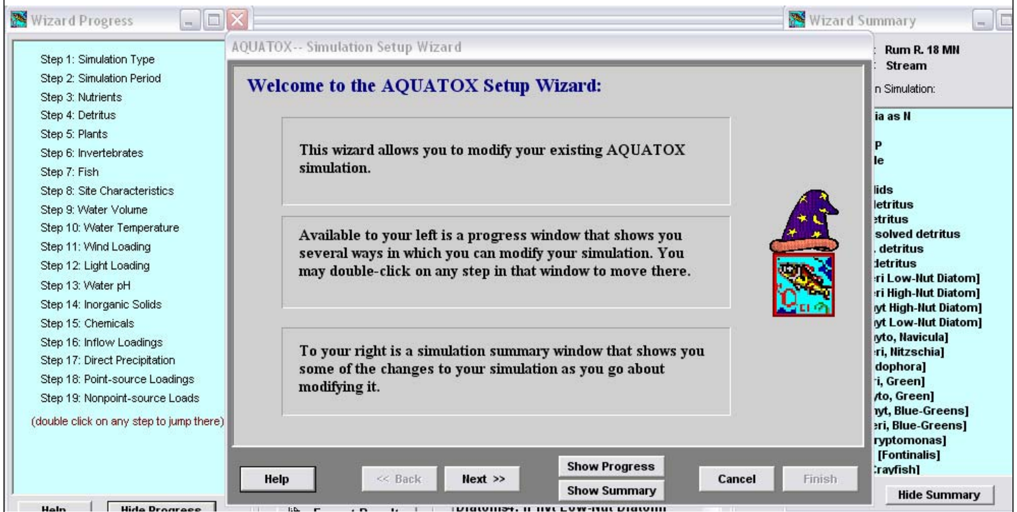
Rum18 MN.aps

Main Study Window



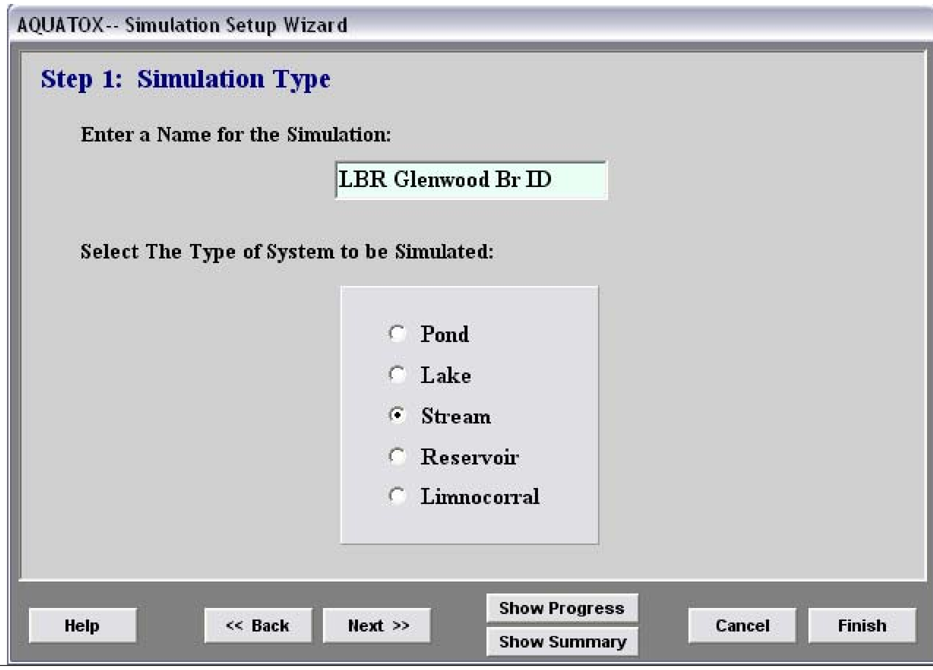
The main study window is the first thing you see when you load an AQUATOX file. Each of these big buttons can be used to view or modify a different portion of the simulation's parameterization. The tool-bar may also be used in this manner as the menu items at the top of the screen. Note that you may see the purpose of each tool-bar option by "hovering" your mouse cursor over each of the buttons. Additionally, the complete list of state variables within a simulation are listed to the right of the screen. By double-clicking on any of these variables you can look at the initial conditions, loadings, and underlying data that represent each state variable. However, to start, we are going to use the most user-friendly portion of the AQUATOX interface which is the Wizard. The Wizard is not comprehensive in that you cannot modify every portion of an AQUATOX simulation. However, it presents the most important characteristics of an AQUATOX simulation and is a great way to start as a beginner. Click on the Wizard button now.

AQUATOX Setup Wizard



The simulation setup wizard is composed of three windows: “Progress” allows you to see each of the steps within the wizard and, by double clicking on any one of these steps you can jump to a specific step. The main window in the center is where you’ll be doing most of your work examining and modifying parameters. The “Wizard Summary” window shows you the current list of state variables contained within your simulation as you go through the modification process.

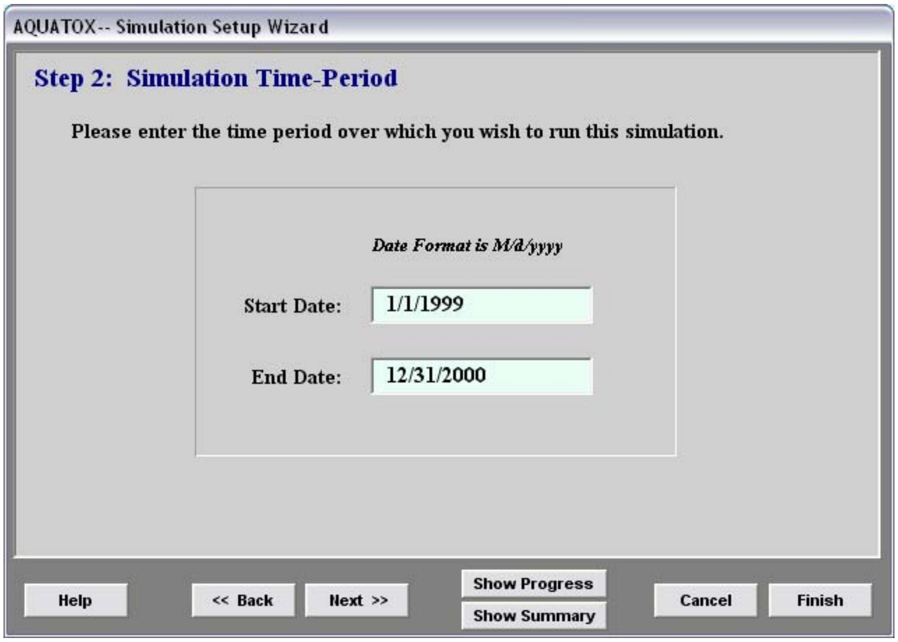
Step 1: Simulation Type



We’ll start with the most basic change, and that is the name of the simulation. Change to **LBR Glenwood Br ID** for Lower Boise River, Glenwood Bridge, Idaho.

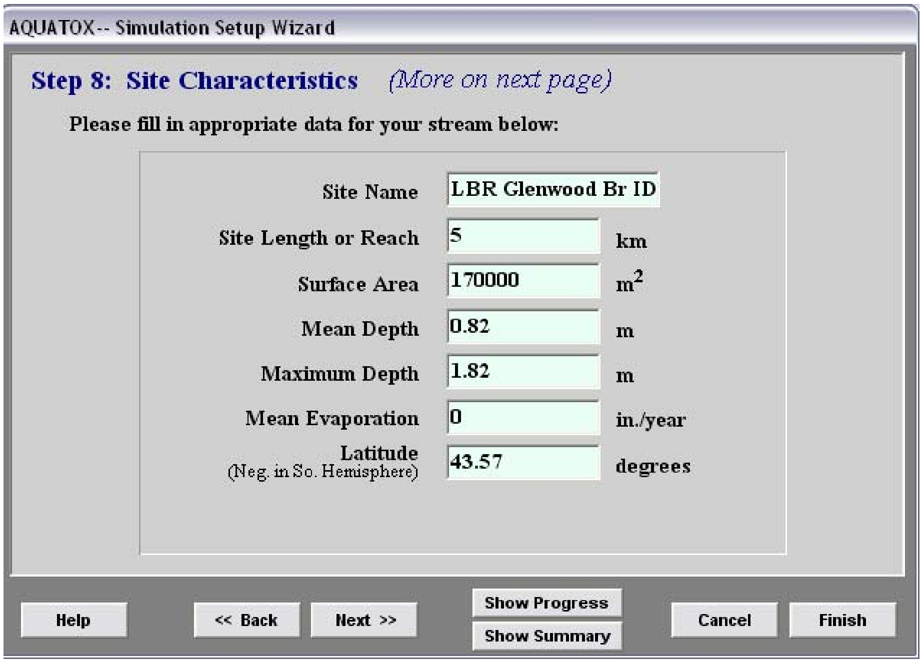
Check to make sure that the water body type selected is “Stream”. The choice of water body type governs the physical processes that operate, and in some cases, availability of particular user options.

Simulation Time-Period



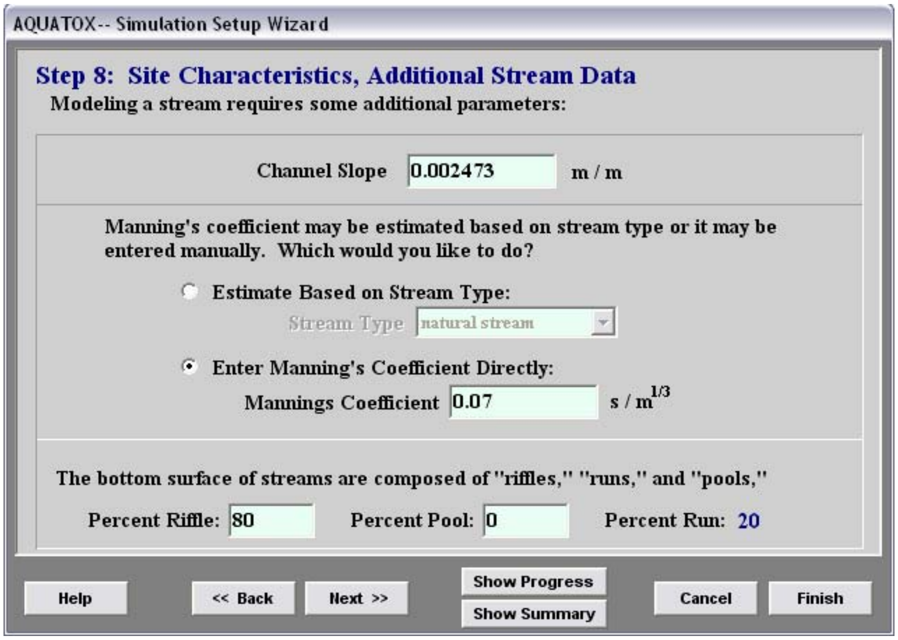
Next we'll move to the simulation time-period. We will simulate two years make sure the dates match the dates shown here. Next we're going to jump to the site characteristics so double click on **Step 8: Site characteristics** in the "Progress" window.

Site Characteristics



We are modeling LBR Glenwood Bridge so the site name should be changed to match the simulation name, We will model an arbitrary 5 km reach length (shorter reaches increase the simulation time because of the effects of the shorter residence time on the differential equation solver). The surface area is 170,000 m. Average Mean Depth is 0.82 meters. This can be replaced later by daily values if we have gage data or a watershed simulation to populate this as a time-series. (The mean depth affects several portions of the model including the light climate for bottom-dwelling plants.) The maximum depth is set at 1.82 meters for the site. We'll set the evaporation to zero for now as this is far-outweighed by inflow and outflow of water in calculating a water balance for this small segment of river. The Latitude should be set to 43.57 degrees, which affects the photoperiod when calculating photosynthesis.

Site Characteristics *(cont.)*

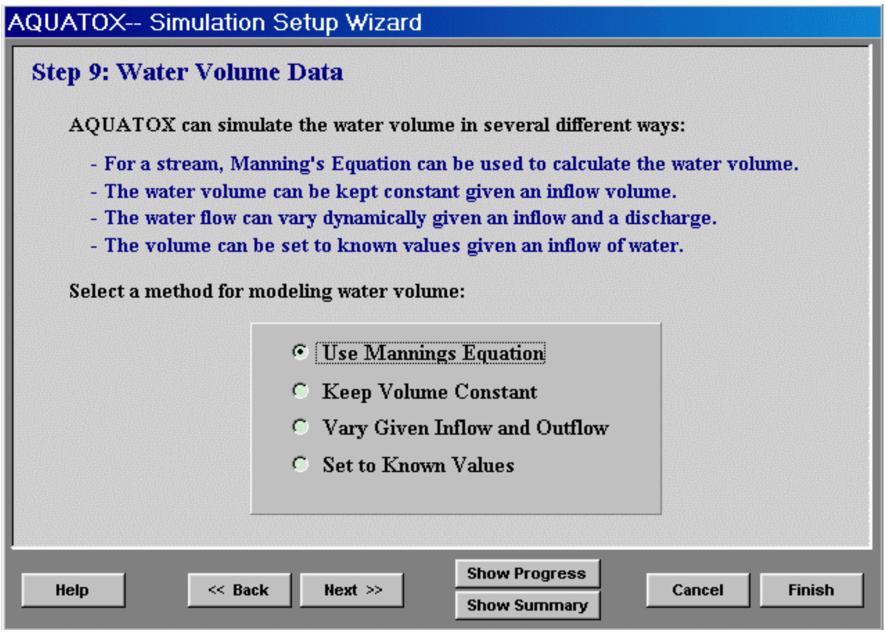


We set the **channel slope** to 0.002473 based on measured hydraulic data from the site; this parameter affects the scour and deposition of detritus and plants from and to the stream's bottom.

Manning's coefficient can affect the water volume of the site if Manning's equation is used for this calculation. It could be estimated by the software based on the fact that this is a natural stream; however, based on a spreadsheet calibration tool that we will use shortly, we will see that the best fit is with a roughness value of **0.07**, which is reasonable for a cobblestone bed**.**

Based on pebble counts for the site we'll set the **Percent Riffle** of the site to 80% and the **Percent Pool** of the site to 0% (the percent run auto-calculates); these parameters affect the available habitat for different organisms that may be limited by water velocity.

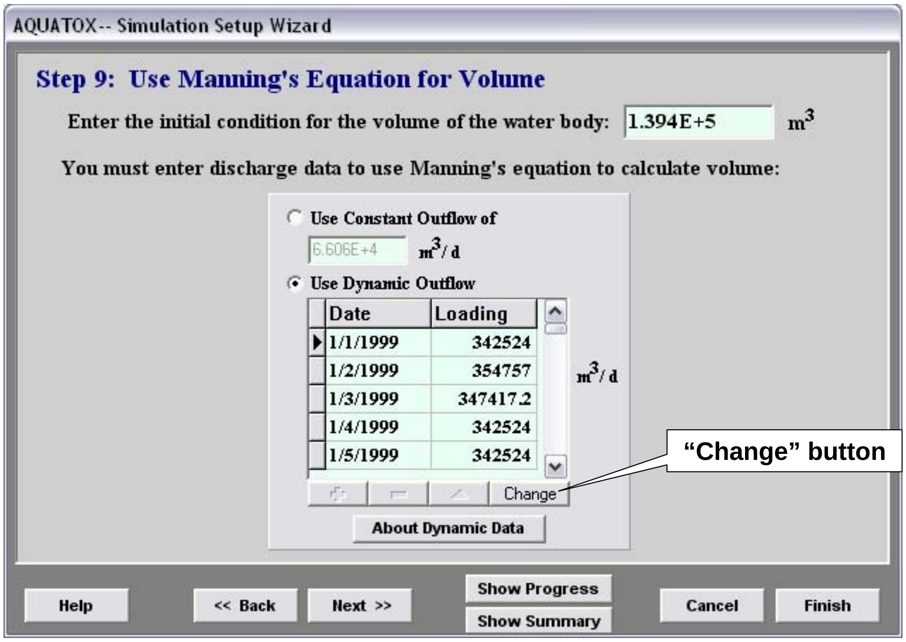
Water Volume Choices



Notes: The four options for modeling water volume are shown on this screen. The Manning's Equation Method (for streams only) requires discharge data. Inflow data and site volume are calculated using Manning's Equation. Careful attention should be given to the "Channel Slope" and "Manning's Coefficient" parameters entered in the "Stream Data" screen (within the site underlying data screen.), or in the previous Wizard screen. The *Keep Water Volume Constant* method requires inflow data. Discharge is calculated based on inflow and evaporation. If you choose to *Vary Given Inflow and Outflow*, volume is calculated based on inflow, outflow and evaporation. The *Utilize Known Values Method* requires a time-series of known volumes and inflow data. Outflow is calculated taking evaporation into account.

In this case, we have flow data only from the USGS gage so the Use Manning's Equation option will be most useful.

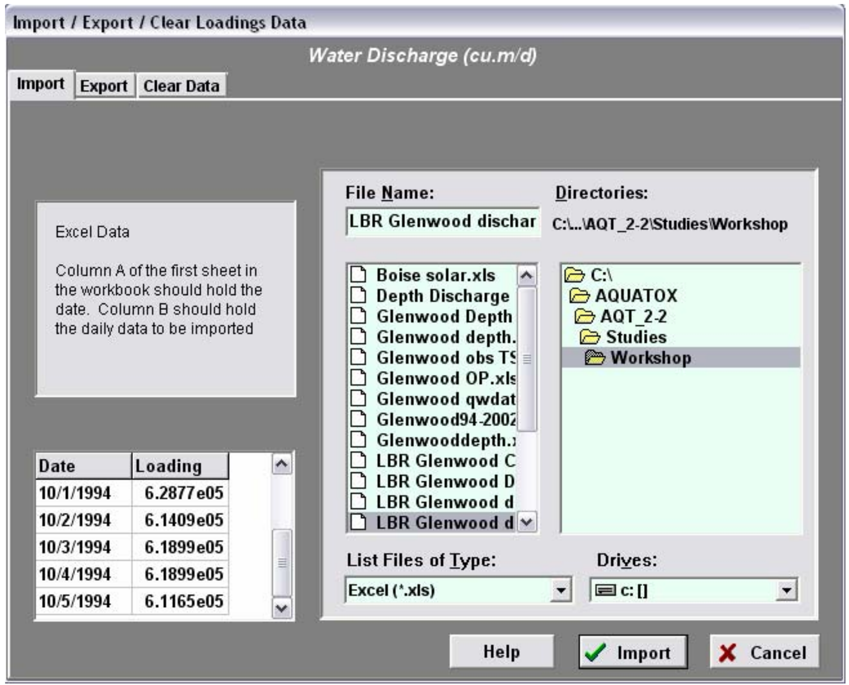
Using Manning's Equation



The initial condition is not particularly important as the Manning's calculation will take place once the simulation starts. However, based on the mean depth and surface area, we'll set this value to 1.394e5.

Below you can see what will soon become a familiar sight: the AQUATOX loadings interface. You have two options when modeling loadings, using a constant loading each day of the simulation or entering a "dynamic" loading based on an entered or imported time-series. You can use the buttons at the bottom of the interface ("+" "-" "^") to manually edit or produce a time-series. Probably more efficient will be to create a time-series externally and to import this using the "change" button.

Import / Export / Clear Loadings



Using the interface shown here, you can import time-series loadings, or by clicking the two tabs at the top you can bring up interfaces to export or clear loadings. The formats available for import (click on downward facing arrow by **List Files of Type**) comma delimited, tab delimited, DBase, Paradox database, Excel, or in the case of water flows, USGS flow data as downloaded from the Internet. However, USGS has made their format more general, making it difficult to do an automatic conversion; therefore, we will import a file captured and converted earlier from the USGS Web site.

Import **LBR Glenwood discharge.xls**

Once you have imported the file you must click on “Next” in the Wizard for it to actually be linked.

Exercise: Familiarize Yourself with the Technical Documentation

Q: How is Manning's Equation Utilized to Estimate Volume?

A:

Table 1. Computation of Volume, Inflow, and Discharge

Method	Inflow	Discharge
Constant	*InflowLoad*	*InflowLoad - Evap*
Dynamic	*InflowLoad*	*DischargeLoad*
Known values	*InflowLoad*	*InflowLoad - Evap + (State - KnownVals)/dt*
Manning	*ManningVol - State/dt + DischargeLoad + Evap*	*DischargeLoad*

The variables are defined as:

InflowLoad = user-supplied inflow loading (m^3/d);
DischargeLoad = user-supplied discharge loading (m^3/d);
State = computed state variable value for volume (m^3);
KnownVals = time series of known values of volume (m^3);
dt = incremental time in simulation (d); and
ManningVol = volume of stream reach (m^3), see (4).

Figure 14 illustrates time-varying volumes and inflow loadings specified by the user and discharge computed by the model for a run-of-the-river reservoir. Note that significant drops in volume occur with operational releases, usually in the spring, for flood control purposes.

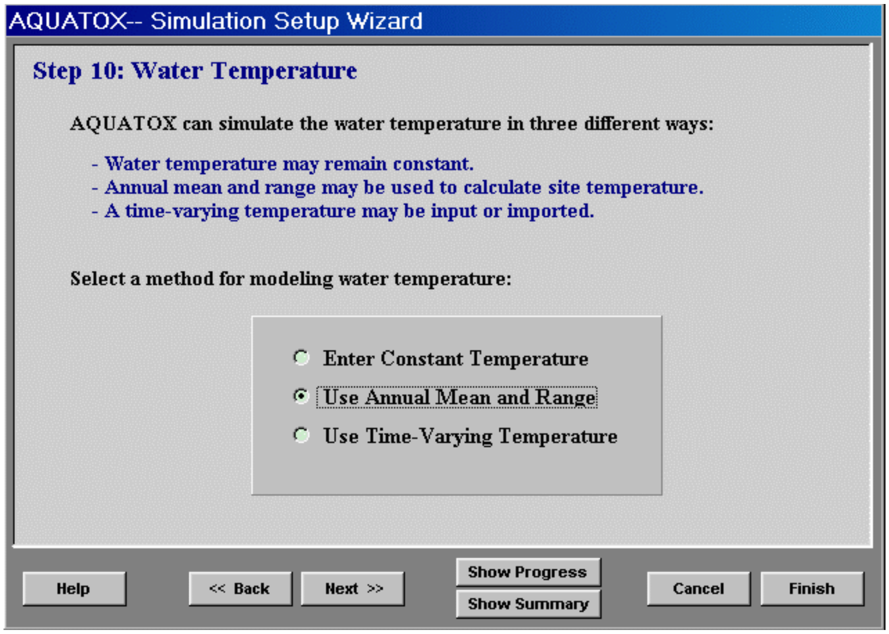
The time-varying volume of water in a stream channel is computed as:

$$ManningVol = Y \cdot CLength \cdot Width \qquad (4)$$

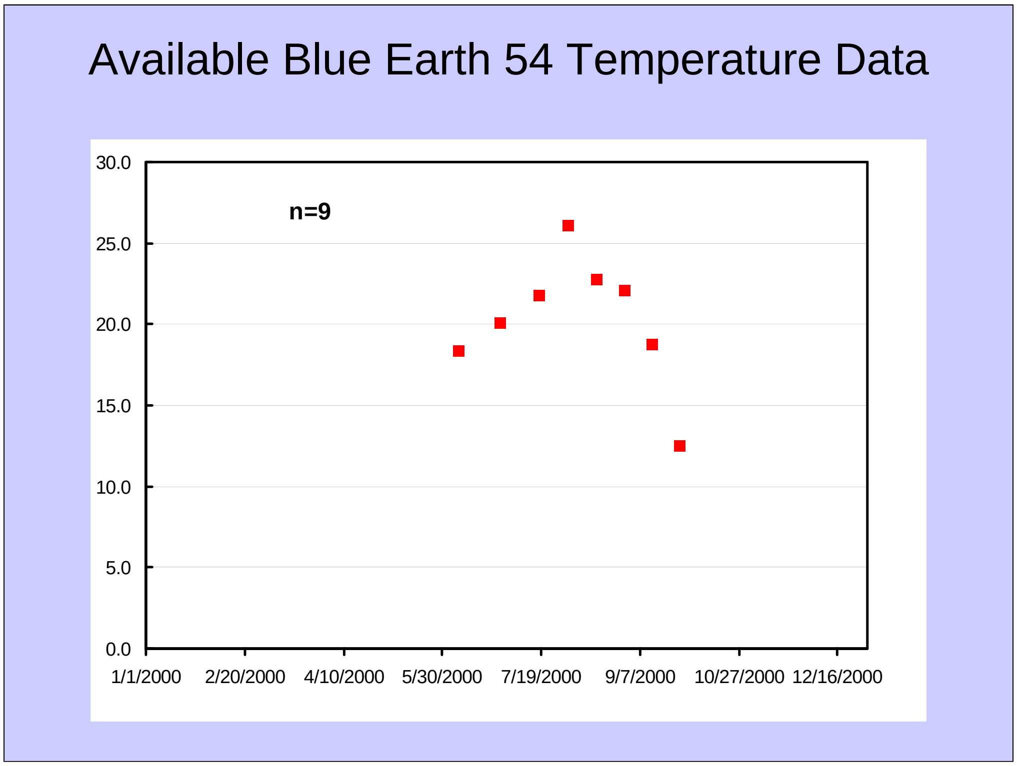
When you come across a question for which you need more information, your first resource should be the AQUATOX technical documentation. We will now take a break from using the wizard to navigate to the relevant file on your computer and spend a moment perusing it and the Release 2.1 technical addendum.

There is also an in-depth users manual that provides an introduction to the AQUATOX interface. We will open up this document as well.

Water Temperature Choices

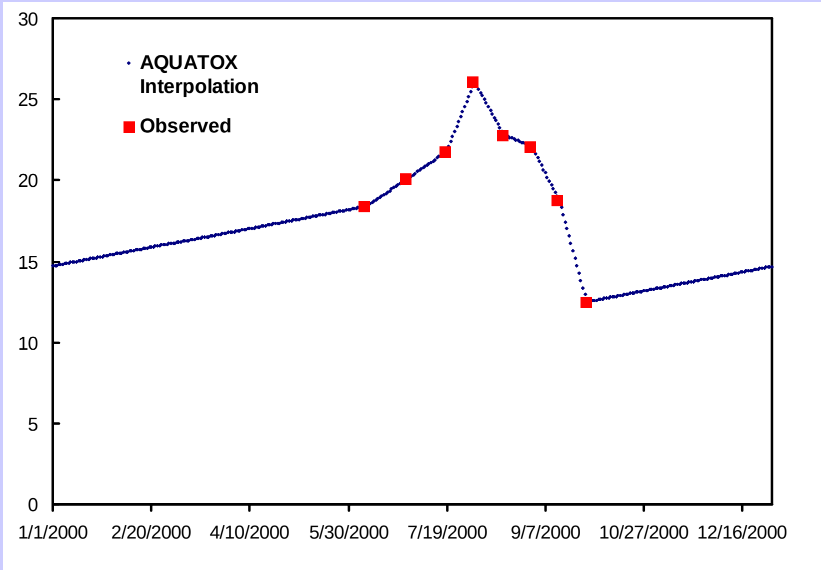


Temperature can be modeled as a constant, using dynamic data, or using annual means and ranges. In this case, our choice depends on the nature of the data that we have. **We will deviate from loading Glenwood Bridge data for the moment in order to illustrate issues to consider in using sparse data**. Our example is Blue Earth River, another MN river used in calibrating AQUATOX.



This graph shows the nine available temperature data points for mile 54 of the Blue Earth river. Now we could import these data into AQUATOX as dynamic temperature data, but this is a good time to illustrate one important aspect of AQUATOX dynamic data:

AQUATOX Interpolates Dynamic Loadings on an Annual Basis

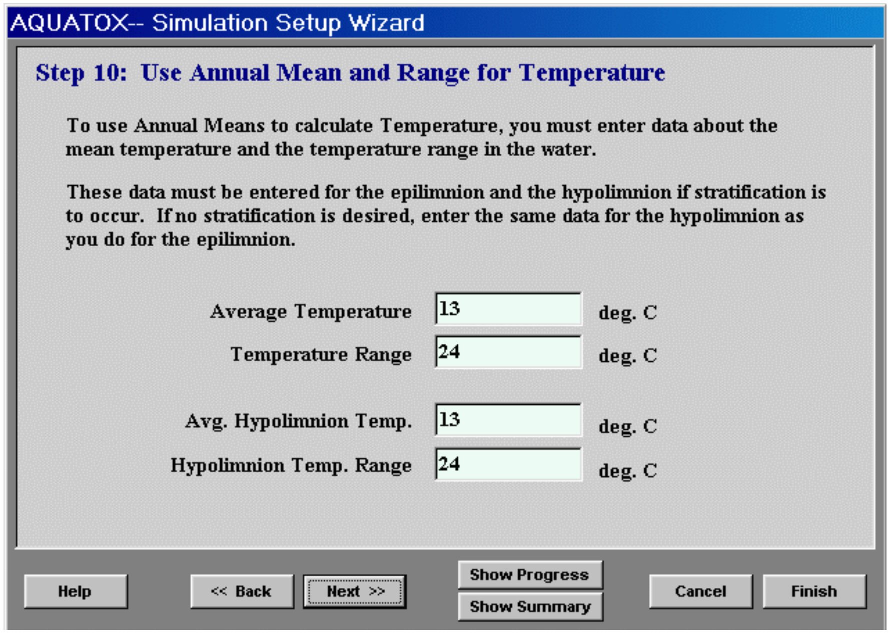


This graph shows actual simulation results for Temperature when the set of 9 observed data-points are simply loaded into the simulation. AQUATOX will linearly interpolate between available data-points when a limited set of dynamic data are available. As you can see, this interpolation takes place between years when there are no relevant data at the beginning or end of a simulation.

This interpolation can be important if you are trying to include a “spike” loading of toxicant or other perturbation. You must put dates with zero loadings on each side or there will be an unintended effect due to interpolation.

Getting back to temperature, we can look at the third option, using annual means and ranges.

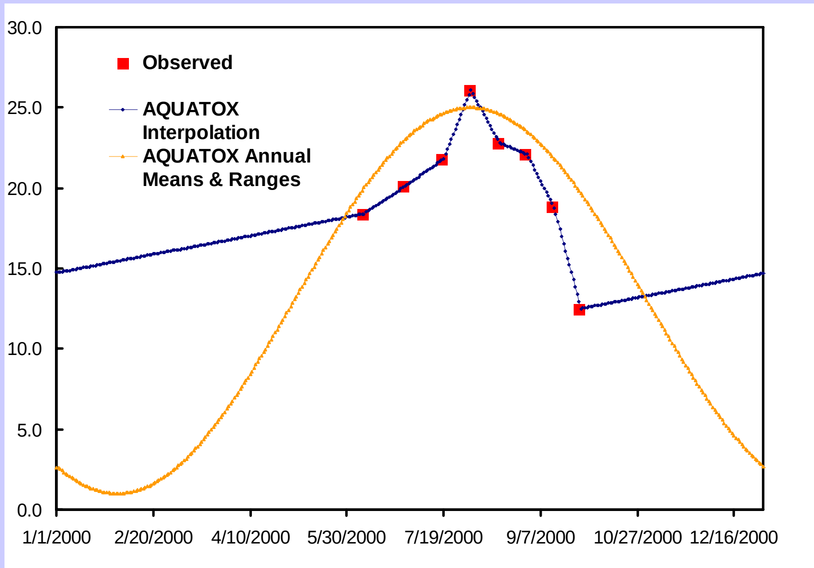
Using Annual Means and Ranges



Looking at observed data for Blue Earth, we have a maximum value of 26.1 C but this is a bit of an outlier. So assuming that we would want a maximum temperature of around 25 degrees and a minimum of 1 degrees in the Minnesota winter, we have an average of 13 and a range of 24 degrees (max – min).

