AQUATOX Training Workshop

Web Training Materials, August 2012

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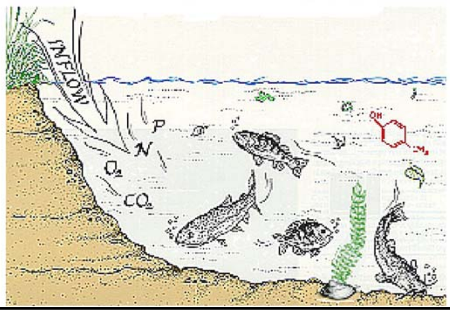


Introduction

- 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.

CD Setup: Files, Installation

- Data Folder
- Documents Folder
- Presentation Folder
- References Folder
- Reprints Folder
- AQUATOX Installation
  - » Which Installs to…

For purposes of the workshop, the **Data** folder and subfolders contain all of the raw data sets that we will be using to run various simulations within AQUATOX.

The **Documents** folder contains a Users Guide, Technical Documentation, and Validation Reports in PDF format (all the published documentation).

Also on the CD are: the **Presentation** folder with all the presentation material for the workshop, the **References** folder with reports containing useful parameter values, and the **Reprints** folder with some published papers on AQUATOX for the use of the participants.

We will discuss the AQUATOX file structure that is created when the AQUATOX installation program is run. Installation must be done by a systems administrator.

Potential Applications for AQUATOX

- Many waters are impaired biologically as well as chemically
- Managers need to know:
  - Most important stressor?
  - Implications of possible pollution control and/or restoration measures?
    - Differences in biotic communities
    - Improved water quality
  - Unintended consequences?
  - Recovery time?
  - Uncertainty around predictions?
- Science vs policy decisions

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 water bodies that don't fully support the aquatic life uses as designated in their state water quality standards.

As of early 2009, of the waters that have been assessed, 44% of rivers and streams, 59% of lakes, reservoirs and ponds, and 35% of estuaries were impaired for one or more of their designated uses. Commonly reported causes of impairment included nutrients, siltation, organic enrichment, 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.

An important point to be made is that the model will provide projections of possible outcomes; the decision of whether any of the outcomes is "acceptable" is a policy decision. One of the most valuable applications of AQUATOX is to evaluate the potential implications and ramifications of various management options.

Regulatory Endpoints Modeled

- Nutrient and toxicant concentrations
- Biomass
  - plant, invertebrate, fish
- Chlorophyll a
  - phytoplankton, periphyton, moss
- Biological metrics
- Total suspended solids, Secchi depth
- Dissolved oxygen
  - daily minimum and maximum
- 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. It should be reiterated that the model output does not by itself provide an answer as to the acceptability of the results; the decision of which measures to adopt, if any, is a policy decision. AQUATOX provides the ability to evaluate potential implications of different courses of action.

We'll discuss the different kinds of AQUATOX output in more detail a little later.

Potential Applications
nutrients

- Develop nutrient targets for rivers, lakes and reservoirs subject to nuisance algal blooms
- Evaluate which factor(s) is controlling algae levels
  - nutrients, suspended sediments, grazing, herbicides, flow
- Evaluate effects of agricultural practices or land use changes
  - 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?
  - Linkage to watershed models in BASINS

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. We'll explore this in greater detail later.

The model has been, or is being, used in assessing nutrient impacts on various waterbodies including the Cahaba River Alabama, the Lower Boise River Idaho, Indian Creek Indiana, Tenkiller Lake Oklahoma, three rivers in Minnesota, twenty streams in northern Florida, Venice Lagoon Italy, and Vitória Bay Brazil.

Potential Applications of AQUATOX
toxic substances

- Ecological risk assessment of chemicals
  - 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?
- Bioaccumulative compounds
  - Calculate BAFs and tissue concentrations
  - Estimate time until fish are safe to eat after remediation

The model can represent up to 20 organic chemicals simultaneously. It considers degradation pathways, bioaccumulation, and ecotoxicity.

AQUATOX has been, or is being, used in assessing bioaccumulation and toxic impacts on various waterbodies including mesocosms in Minnesota and France, Lake Hartwell Georgia, the Songhuajiang River China, Galveston Bay Texas, the Tajan River Iran, and Skensved stream Denmark.

Potential Applications
aquatic life support

- Evaluate proposed water quality criteria
  - Differences in biotic communities?
  - Support designated use?
- Estimate recovery time of community after reducing pollutants
- Evaluate potential responses to invasive species and mitigation measures
  - Impacts on native species?
  - Changes in ecosystem "services"?
- Evaluate possible effects of climate change
  - Link to climate and/or watershed models

AQUATOX is being, or has recently been, used in assessing the impacts of zebra mussels and the potential impacts of climate change on Lake Onondaga New York, and the impacts of the Deepwater Horizon oil spill on Mississippi Sound.

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 panels and in several published model reviews
- Distributed by US EPA, Open Source code

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 Releases 2.1 and 2.2. Release 3, which was issued in September 2009, is a powerful version, which can model linked segments, layered sediments, and estuaries, with significantly improved graphing and statistical capabilities. Release 3.1 is in Beta test now and will probably be issued in Spring, 2011.

Acceptance of AQUATOX

- Has gone through 2 EPA-sponsored peer reviews (following quotes from 2008 review):
  - "model enhancements have made AQUATOX one of the most exciting tools in aquatic ecosystem management"
  - "this is the first model that provides a reasonable interface for scientists to explore ecosystem level effects from multiple stressors over time"
  - "the integration of ICE data into AQUATOX makes this model one of the most comprehensive aquatic ecotoxicology programs available"
  - it "would make a wonderful textbook for an ecotoxicology class"
- Is gradually appearing in open literature

Mauriello, D.A., and R.A. Park. 2002. An adaptive framework for ecological assessment and management. In: Integrated Assessment and Decision Support (A. E. Rizzoli and A.J. Jakeman, eds.) International Environmental Modeling and Software Society, Manno, Switzerland. pp. 509-514.

Rashleigh, B. 2003. Application of AQUATOX, a process-based model for ecological assessment, to Contentnea Creek in North Carolina. *Journal of Freshwater Ecology* 18 (4): 515- 522.

Carleton, J. N., M. C. Wellman, P. A. Cocca, A. S. Donigian, R. A. Park, J. T. Love, and J. S. Clough. 2005. Nutrient Criteria Development with a Linked Modeling System: Methodology Development and Demonstration. *TMDL 2005*. Water Environment Federation, Alexandria, Virginia, pp. 1-25.

Carleton, J. N., R. A. Park, and J. S. Clough 2009. Ecosystem Modeling Applied to Nutrient Criteria Development in Rivers. Environmental Management (on-line July 28, 2009).

Park, R. A., J. S. Clough, M. C. Wellman, and A. S. Donigian. 2005. Nutrient Criteria Development with a Linked Modeling System: Calibration of AQUATOX Across a Nutrient Gradient. *TMDL 2005*. Water Environment Federation, Alexandria, Virginia, pp. 885-902.

Rashleigh, B., M.C. Barber, and D.M. Walters. 2005. Foodweb modeling for PCBs in the Twelvemile Creek Arm of Lake Hartwell. Pages 301-304 *in*: K.J. Hatcher (Ed.), Proceedings of the Georgia Water Resources Conference, April 25-27, Athens, Georgia.

Rashleigh, B. 2007. Assessment of lake ecosystem response to toxic events with the AQUATOX model. Pages 293–299 in: I.E. Gonenc, V.

Koutitonsky, B. Rashleigh, R. A. Ambrose, and J. P. Wolfin (eds) 2007. *Assessment of the fates and effects of toxic agents on water resources.* Springer, Dordrecht, The Netherlands.

Sourisseau, S., A. Basseres, F. Perie, and T. Caquet, 2008. Calibration, validation and sensitivity analysis of an ecosystem model applied to artificial streams. *Water Research* 42:1167-1181.