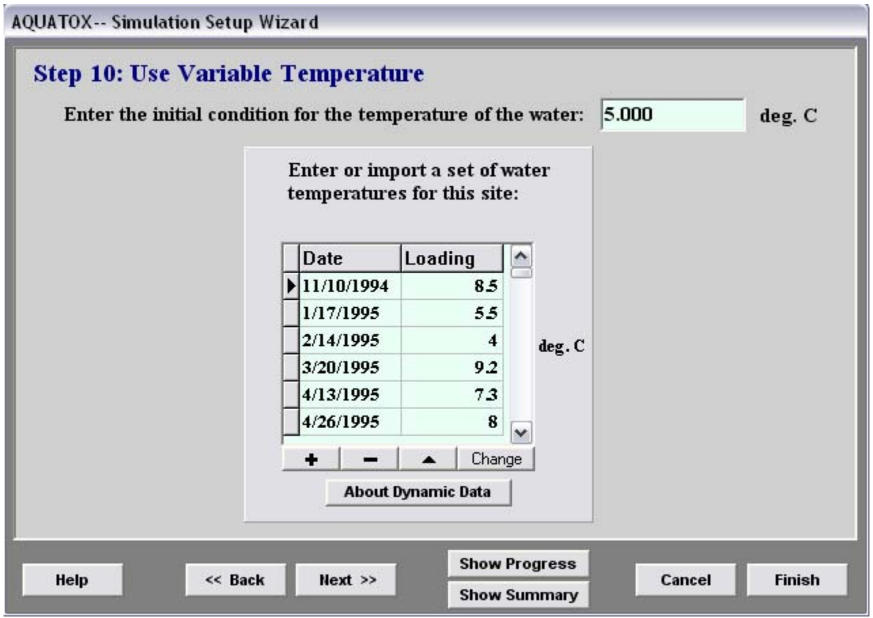
Note that because this is not a lake, the hypolimnion temperature is irrelevant so we would just enter the same values for epilimnion temperature.

Results with Annual Means & Ranges



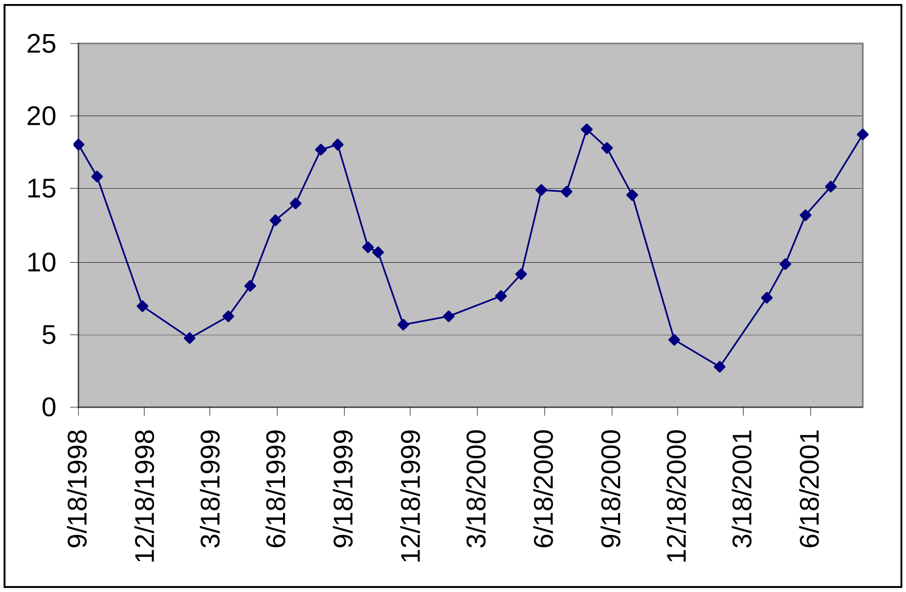
This graph shows how AQUATOX models temperature using the parameters we just provided. Though it does not hit the data points perfectly it is more important that the long winter dormancy period is properly modeled than the summer data gets represented perfectly.

Import observed temperature



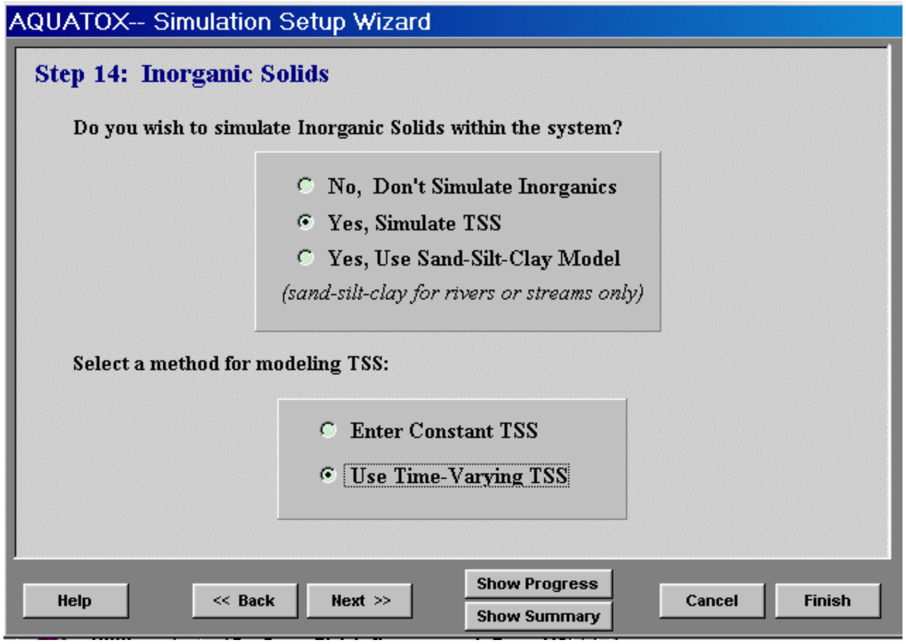
Getting back to our Glenwood Bridge example, we have a time series of observed temperature data that we will use. Those are imported into the study from **LBR Glenwood Temp.xls**.

A segment of the observed temperature



The observed USGS data are judged sufficient to define the time course for temperature.

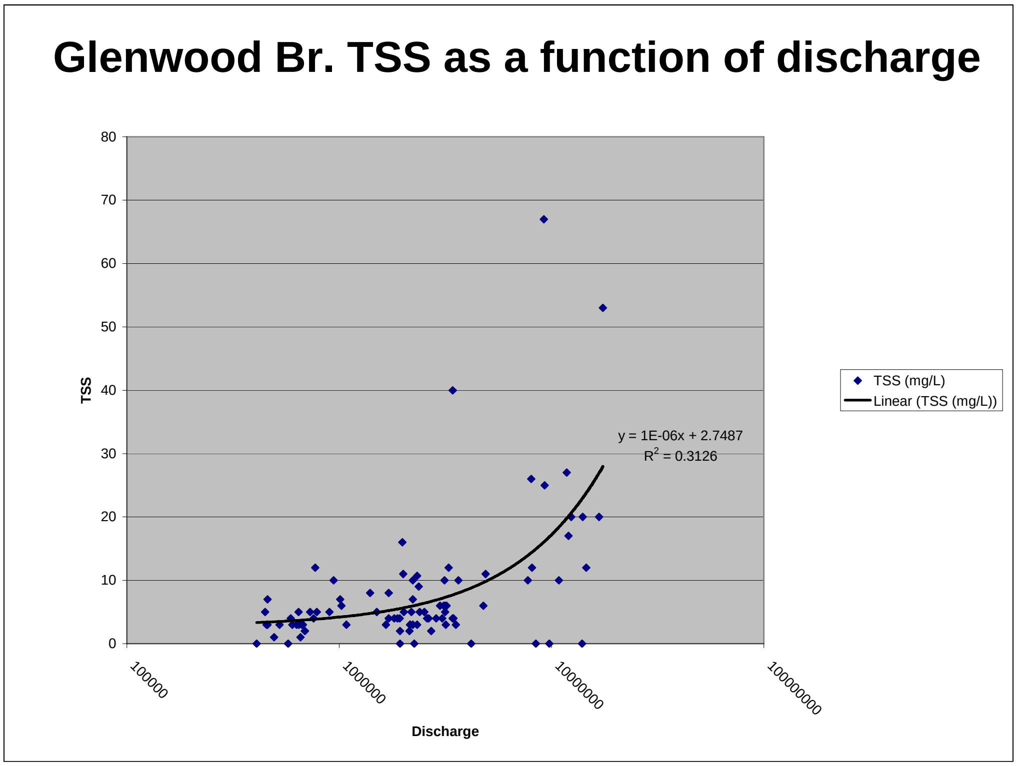
Inorganic Solids Setup



Next we're going to jump to Inorganic Solids as the stream model is not sensitive to wind loadings. Double click on the **Step 14** text to jump within the Wizard. We will select to load time-varying TSS.

The three options for modeling inorganic sediments are to exclude organic sediments, model TSS as a non-reactive time-series, or to include the sand-silt-clay model which we will discuss on Day 3.

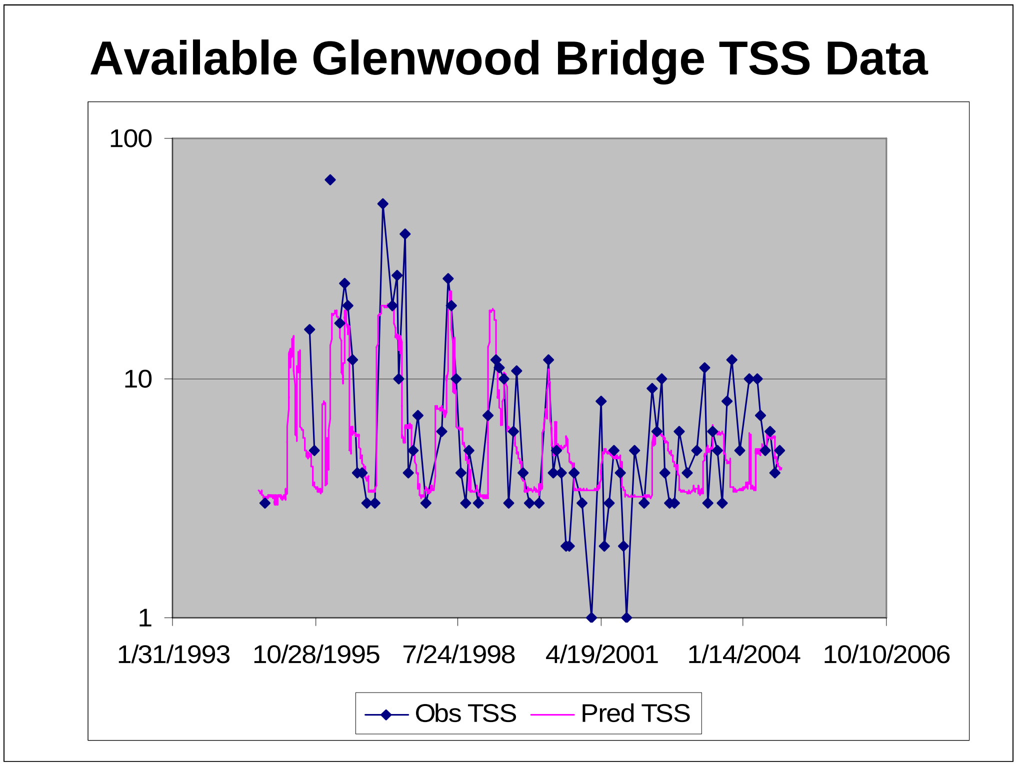
See Chapter 6 of the technical documentation for more information on these models.



Moving back to the slideshow for a moment, we see a weak relationship with much scatter between water discharge and observed total suspended sediment (not solids). This is a managed river with controlled releases and occasional flushing of sediment from upstream impoundments.

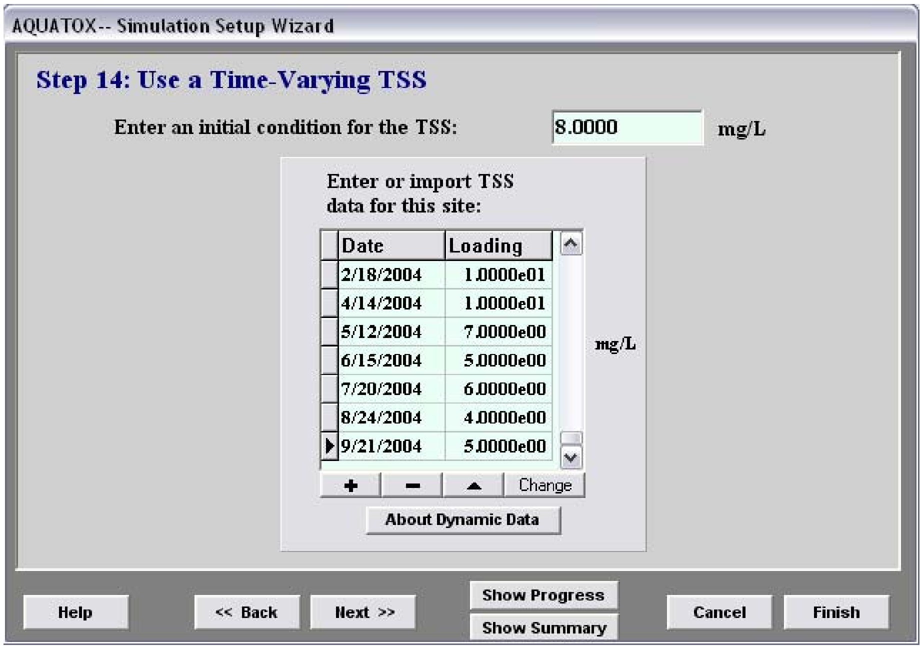
A TSS of 20 (mg/L), corresponds to a light extinction of 3.4 (1/m). This, in turn, corresponds to an estimated Secchi depth of 0.56m. It is clear how important TSS can be to algal growth given these facts. Because the model is so sensitive to low TSS modeling “average” conditions is not acceptable.

When modeling a relatively data-sparse river (and this is the case with the vast majority of rivers that you will encounter), linkage to a Hydrology/Watershed model is a powerful tool, and is likely to be more precise than the simple relationships that you will put together with data. However, we have no such model results to link for the Boise River.



Plotting the interpolated observed TSS with the results predicted by the empirical model, we see that the sparse observed data are preferable to estimates that miss both high and low values.

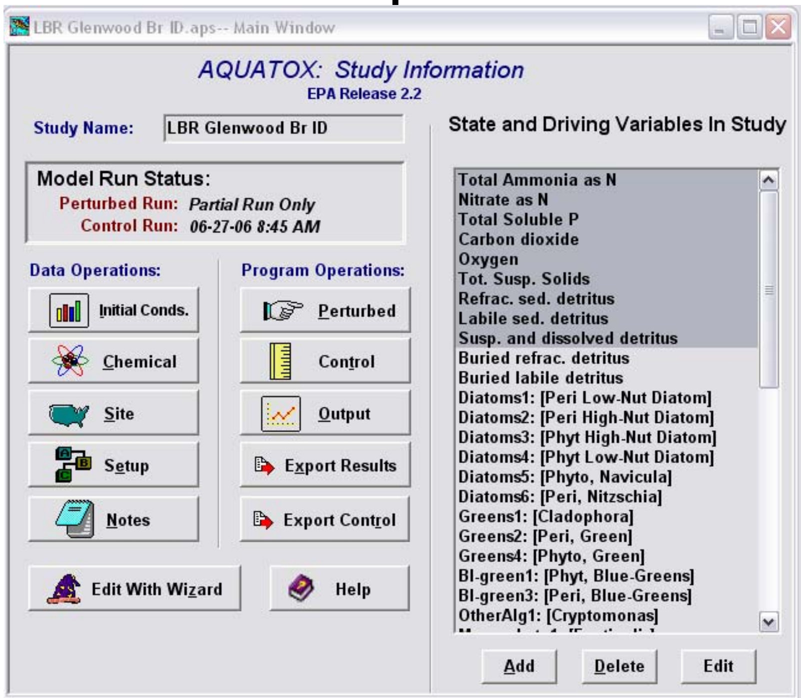
Import Time Varying TSS Input



Use the “change” button to import the file **Glenwood obs TSS.xls.**

Next, we’re going to modify inflow loadings. You may use the wizard screen to input inflow loadings, but as mentioned previously there are some subtleties in the interface that are not captured by the wizard. We’ll go into the state variable list to import these loadings. Select “Finish” after the import is complete and “yes” that you’d like to save changes.

Select Multiple Variables



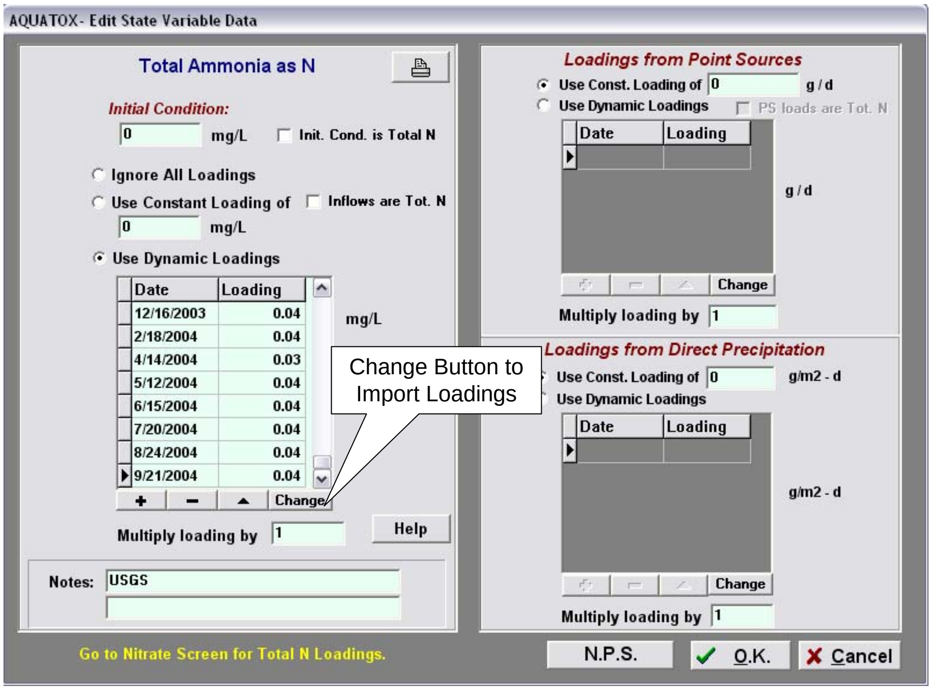
Click "Finish" to exit the Wizard and save your changes. Save the study as **LBR Glenwood Br ID.aps** before proceeding.

You may use the wizard screens to input inflow loadings, but as mentioned previously there are some subtleties in the interface that are not captured by the wizard. We'll go into the state variable list to import these loadings.

It is very useful to select multiple items from a list using standard windows shift-click and control-click options. This can be useful when editing state variables and also producing output within AQUATOX.

In this case, we select the first nine variables within AQUATOX in which all nutrient and organics state variables are held.

Ammonia Loadings

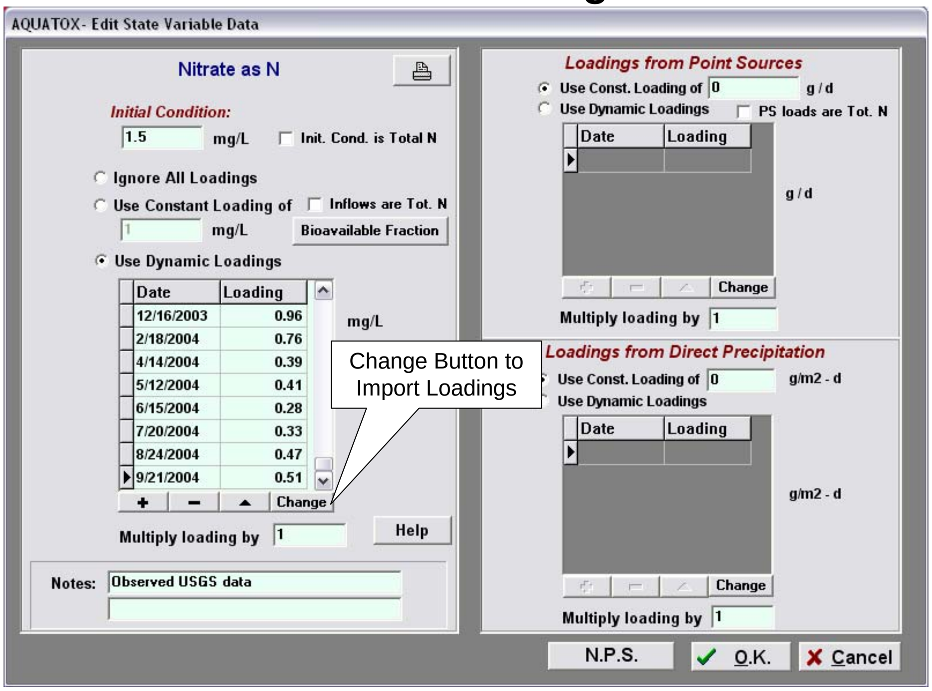


For ammonia select the **Dynamic Loadings** radio button and import observed values (**LBR Glenwood NH4.xls**) downloaded from the USGS Web site.

Note, de-select **Init Cond is Total N** and **Inflows are TotN**.

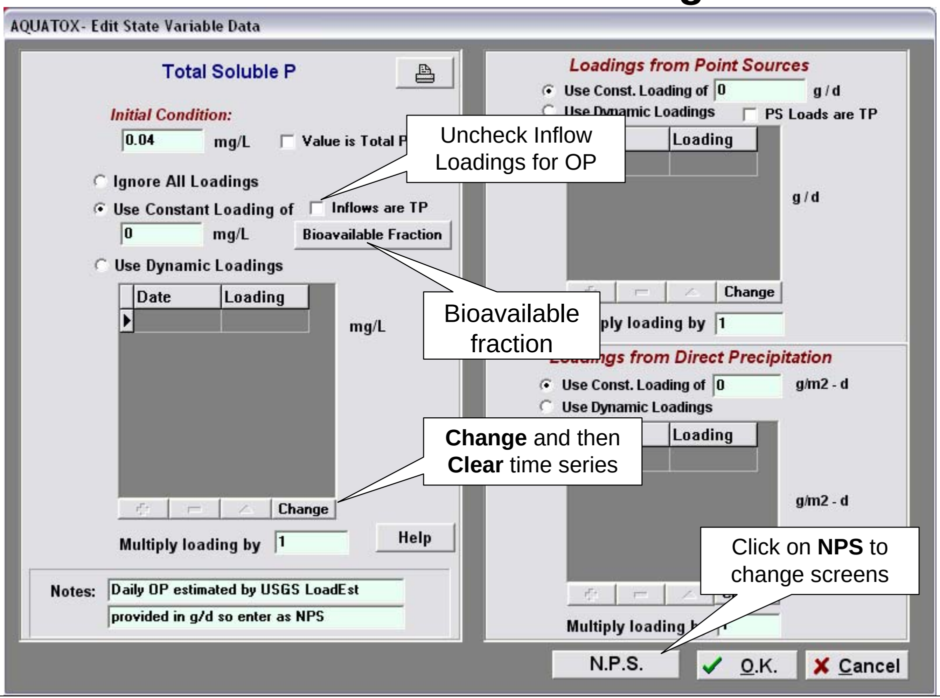
For bookkeeping purposes (so you know the source of the loadings in your simulation in the future) it is best to update the notes field at the bottom of each screen as you change a loading.

Nitrate Loadings



Nitrate as N: Select the **Dynamic Loadings** radio button and import **LBR Glenwood NO3.xls**. Initial conditions are much less important for stream simulations in which water flows through the system several times each day so we do not have to worry about being precise for that parameter. Alternatively, we could import total N loadings.

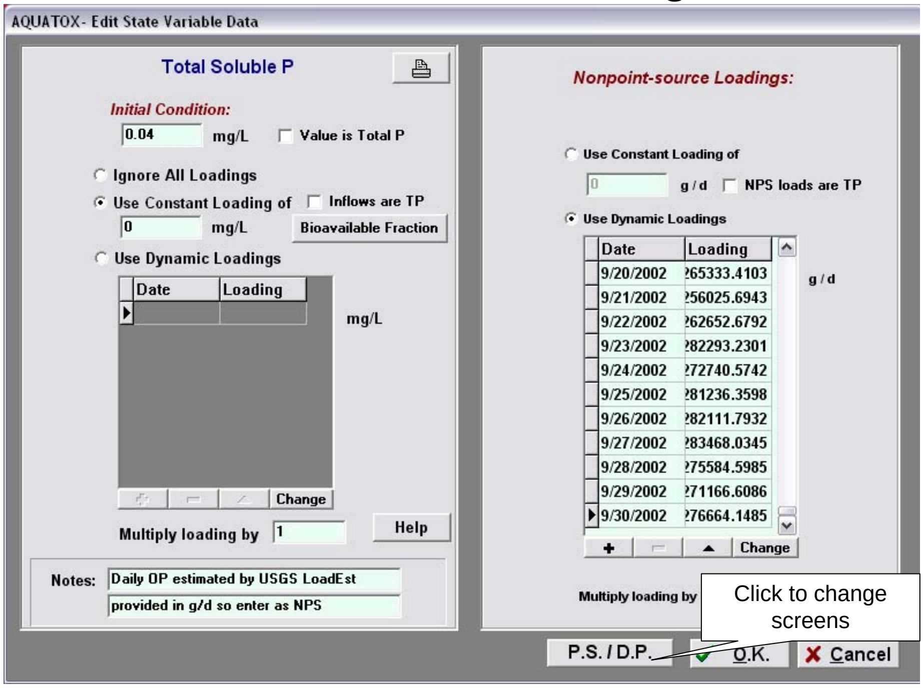
Total Soluble P Loadings



This will require several steps to modify the previous loading options. The input data are orthophosphate, so uncheck the box for **Inflows are TP**, set **Constant Loading** to 0; click on **Change** button to then **Clear** dynamic loadings. Click on **NPS** to change screens. The estimated OP values were obtained by regression using the USGS LoadEst program; they are in g/d and could be input as either point-source loadings or nonpoint-source loadings; we will choose the latter so that point-source loadings can be added at a later date if desired.

Bioavailable Fraction provides a way to modify the loadings if part is unavailable. This is more applicable to TP; we will assume that all OP is available

Total Soluble P Loadings



Import **Glenwood OP.xls** as Nonpoint-source Loadings.

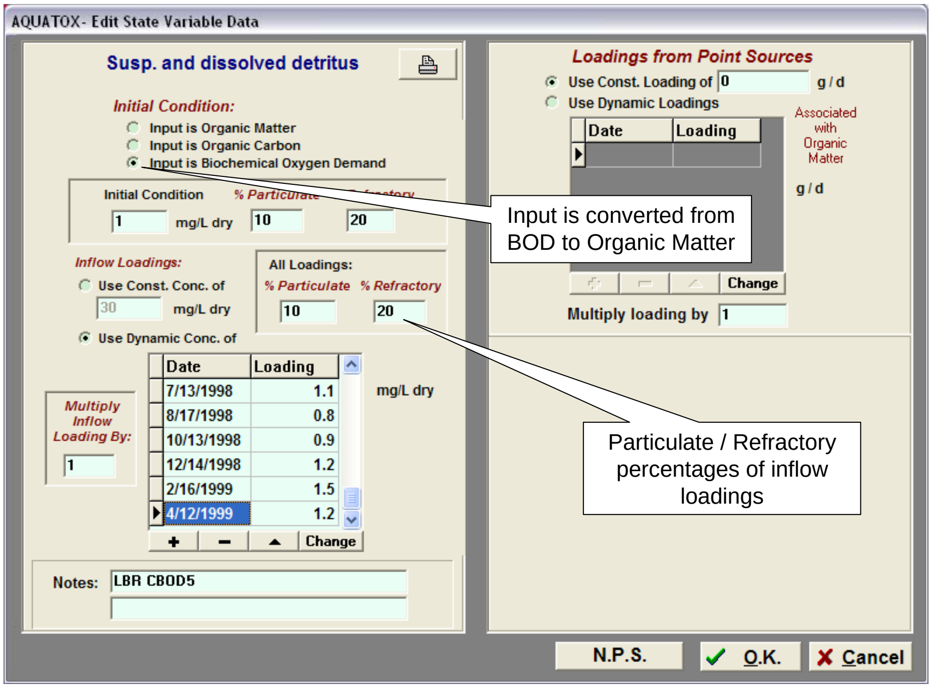
Next, for **Carbon Dioxide**, in the absence of other data, keep the default assumption of an inflow load of 0.7 mg/L.

For **Oxygen**, import available DO values (**LBR Glenwood DO.xls**). Oxygen concentrations in the stream will be dominated by these loadings due to the frequency which water flows into and out of the reach.

TSS: This shows us the values we've imported from the wizard. You probably should clean up the notes fields.

Sedimented Detritus (two screens): Keep constant at initial condition levels

Suspended and Dissolved Detritus



Suspended and Dissolved Detritus: Select input as BOD. Import **LBR Glenwood CBOD5.xls.**

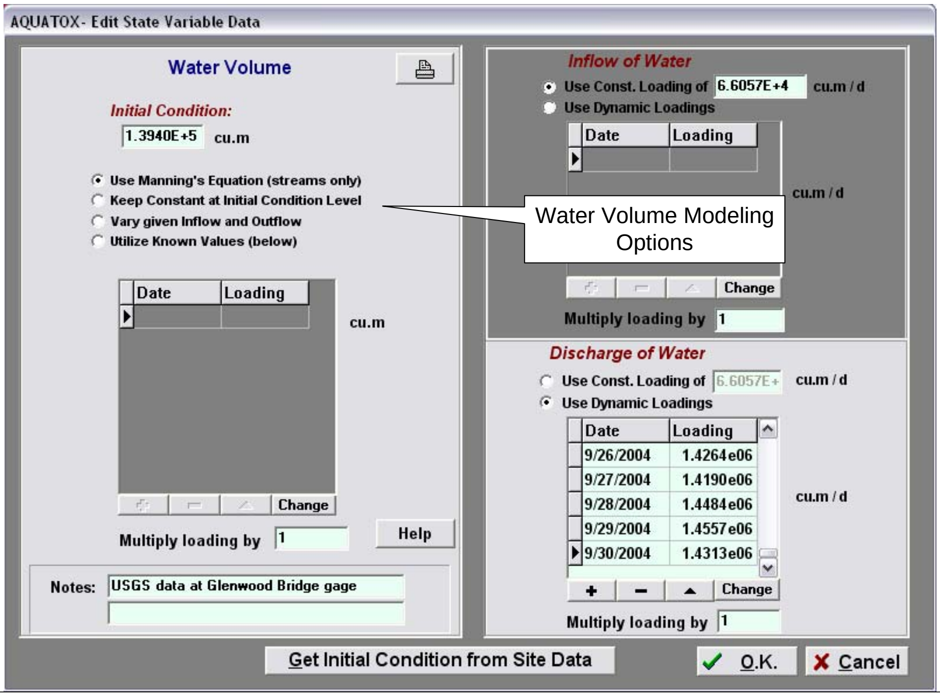
Input may be entered as Organic Matter, or may be converted from inputs of Organic Carbon or BOD. If BOD is entered, inflow loadings of phytoplankton, which contribute to BOD, are subtracted before converting to the model’s internal organic matter units. The conversions used are:

Organic matter = BOD * 0.74

Organic matter = organic carbon * 1.9

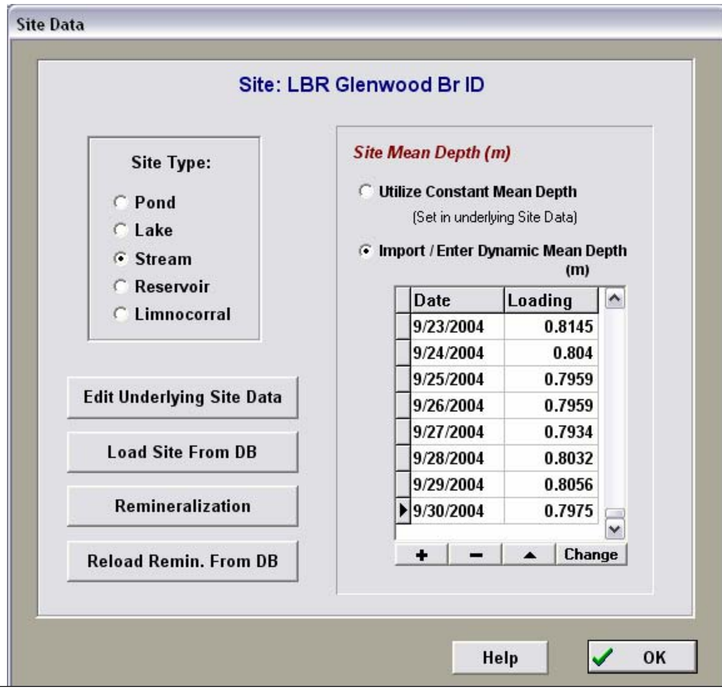
Using the percentage entry boxes, organic matter loadings must also be split into four compartments: Particulate Refractory Detritus, Particulate Labile Detritus, Dissolved Refractory Detritus, and Dissolved Labile Detritus. (Labile detritus is organic matter that decomposes at a much faster rate than refractory detritus.) A general default value for percent particulate is 10%. Because the basis is BOD5, a value of 20% for refractory is reasonable.

Water Volume Screen



In the interest of completeness, we should go to the water volume screen and update the notes field.

Water Depth



Finally, we want to calculate and enter dynamic water depth as a function of discharge. On the Main Screen, click on Site. The time series can be imported into the first screen. Import: **Glenwood Depth Discharge calibration.xls**.

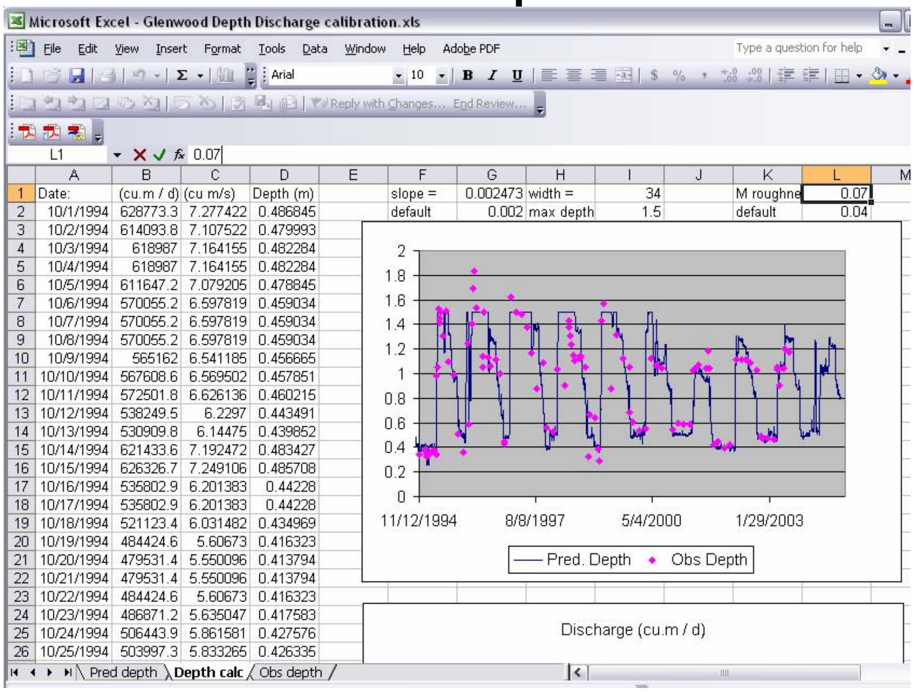
The model imports the first two columns from the first worksheet, which is **Pred Depth**. Save the study as before, **LBR Glenwood Br ID.aps**. This file should correspond to **LBR Glenwood 1.aps**, which is on your CD and in your Study directory.

The model will take about 10 minutes to run, so click on **Control** in the Main Screen to start. We'll look at the results in Lab 3.

To summarize what we've accomplished so far, we are going through the steps you would need to go through to produce a new AQUATOX application to an existing site:

- We identified a surrogate site to use as a template
- We modified the physical characteristics of the surrogate site to match "our site"
- We modified the nutrients, organics loadings, and turbidity using data from "our site."
- We have not yet modified the biota.
- However, if the biota are not dramatically different from site to site we may still get a decent simulation, just by using the physical characteristics, nutrient, and organics loadings from "our site."

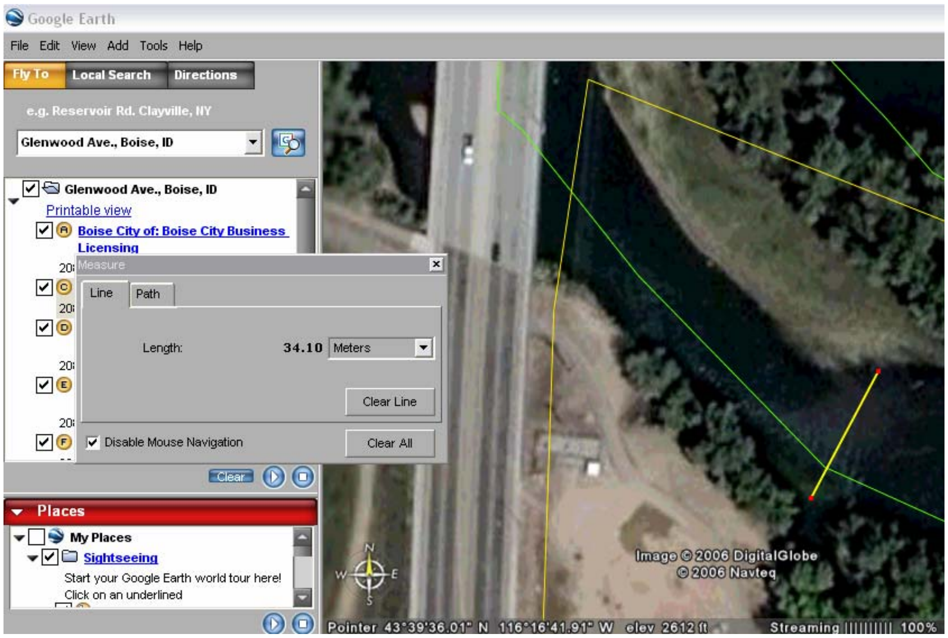
Water Depth



Now, let’s see how the dynamic depth was estimated. Open **Glenwood Depth Discharge calibration.xls**.

The model imports the first two columns from the first worksheet, which is **Pred Depth**. The calculations are done in sheet 2, **Depth calc**. To calibrate depth, the objective is to vary one or more parameters so that the estimated depth corresponds to the observed values (purples dots). We have measured values for slope (G1) and width (I1). However, we should vary the Manning’s roughness coefficient (L1) from the default value of 0.04—try it! A value of 0.07, which is near the upper end of the normal range of values, seems to give the best fit. The computations are performed in Column D and flow to Column B in the **Pred depth** worksheet.

Tip: use Google Earth to get width



Tip: if you do not have the channel width, you can obtain it by locating the site with Google Earth and using the Measure tool to obtain the width. In this example the measurement is made at the riffle upstream from Glenwood Bridge.

Modeling Plants with AQUATOX

- Equations
- Parameters
- Phytoplankton
- Periphyton
- Macrophytes
- Moss

See Chapter 4 of the Technical Documentation.

Plant Derivatives

$$\frac{dBiomass_{phyto}}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation \pm \underbrace{Sinking - Washout \pm TurbDiff}_{\text{free floating plants}}$$

$$\frac{dBiomass_{peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation - \underbrace{Slough}_{\text{bottom dwelling}}$$

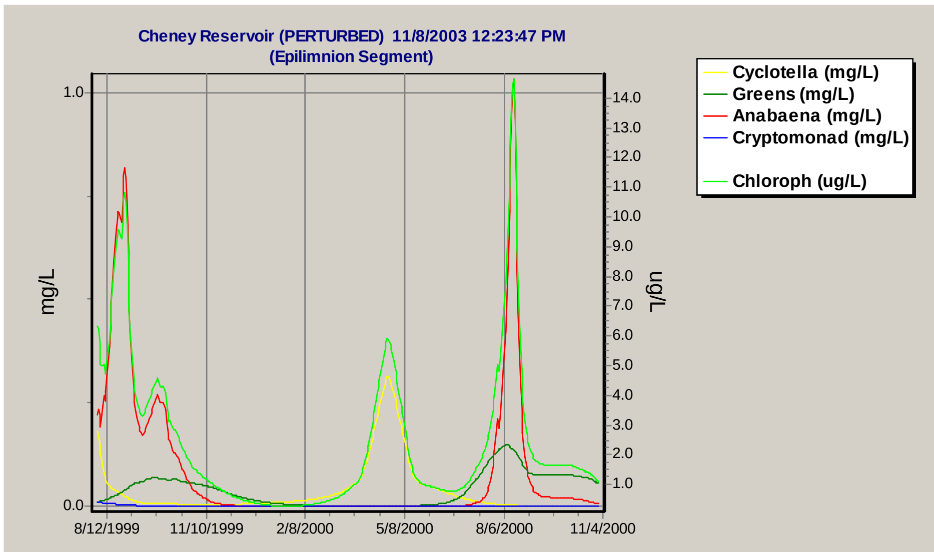
These equations are provided just to give a look at general model setup. Each state variable is subject to such a derivative. Additionally, these terms make up the basis for graphing "rates" for each organism.

Rates for state variables are output in units of percentage of mass using the following equation:

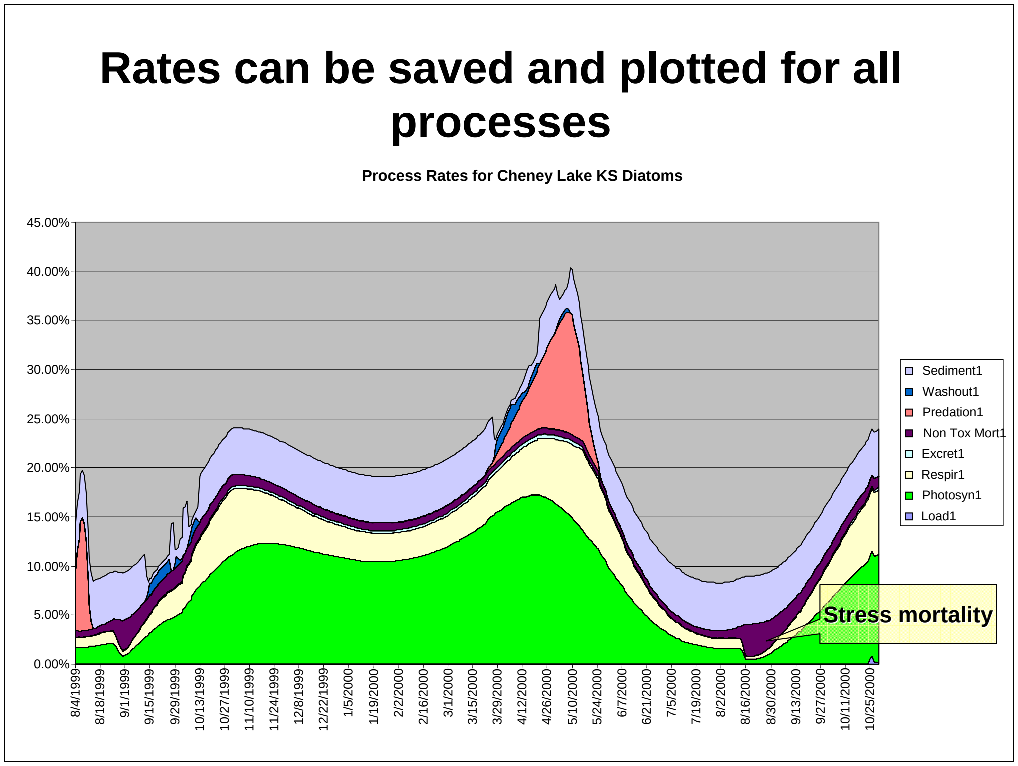
Rate *(fraction/day)* **= Rate** *(mass/day)* **/ State** *(mass)*

(To express in units of percentage, this fraction is multiplied by 100 by Excel)

Phytoplankton Biomass Shows Succession chlorophyll *a* summarizes response



One advantage of AQUATOX is that we can model as many as six groups in each of four different phytoplankton taxa (diatoms, greens, blue-greens, and others). The results are then converted to chlorophyll a to summarize the results and to provide a means for comparison with observed data.

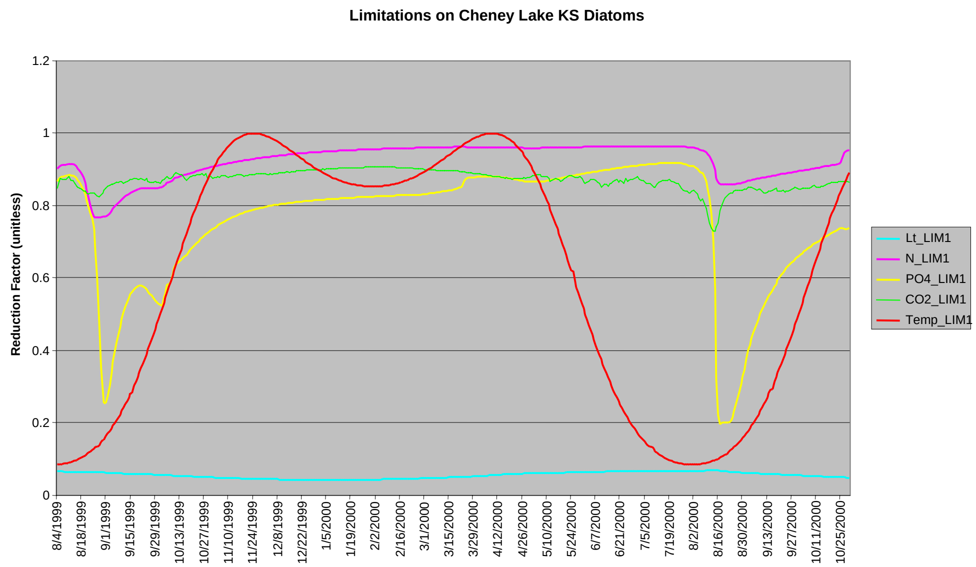


When you choose to "save rates," you are looking at each of the elements of the state variable's derivatives (e.g. the plant derivatives shown previously) to get an idea of what is causing the concentration of this state variable to increase or decrease. Examining rates gives us a window into the inner workings of AQUATOX and this can helps us understand why the model is making the predictions that it is making.

We like to use area graphs for rates because you can readily see the additive (or subtractive) nature of various processes. Think of an area graph as a continuous pie chart. The rates are expressed as percent of biomass (or concentration) at each time. These and the limitation plots that follow were created with Excel using rate files that were saved during the simulation. To save the rates click on **Setup** then **Rate Specifications** *prior to running the simulation*. Be sure to click on **Save Rates** when you have made your choices.

Stress mortality occurs twice in this simulation of diatoms in a Kansas lake. As you'll see in the following slide, it occurs when nutrients are strongly limiting.

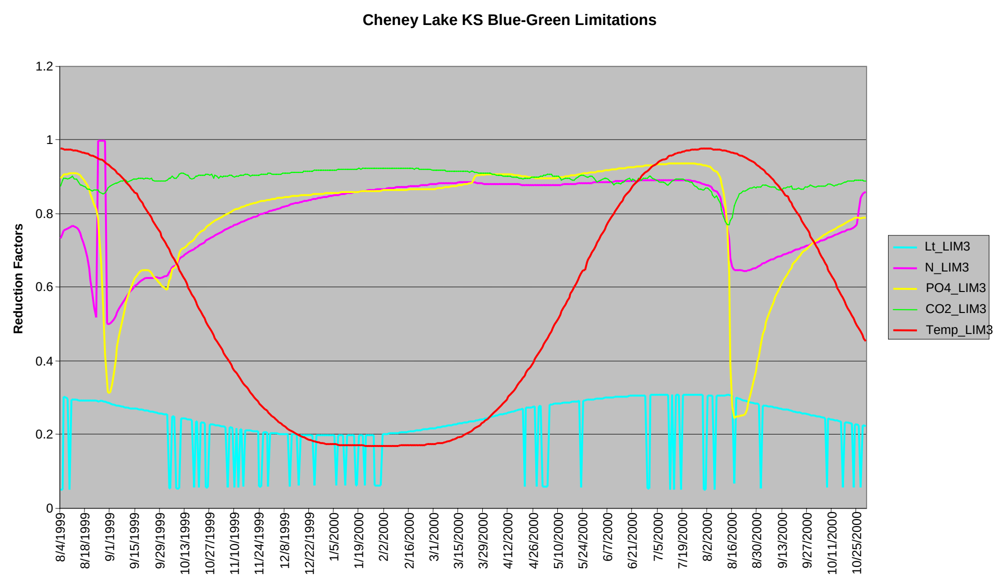
Time-varying limitations to photosynthesis also can be analyzed



Light is uniformly limiting in this well mixed lake. Temperature limits diatoms in the summer, and phosphate is limiting when blue-green algal blooms occur. This latter limitation leads to increased (stress) mortality.

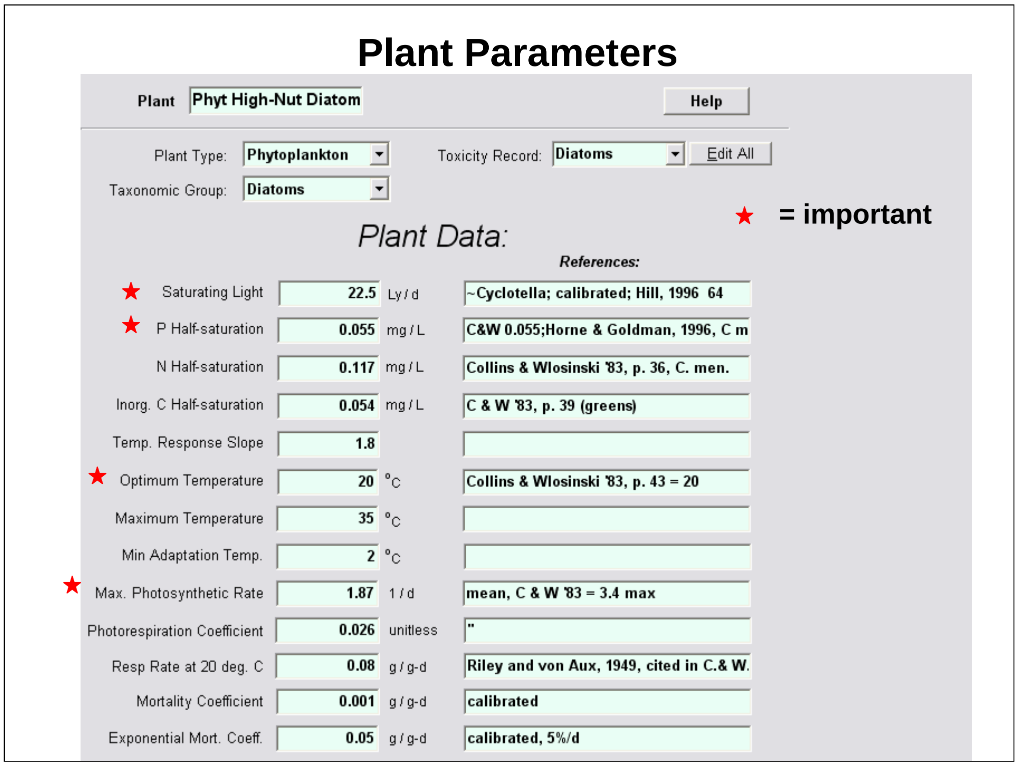
In the model, each limiting factor can have a value between 0 and 1, 0 if totally limiting and 1 if not limiting. See Equations 32 and 33 in the *AQUATOX Technical Documentation*.

Limitations on various groups can be compared



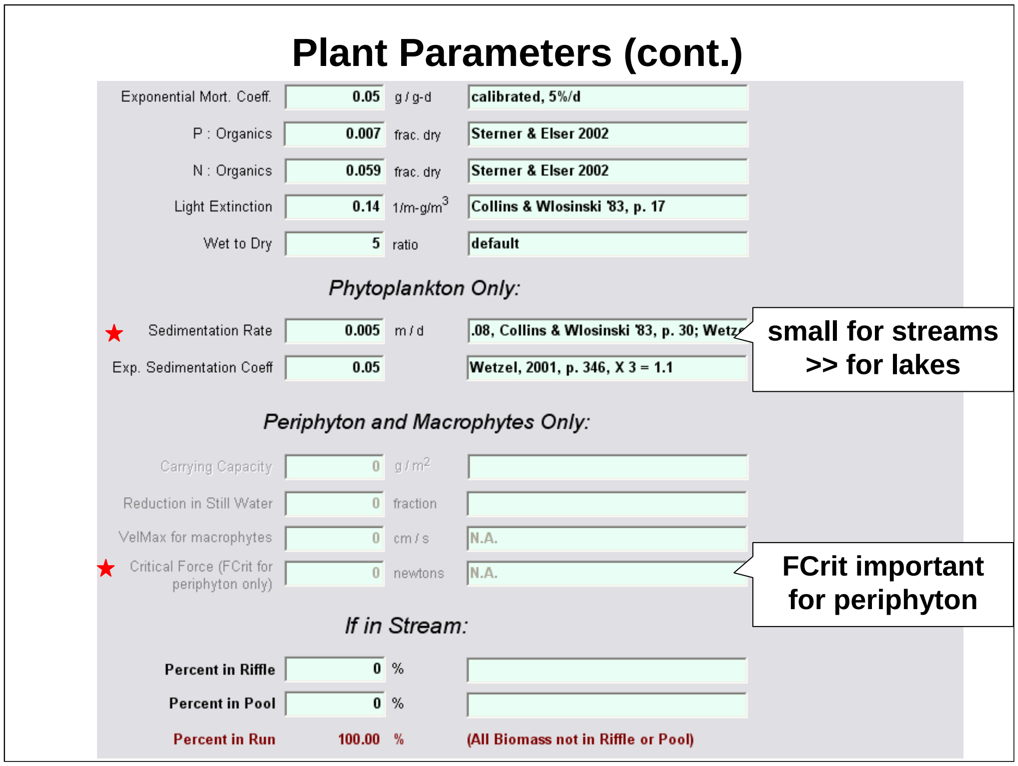
Compare this plot with the previous one. The blue-greens are warm-water forms, so they have optimal temperature during the summer--out of phase with the diatoms. Light is not as limiting as for diatoms most of the time because the blue-greens are assumed to float in the top 1/4 m except when wind exceeds 3 m/s and Langmuir circulation is assumed to occur, thus causing the algae to be drawn deeper in the water column.

Note that temperature limitation occurs at both high and low temperatures.



By double-clicking on a state variable and choosing to **Edit Underlying Data**, you can inspect and change, if necessary, any parameters. Keep in mind that the default parameters have been carefully established, so be careful in what you change. We will try to highlight those parameters that are most likely to need calibrating, based on model sensitivity and the wide range of values reported in the literature.

As an introduction to modeling plants, we will go fairly quickly through these parameters and will focus on the most important parameters for calibration.



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The phytoplankton mortality coefficient may be adjusted for a particular site, and exponential mortality coefficient (which increases the mortality for suboptimal conditions) may need to be adjusted if blooms crash too quickly or not quickly enough. Occasionally the extinction coefficient may need to be increased if algal growth is too strong--that is the principal means of negative feedback, and can vary among groups.

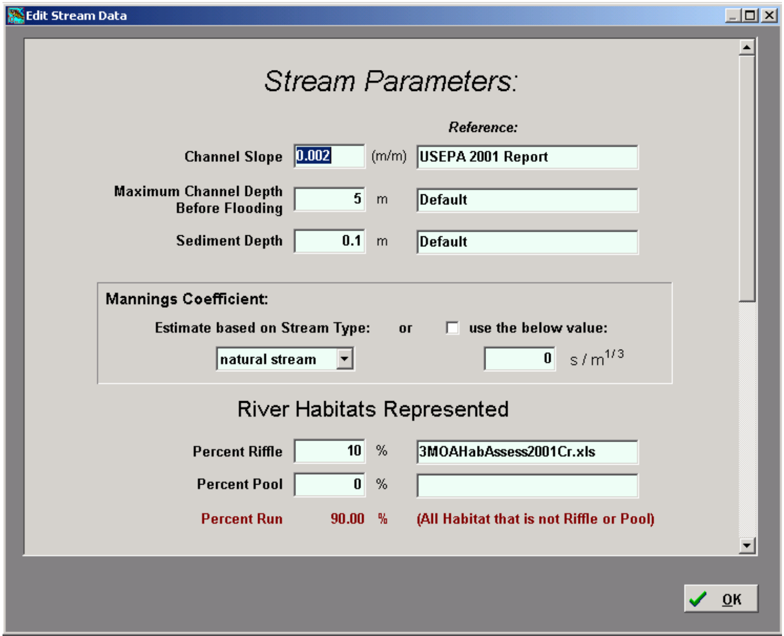
Global vs. Site-Specific Plant Parameters

Most plant parameters may be assumed to be global as a plant species is not assumed to differ from one site to another.

Some plant parameters reflect site characteristics and may need to be calibrated for your site.

- Critical Force for Periphyton -- reflects site's substrate
- Carrying Capacity for Macrophytes -- reflects habitat
- Optimum Temperature -- reflects cold-/warm-water species
- Mortality Coefficients -- reflect quality of habitat

Habitats are characterized in the Site/Stream Parameters screen



Percent habitat parameters affect the simulations in two ways: as limitations on photosynthesis and consumption and as weighting factors for water velocity (see Section 3.2 of the Technical Documentation). Each animal and plant is exposed to a weighted average water velocity depending on its location within the three habitats. This weighted velocity affects all velocity-mediated processes including entrainment of invertebrates and fish, breakage of macrophytes and scour of periphyton. The reaeration of the system also is affected by the habitat-weighted velocities.

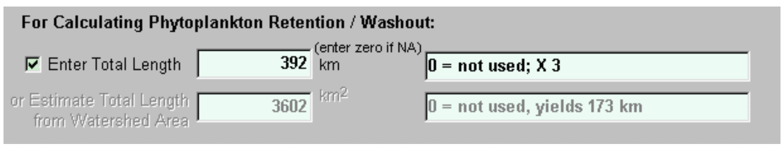
Difference Between Library Parameters and "Underlying Data"

- Libraries
  - are not attached to a simulation
  - are not saved when a simulation is saved
  - have no effect on simulation results
  - independent databases that may be loaded into a simulation or saved from a simulation for later reference
- Underlying Data
  - are attached to a simulation; are loaded and saved when a simulation is loaded and saved
  - will affect simulation results
  - are independent from Libraries, i.e. changing these parameters has no effect on Libraries

An important design consideration is that a study file is self-contained with parameter sets, site constants, loadings, and results that can be saved together. On the other hand, libraries are general resources that can be saved from successful calibrations, edited, and loaded into studies as needed; they are gradually growing in size.

Modeling Phytoplankton

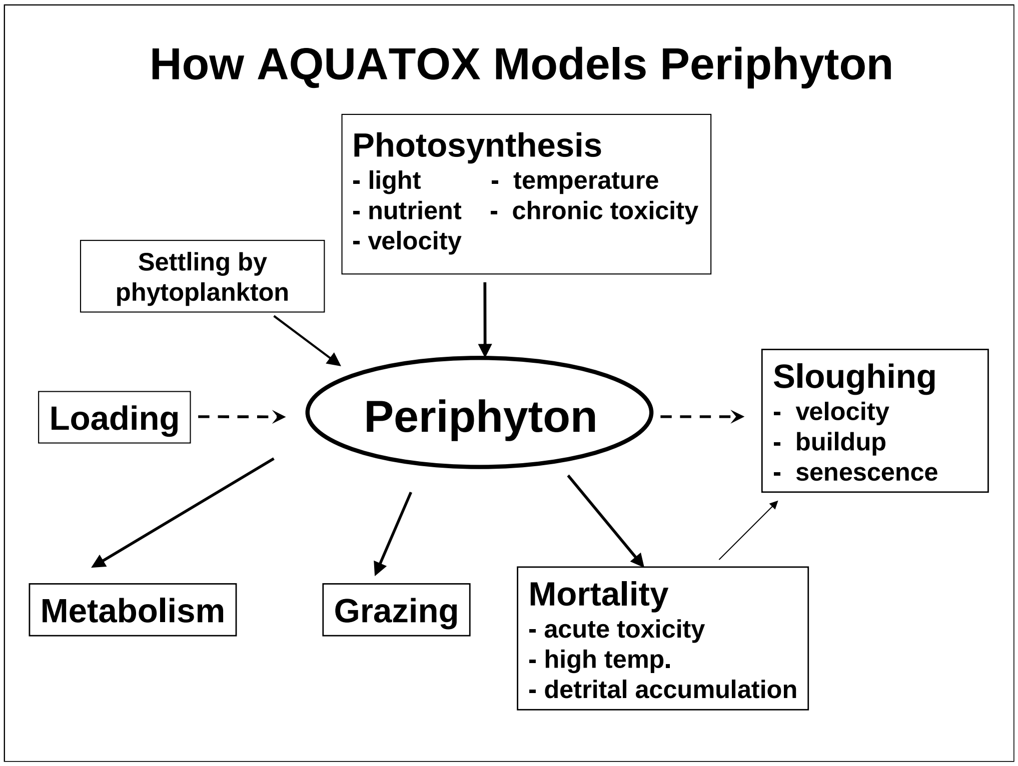
- Phytoplankton may be greens, blue-greens, diatoms or “other algae”
- Subject to sedimentation, washout, and turbulent diffusion
- In stream simulations, assumptions about flow and upstream production are important



Because the phytoplankton (and zooplankton) in a particular reach may have washed in from upstream, residence time in the upstream reaches is important. However, phytoplankton usually experience a longer residence time than the mainstem water because of growing in backwater eddies. Therefore, one should usually use an effective length of upstream river that is twice or even three times the actual length. AQUATOX uses a simple empirical relationship to compute length based on watershed area; that can be used in the absence of information on the actual length.