Park, R. A., J. S. Clough, and M. C. Wellman. 2008. AQUATOX: Modeling environmental fate and ecological effects in aquatic ecosystems. *Ecological Modelling* 213: 1-15 (24 April 2008)

Lei, B., S. Huang, M. Qiao, T. Li, and Z. Wang. 2008. Prediction of the environmental fate and aquatic ecological impact of nitrobenzene in the Songhuajiang River using the modified AQUATOX model. *Journal of Environmental Sciences 20: 1-9.*

Comparison of Dynamic Risk Assessment Models

State Variables & Processes	AQUATOX	CATS	CASM	Qual2K	WASP7	EFDC-HEM3D	QEAFdChn	BASS	QSim
Nutrients	X	X	X	X	X	X			X
Sediment Diagenesis	X			X	X	X			
Detritus	X	X	X	X	X	X			X
Dissolved Oxygen	X		X	X	X	X			X
DO Effects on Biota	X								X
pH	X			X					X
NH4 Toxicity	X								
Sand/Silt/Clay	X				X	X			
SABS Effects	X								
Hydraulics						X			X
Heat Budget				X	X	X			X
Salinity	X				X	X			
Phytoplankton	X	X	X	X	X	X			X
Periphyton	X	X	X	X	X				X
Macrophytes	X	X	X						X
Zooplankton	X	X	X						X
Zoobenthos	X	X	X						X
Fish	X	X	X					X	X
Bacteria			X						X
Pathogens				X		X			
Organic Toxicant Fate	X	X			X			X	
Organic Toxicants in:									
Sediments	X	X			X	X			
Stratified Sediments	X				X	X			
Phytoplankton	X	X							
Periphyton	X	X							
Macrophytes	X	X							
Zooplankton	X	X					X		
Zoobenthos	X	X					X		
Fish	X	X					X	X	
Birds or other animals	X	X							
Ecotoxicity	X	X	X					X	
Linked Segments	X			X	X	X	X		X

AQUATOX has a very complete coverage of plants and animals with the capability to model Diatoms, Greens, Cyanobaceria, 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.

Park, R. A., J. S. Clough, and M. C. Wellman. 2008. AQUATOX: Modeling environmental fate and ecological effects in aquatic ecosystems. *Ecological Modelling* 213: 1-15 (24 April 2008)

Comparison of Bioaccumulation Models: Biotic State Variables

Table 3.2. Comparison of Bioaccumulation State Variables

BIOTIC 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
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. 2005

Imhoff, J. C. et al. (2005). “Comparison of Chemical Bioaccumulation Models to Assist in Model Selection for Ecological Assessments and TMDL Development.” *Managing Watersheds for Human and Natural Impacts*, Williamsburg, Virginia, USA, 126-126.

What AQUATOX does *not* do

- It does not model fate of metals
  - **Hg was attempted, but unsuccessful**
- It does not model bacteria or pathogens
  - **microbial processes are implicit in decomposition**
- It does not model temperature regime and hydrodynamics
  - **temperature is a driving variable**
  - **easily linked with hydrodynamic model**

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.

The toxic effects of metals could be examined, but not the environmental fate; this has been done on at least one reservoir in Florida, where the effects of copper sulfate were examined.

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. However, the Di Toro sediment diagenesis model is available as an option in Release 3, though it does require additional parameters.

Di Toro, D. M. 2001. Sediment Flux Modeling. Wiley-Interscience, New York.

Model has been used with flow field simulated by EFDC.

AQUATOX Structure

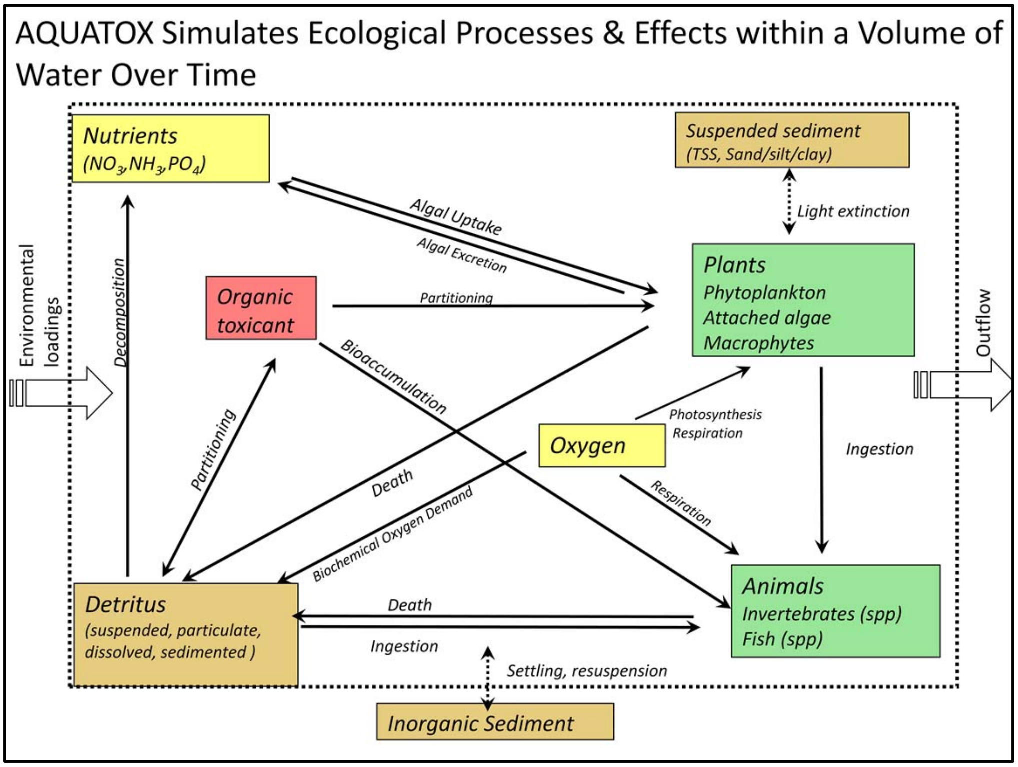
- Time-variable
  - variable-step 4th-5th order Runge-Kutta
    - usually daily reporting time step
    - can use hourly time-step and reporting
    - fixed-step-size option also available
- Spatially simple unless linked to hydrodynamic model
  - thermal stratification
  - salinity stratification (based on salt balance)
- Modular and flexible
  - written in object-oriented Pascal (Delphi)
  - model only what is necessary (flask to river)
  - multi-threaded, multiple document interface
- 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 several years. The results are integrated over the specified time period.

Stratification with two layers can be modeled based on temperature differences or specified dates.

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.



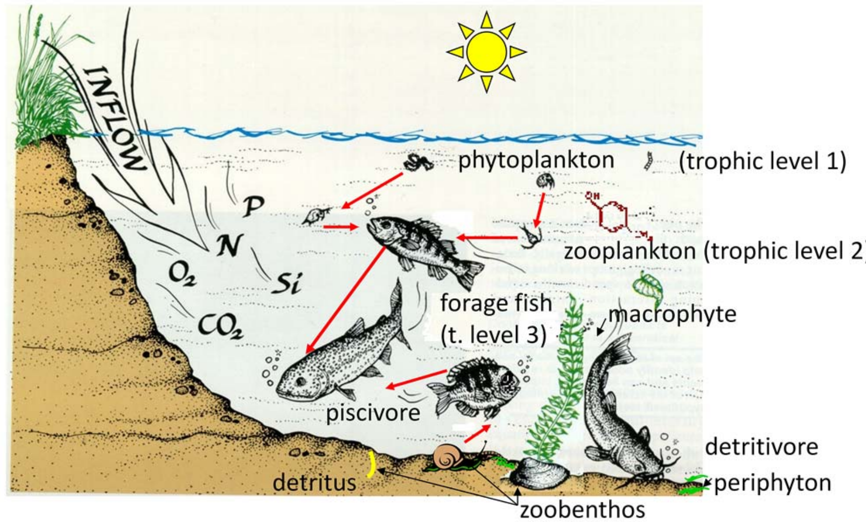
This is a simplified flow chart of the physical, chemical and biological processes simulated by AQUATOX.