Modeling Periphyton

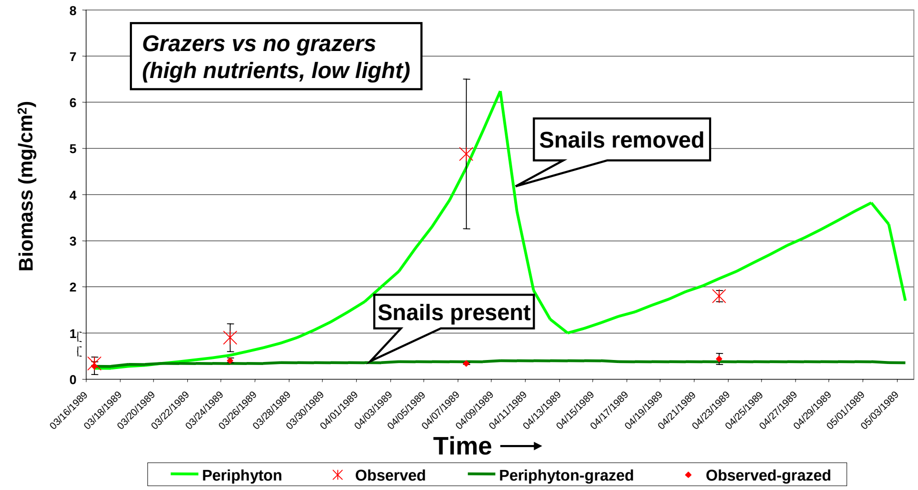
- Periphyton are not simulated by most water quality models
- Periphyton are difficult to model
  – include live material and detritus
  – stimulated by nutrients
  – snails & other animals graze it heavily
  – riparian vegetation reduces light to stream
  – build-up of mat causes stress & sloughing, *even at relatively low velocity*
- Many water body impairments due to periphyton



Note that periphyton and phytoplankton are linked, to better reflect reality, and to better correspond to monitoring data. This affects the chlorophyll *a* observed in the water column during a periphyton sloughing event. (This will be discussed in greater detail during Laboratory #3.)

Several Independent Factors Affect Periphyton

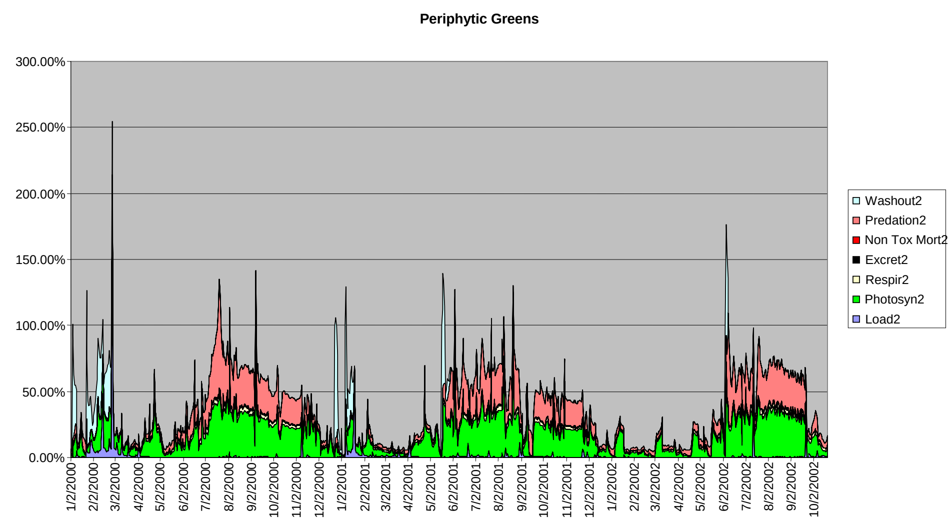
One important factor is Grazing by Snails



This and the following graph were the result of a model validation exercise utilizing a comprehensive dataset from a series of experiments that manipulated nutrient levels, ambient light and grazing pressure by snails Rosemond, 1993). The model was calibrated using the experimental results, and then validated against ambient stream conditions.

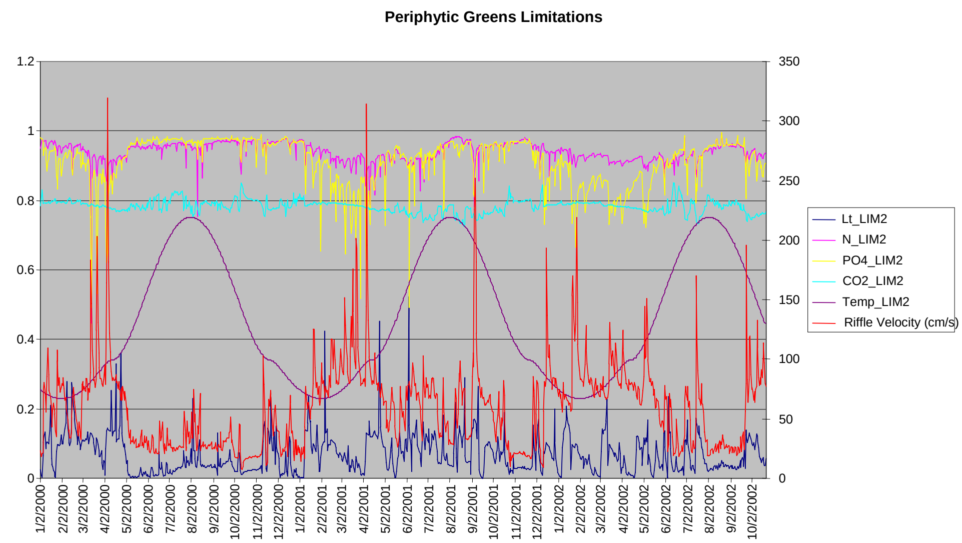
Rosemond, A. D. 1993. Seasonality and Control of Stream Periphyton: Effects of Nutrients, Light, and Herbivores. Pages 185. Vanderbilt University, Nashville, Tenn.

Sporadic Sloughing and Intense Grazing Characterize Periphyton



By plotting the rates we can see that in this simulation of Cahaba River AL photosynthesis is offset by grazing with sporadic sloughing.

Self-shading is important limitation, followed by winter temperature & nutrients



Light limitation is also caused by high suspended solids associated with high discharge (indicated by riffle velocity). Velocity also is responsible in part for sloughing of periphyton. In this high-nutrient stream carbon limitation often prevails, with sporadic phosphorus limitation occurring when blooms follow moderate runoff events.

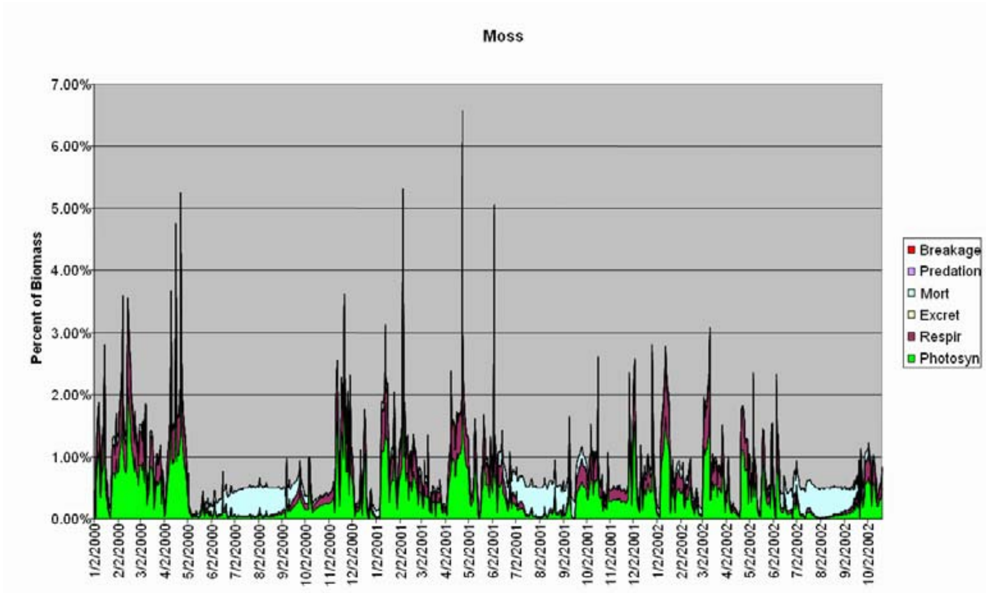
Modeling Macrophytes

- Macrophytes are assumed to be rooted
- Can have significant effect on light climate and other algae communities
- Root uptake of nutrients is assumed and mass balance tracked
- May act as refuge from predation for animals
- Moss are a special category

Free floating macrophytes are included in Release 3.

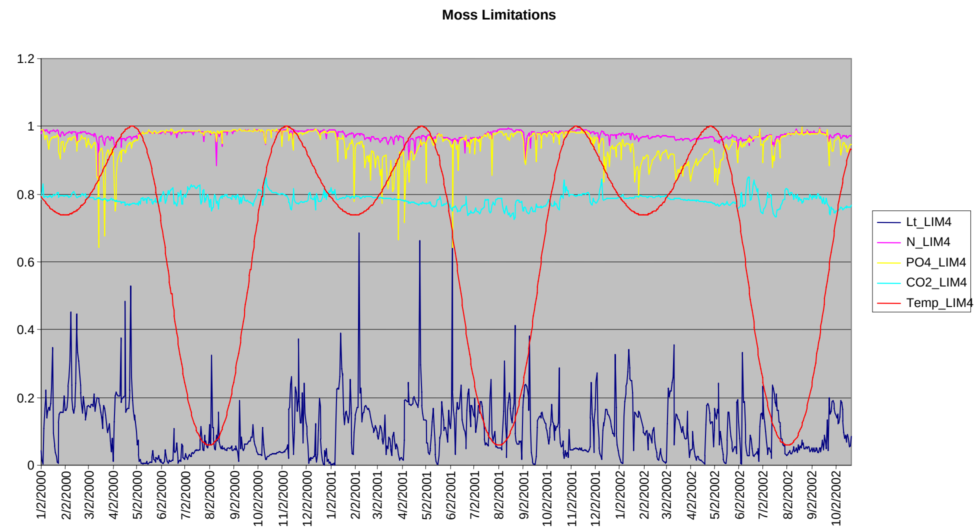
The macrophyte leaves can provide significant surface area for periphyton growth

Moss are stable component with little grazing or breakage, only summer die-back



In some streams moss form the “big slow” compartment. They grow slowly, are not subject to much herbivory, have low mortality rates, and when they die back in the summer or are scoured by storm events the detritus breaks down slowly. They are somewhat sensitive to nutrients levels in the water column.

Moss light limitation decreases when sloughing removes periphyton; summer temperature causes die-back



Moss are adapted to low light, but they are affected by periphyton. As parameterized, they are adapted to cold temperatures and exhibit summer die-back.

Modeling Animals with AQUATOX

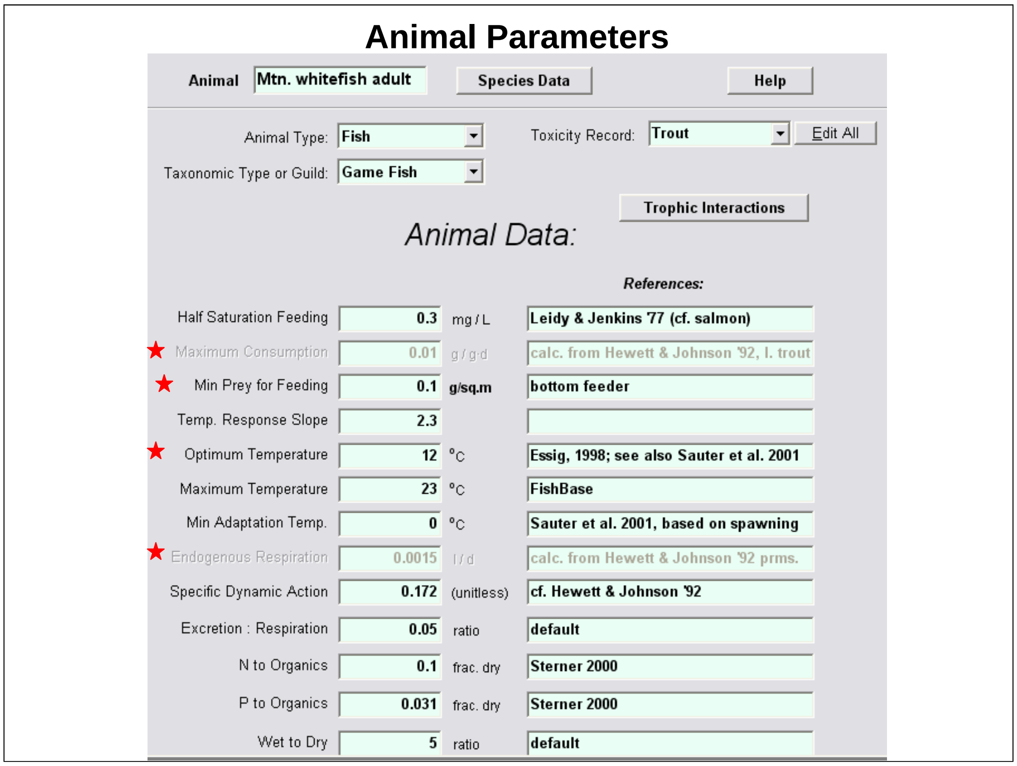
- Equations
- Parameters
- Zooplankton
- Zoobenthos
- Fish

Animal Derivatives

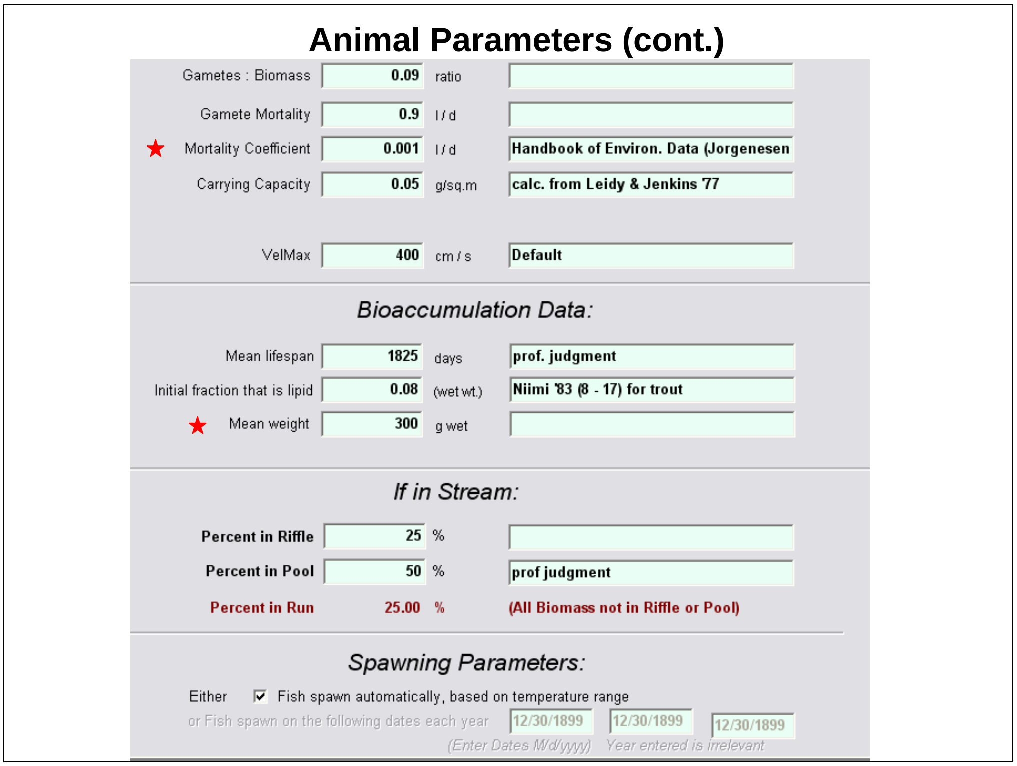
$$\frac{dBiomass}{dt} = Load + Consumption - Defecation - Respiration$$
$$- Excretion - Mortality - Predation - GameteLoss$$
$$- Washout \pm Migration - Promotion + Recruit - Entrainment$$

Note: *Promotion* includes emergence of aquatic insects

These equations are provided just to give a look at general model setup. Each state variable is subject to such a derivative. Additionally, these terms make up the basis for graphing “rates” for each organism.

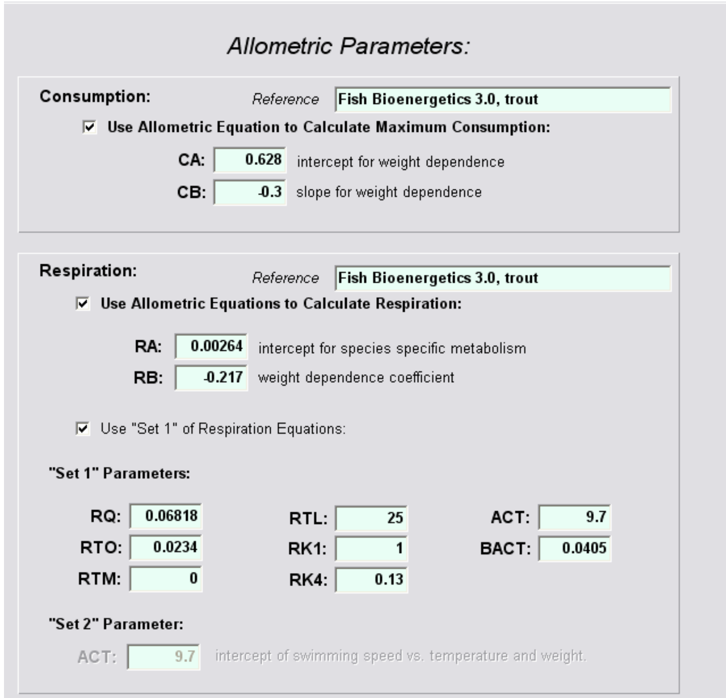


Sensitive parameters include maximum consumption rate and respiration rate if not calculated based on weight (see slide below).



Mortality is often a site-specific response and is therefore subject to calibration.

Animal Parameters (fish-specific allometric parameters)



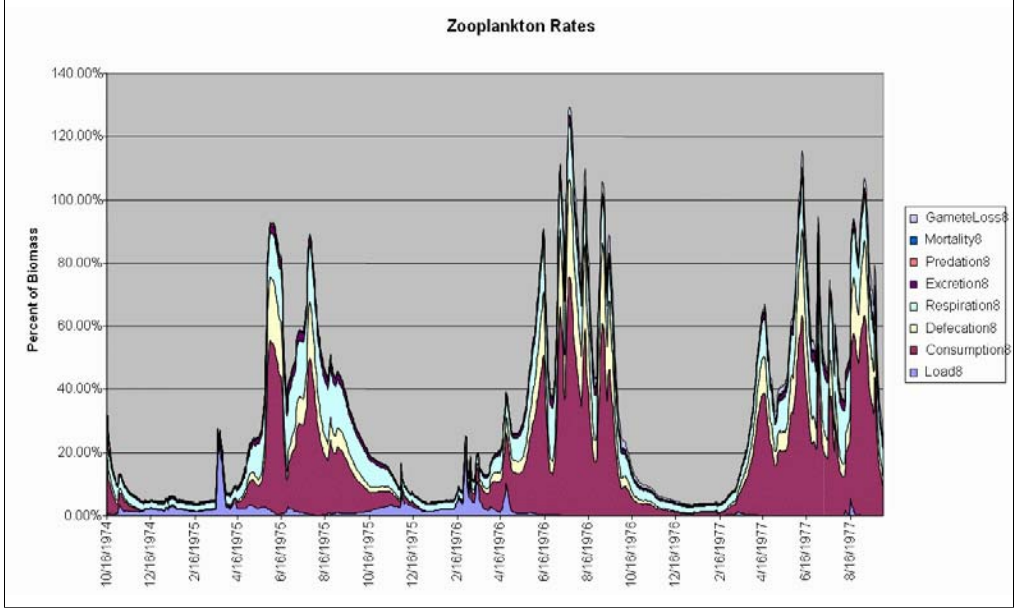
Allometric: change in metabolic rate in relation to the size of the organism.

In this case consumption and respiration are a function of the species mean weight in fish.
The parameter values are taken from the Wisconsin Bioenergetics Model (Hewett and Johnson, 1992; Hanson et al., 1997).

Hewett, S. W., and B. L. Johnson. 1992. Fish Bioenergetics 2 Model. Pages 79. University of Wisconsin Sea Grant Institute, Madison.

Hanson, Paul C., Timothy B. Johnson, Daniel E. Schindler, and James F. Kitchell. 1997. Fish Bioenergetics 3.0. Madison: Center for Limnology, University of Wisconsin.

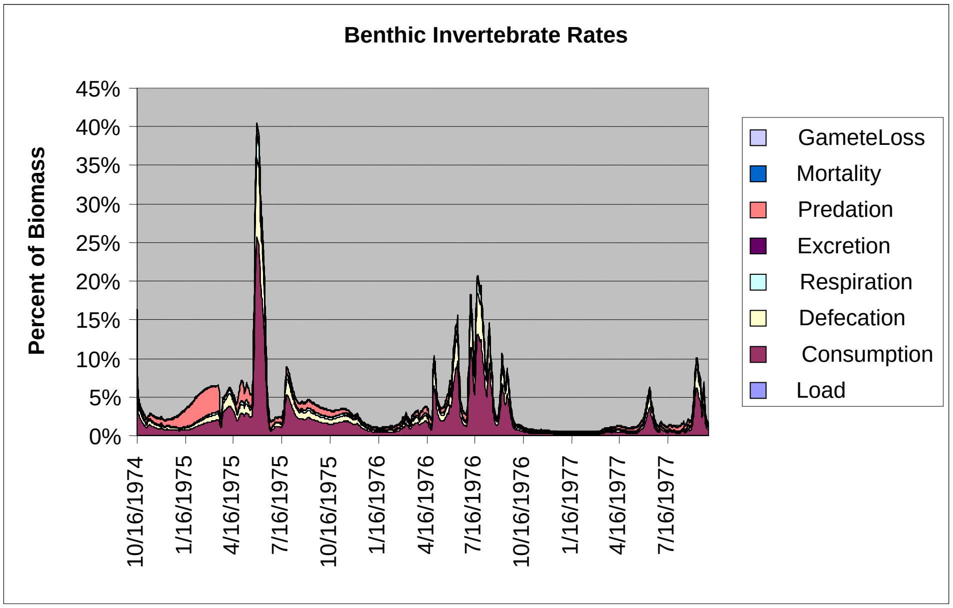
Zooplankton Consumption is tied to Phytoplankton Productivity



In Coralville Lake loadings of zooplankton from upstream can be significant at times.

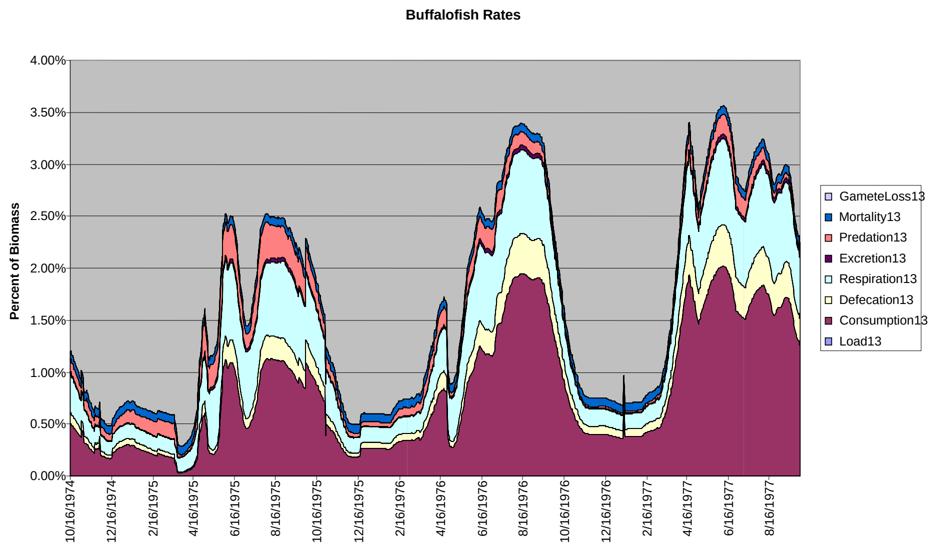
Consumption is heaviest during phytoplankton blooms, although detritus is a secondary source of food. (Without detritus as an alternate food source zooplankton would not be sustained.)

Benthic Invertebrates also tied to Phytoplankton Productivity through Detritus



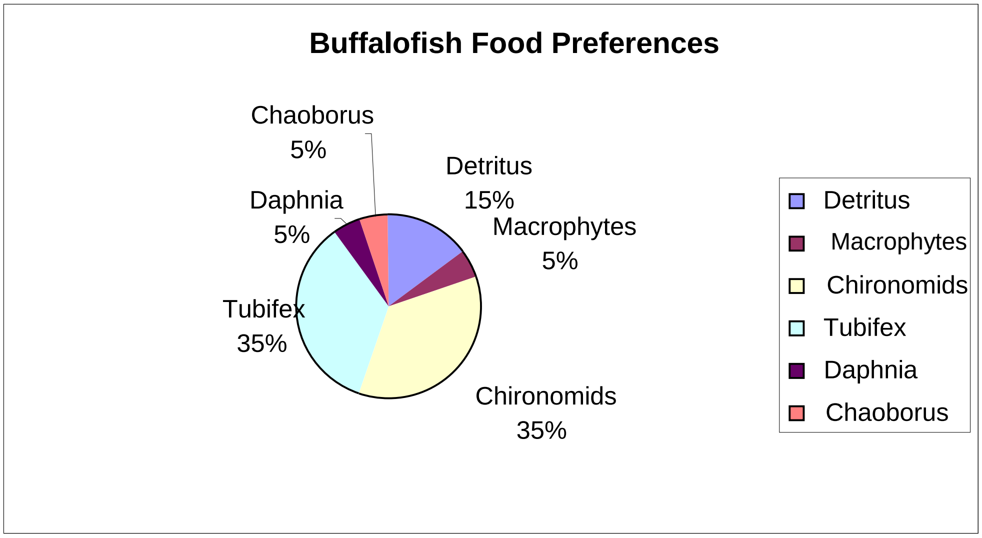
Note heavy predation loss early in simulation. High consumption occurs when algal blooms crash and detritus settles to the bottom.

Fish exhibit seasonal patterns based on food availability and temperature



Buffalofish were a very important component of the Coralville Lake ecosystem. They supported a thriving commercial fishery until high levels of dieldrin were detected in their tissue. In this simulation, predation of young buffalofish by bass declined as the bass were killed off by dieldrin. (The simulation starts with dieldrin concentrations in fish at zero, but those increase as a consequence of bioaccumulation.)

Animals have food preferences, but can switch feeding based on availability



The user can specify food preferences and egestion rates for each animal group. Prey switching is simulated as availability of preferred prey declines.

Trophic Matrix for Buffalofish

AQUATOX-- Trophic Interactions

Trophic Interactions of Buffalofish:

	Preference (ratio)	Egestion (frac.)	References:
R detr sed	0	0	
L detr sed	0.15	0.3	L & J '77, Table 9
R detr part	0	0	
L detr part	0	0.5	
Cyclotella nan	0	0	
Greens	0	0	
Blue-greens	0	0	
Dinoflagellate	0	0	
Myriophyllum	0.05	0.8	L & J '77, Table 9
Chironomid	0.35	0.158	IA DNR Web page: do feed on benthos
Tubifex tubife	0.35	0.158	
Daphnia	0.05	0.158	
Rotifer, Brach	0	0	
Chaoborus	0.05	0.158	
Bluegill	0	0	
Shad	0	0	
Buffalofish	0	0	
Buffalofish22	0	0	
Largemouth Bas	0	0	
Largemouth Ba2	0	0	
Walleye	0	0	

View all data · View Organisms in Current Study Only · Print

Save Matrix to a File · Load Matrix from a File · Help · OK

The preference values do not have to add up to 1 because the model automatically normalizes the values based on the organisms in the current study. The egestion fraction is the fraction not assimilated; the higher the value, the lower the nutrition.

Exported Trophic Matrix

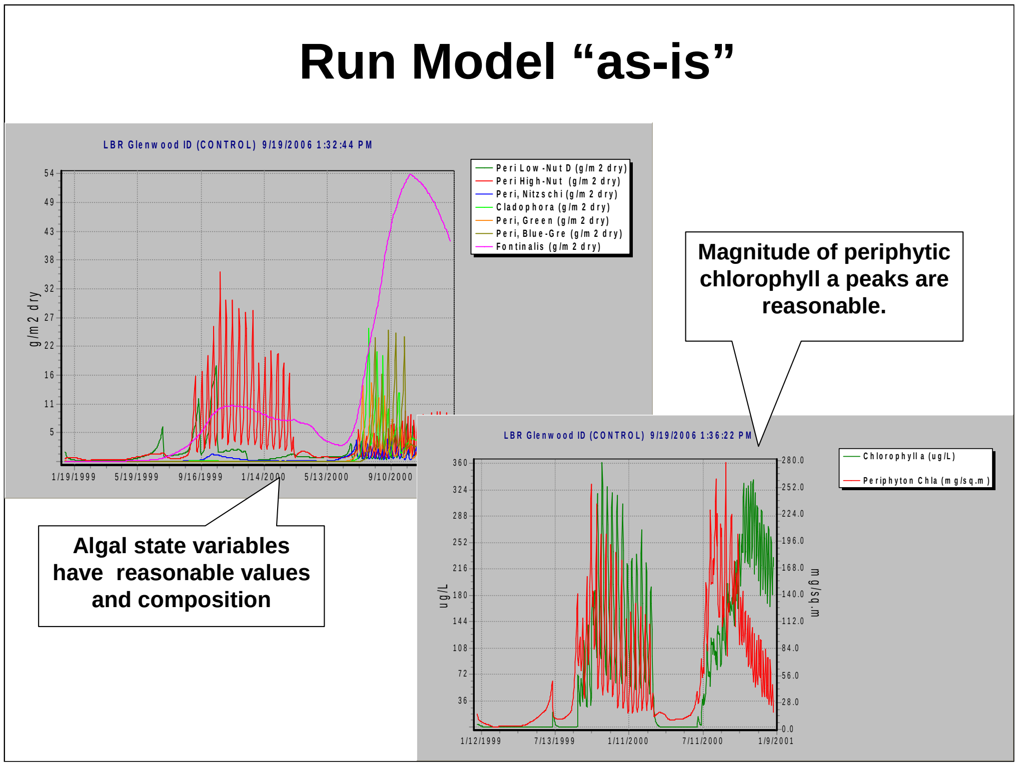
Trophic interaction matrices may be exported to Excel to check appropriateness of overall parameterization. Interactions are normalized to 100% depending on species in the given simulation.