Processes Simulated

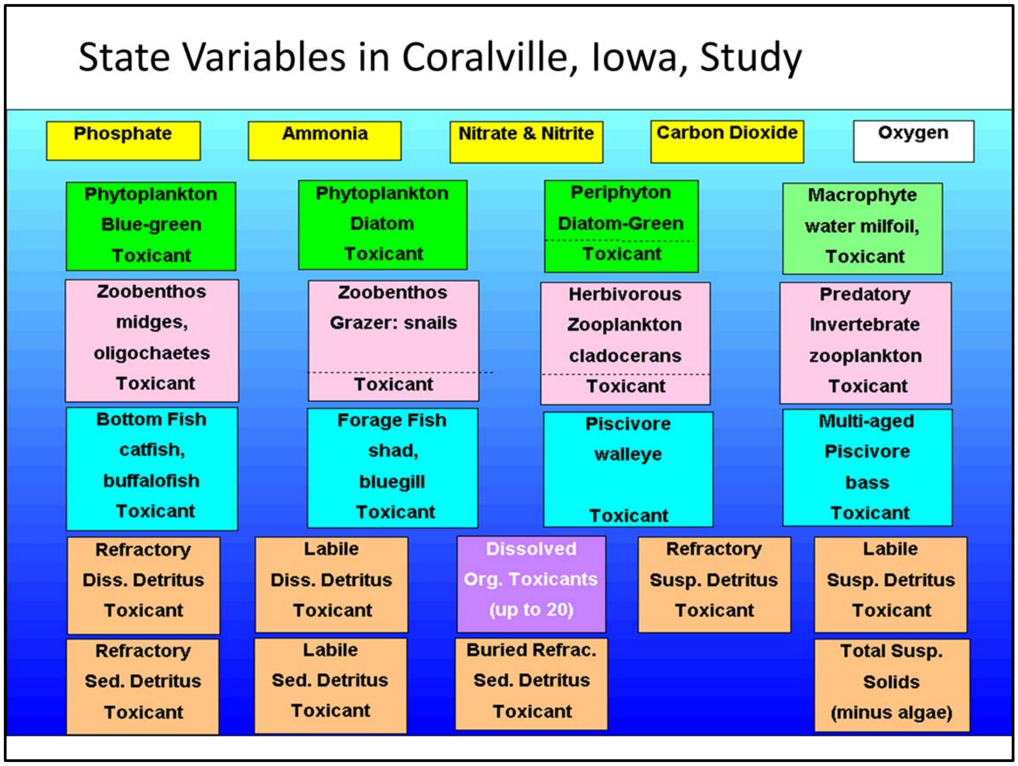
- **Bioenergetics**
  - **feeding, assimilation**
  - **growth, promotion, emergence**
  - **reproduction**
  - **mortality**
  - **trophic relations**
  - **toxicity (acute & chronic)**
- **Environmental fate**
  - **nutrient cycling**
  - **oxygen dynamics**
  - **partitioning to water, biota & sediments**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

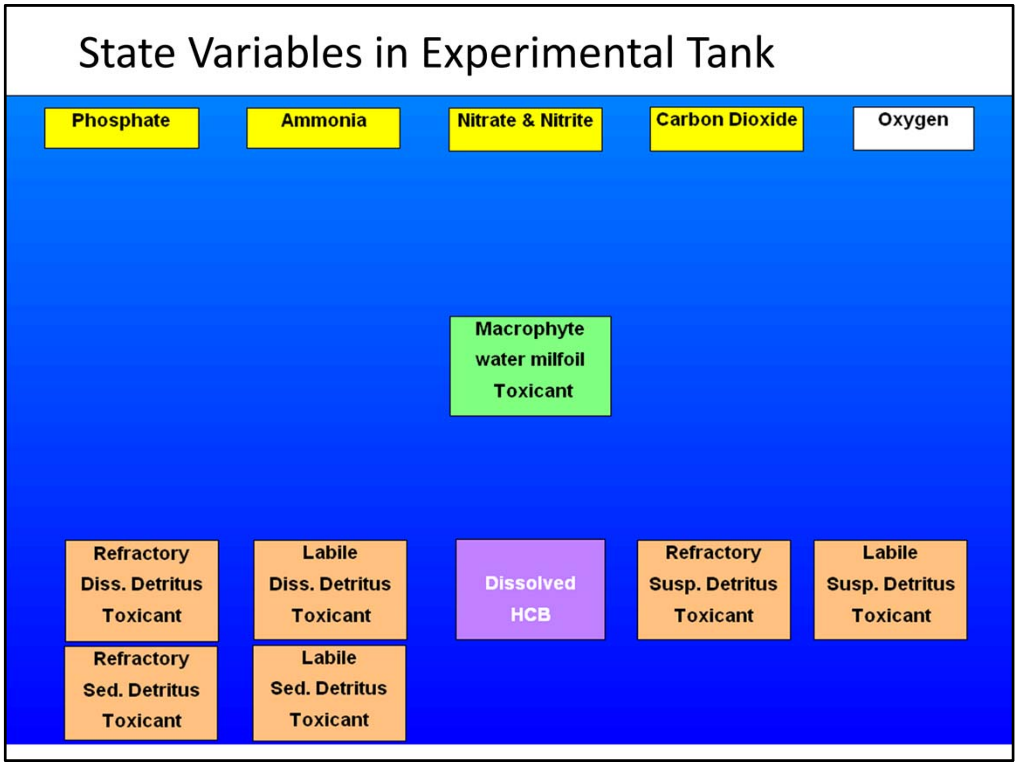


The ecosystem consists of abiotic and biotic components. Phytoplankton, periphyton, and macrophytes are the primary producers, fixing organic matter from nutrients and sunlight. As such they are the first trophic level. Zooplankton and many zoobenthos are primarily herbivores, thus they are the second 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 simulating 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

It has been our design philosophy to make AQUATOX as general as possible, with parameters that are “global”, i.e., that do not change from site to site. For example, the maximum photosynthesis rate of an algal species should be intrinsic to the group, although the actual photosynthesis rate will be affected by site-specific environmental conditions. Site conditions will obviously be different, and require input.

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, tributary inputs
- Multiple sediment layers with pore waters
- Sediment Diagenesis Model
- Diel oxygen and low oxygen effects, ammonia toxicity
- Interspecies Correlation Estimation (ICE) toxicity database
- Variable stoichiometry, nutrient mass balance, TN & TP
- Dynamic pH
- Biota represented by guilds, key species
- Constant or variable loads
- Latin hypercube uncertainty, nominal range sensitivity analysis
- Wizard & help files, multiple windows, task bar
- Links to HSPF and SWAT in BASINS

Because you may have been using an earlier version of the model, it is instructive to highlight the capabilities of successive versions.

• Release 1 from 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 April 2004.

• Release 2.1, issued in October, 2005, and Release 2.2 in October 2006 improved eutrophication analysis.

• Release 3 is a much more powerful version, which can model linked segments, layered sediments, and estuaries. It underwent a very favorable peer review and was issued on the EPA web site in August 2009.

http://water.epa.gov/scitech/datait/models/aquatox/index.cfm

Recent enhancements to BASINS 4 will necessitate modifications to the linkage to SWAT; at this time the SWAT linkage works with BASINS 3.1 but not BASINS 4.

Release 3.1

- 64-bit-compatible software installer
- Updated Interspecies Correlation Estimation toxicity regressions
- Improved uncertainty & sensitivity output
- Additional outputs for diagenesis & bioaccumulation
- Improved database export & search capabilities
- More flexible linkage to HSPF watershed model
- Addition of sediment-diagenesis "steady-state" mode to significantly increase model speed
- Modification of denitrification code in goal of simplifying calibration and alignment with other models;
- Enabled importation of equilibrium CO2 concentrations to enable linkage to CO2SYS and similar models;
- New BOD to organic matter conversion relying on percent-refractory detritus input

Download available at EPA AQUATOX page

Additional capabilities are available in Release 3.1 as compared to Release 3, including:

Modifications to PFOS model to be more flexible:

• Elimination rates (K2s) are editable for animals and plants;

• Improved gill-uptake equation for invertebrates;

Bioaccumulation and toxicity modeling improvements:

• Optional alternative elimination-rate estimation for animals based on Barber (2003) ;

• Updated ICE (toxicity regressions) based on new EPA models released in February 2010 and improved AQUATOX ICE interface

Improved sensitivity and uncertainty analyses

• "Output to CSV" option for uncertainty runs so that complete results for every iteration may be examined;

• Allowed for non-random sampling for "statistical sensitivity analyses;"

• For sensitivity analysis, implemented a "reverse tornado" diagram (a.k.a. "effects diagram") that shows the effects of each parameter change on the overall simulation;

Database Improvements

• AQUATOX database search functions dramatically improved.

• "Scientific Name" added to Animal and Plant databases.

Interface and Data Input Improvements

• Software and software installer is 64-bit OS compatible;

- Added an option in the setup screen to trigger nitrogen fixation based on the N to P ratio.
- Addition of output variables to clarify whether photosynthesis is sub-optimal due to high-light or low-light conditions.
- Time varying evaporation option in the "site screen," with linkage from the water volume screen
- Grid mode within a study. In other words, all animal, plant, and chemical parameters in a study can be examined, edited, and exported to Excel simultaneously
- Updated HSPF WDM file linkage to be more generally applicable (doesn't require use of WinHSPF).
- Enabled hourly loadings for the following variables: All nutrients, CO_2, Oxygen, Inorganic suspended sediments (sand/silt/clay), TSS, Light, Organic Matter
- Other minor interface improvements.

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.

What are the Analytical Capabilities?