	Mayfly (Baetis	Gastropod	Shiner	Bluegill	Stoneroller	YOY LMB	Adult LMB
R detr sed		3.1%			8.3%		
L detr sed	10.0%	3.1%			8.3%		
R detr part						50.0%	
L detr part			18.2%	8.7%		50.0%	
Peri Low-Nut D	30.0%	34.4%	9.1%		20.8%		
Phyt Low-Nut D			9.1%				
Peri Hi-Nut Di	30.0%	34.4%	9.1%		20.8%		
Peri, Green wa	30.0%	25.0%	9.1%		33.3%		
Phyto, Green			9.1%				
Fontinalis					8.3%		
Mayfly (Baetis			36.4%	34.8%			17.8%
Gastropod				21.7%			
Shiner				34.8%			21.7%
Bluegill							21.7%
Stoneroller							21.7%
Largemouth Bas							17.0%
Largemouth Ba2							

AQUATOX models **prey switching** based on prey biomasses: During each time-step of the simulation, prey species are assessed to see if they exceed the minimum prey threshold (BMIN). If there is insufficient prey for feeding, that compartment is zeroed out and the normalization to 100% continues with other existing species.

Lab 3: Choice of Biota, Calibration of Glenwood Bridge, Lower Boise River, ID

- Check initial run with Rum River state variables
- Change Total Length for phytoplankton
- Change fish to reflect Boise R. species
- Minor calibration
- Demonstration of continued “tweaking” of parameters



Open **LBR Glenwood Br ID.aps**, which you ran in Lab 2.

Our initial examination of results is somewhat encouraging. The observed composition consists of abundant centric (high-nutrient) and pennate (low-nutrient) diatoms, abundant greens, including common *Cladophora* (a macroalga), and a few significant blue-greens peaks in year 2. Of these, only blue-greens are not well represented in the simulation.

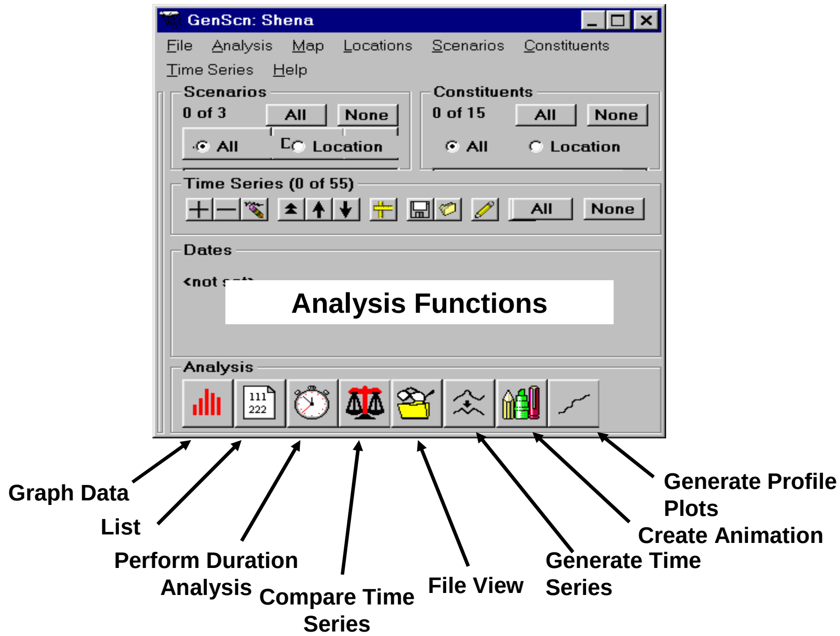
The periphyton likely are going through buildup that is too rapid and sloughing events that are too frequent, however.

Observed chlorophyll a levels are comparable to those predicted. Let’s examine those results against observed data using GenScn.

These results have also been saved as **LBR Glenwood 1b.aps**

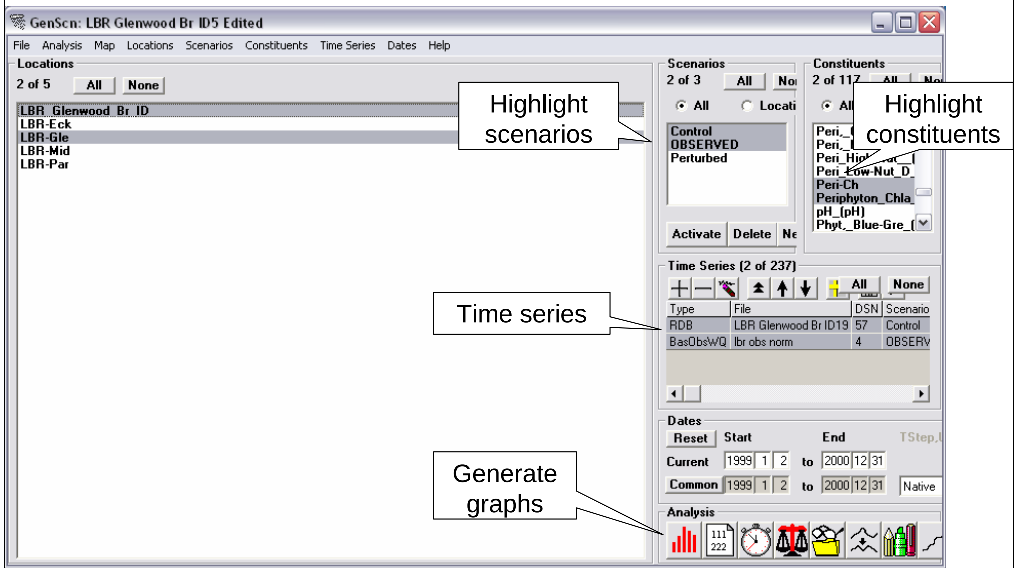
GenScn

Interface for scenario development & data post-processing



GenScn is a tool for processing, analyzing and comparing time series data, which is very useful when dealing with the volumes of output data generated by dynamic models such as HSPF, SWAT, and AQUATOX. However, it is somewhat confusing to use, so we will provide you with "cookbook" instructions to follow at a later date.

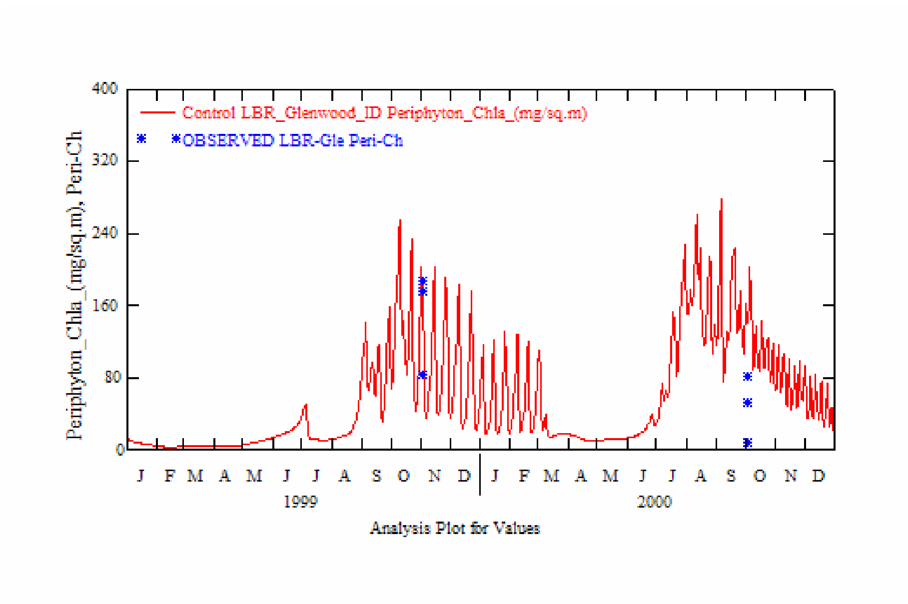
GenScn is part of the BASINS system and can be used to plot and analyze results



To plot observed and predicted values in GenScn:

1. go to main window of study
2. click on **File, Export to Genscn**
3. in GenScn, click on **File, Edit Project**
4. for File Type pick **BasObsWQ,** then **Add From File,** Select **LBR OBS Norm.dbf,** Open, then **OK**
5. highlight **LBR-Glen** and **LBR Glenwood Br ID,** then under Scenarios highlight **OBSERVED** and **Control**, then under Constituents highlight **Peri-Chl,** and **Periphyton_Chla**
6. click "+" and then **All** under **Time Series**
7. click **Generate Graphs** (far left) icon under **Analysis**
8. click **Generate** in **Graphs** screen
9. you can click on symbol or legend in graph if you wish to change from default

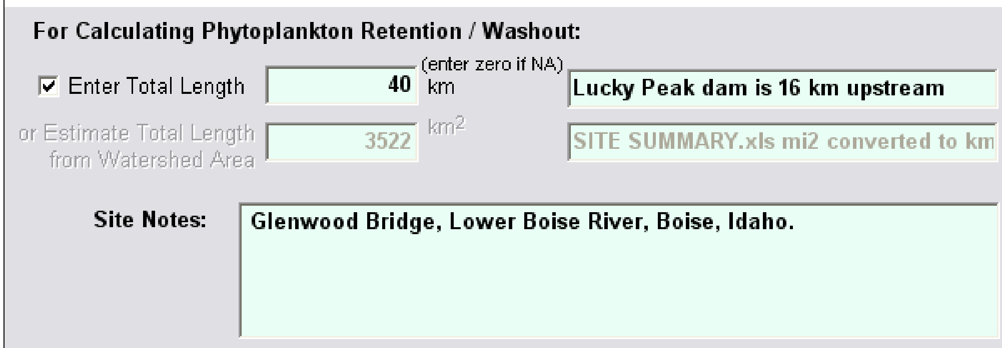
Using GenScn we see that the fit to observed periphytic chlorophyll is fairly good



We chose 1999 and 2000 because the hydrology is quite different for those two years. The fit for 1999 is quite good based on visual inspection. The fit for 2000 is not as good, but this is with Rum River state variables and parameters. Let's make some changes, especially to the fish, and then revisit the fit.

Note: the observed data are stored as a dBase file **LBR OBS Norm.dbf**. The periphyton data have been normalized by correcting for available substrate, recognizing that the periphyton are collected from cobbles and that usually they occur on hard substrates such as cobbles and gravel and not sand. Pebble counts were used to determine the percentage available substrate.

Change Length in Site Screen



Length is used to calculate phytoplankton and zooplankton retention time

Set the total length to 40 km, which accounts for longer residence time (~length) due to Diversion and Barber impoundments.

Phytoplankton and zooplankton can quickly wash out of a short reach, but they may be able to grow over an extensive reach of a river, including its tributaries. Somehow the volume of water occupied by the phytoplankton needs to be taken into consideration. To solve this problem, AQUATOX takes into account the “Total Length” of the river being simulated so that phytoplankton and zooplankton production upstream can be estimated. Then, to simulate the inflow of phytoplankton from upstream reaches phytoplankton upstream loadings are estimated.

An integral assumption in this approach is that upstream reaches being modeled have identical environmental conditions as the reach being modeled and that plankton production in each mile up-stream will be identical to plankton production in the given reach.

Modify biotic assignments

(Remove Macrophyte Fontinalis)

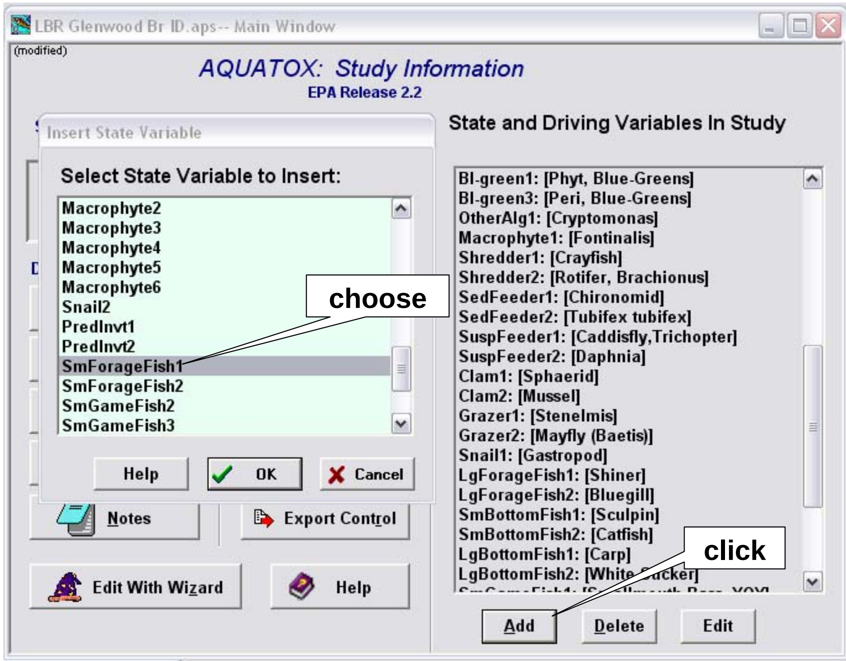
Rum River MN		Lower Boise R. ID
		chiselmouth
		dace
shiner		shiner
bluegill	→	pikeminnow
sculpin		sculpin
catfish		catfish
carp		carp
white sucker		white sucker
smallmouth bass (2)	→	largemouth bass (2)
walleye	→	rainbow trout (2)
		mountain whitefish (2)

Fish species may change considerably from one watershed to another, so one should always check the assignments when modeling a new site.   We will demonstrate both how to add new species, as well as replace or modify existing spp in an application.

We can keep the algal and invertebrate designations the same for the most part. However, be alert for invasive species; the New Zealand mud snail is one that first appeared at Glenwood Bridge in 2003.

Also, as shown above, remove Fontinalis from the MN Rivers simulation. This is not well calibrated for the Lower Boise river and its rapid growth is contributing to the rapid growth of periphyton.

Add fish



There are three ways to modify the types of biota in the system.

1. Add a species “manually” through the main interface.
2. Replace an existing species with a different set of “underlying data”
3. Modify the species using the wizard (usually easiest).

We will demonstrate all three procedures within this exercise.

To add a fish “manually” click on **Add** and select the **State Variable to Insert**. We have another bottom fish to add, chiselmouth. We already have 4 bottom fish so we will add a small forage fish and assign chiselmouth to that designation. This illustrates an important point: the guild labels are just to help you organize the state variables; chiselmouth is a bottom fish, and it is large; however, these characteristics are imparted by the parameters that we use, not by the nominal guild name. The only exception is that dietary assimilation of toxicants by large game fish is more efficient than for other fish (this will be a function of weight in Release 3).

The choice of Animal Type (found on the parameter screen) can be important for invertebrates, however, because some of the ecological processes that affect them differ slightly. See p. 4-1 in the **Technical Documentation** for the differences in processes for the different plant and animal types.

Choose fish from list of animals in Library

Once you have added an organism, **double-click** on the name to open the loading screen and **set the initial condition**. Initial conditions are not important for plants and invertebrates, but fish respond slowly and the initial condition may require a "spin-up" period to obtain a stable value.

We will start with a value of 0.1 for chiselmouth.

To add a species not in the Library

mountain whitefish:

- load a similar species or group (trout in this case)
  - use GridMode to find best match in Library
- go to a parameter source, such as FishBase.Org, to check food preferences, temperature preferences, mean weight
- Google species to find more specific information online
  - changed TOpt based on Essig, 1998; TMin based on Sauter et al. 2001

New Zealand mud snail (Potamopyrgus):

- used gastropod as template
- all additional information in Hall et al., 2003

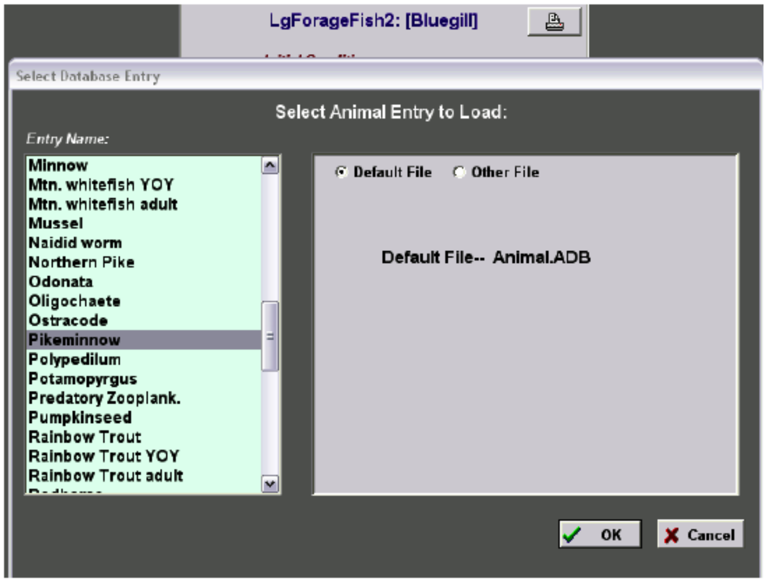
Always start with the closest species or group because many parameters extend across groups. In a later lecture we will cover examples of general sources of parameters. The Internet is a great source if general information and specific parameter values, and it is improving daily.

In Library can choose GridMode to see all species at once

	Max Consumpt	Max Consumpt Reference	Min Prey	Min Prey Reference
Mtn. whitefish YOY	0.01	calc. from Hewett & Johnson '92, l. trout	0.25	
Mtn. whitefish adult	0.01	calc. from Hewett & Johnson '92, l. trout	0.1	bottom feeder
Mussel	0.05	Anadonta (Pusch et al., 2001, p. 320)	0	filter feeding mollusc
Naidid worm	0.25	prof judgment, calibrated	0.1	
Northern Pike	0.05	calc. from Hewett & Johnson '92 prms.	0.25	prof. judgement
Odonata	0.09	Leidy and Ploskey, 1980	0.1	prof. judgment
Oligochaete	0.5	prof judgment	0	
Ostracode	1.2	est. to be 1/2 cladoceran	0.06	twice cladoceran
Pikeminnow	0.05	Collins & Wlosinski 1983	0.25	prof. judgment
Polypedilum	0.7	McIntire & Colby p. 172	0.1	prof. judgment
Potamopyrgus	0.17	Hall et al., 2003, Frontiers in Ecology 1:8	0.7	(McIntire et al. 1996 = 0.7)
Predatory Zooplank.	1.1	Leidy & Ploskey, '80, p. 87	0.1	est. from Leidy & Ploskey, '80, p. 86
Pumpkinseed	0.05	Hewett & Johnson '92 calc. (Dace)	0.25	prof. judgement
Rainbow Trout	0.01	calc. from Hewett & Johnson '92, l. trout	0.25	
Rainbow Trout YOY	0.01	calc. from Hewett & Johnson '92, l. trout	0.25	
Rainbow Trout adult	0.01	calc. from Hewett & Johnson '92, l. trout	0.25	
Redhorse	0.06	Leidy & Jenkins '77	0.25	prof. judgment
Riffle beetle, Sten	0.5	McIntire & Colby p. 172	0.2	prof judgment
Rotifer, Brachionus	3.4	from sev. papers, extrapolated from growth	0.3	Walz. 1995, p. 441
Rotifer, Keratella	3.438	Collins & Wlosinski 9183, p. 45 (B.r.)	0.06	Walz, 1995, p. 441

To quickly scan (and edit) a Library click on **GridMode** at the top of the Library screen.

Replacing One Fish Species with Another



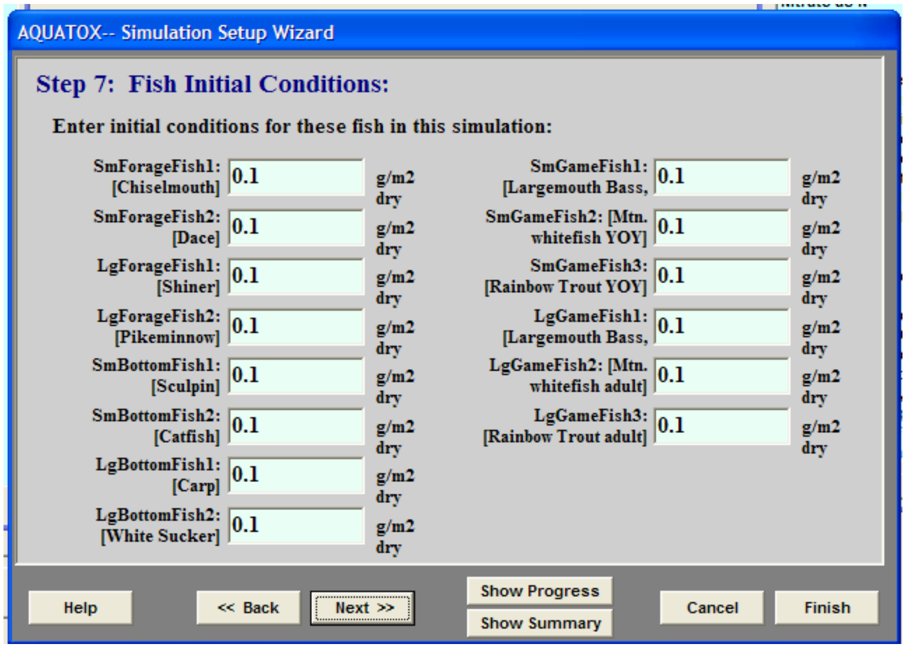
To replace an existing animal in the simulation with another, open the loading file for the original species and click on **Load Data** to bring up the screen to select the animal or plant entry, then choose the alternate species or group **and click OK**. We will do this to replace bluegill with pikeminnow.

Load **Pikeminnow** into existing LgForageFish2 (previously bluegill)

Using the Wizard to Modify Biota

1. Remove smallmouth bass (2 lines).
2. Remove walleye.
3. Add **Largemouth Bass** as a size-class gamefish (**Largemouth Bass YOY** and **Largemouth Bass, Lg**)
4. Add **Mountain Whitefish** as a size-class gamefish (**Mtn. whitefish YOY** and **Mtn. whitefish adult**)
5. Add **Rainbow Trout** as a size-class gamefish (**Rainbow Trout YOY** and **Rainbow Trout adult**)
6. Add **Dace** as a single-compartment small forage fish

Set Fish Initial Conditions



Using the wizard interface allows us to enter initial conditions for all fish species on a single screen.

We'll set all initial conditions to 0.1 for use in a spin-up.

We will revisit these initial conditions later.

Examine Trophic Interactions

Select “Export Trophic Interactions” from the Study Menu:

	Dace	Shiner	Pikeminno	Sculpin	Catfish	Carp	White Suck	Largemout	Mtn. whitef	Rainbow Tr	Largemout	Mtn. whitef	Rainbow Tr
Crayfish			11.1%										
Rotifer, Brach													
Chironomid	25.0%	7.1%	5.6%	81.2%	29.1%	11.1%	6.0%	55.9%	42.7%	25.0%	0.3%	9.4%	14.6%
Tubifex tubife						33.3%	6.0%		6.1%	25.0%		6.8%	14.6%
Caddisfly,Tric	50.0%	21.4%	5.6%	8.9%	1.8%		8.0%	38.2%	2.4%	12.5%	0.3%	7.7%	7.3%
Daphnia		21.4%							48.8%	12.5%		1.7%	7.3%
Sphaerid						11.1%	6.0%						
Mussel							6.0%						
Stenelmis	25.0%	14.3%	5.6%				8.0%				11.0%	1.7%	
Mayfly (Baetis		21.4%		8.9%						25.0%		6.0%	
Gastropod												25.6%	
Chiselmouth			11.1%								17.2%	1.7%	
Dace			11.1%								9.9%	1.7%	
Shiner			11.1%	1.0%	29.1%						13.4%	1.7%	11.6%
Pikeminnow											13.4%	1.7%	11.6%
Sculpin			11.1%									0.9%	
Catfish												0.9%	
Carp												0.9%	5.5%
White Sucker												0.9%	5.5%
Largemouth Bas			11.1%		29.1%						10.5%	10.3%	7.3%
Mtn. whitefish			11.1%									10.3%	7.3%
Rainbow Trout												10.3%	7.3%
Largemouth Ba2											10.5%		
Mtn. whitefis2											13.4%		
Rainbow Trout2													

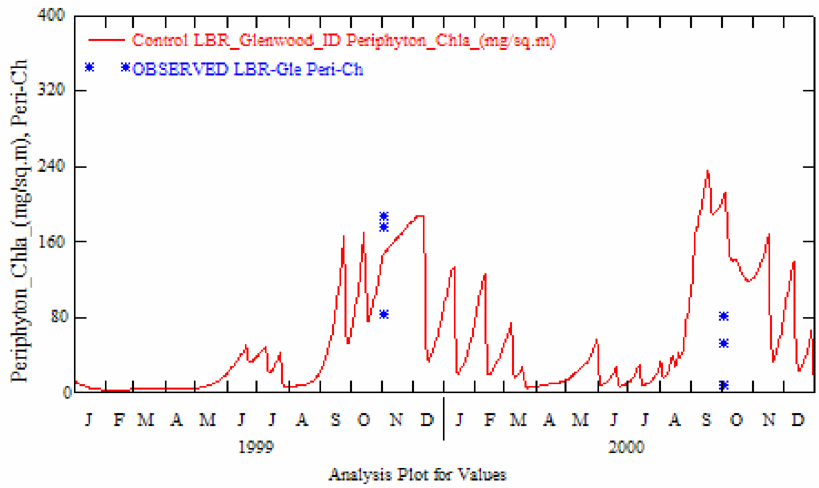
An examination of trophic interactions is usually a wise step. This has some suspicious entries (such as sculpin only being preyed upon by pikeminnows and mountain whitefish) , but we will let it go for now.

We are ready to run

We are not actually going to run this simulation during the workshop, because it is just an intermediate step and will take roughly 25 minutes to execute. If you'd like to run the simulation on your own now or later, please save the file now as an intermediate step. (We will be modifying the existing study and running it shortly.)

Your simulation now should match the file **LBR Glenwood 2.aps**"

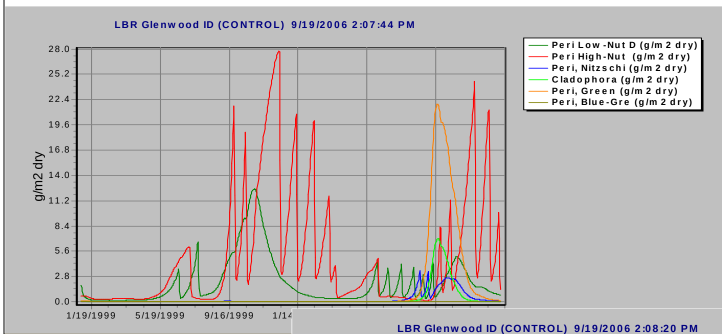
Compare Results to Observed Data using GenScn

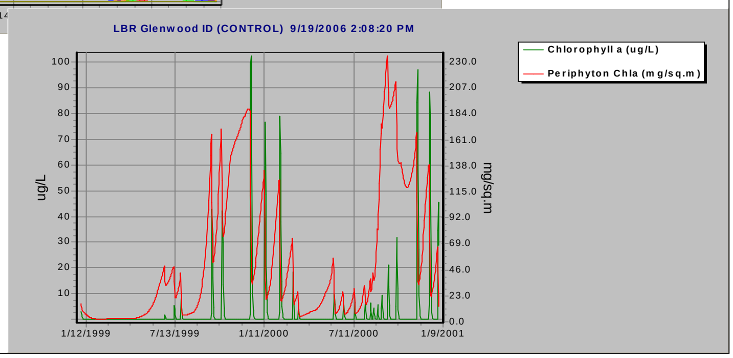


Same procedure performed previously. The results have changed as a result of top-down control. With data from only two dates, we are not in a position to state whether this is an improvement or not!

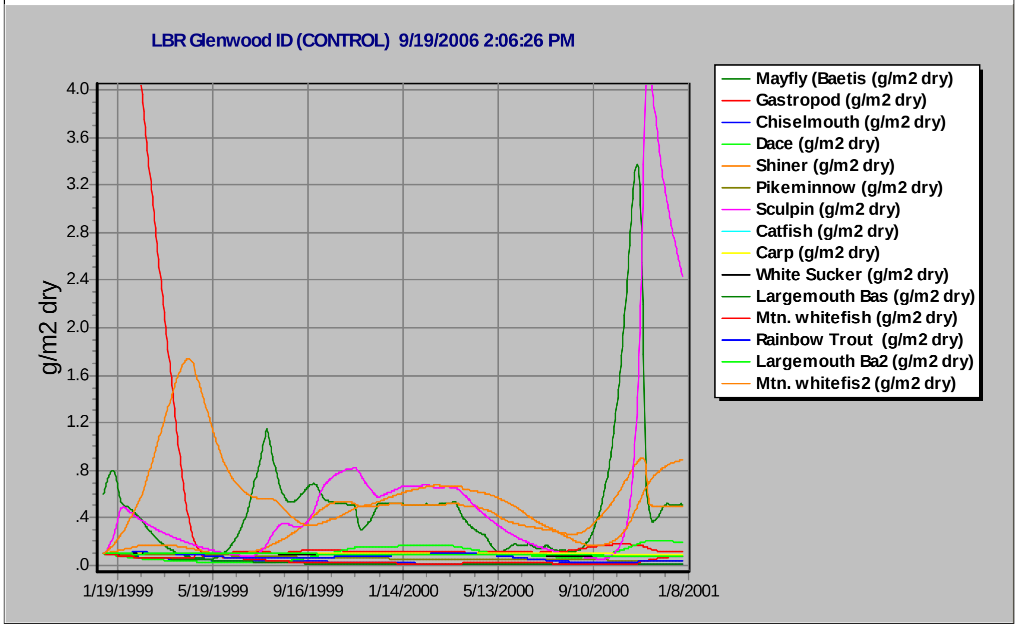
However, the extreme variations in biomass due to periphyton buildup and sloughing is no longer present which is a good thing.

High-nutrient diatoms dominate

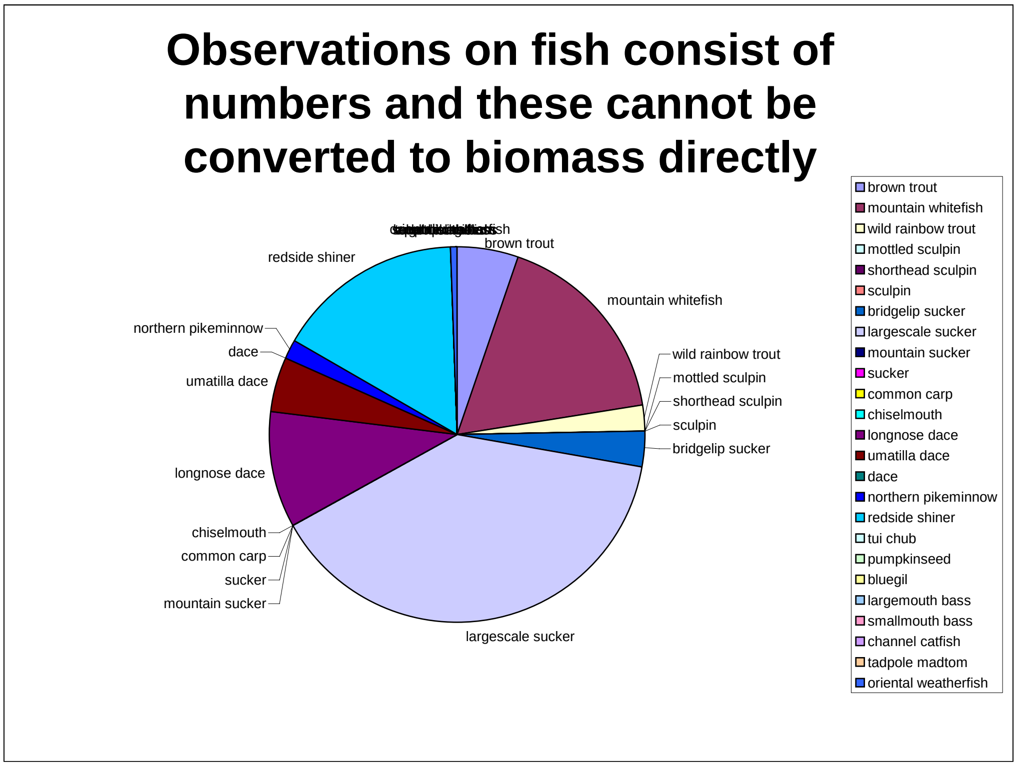




Fish show transient dynamics



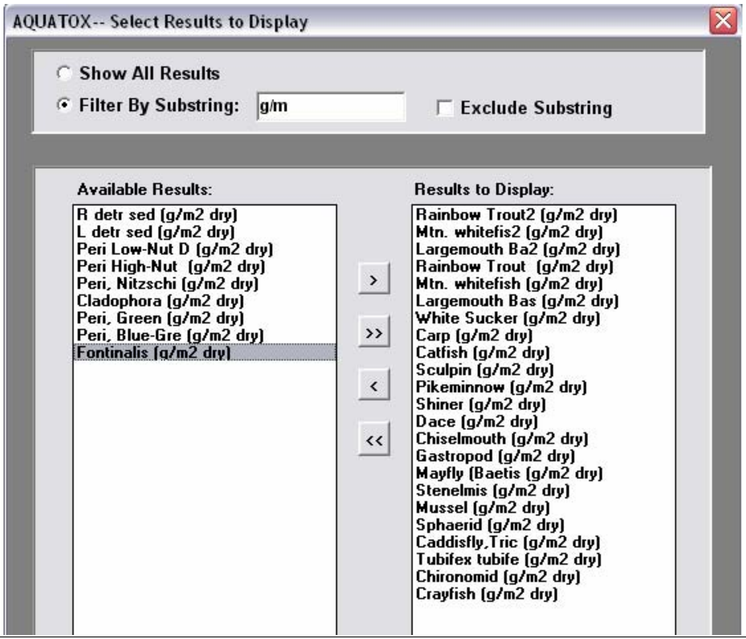
The initial condition for snails is 9 g/m2, which is obviously too high; however, they virtually disappear, suggesting that predation as simulated is greater than in reality.