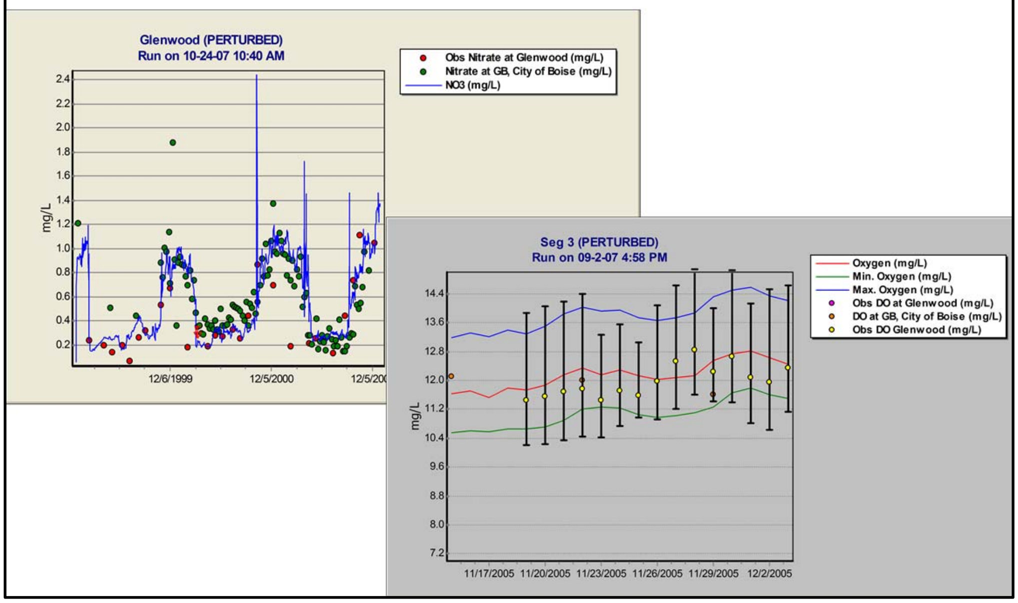
- Graphical Analysis
  - Comparison of model results to Observed Data
  - Graph types and graph libraries
- Control-Perturbed Comparisons
- Process Rates
- Limitations to Photosynthesis
- Sensitivity Analysis
- Uncertainty Analysis

We now switch out of the laboratory and into an overview discussion of the analytical capabilities. Each of these capabilities will be explored in more detail as the course continues; this section is just intended to provide an overview.

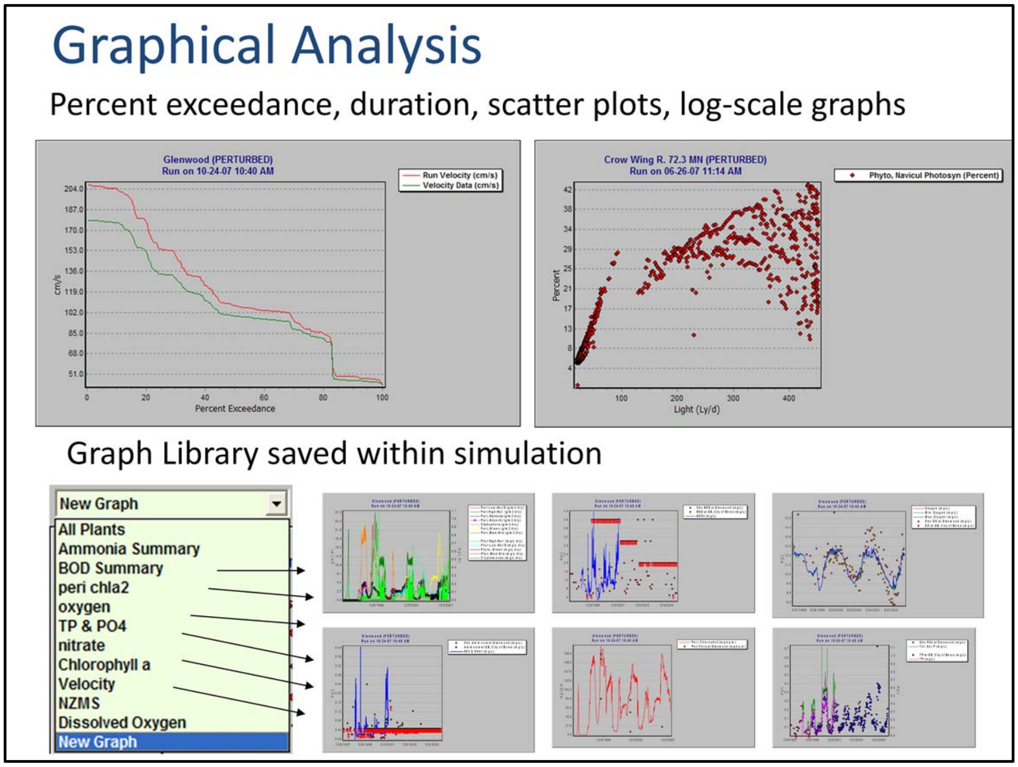
AQUATOX is a very powerful analytical tool that permits the user to elucidate model behavior and explore relationships at different levels of resolution. The transparency of the model constructs and applications support good modeling practice as required by decision makers.

Graphical Analysis

Compare observed data to model output



Observed data, including ranges and non-detects, can be imported and plotted with model output.

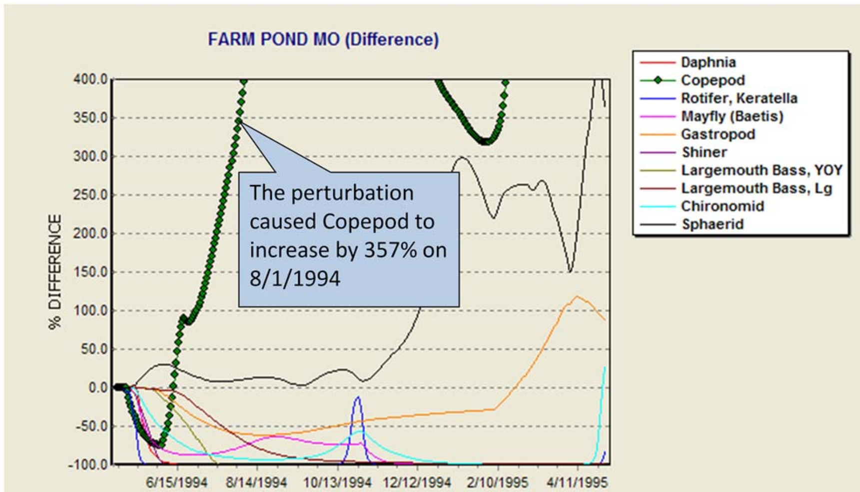


Fully integrated graphical output includes specialized graphs such as percent exceedance and duration graphs desired by decision makers.

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 (in this case, addition of Esfenvalerate) 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 animals in the simulation (graph above). Note that several animals go extinct. Why do you suppose the Copepod does so well given the perturbation?

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 biologically unimportant.

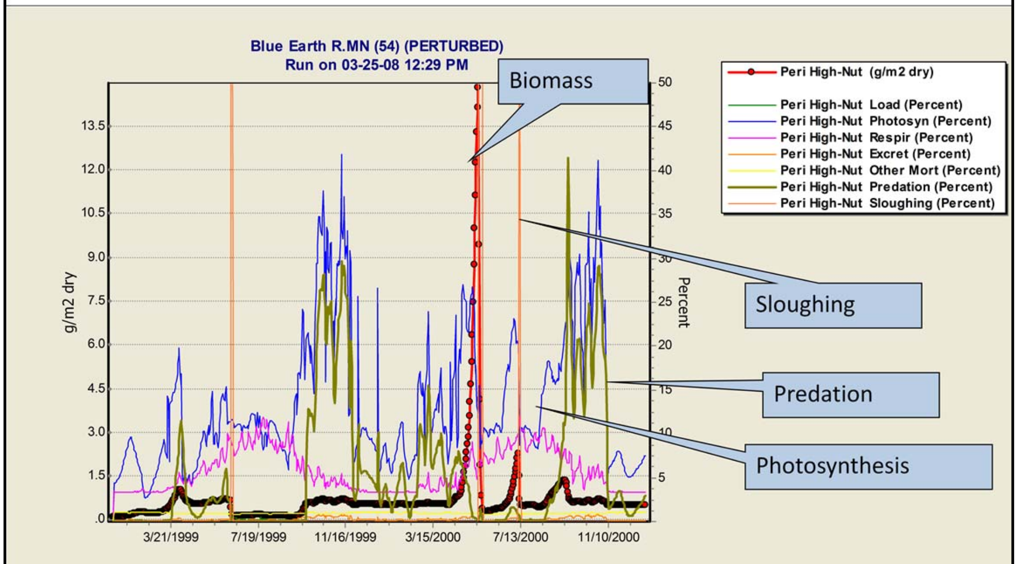
Process Rates

- Concentrations of state variables are solved using differential equations
  - For example, the equation for periphyton concentrations is:

$$\frac{dBiomass_{Peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion$$
$$- Mortality - Predation + Sed_{Peri}$$