We have percentage distributions for fish at Glenwood Bridge from USGS; these cannot be used directly to calibrate the model. However, allowing for differences in mean weight, the community is dominated by suckers, minnows, and mountain whitefish; brown trout, which we have not modeled, seem to exceed rainbow trout. We should probably add brown trout, but at this time let's consider them as lumped with rainbow trout and add gastropods (a prey item for brown trout) to the rainbow trout preference matrix for this study.

There are several species plotted together at the top of the chart because they are present in very low numbers; we will ignore them.

Obtain tabular output



While still in the Output window, click on the **Perturbed Simulation** tab. Click on **Choose Variables**, use “g/m” as a filter substring to limit the list. Choose the invertebrates and fish for tabulation.

Use the end values as initial conditions

Change Variables

Control Simulation: Results

Help | Print

Save Table to Excel

	Chiselmouth (g/m2 dry)	Dace (g/m2 dry)	Shiner (g/m2 dry)	Pikeminnow (g/m2 dry)	Sculpin (g/m2 dry)	Catfish (g/m2 dry)
12/14/2000	0.0169	0.2056	0.5018	0.0422	2.9683	0.0719
12/15/2000	0.0169	0.205	0.5021	0.0422	2.9326	0.0719
12/16/2000	0.0168	0.2044	0.5023	0.0422	2.8965	0.0719
12/17/2000	0.0167	0.2039	0.5025	0.0421	2.86	0.0719
12/18/2000	0.0167	0.2033	0.5025	0.0421	2.824	0.0719
12/19/2000	0.0166	0.2028	0.5026	0.0421	2.7896	0.0719
12/20/2000	0.0165	0.2023	0.5026	0.0421	2.7552	0.072
12/21/2000	0.0165	0.2019	0.5026	0.042	2.7231	0.072
12/22/2000	0.0164	0.2014	0.5026	0.042	2.6921	0.072
12/23/2000	0.0163	0.2009	0.5026	0.042	2.6614	0.072
12/24/2000	0.0163	0.2005	0.5026	0.042	2.6318	0.072
12/25/2000	0.0162	0.2001	0.5026	0.0419	2.6025	0.072
12/26/2000	0.0162	0.1997	0.5026	0.0419	2.5738	0.072
12/27/2000	0.0161	0.1993	0.5026	0.0419	2.5454	0.072
12/28/2000	0.016	0.1989	0.5025	0.0419	2.5177	0.072
12/29/2000	0.016	0.1985	0.5022	0.0418	2.4916	0.072
12/30/2000	0.0159	0.1982	0.5017	0.0418	2.4647	0.072
12/31/2000	0.0159	0.1979	0.5016	0.0418	2.4371	0.072

The key end values from the table are:

Gastropod 0.1

Chiselmouth 0.02

Dace 0.2

Shiner 0.5

Pikeminnow 0.04

Sculpin 2.4

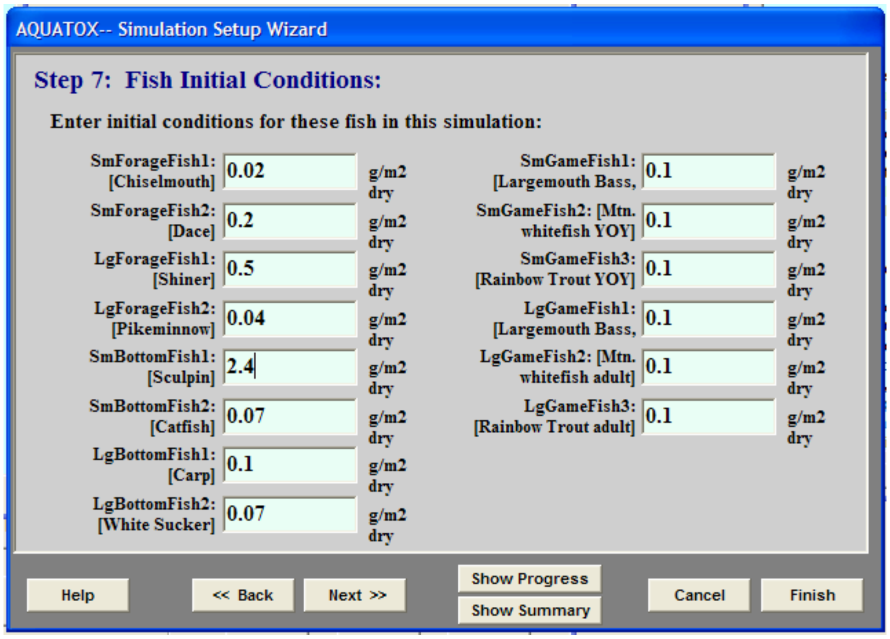
Catfish 0.07

Carp 0.1

White sucker 0.07

The quickest way to input these is to use the Wizard.

Use the wizard to change initial conditions



Change gastropods from 9 to 0.1 in previous screen.

Change the fish initial conditions accordingly, including making all the adult game fish 0.1.

Reexamine Trophic Interactions

Select “Export Trophic Interactions” from the Study Menu:

	Dace	Shiner	Pikeminnow	Sculpin	Catfish	Carp	White Suck	Largemout	Mtn. whitef	Rainbow Tr	Largemout	Mtn. whitef	Rainbow Tr
Crayfish			11.1%										
Rotifer, Brach													
Chironomid	25.0%	7.1%	5.6%	81.2%	29.1%	11.1%	6.0%	55.9%	42.7%	25.0%	0.3%	9.4%	14.6%
Tubifex tubife						33.3%	6.0%		6.1%	25.0%		6.8%	14.6%
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Sphaerid						11.1%	6.0%						
Mussel							6.0%						
Stenelmis	25.0%	14.3%	5.6%				8.0%				11.0%	1.7%	
Mayfly (Baetis		21.4%		8.9%						25.0%		6.0%	
Gastropod												25.6%	
Chiselmouth			11.1%								17.2%	1.7%	
Dace			11.1%								9.9%	1.7%	
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Pikeminnow											13.4%	1.7%	11.6%
Sculpin			11.1%									0.9%	
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Carp												0.9%	5.5%
White Sucker												0.9%	5.5%
Largemouth Bas			11.1%		29.1%						10.5%	10.3%	7.3%
Mtn. whitefish			11.1%									10.3%	7.3%
Rainbow Trout												10.3%	7.3%
Largemouth Ba2											10.5%		
Mtn. whitefis2											13.4%		
Rainbow Trout2													

Going back to the trophic interactions matrix we see that there are alternate predators for mayflies (which could damp down the sculpin response). Snails are preyed on too heavily by mountain whitefish, but should also have some predation pressure from rainbow trout—although the true snail predator is brown trout, which we are not modeling. Finally, sculpin are subject to predation by catfish, bass, and rainbow trout.

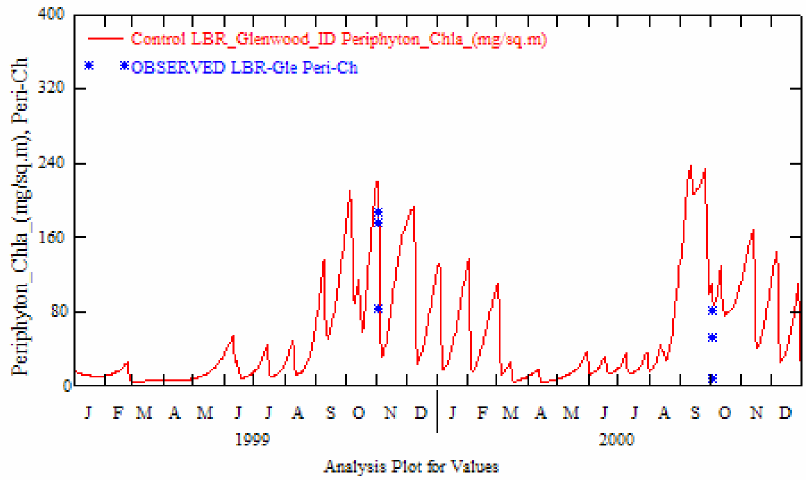
Suggested changes to preference values

- Dace: mayfly = Stenelmis value
- Pikeminnow: mayfly = Stenelmis
- Bass (adult): sculpin = shiner
- Mtn. whitefish (adult): gastropod = mayfly
- Rainbow trout (adult): mayfly = caddisfly
- Rainbow trout (adult): Tubifex → 0
- Rainbow trout (adult): Sculpin = shiner

We will make those changes to the preferences. Ordinarily we would not make so many changes at once, but the fish are not well calibrated, and we are anxious to see what the effects would be. (If you don't agree with our changes, feel free to make your own.) Not all preference values are normalized in the input screen; therefore, we'll equate the preferences to other prey.

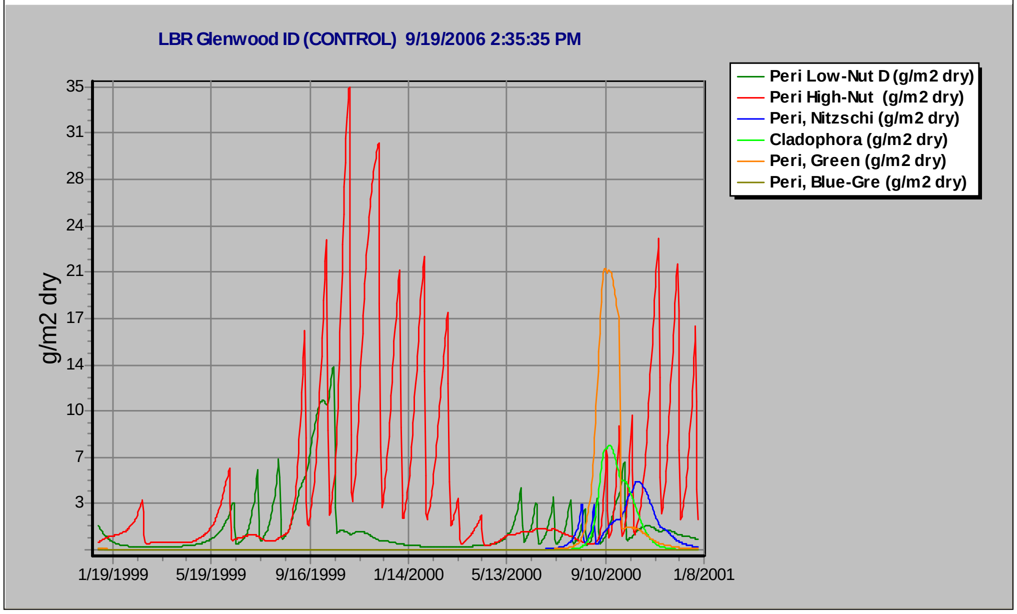
Save the changes and re-run the simulation as "Control." This may take 20 minutes, so start the simulation and then break or go on to the next lecture.

Results with changes to fish preferences and initial conditions



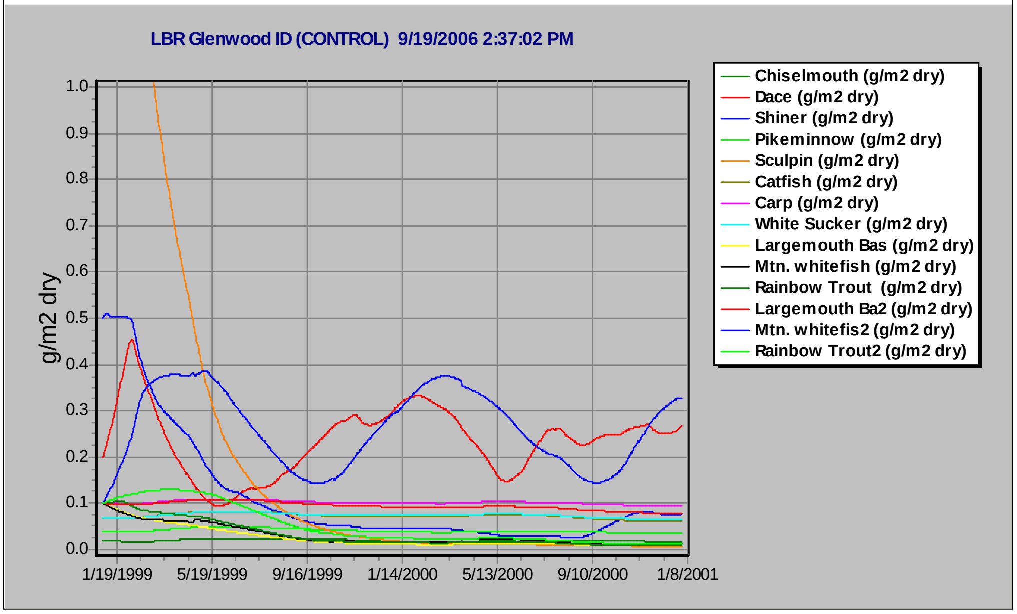
This appears to be marginally better.

Algal composition is still good



What is missing in the simulation are the periphytic blue-greens, which are abundant at the site. If you want an exercise on your own, try calibrating the blue-greens. Hint: you might consider these blue-greens to be adapted to colder water.

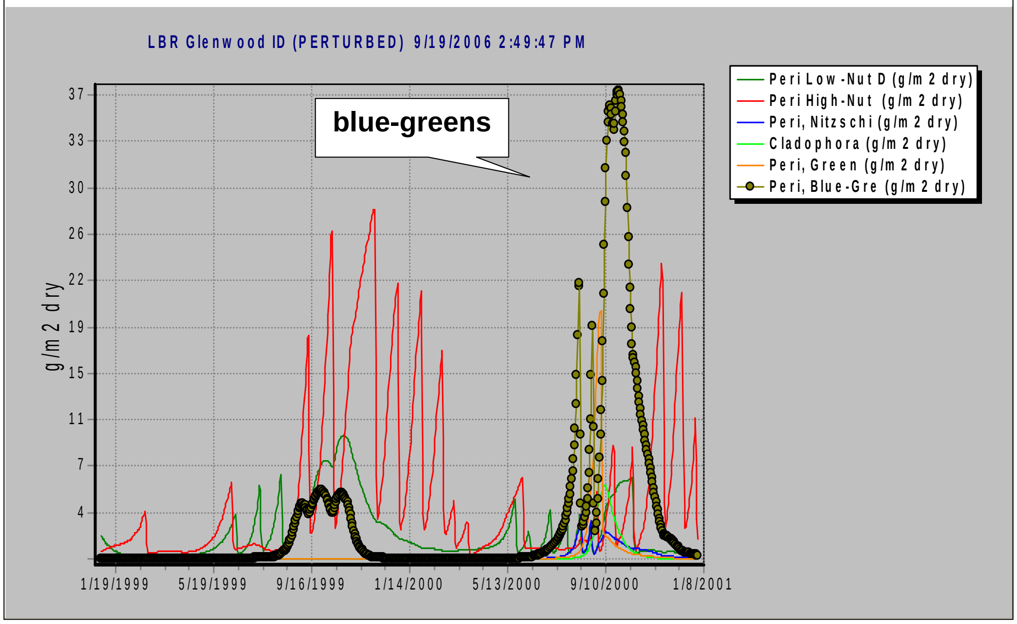
Fish still exhibit transient behavior but not explosive increases in biomass



We could decrease sculpin initial conditions, but they only affect the first 6 months. Following the transient period, dace and mountain whitefish are dominant, which corresponds to the pie chart distribution; sphaerid bivalves are also predicted to be important, which may mean the predation preferences may not be correct. Bass and rainbow trout have lower biomasses; the bass optimum temperature may be too low because one would expect even lower biomass levels. We will stop our simulations here; the next three slides show the effects of changing the optimum temperature for periphytic blue-greens.

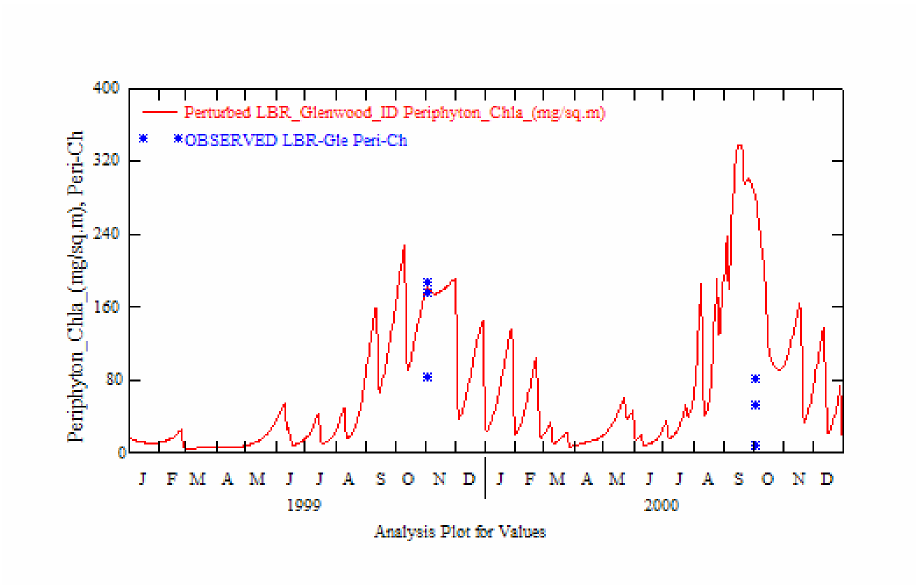
Save the results. They are also saved in your directory as **LBR Glenwood 3.aps**.

“Coldwater” blue-greens improve composition

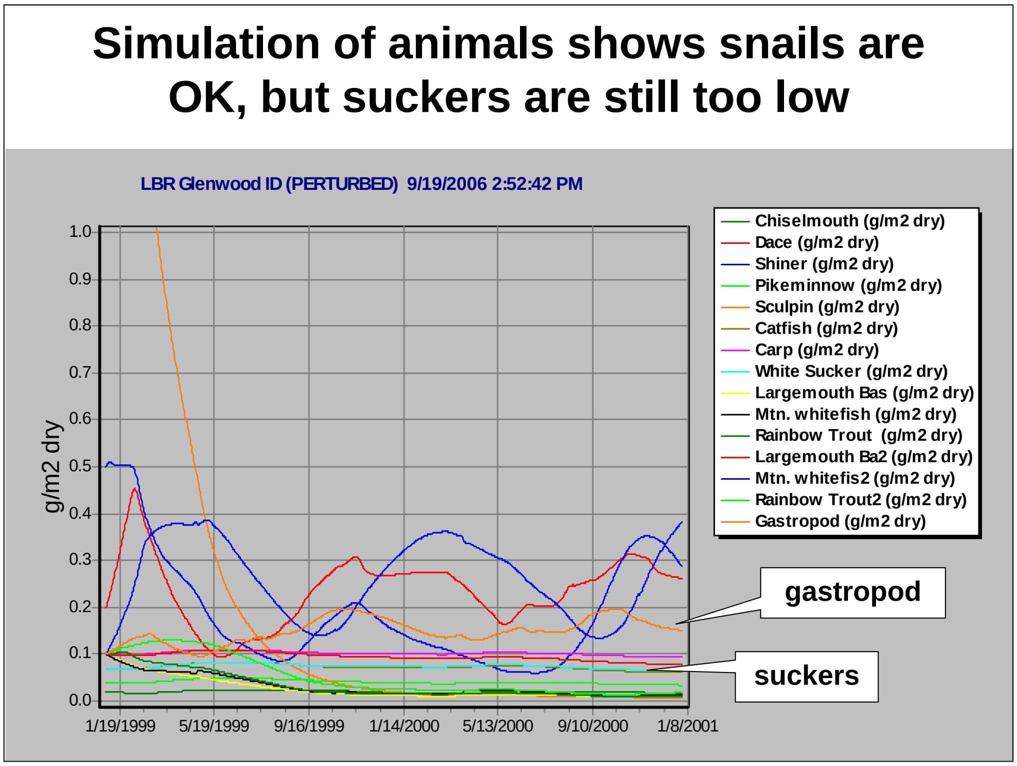


If you had tweaked the blue-greens this is what you might have found. Changing the optimum temperature for periphytic blue-greens from 30 to 20 degrees improves the composition, but provides a worse fit to chlorophyll a. This is saved as **LBR Glenwood 3 bl-gr.aps**. Admittedly, a 10 degree change is rather drastic.

Similar fit to chlorophyll with “coldwater” blue-greens



Periphyton Chlorophyll a seems more overpredicted in 2000.



Inspection of a plot of the animals indicates that the prior change in predation of snails had the desired effect of maintaining their biomass. However, recall that suckers are important at Glenwood Bridge, and they are underrepresented in the simulation. That too could be the subject of continued calibration.

We will stop fiddling with the Glenwood Bridge study, but you are welcome to continue in your spare time.

We have now completed the first set of steps that enable you to apply an AQUATOX simulation to your new site. If you have a site to model with AQUATOX, you would be well served to follow the steps in Labs 2 and 3 closely.

Within these labs we have set up your site's physical characteristics, its nutrient and organic matter loadings, and we have set up your site's biotic composition as well.

The next steps you might take would be comparing your simulation against observed data in an iterative calibration process (if necessary). If you have an independent set of data you could then validate your calibrated model against those data points. Finally, you can use the calibrated (or validated) model to play "what if" games or forecast what the effects of changing conditions might be in your system. Of course, you can also examine the effects toxicants might have on the system as we will discuss in detail on day three.

Model Performance

Sources of Parameter Values

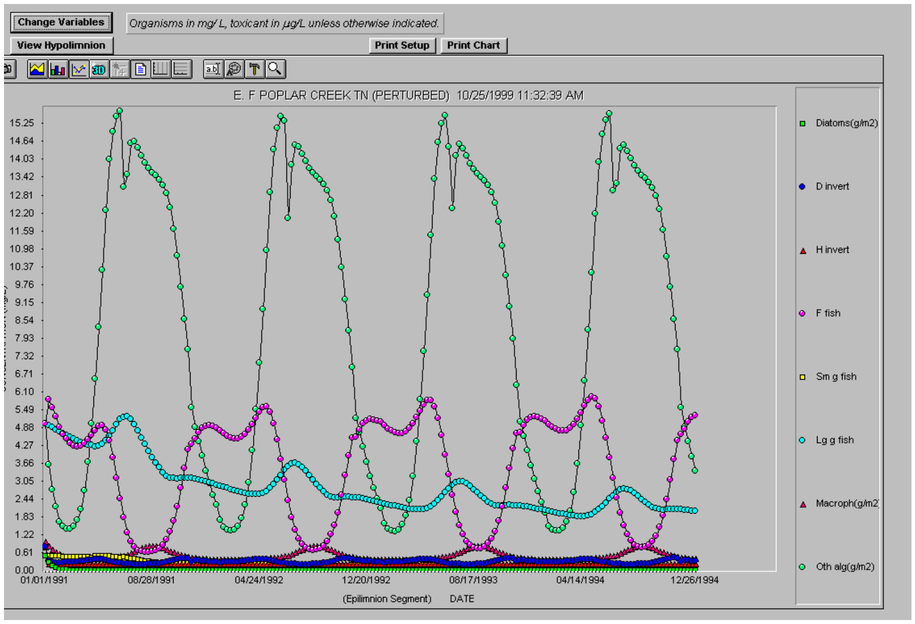
Calibration Strategy for Minnesota Rivers

We will cover three somewhat related areas in this lecture.

Weight-of-Evidence for Model Performance— Limited by Quantity and Quality of Data

- Reasonable behavior based on general experience
- Visual inspection of data points and model plots
- Do model curves fall within error bands of data?
- Do point observations fall within model bounds obtained through uncertainty analysis?
- Regression of paired data and model results—is there concordance, bias?
- Comparison of mean data and mean model results
- Comparison of frequency distributions
  - Relative bias
  - F test
- Kolmogorov-Smirnov test of cumulative distributions

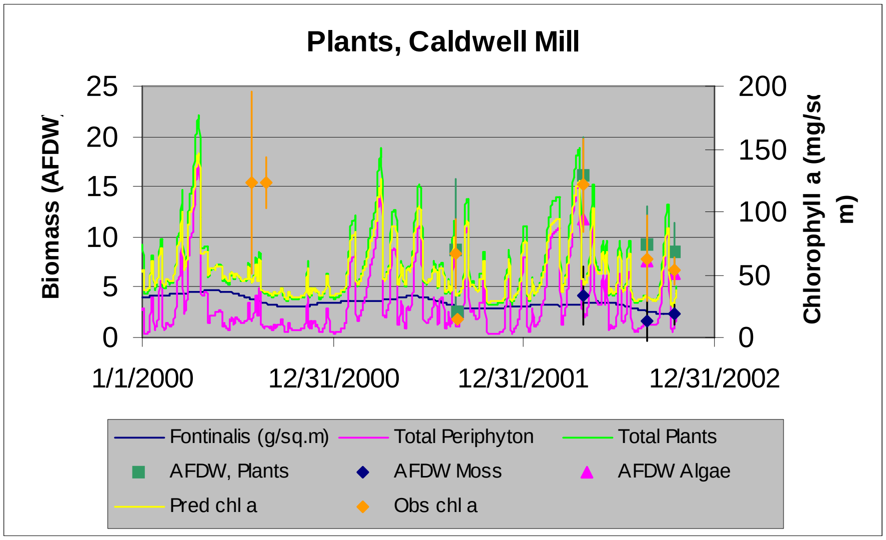
Reasonable ecosystem behavior test



In the absence of data, we can run a multiple-year simulation and look for stability and reasonableness of biomass values.

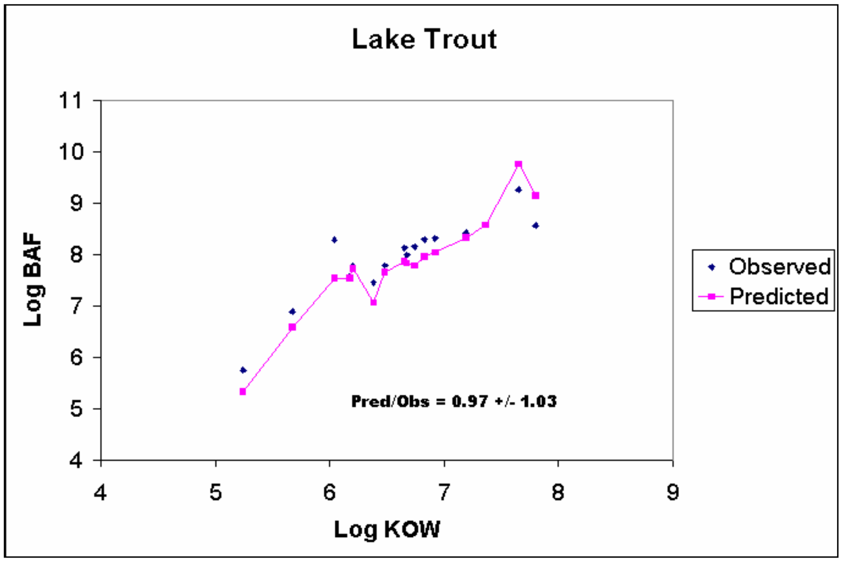
The model was calibrated for Caldwell Mill, Cahaba River, Ala.

Once past the transient conditions of 2000, the fit was acceptable



Visual inspections of fits of predictions to observed data are useful in evaluating how well patterns are represented, with allowance for the vagaries of widely spaced data points. Although not quantitative, they contribute considerably to the weight of evidence that the model is representing the periphyton dynamics realistically. The model was calibrated with data from Caldwell Mill. Beyond the transient conditions of the year 2000, the model seems to give a reasonable fit to the observed data, considering the spread in the observations as indicated by the error bars (+/- 1 standard deviation).

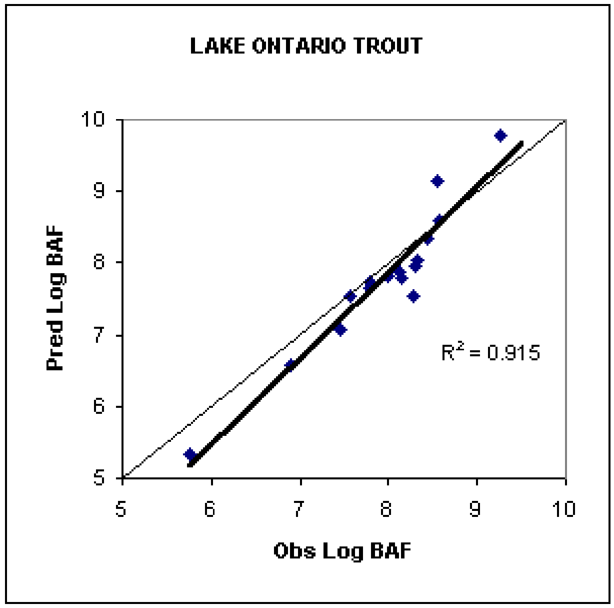
AQUATOX validation with Lake Ontario PCB data



U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports. Washington, DC.

Inspection of the concordance of observed and predicted bioaccumulation factors suggests that the fit is reasonable.

Regression of Lake Ontario observed and predicted PCB BAFs



However, regression shows that the correlation may be very good, but the slope indicates that there is systematic bias in the relationship.