- Individual terms of these equations may be saved internally, and graphed to understand the basis for various predictions

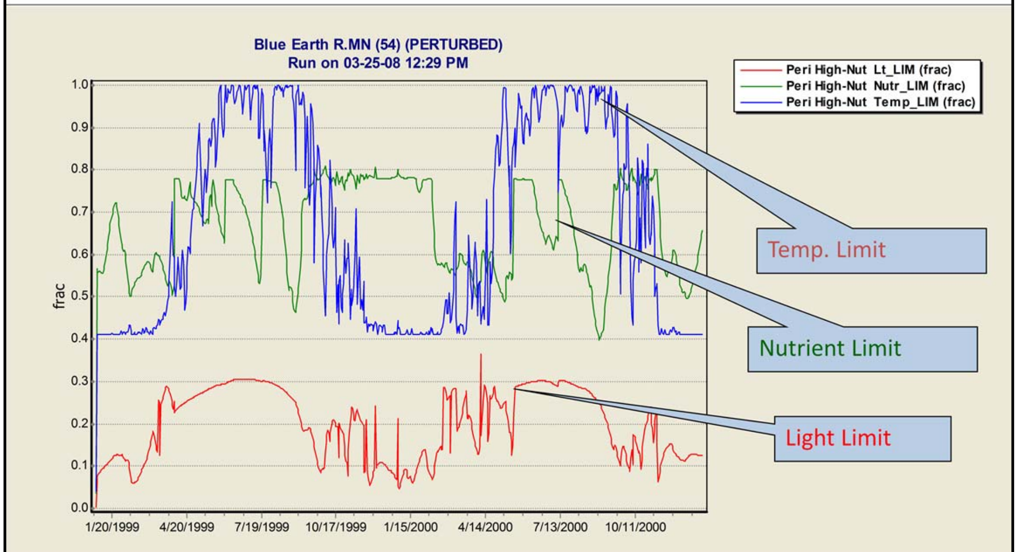
Rates Plot Example: Periphyton



The red line with red circles represents the biomass. The user may wonder why there is such a large bloom of periphyton predicted in the second year. The answer may be ascertained by examining the rates.

The answer is not explained by photosynthesis rates, in blue, which remain cyclical but consistent over the course of the simulation.
The answer is explained by predation (i.e., grazing) which drops down dramatically in the second year.
There are also three sloughing events worth noting in which periphyton is sloughed and transported downstream.

Limitations to Photosynthesis May also be Graphed

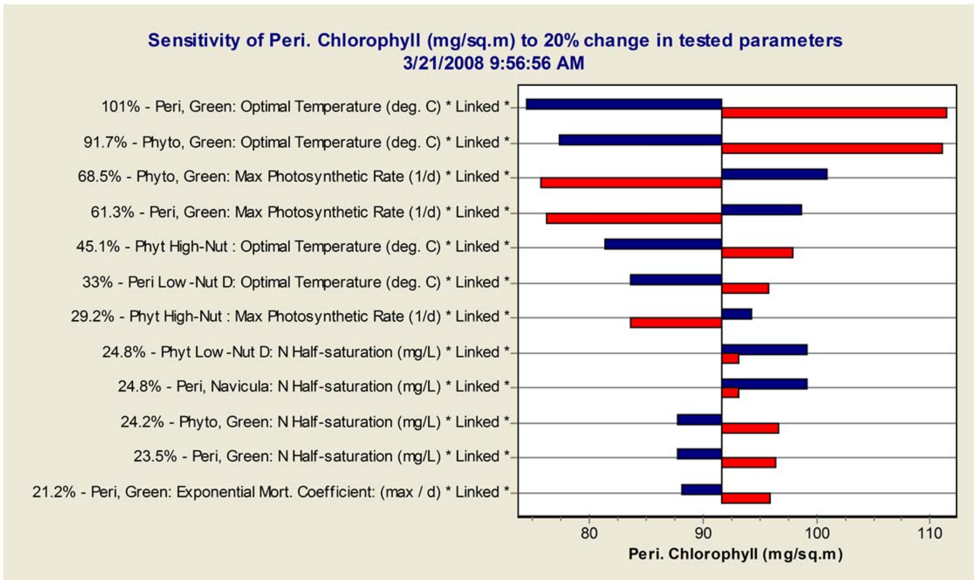


Light limitation means that the plant photosynthesis rate is less than one third of the PMax. The temperature limitation reduces photosynthesis during winter months.

PProdLimit = LtLimit · NutrLimit · Tcorr

A limitation value of 1.0 means that there is no limitation

Integrated Nominal Range Sensitivity Analysis with Graphics

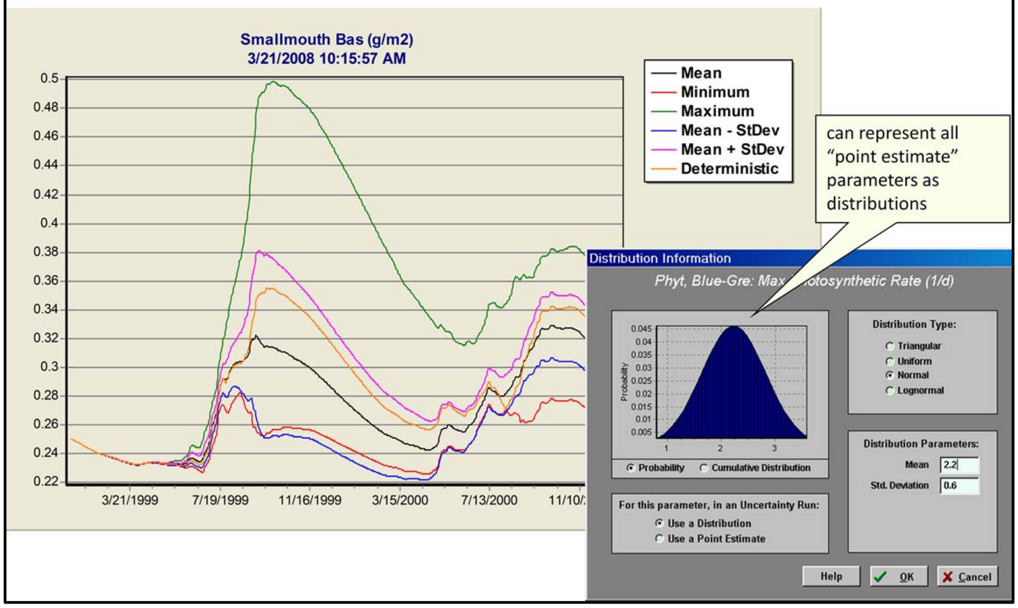


Now we will briefly discuss some of the Sensitivity and Uncertainty graphs that can be generated:

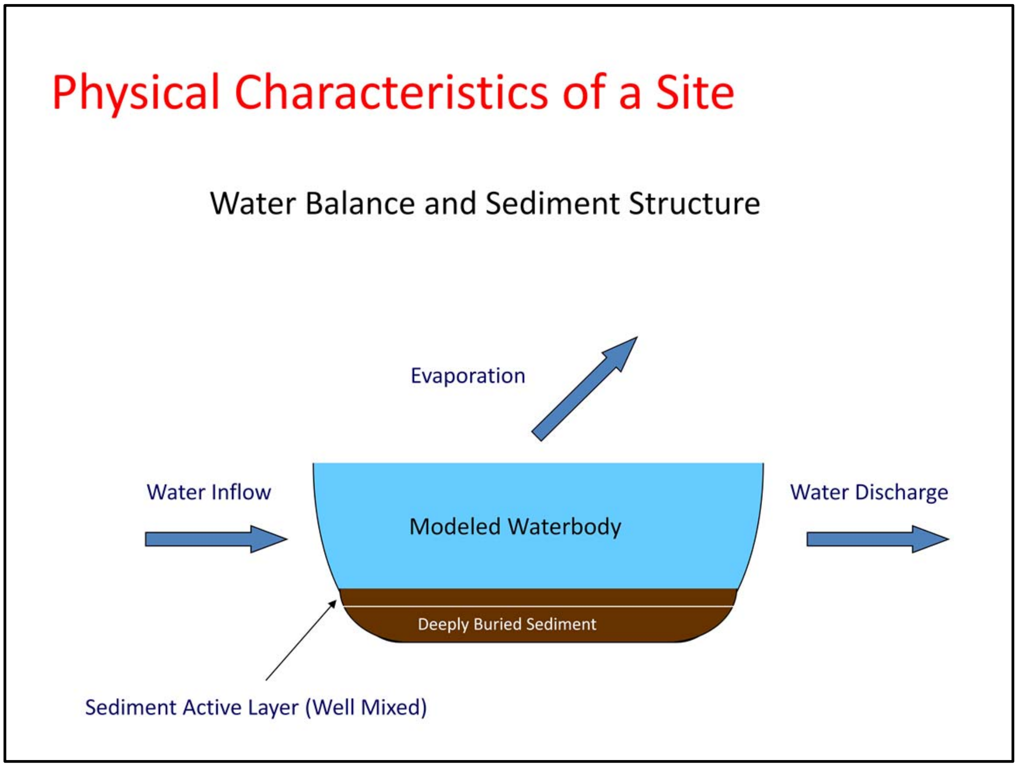
AQUATOX can automate a nominal range sensitivity analysis (also known as a "one-at-a-time" sensitivity analysis), in which multiple parameters are changed by a given percentage. The sensitivity of model output to the different perturbations can then be compared.

The end result is referred to as a “Tornado Diagram.” Tornado diagrams may be produced within the AQUATOX output window. When interpreting a tornado diagram, the vertical line at the middle of the diagram represents the deterministic model result. Red lines represent model results when the given parameter is reduced by the user-input percentage while blue lines represent a positive change in the parameter.

Integrated Latin Hypercube Uncertainty Analysis with Graphics



These model results represent summary statistics for each time-step of the simulation based on the Monte-Carlo analysis. The deterministic line plotted represents a single scenario run with "point estimate" values replacing each distribution. All other lines are statistics derived from all of the scenarios run during the analysis.

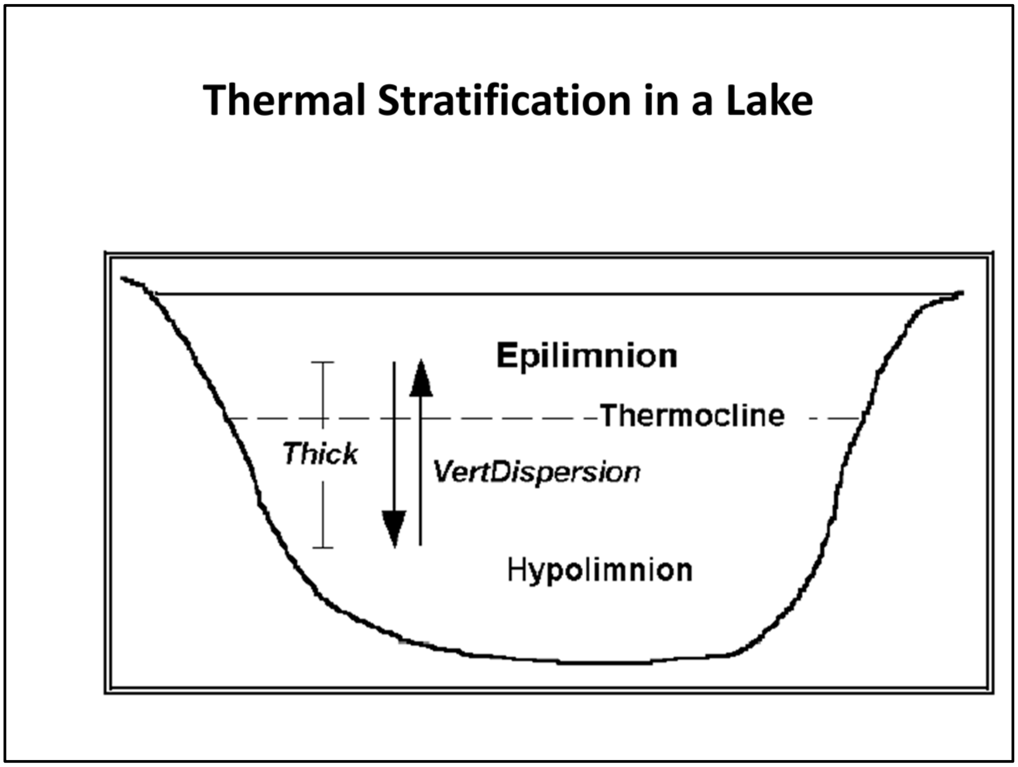


Water balance is defined as a function of inflow, evaporation, and discharge. We will discuss the various mechanisms for modeling water balance in a future slide. The modeled waterbody or river segment is assumed to be well mixed. Evaporation is a function of the site's surface area and the mean annual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

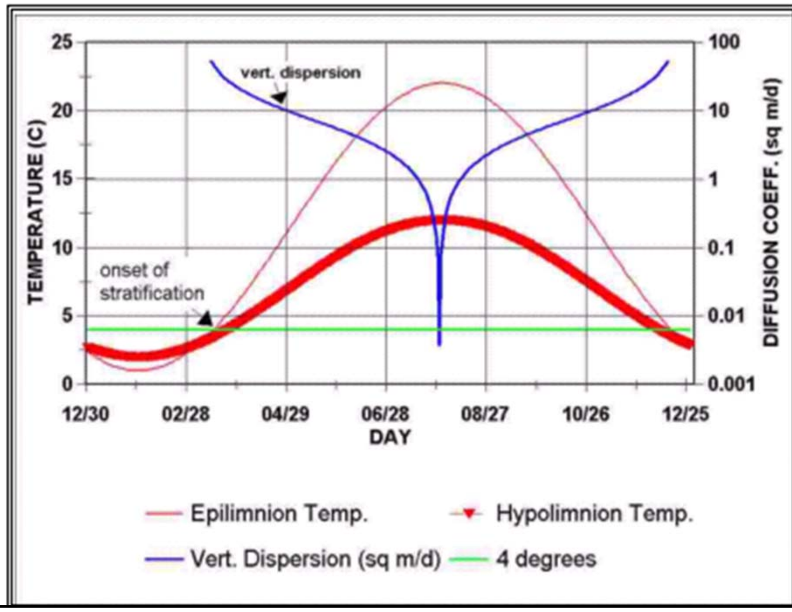
This information covered in Section 3 of the **Technical Documentation**.



Thermal stratification 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).

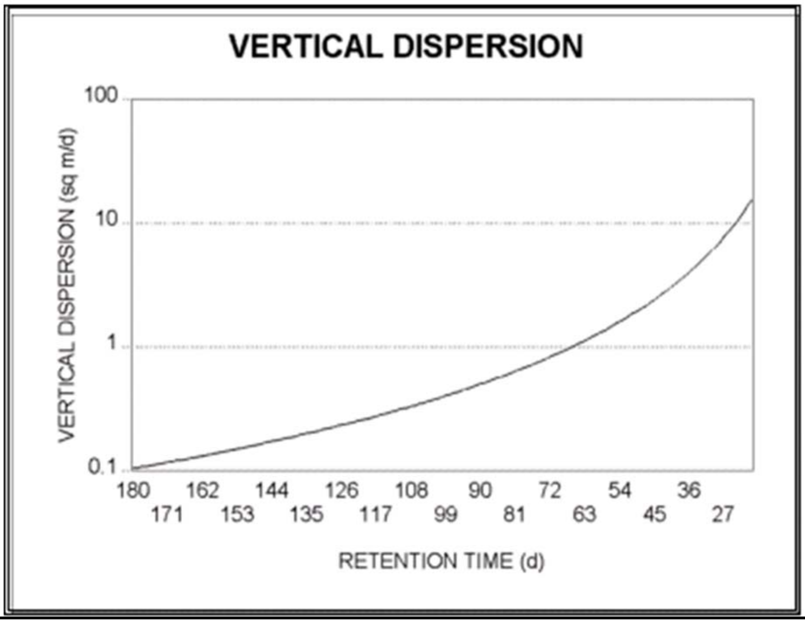
Dividing the lake into two vertical zones follows the treatment of Imboden (1973), Park et al. (1974), and Straškraba and Gnauck (1983). The onset of stratification is considered to occur when the mean water temperature exceeds 4° and the difference in temperature between the epilimnion and hypolimnion 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. However, the user can also specify the date of overturn and stratification and time-varying thermocline depth.