Predicted/Observed Lake Ontario PCB BAFs

AQUATOX (Park, 1999)

	Phyto	Mysids	Trout
Mean	0.53	1.34	0.97
Std Dev	0.51	1.22	1.03

Gobas, 1993, model (results, Burkhard, 1998)

Mean	0.17	0.35	1.23
Std Dev	0.17	0.30	2.20

Thomann et al., 1992, model (results, Burkhard, 1998)

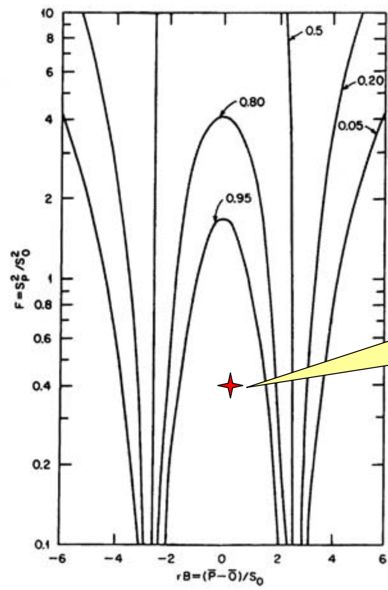
Mean	0.17	0.51	2.52
Std Dev	0.17	0.44	2.79

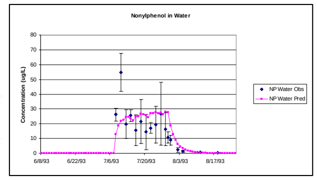
Comparison of the ratios of predicted to observed BAFs indicates that AQUATOX provides better fits for some organisms (but not others) when compared to two other bioaccumulation models. The mysid fit is much better because the modeled position in the food chain is more realistic (predatory zooplankter rather than herbivore).

Statistical Comparison of Means and Variances

$$rB = \frac{(\overline{Pred} - \overline{Obs})}{S_{obs}}$$

$$F = \frac{S^2{}_{pred}}{S^2{}_{obs}}$$





Overlap between distributions based on relative bias, rB, and ratio of variances, F.
Isopleths assume normal distributions; from Bartell et al., 1992.

In this example, the predicted and observed concentrations of nonylphenol in a mesocosm was compared (Park and Clough, 2005).

Park, R. A., and J. S. Clough. 2005. Validation of AQUATOX with Nonylphenol Field Data (Unpublished Report). U.S. Environmental Protection Agency, Washington, DC.

Two measures help answer the question: how much overlap is there between data and model distributions? Relative bias is a robust measure of how well central tendencies of predicted and observed results correspond; a value of 0 indicates that the means are the same (Bartell et al. 1992):

rB = *(Pred_Bar – Obs_Bar)/SObs_*

where:

rB = relative bias (standard deviation units);

Pred_Bar = mean predicted value;

Obs_Bar = mean observed value; and

Sobs = standard deviation of observations.

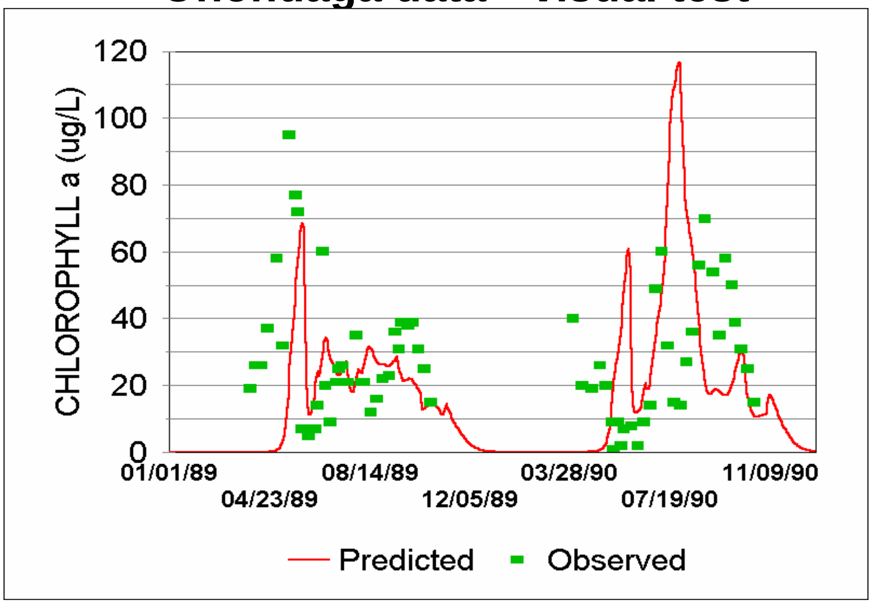
The F test is the ratio of the variance of the model and the variance of the data. A value of 1 indicates that the variances are the same:

F = *Var_Pred/Var_Obs*

Very small F values suggest that the observed data may be too variable to determine the goodness of fit; very large F values indicate that the predictions are imprecise (Bartell et al., 1992). Large F values also may indicate that the model is predicting greater fluctuations than can be supported by sparse data. Assuming normal distributions, the probability that the observed and predicted distributions are the same can be evaluated. Putting the two tests together, if a comparison has rB = 0 and F = 1, then the predicted and observed results are identical.

Bartell, S. M., R. H. Gardner, and R. V. O'Neill. 1992. *Ecological Risk Estimation*. Lewis Publishers, Boca Raton, Florida.

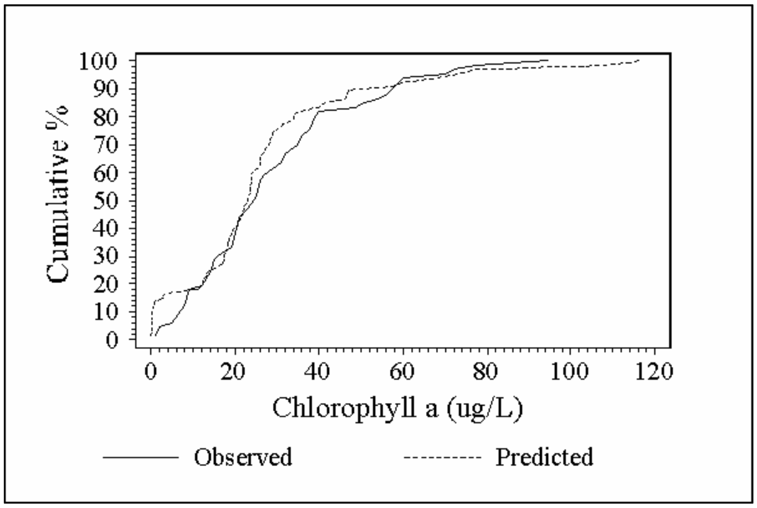
Validation of AQUATOX with Lake Onondaga data—visual test



U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports. Washington, DC.

We will re-visit this example in a later exercise.

Validation with chlorophyll a in Lake Onondaga, NY

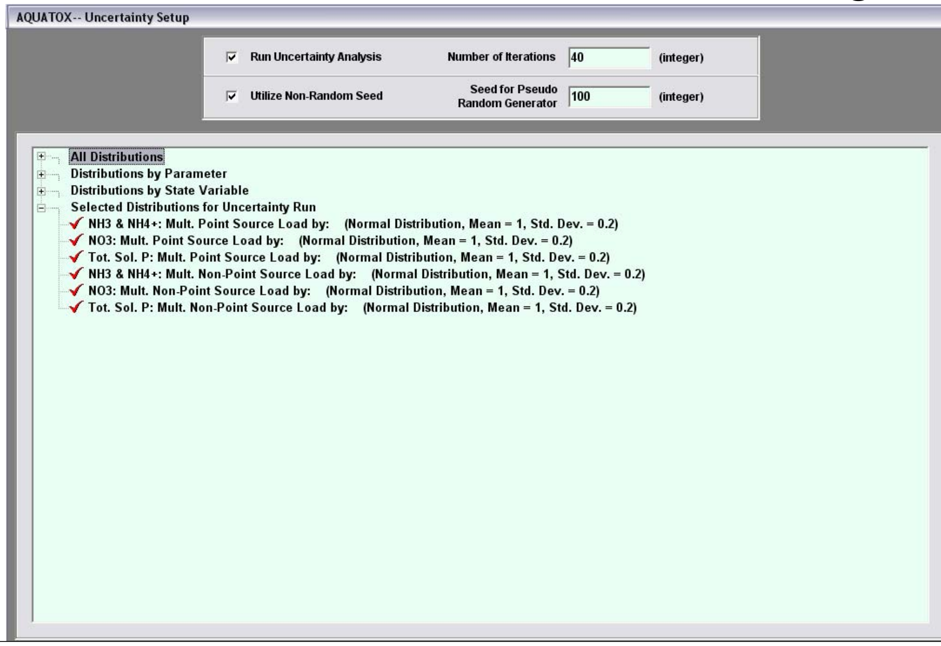


Kolmogorov-Smirnov p statistic = 0.319 (not sign. different)

U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports. Washington, DC.

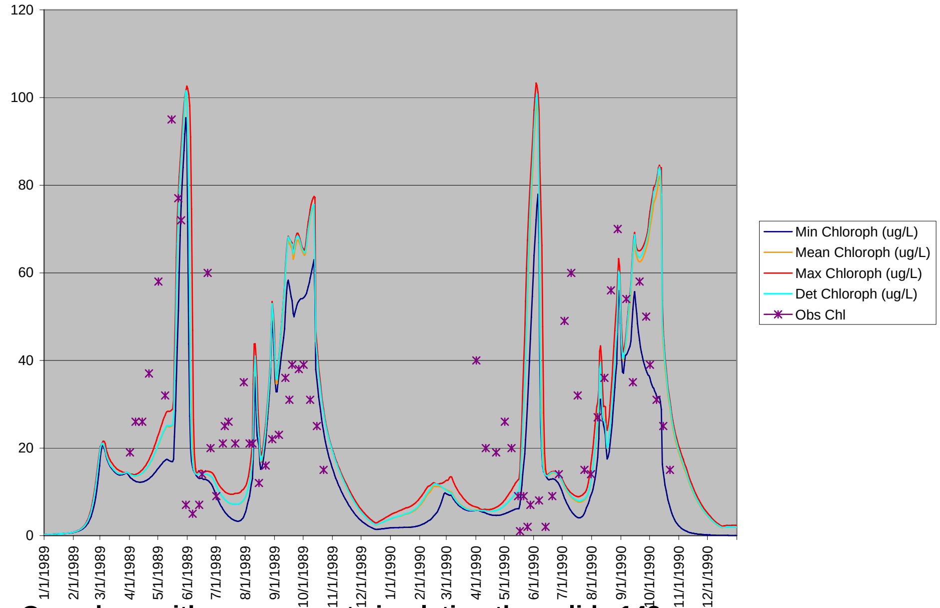
The Kolmogorov-Smirnov statistic is a non-parametric test of whether two datasets differ significantly based on their cumulative distributions. It implied fairly good agreement between the predicted and observed distributions of the chlorophyll *a* values.

We can run uncertainty analysis with distributions around nutrient loadings



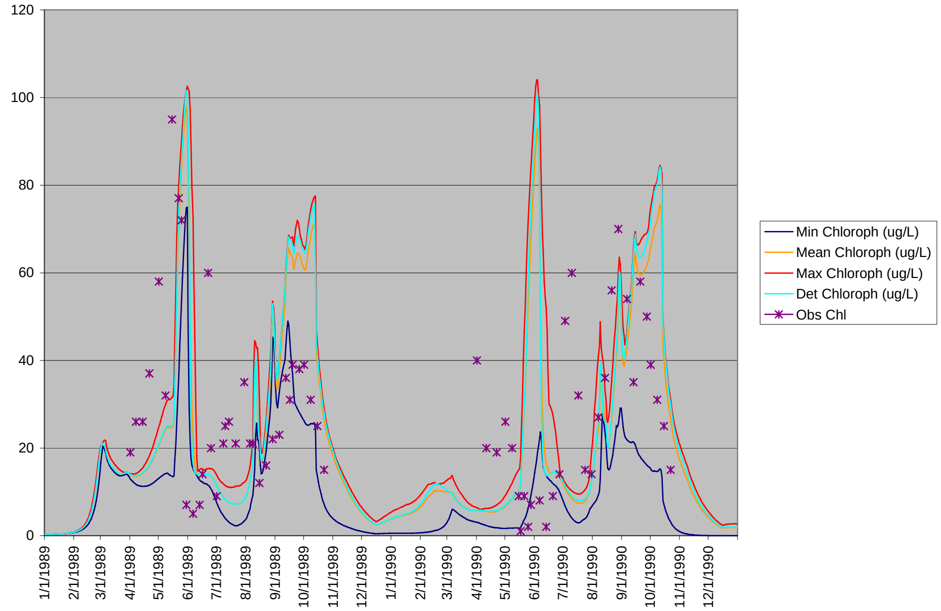
Uncertainty analysis is available to compare envelope of predictions with observed data. For example, still using the Lake Onondaga study, we can provide distributions of values for the nutrient loadings.

Plotting observed points with uncertainty bands for simulation suggests imperfect fit



Lake Onondaga with more recent simulation than slide 143

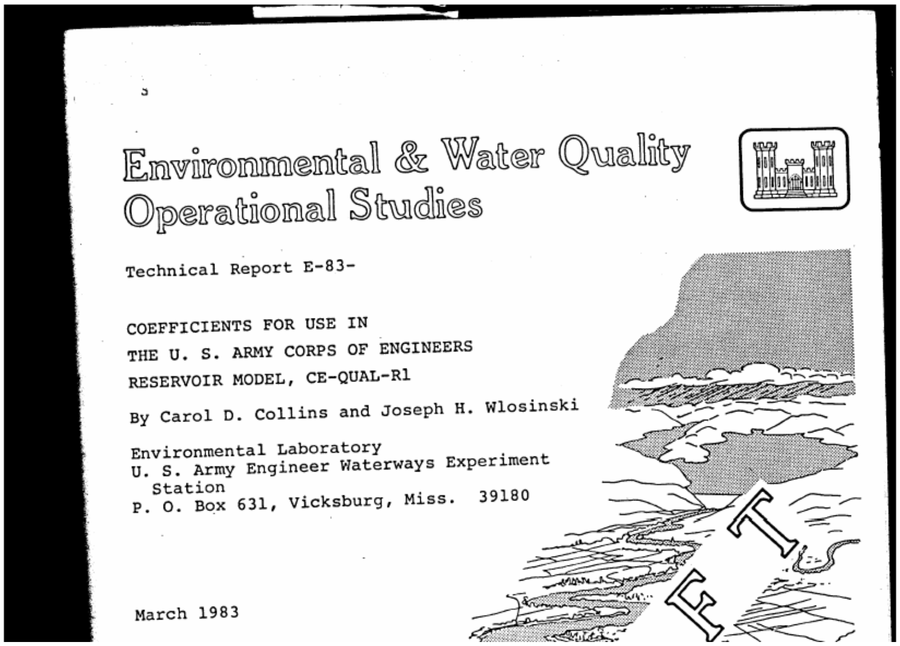
With twice the standard deviations, more of the observed points fall within the envelope



Lake Onondaga with more recent simulation than slide 143

If we double the standard deviations for each of the nutrient loading distributions we can compare the increased envelope of uncertainty with the observed data.

Sources of parameters



Environmental & Water Quality Operational Studies

Technical Report E-83-

COEFFICIENTS FOR USE IN THE U. S. ARMY CORPS OF ENGINEERS RESERVOIR MODEL, CE-QUAL-R1

By Carol D. Collins and Joseph H. Wlosinski

Environmental Laboratory
U. S. Army Engineer Waterways Experiment Station
P. O. Box 631, Vicksburg, Miss. 39180

March 1983

Collins, Carol Desormeau, and Joseph H. Wlosinski. 1983. Coefficients for Use in the U.S. Army Corps of Engineers Reservoir Model, CE-QUAL-R1. Vicksburg, Miss.: Environmental Laboratory, U.S. Army Engineer Waterways Experiment Station.

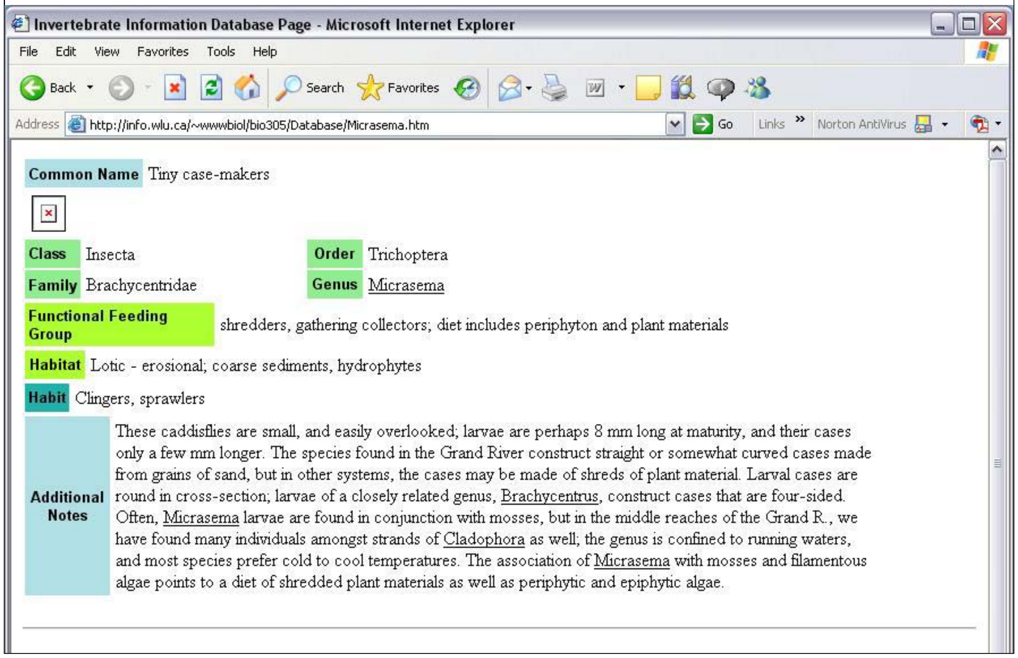
Collins and Wlosinski, 1983, PMax values

Table 5

Gross production rates of phytoplankton (1/day)

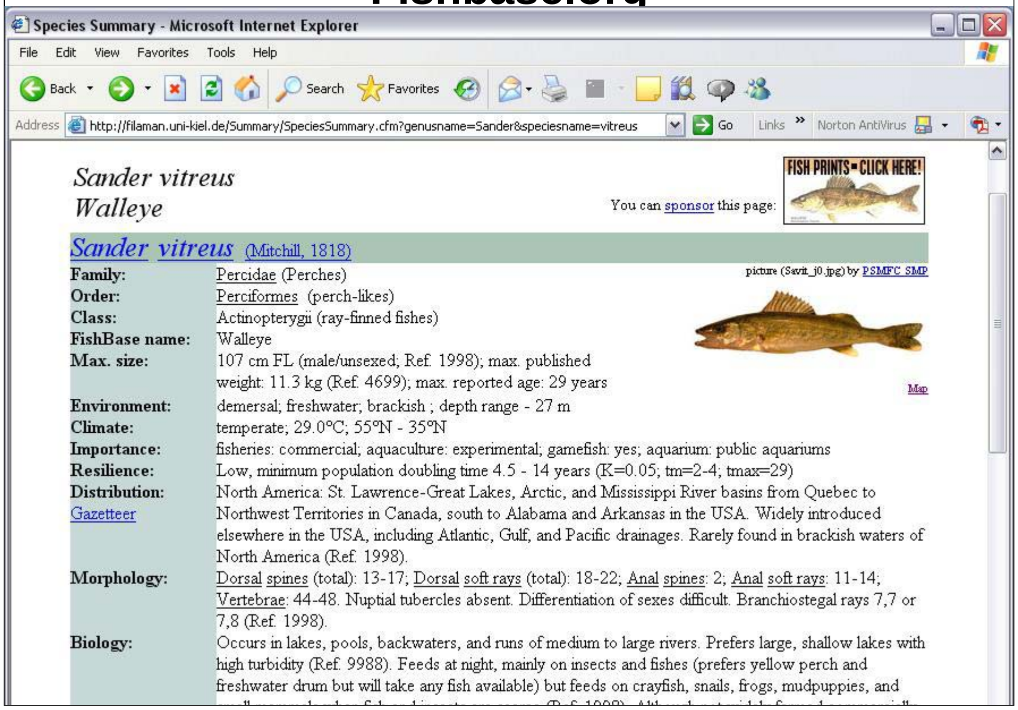
SPECIES	TPMAX	TEMP °C	REFERENCE
DIATOMS			
Asterionella formosa	0.81	20	Holm and Armstrong 1981
Asterionella formosa	0.69	10	Hutchinson 1957
Asterionella formosa	1.38	20	Hutchinson 1957
Asterionella formosa	1.66	25	Hutchinson 1957
Asterionella formosa	1.71	20	Fogg 1969
Asterionella formosa	0.28	4	Talling 1955
Asterionella formosa	0.69	10	Talling 1955
Asterionella formosa	1.38	20	Talling 1955
Asterionella formosa	2.2	20	Hoogenhout and Amesz 1965
Asterionella formosa	1.9	18.5	Hoogenhout and Amesz 1965
Asterionella japonica	1.19	22	Fogg 1969
Asterionella japonica	1.3	18	Hoogenhout and Amesz 1965
Asterionella japonica	1.7	25	Hoogenhout and Amesz 1965
Biddulphia sp.	1.5	11	Castenholz 1964
Coscinodiscus sp.	0.55	18	Fogg 1969
Cyclotella meneghiniana	0.34	16	Hoogenhout and Amesz 1965
Cyclotella nana	3.4	20	Hoogenhout and Amesz 1965
Detonula confervacea	0.62	2	Smayda 1969
Detonula confervacea	1.4	10	Hoogenhout and Amesz 1965
Ditylum brightwellii	2.1	20	Paasche 1968
Fragilaria sp.	0.85	20	Rhee and Gotham 1981b
Fragilaria sp.	1.7	11	Castenholz 1964
Melosira sp.	0.7	11	Castenholz 1964
Navicula minima	1.4	25	Hoogenhout and Amesz 1965
Navicula pelliculosa	2.0	20	Hoogenhout and Amesz 1965
Nitzschia closterium	1.66	27	Harvey 1937
Nitzschia palea	2.1	25	Hoogenhout and Amesz 1965
Nitzschia turgidula	2.5	20	Paasche 1968
Phaeodactylum tricornutum	1.66	25	Fogg 1969
Phaeodactylum tricornutum	2.7	19	Hoogenhout and Amesz 1965
Rhizosolenia fragillissima	1.20	21	Ignatiades & Smayda 1970
Skeletonema costatum	1.26	18	Fogg 1969
Skeletonema costatum	2.30	20	Jorgensen 1968
Skeletonema costatum	1.52	20	Steemann-Nielsen and Jorgensen 1968
Skeletonema costatum	1.23	20	Jitts et al. 1964

Invertebrate Information Database



http://info.wlu.ca/~wwwbiol/bio305/Database/Micrasema.htm

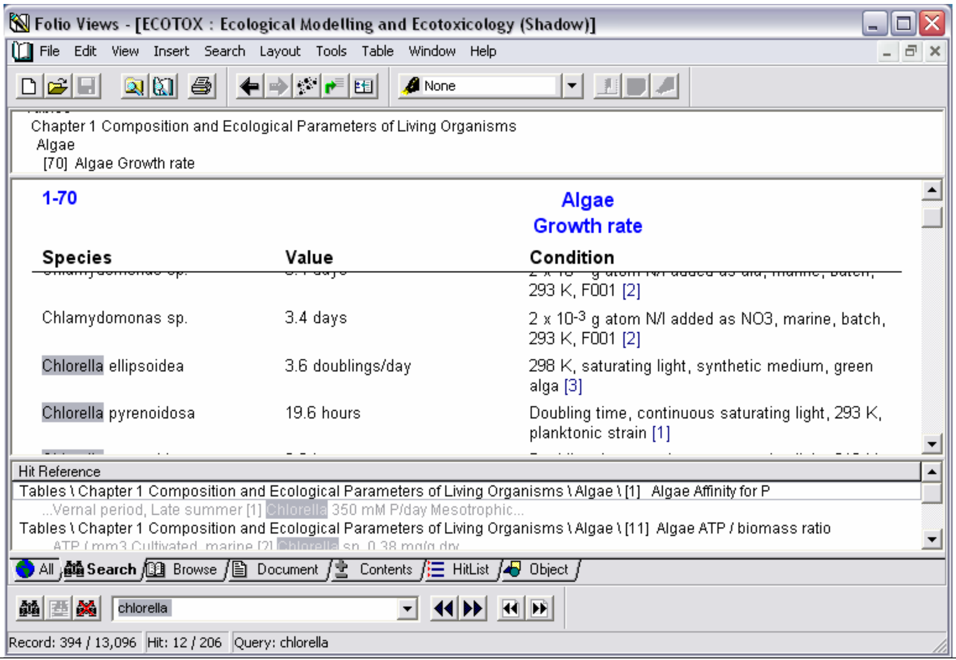
Fishbase.org



The German mirror Web site is often faster than the primary Web site, especially in the afternoon:

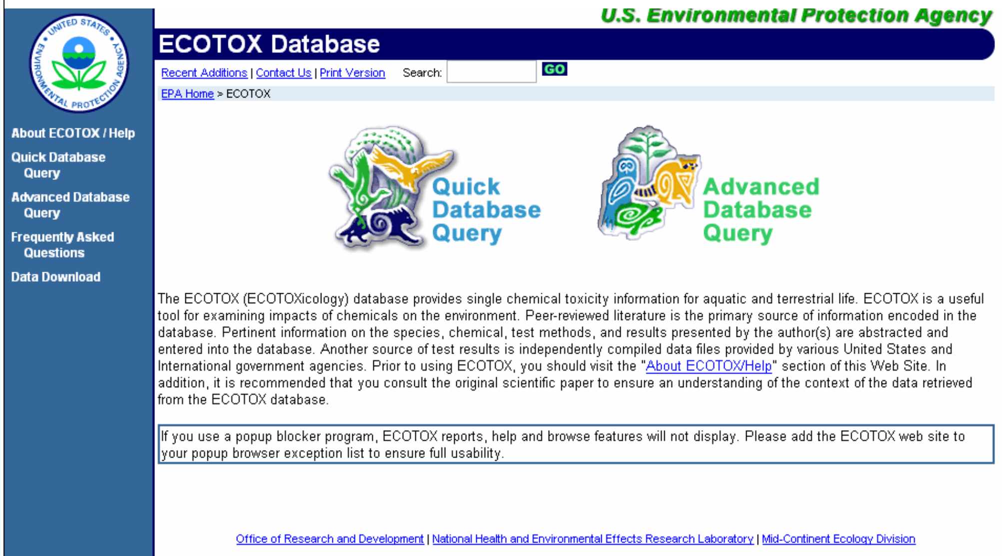
http://filaman.uni-kiel.de/Summary/SpeciesSummary.cfm?genusname=Sander&speciesname=vitreus

ECOTOX (Elsevier product)

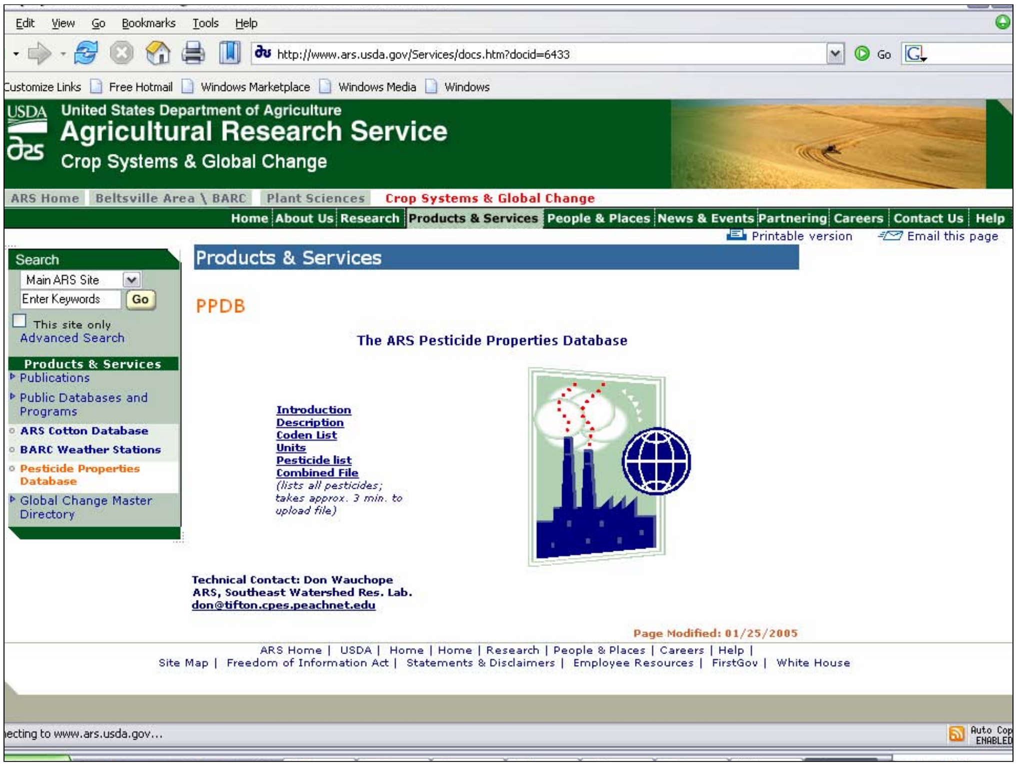


This is an expensive database, but it provides a useful survey of parameter values. Be careful of calibrated values mixed in with values observed from careful experiments.

ECOTOX (EPA Database)

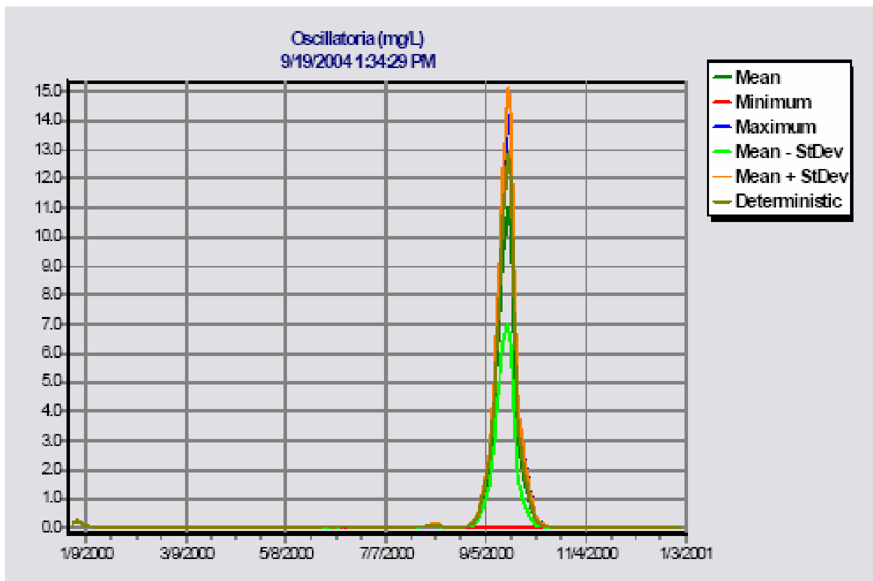


This is a comprehensive database of toxicity parameters that is constantly updated.



The ARS Pesticide Properties Database is quite useful:
http://www.ars.usda.gov/Services/docs.htm?docid=6433

Sensitivity analysis of blue-green to saturated light parameter (74+-30)



Sensitivity of blue-green algae in Blue Earth River MN was used to analyze the response to variations in the saturated light parameter. This was used to determine an appropriate value based on observed ranges in values.

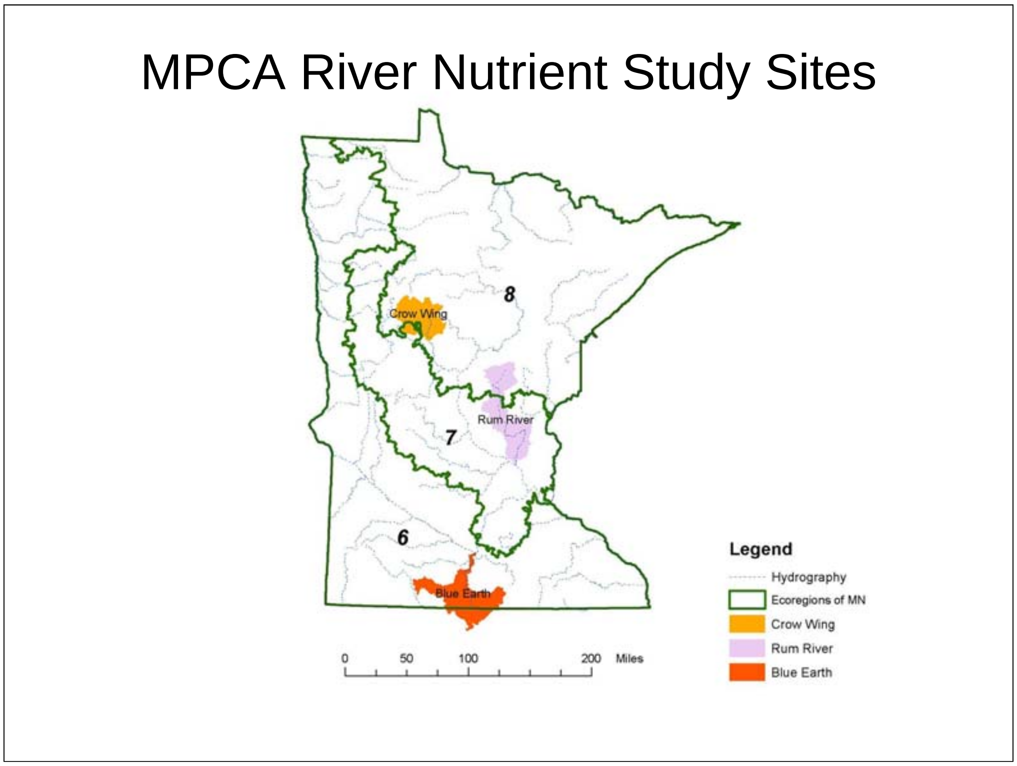
Calibration Strategy for Minnesota Rivers

- Must be able to simulate *changing* conditions!
- Add plants and animals representative of both low- (Crow Wing) and high-nutrient (Blue Earth) rivers
- Iteratively calibrate key parameters for each site and cross-check to make sure they still hold for other site
- When goodness-of-fit is acceptable for both sites, apply to an intermediate site (Rum River) and reiterate calibration

First the model was calibrated against observed data for the Blue Earth River, then the same parameter set was used to simulate the Crow Wing River. Adjustments were made to parameters, especially for the low-nutrient algae, until a suitable fit was obtained, and then the new values were used to simulate the Blue Earth River, and further adjustments were made. This iterative approach proceeded until both sites were suitably represented by the same parameter set.

The next step was to attempt to validate the two-site calibration with data from the Rum River. HSPF was not run for the Rum River basin; a stand-alone implementation was used with the same parameter set. However, the fit was not satisfactory. A combination of moderate nutrients and low turbidity seems to favor green algae in ways not predicted by the experience with the low- and high-nutrient sites, and additional calibration was indicated. So, rather than using the site for validation, the decision was made to calibrate across all three sites.

To avoid reentering parameter values between sites and to speed up the calibration, a modification was made to AQUATOX Release 3, which is in beta test now. Release 3 represents linked segments sharing a common parameter set. The model was made more general so that separate, unlinked sites could be simulated simultaneously with a common parameter set. Thus, the effect of a change in a parameter value could be evaluated across all three sites and changed accordingly. A one-year simulation for the three riverine sites takes about 45 minutes on a Pentium 4 2.8 GHz machine. The procedure is not only efficient, it facilitates comparisons among the three sites.



The Blue Earth River watershed is located in the Western Corn Belt Plains, part of the Aggregate Nutrient Ecoregion 6. The upper Crow Wing River watershed is located in the Northern Lakes and Forests, part of the Aggregate Nutrient Ecoregion 8. The Rum River watershed is located in the North Central Hardwood Forests.

Rum River, Minnesota

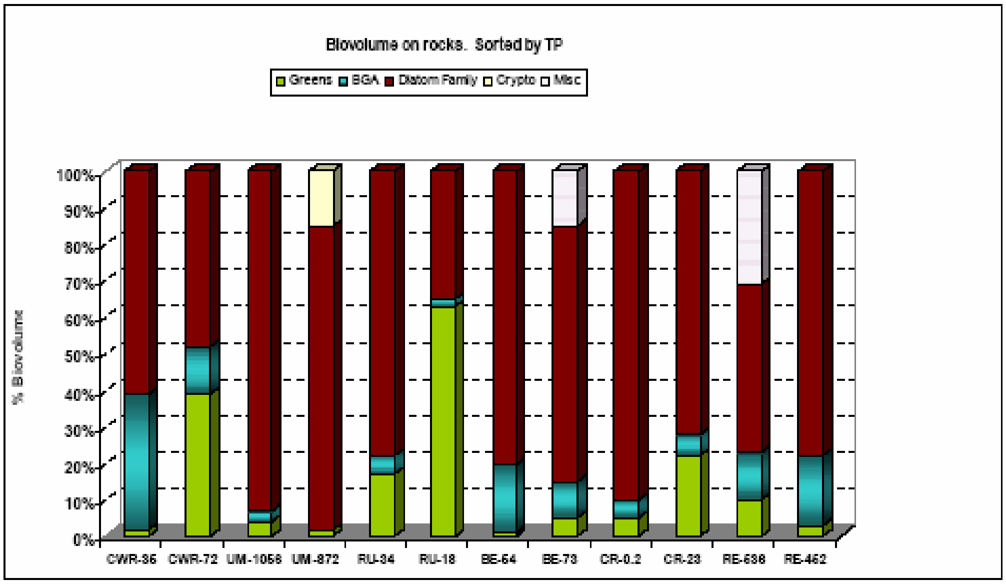
(Heiskary & Markus, 2003)

All three rivers are shallow and are capable of supporting diverse periphyton communities, which vary in composition according to their position on a nutrient gradient.

Periphyton percent biovolume on rock

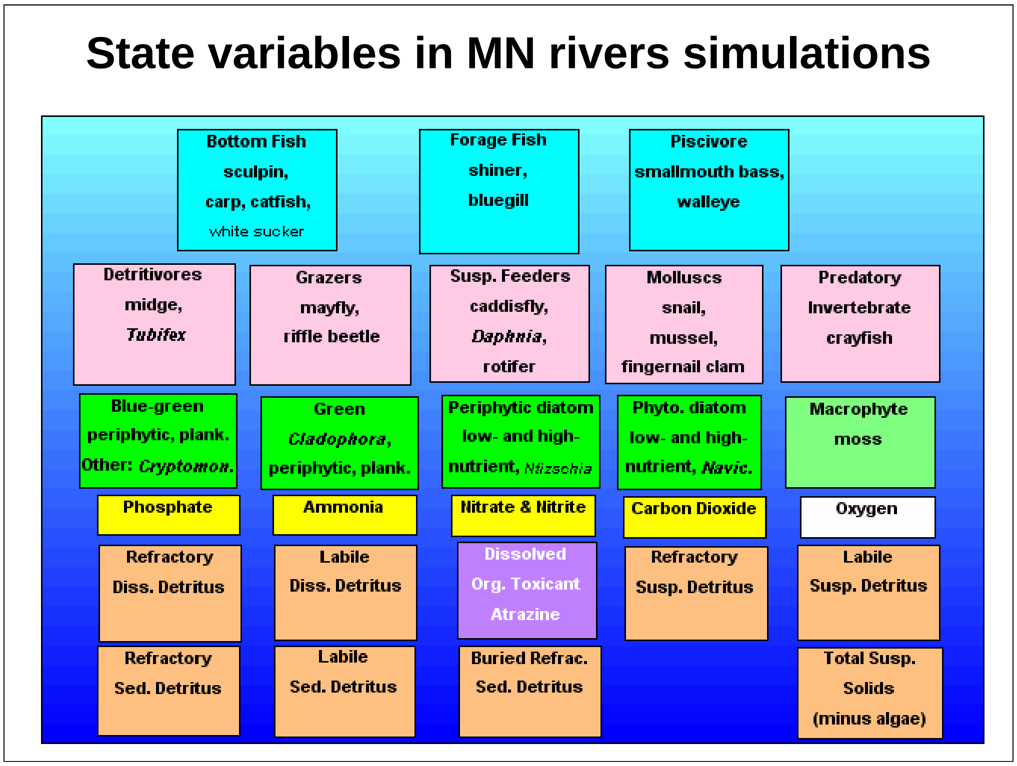
Sites sorted based on summer-mean TP for 2000

(Heiskary & Markus, 2003)



CWR: Crow Wing, UM: Upper Mississippi, RU: Rum, BE: Blue Earth, CR: Crow, RE: Red.

The Crow Wing River has relatively low levels of nutrients and low turbidity. The Rum River has moderate levels of nutrients and low turbidity. The Blue Earth River has high levels of nutrients and periodically high turbidity.

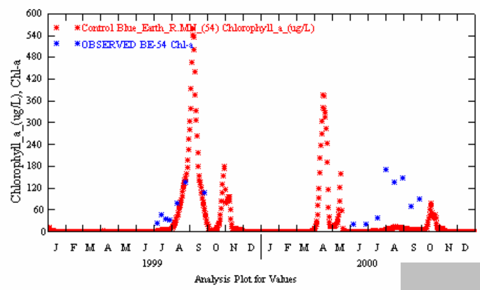


State variables were chosen to represent both the nutrient-poor, clear-water Crow Wing River and the nutrient-enriched, turbid Blue Earth River. Sculpin, a cold-water fish, was included although conditions in the Blue Earth River are too warm for its continued survival. Because the objective was to obtain a set of state variables that would span the conditions on the Minnesota rivers, the number of state variables is larger than if a single river with static conditions were being simulated. In fact, the number of algal groups is almost double that required if the model were calibrated for present conditions in a single river.

Calibration of Plants

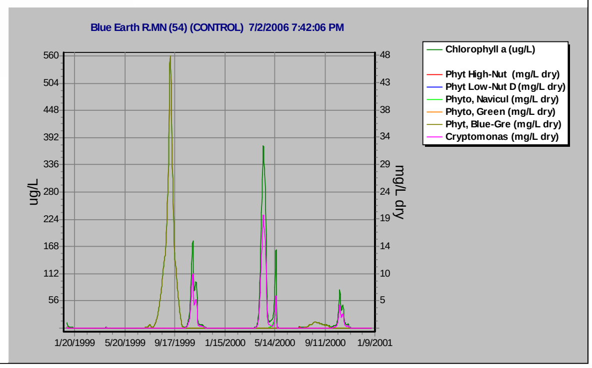
- algae are differentiated on basis of:
  - nutrient half-saturation values
  - light saturation values
  - maximum photosynthesis
- MN project has developed new parameter sets that span nutrient, light, and PMax
- phytoplankton sedimentation rates differ between running and standing water
- critical force for periphyton scour and TOpt may need to calibrated for other sites

Blue Earth River Phytoplankton



it is difficult to simulate the timing of the summer 2000 algal bloom

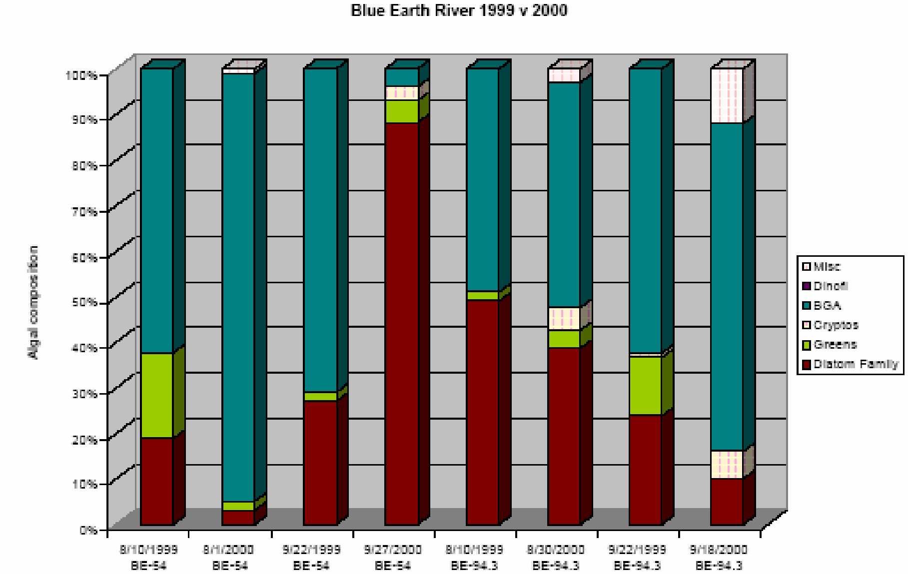
blue-greens, diatoms, and cryptomonads dominate



Calibration of AQUATOX for the Minnesota rivers used the algal variables, chlorophyll *a* and composition, as targets for obtaining best fits. Because there were few data points, suitable calibrations were based on reasonable behavior and appropriate concordance with observed values as determined by graphical comparisons. The predicted invertebrate and fish biomasses were inspected for reasonable values, and adjustments were made as deemed necessary.

Predicted Blue Earth River phytoplankton are dominated by blue-greens, similar to what was observed, and cryptomonads. The latter are not as well supported by the observed data, but the samples do not cover the spring and late fall periods. Diatoms are not as important in the simulation as observed.

Observed phytoplankton dominated by blue-greens, with diatoms, cryptomonads, and greens in Blue Earth River

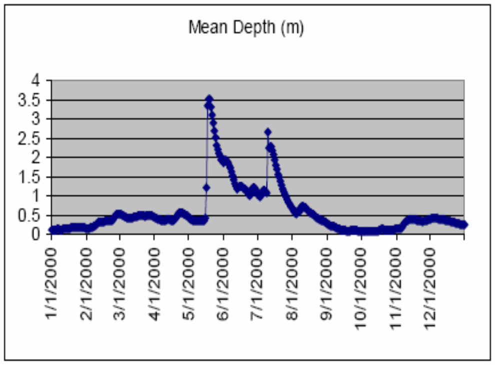


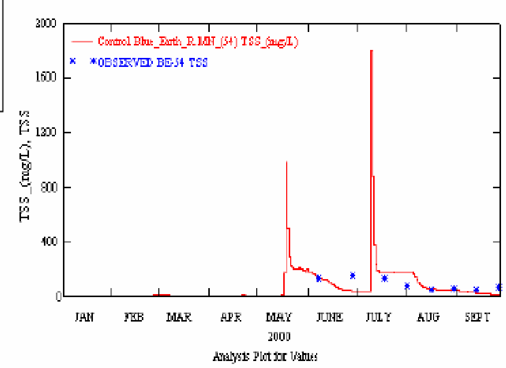
Hydrologic loadings from HSPF may be preventing significant predicted growth in August

- The only gage is at a dam 42 miles downstream and is affected by a small impoundment
- The upstream river may be more “flashy” given the widespread drainage tile fields
- And/or the downstream gage may have been affected by a storm in a tributary watershed
- Therefore the Aug. flow and water depth may have been less than predicted, favoring algae

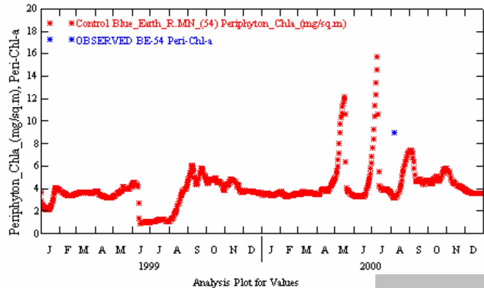
This is the opinion of the ecological modeler, and is not necessarily accepted by the hydrological modelers that ran HSPF.

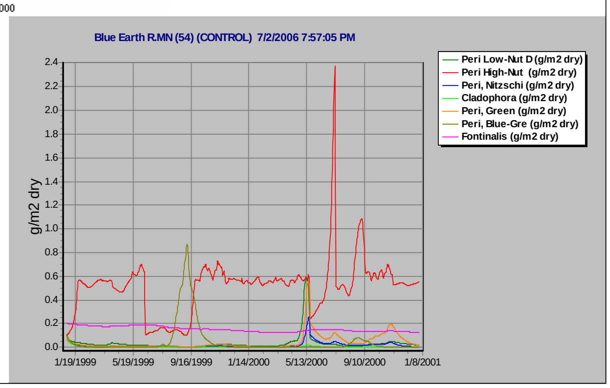
Predicted Depth and Turbidity Preclude Algal Buildup





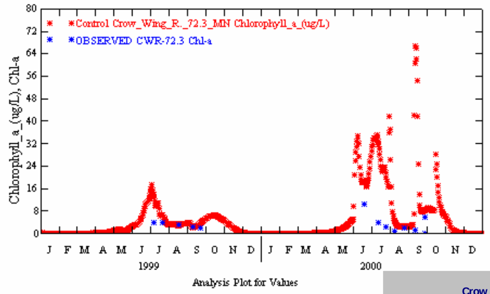
Blue Earth River Periphyton

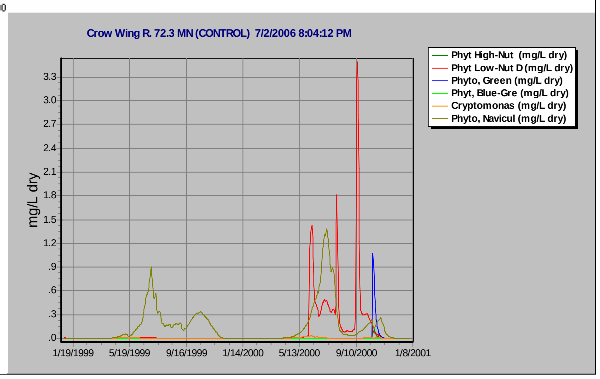




The predicted periphyton in Blue Earth River are dominated by high-nutrient diatoms with lesser amounts of blue-greens and greens as suggested by the observed data. The peak biomass reaches the observed level, but the timing is a little off. Also, it is very difficult to make any firm judgment about the fit of the data, given only one sampling point. Unfortunately scarce data are often the norm.

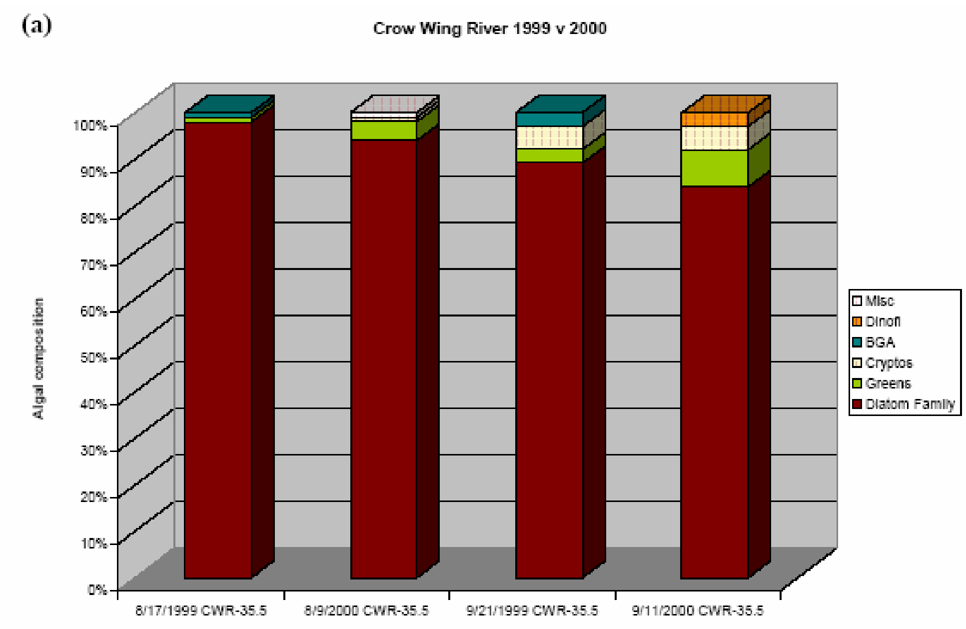
Crow Wing River Phytoplankton





Crow Wing River phytoplankton are dominated by low-nutrient diatoms. Predicted blooms of low-nutrient diatoms and green algae are not supported by the data, but represent transient sloughing events from the periphyton.

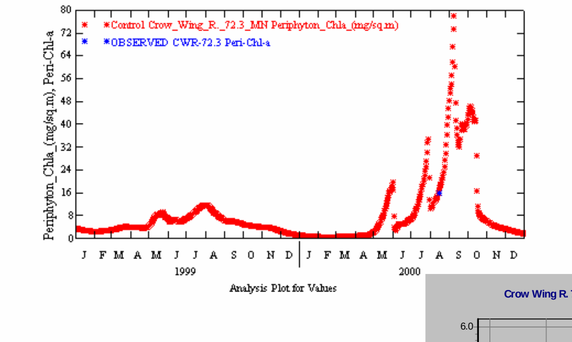
Observed Phytoplankton in Crow Wing River

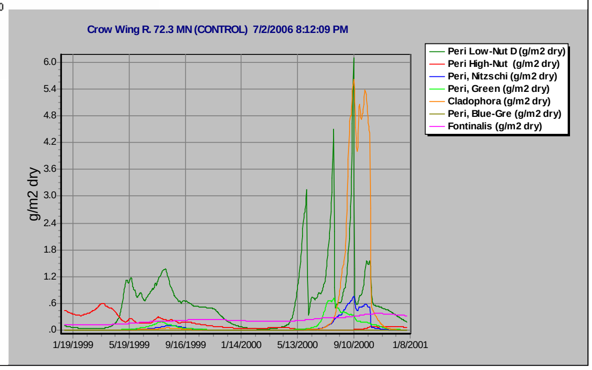


Heiskary, Steven, and Howard Markus. 2003. Establishing Relationships Among In-Stream Nutrient Concentrations, Phytoplankton Abundance and Composition, Fish IBI and Biochemical Oxygen Demand in Minnesota USA Rivers. St. Paul, MN: Minnesota Pollution Control Agency.

Note that these data are from a site downstream from the site modeled.

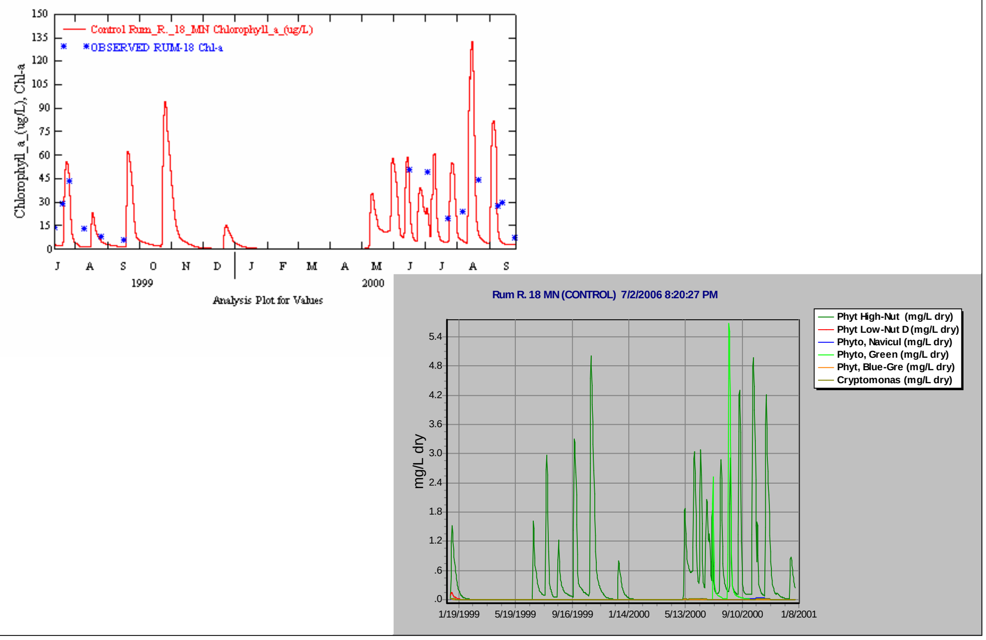
Crow Wing River Periphyton





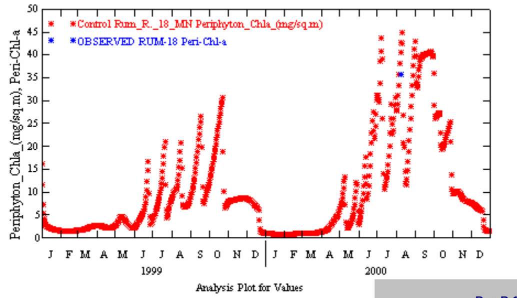
The Crow Wing periphyton are diverse, but are dominated by low-nutrient diatoms and green algae, especially *Cladophora*, similar to what was observed. As with all periphyton samples, there is only one observation for comparison.

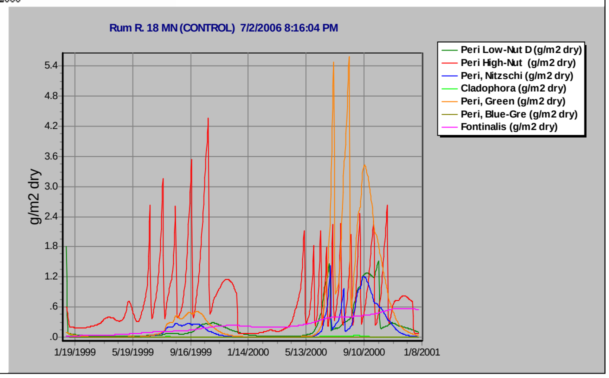
Rum River Phytoplankton



The predicted Rum River phytoplankton are dominated by high-nutrient diatoms in a series of apparent blooms that actually represent sloughing from the periphyton; the blue-greens that are also important in the observed data are not well represented in the simulation. The predicted biomass levels compare favorably with the observations with the exception of a large sloughing event for green algae.

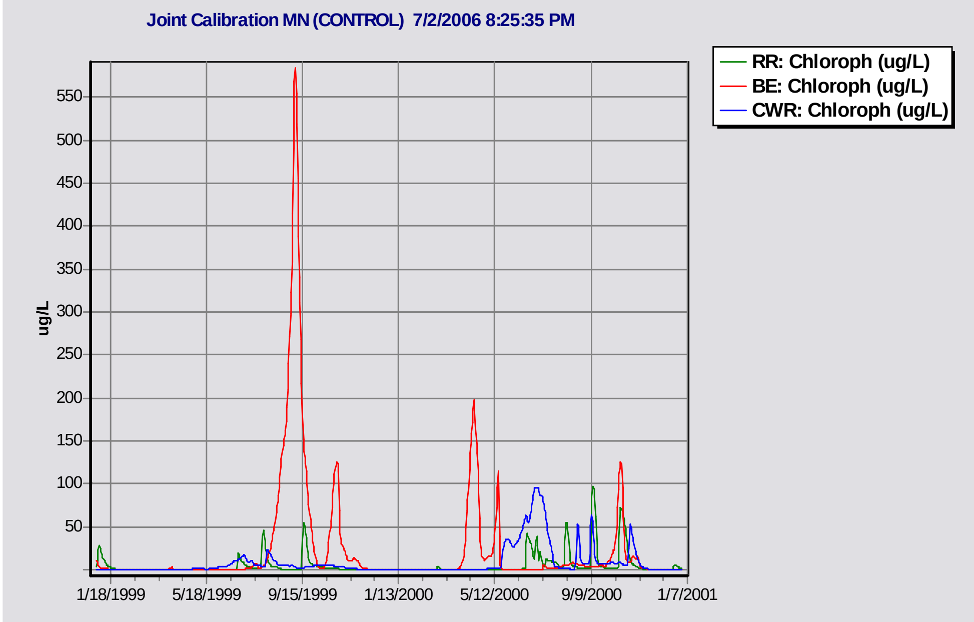
Rum River Periphyton





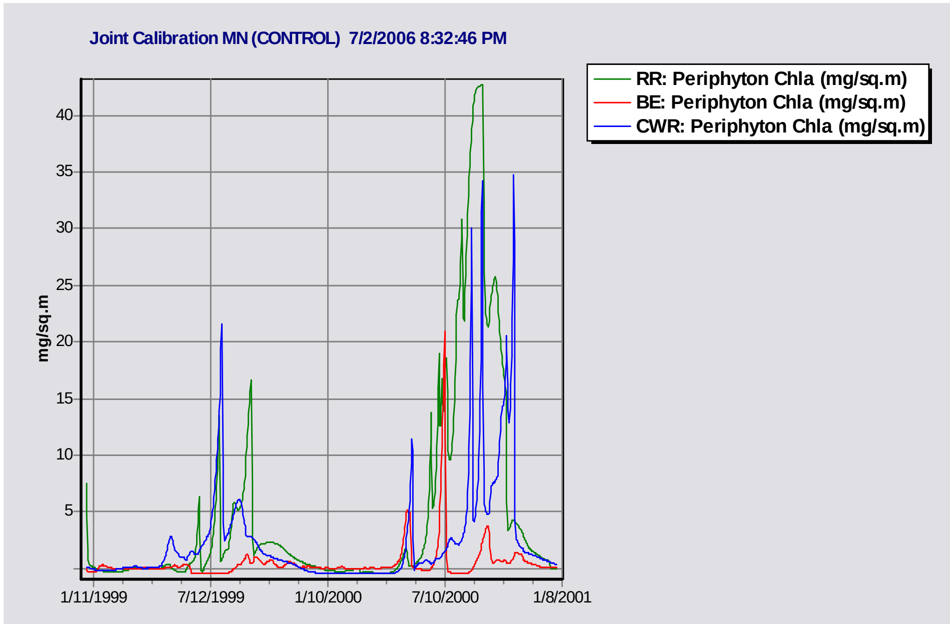
Predicted Rum River periphyton are diverse, are dominated by green algae and high-nutrient diatoms, and exhibit high chlorophyll *a* levels.

Predicted phyto. chl *a* in the Blue Earth, Rum, and Crow Wing Rivers.



The model performs surprisingly well across a wide nutrient and turbidity gradient, as represented by the three Minnesota rivers. AQUATOX Release 3 makes it easy to compare key variables across the sites. For example, it is quite obvious that phytoplanktonic chlorophyll *a* is far greater in the nutrient-enriched Blue Earth River, followed, with one exception, by the moderately enriched Rum River, with generally lower levels being predicted in the nutrient-poor Crow Wing River.

Predicted periphyton chl. *a* in the Blue Earth, Rum, and Crow Wing Rivers



The pattern of predicted chlorophyll *a* for periphyton is not so obvious. The moderately enriched but clear-water Rum River is predicted to have the highest overall level of periphyton. The nutrient-poor, clear-water Crow Wing River and the nutrient-enriched, often turbid Blue Earth River are predicted to have lower levels of periphyton but with occasional blooms. These predictions are in accordance with the single observations of periphyton in the three rivers and with observations across nutrient gradients in other rivers.