Stratification is a Function of Temperature Differences

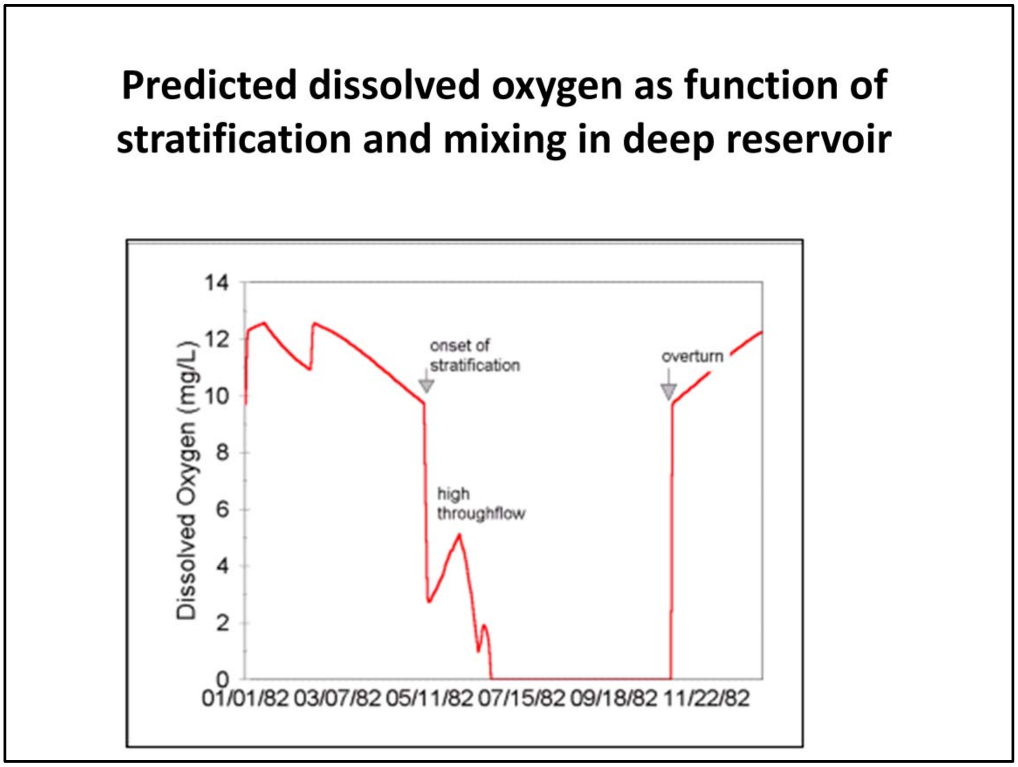


Diffusion between the epilimnion and hypolimnion is a function of the temperature differential. The user specifies the temperatures (or mean and range) for each layer and the model computes when stratification occurs and how much turbulent diffusion occurs.

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.



Anoxia in the bottom waters can occur as a result of decomposition of detritus, as shown in this graph of the hypolimnion.

When anoxia occurs the model assumes that mobile zooplankton and fish migrate to the epilimnion.

Hypoxia can be temporarily reversed by high throughflow from storm runoff.

Reservoir management enhancements

Because reservoirs may be heavily managed, a user may specify:

- a constant or time-varying thermocline depth;
- options as to how to route inflow and outflow water
- the timing of stratification and overturn

Stratification assumptions and equations based on lake characteristics may not be appropriate for modeling reservoirs. Moreover, a lake may have a unique morphometry or chemical composition that renders inappropriate the equations presented previously. For this reason, a "stratification options" screen is available (through the site screen or water-volume screen) that allows a user to specify the characteristics of a stratified system.

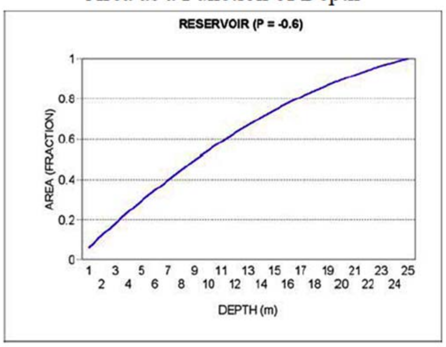
Bathymetric Approximations

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

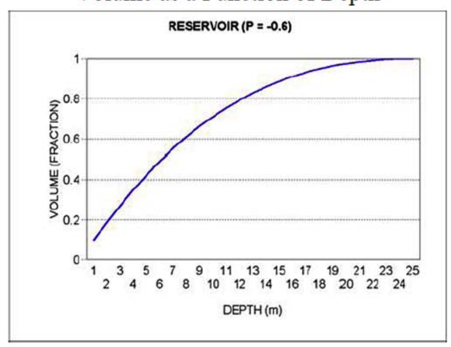
$$P = 6.0 \cdot \frac{ZMean}{ZMax} - 3.0$$

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



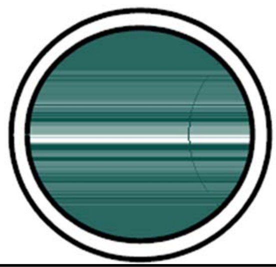
The depth distribution of a water body is important because it determines the areas and volumes subject to mixing and light penetration. The shapes of ponds, lakes, reservoirs, and streams are represented in the model by idealized geometrical approximations, following the topological treatment of Junge (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.

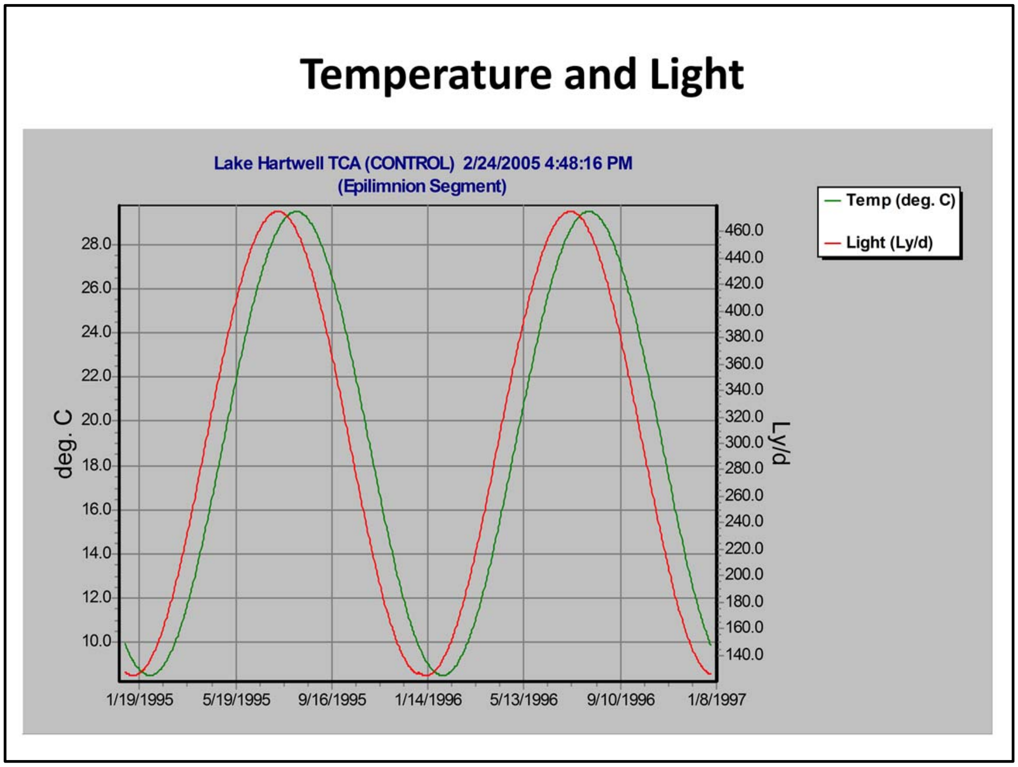
Littoral Fraction

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:

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

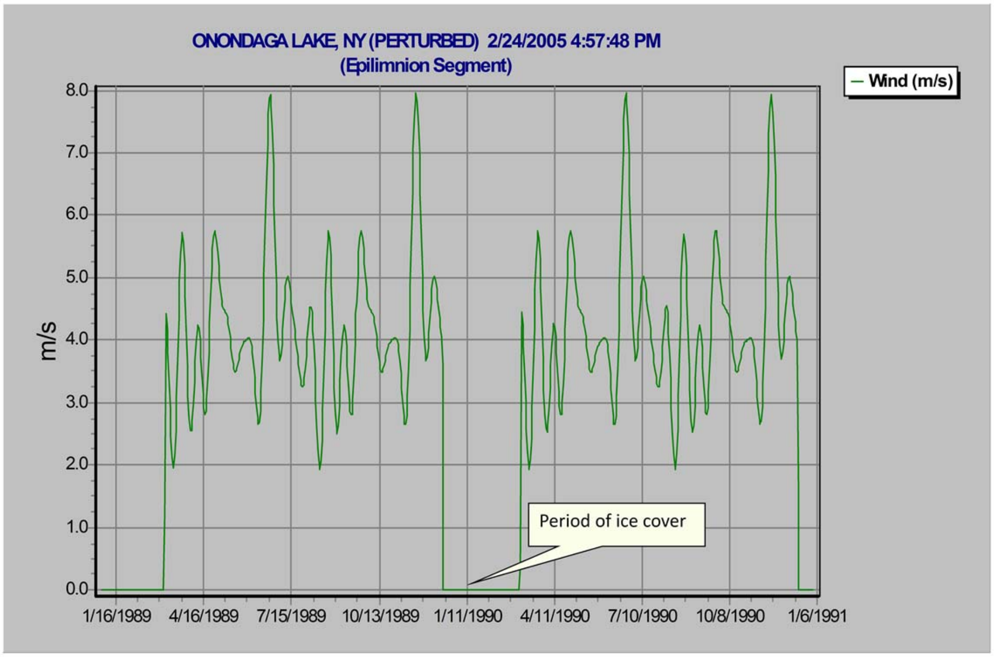
A relatively deep, flat-bottomed basin would have a small littoral area and a large sublittoral area:





Water temperature and incoming light are two very important driving variables in AQUATOX, affecting numerous chemical, physical and biological rates.
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. If site data is not available, a default loading is provided which is based on an annual cycle of data taken from the Buffalo, NY airport. Therefore, it has a 365-day repeat, representative of seasonal variations in wind 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.

Modeling Plants with AQUATOX

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

See Chapter 4 of the Technical Documentation.

Plant Derivatives

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

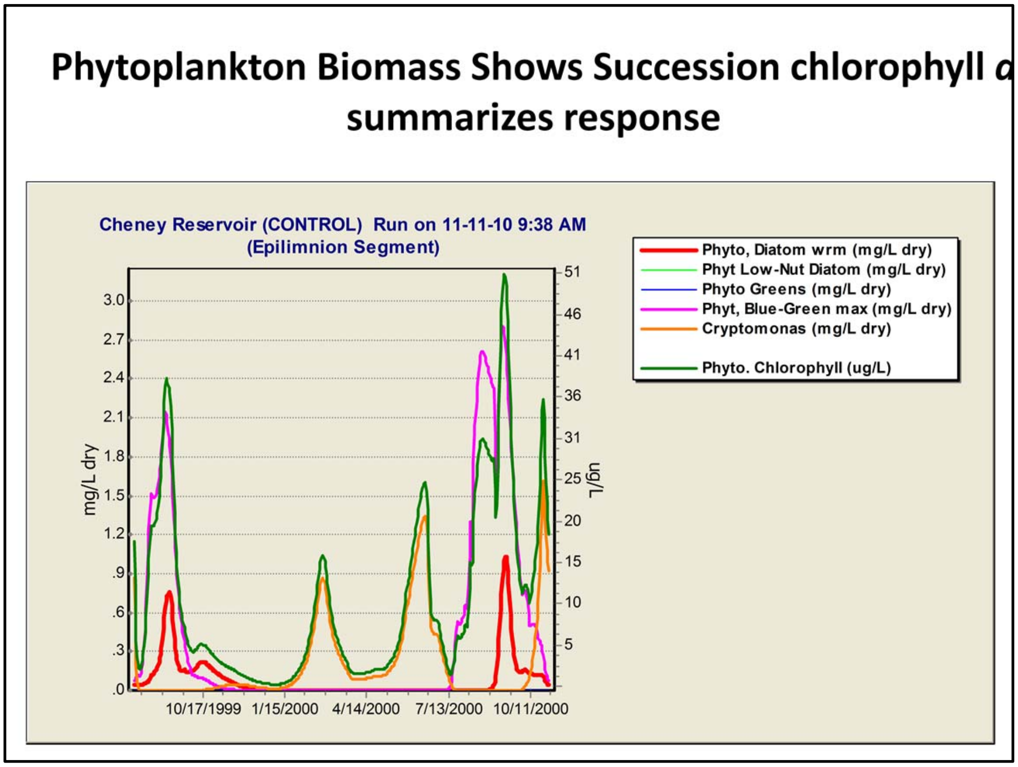
$$\frac{dBiomass_{peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation - \underbrace{Slough}_{\text{bottom dwelling}}$$

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:

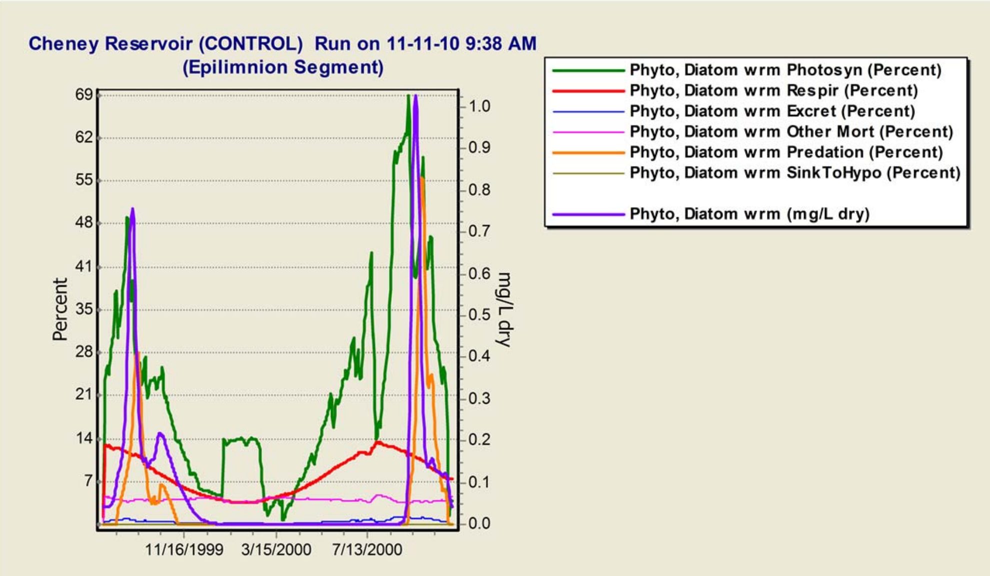
Rate *(fraction/day)* **= Rate** *(mass/day)* **/ State** *(mass)*

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



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

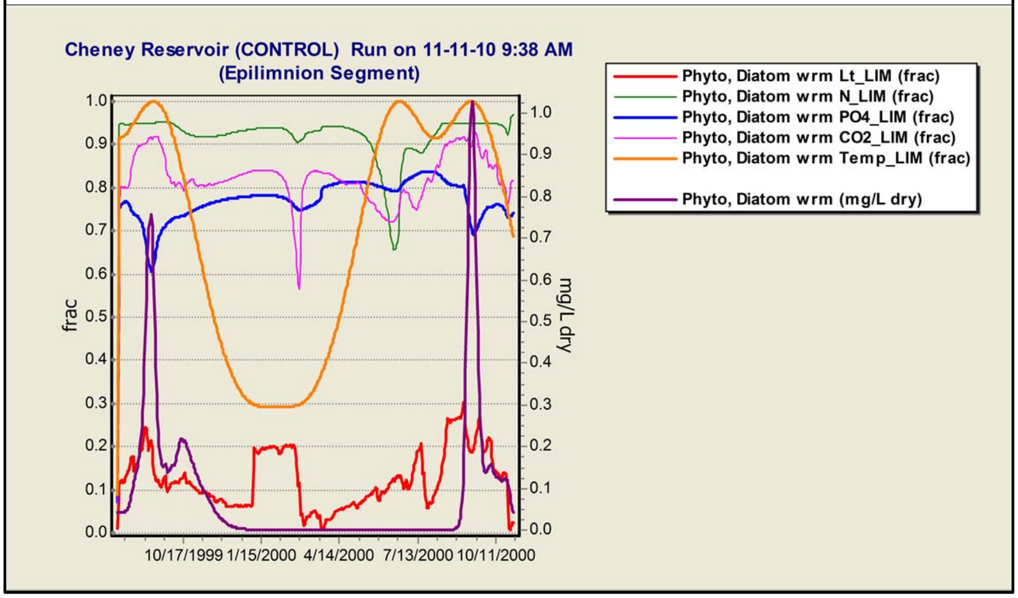
Rates can be saved and plotted for all processes



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.

The rates are expressed as percent of biomass (or concentration) at each time. These and the limitation plots that follow were created in AQUATOX.

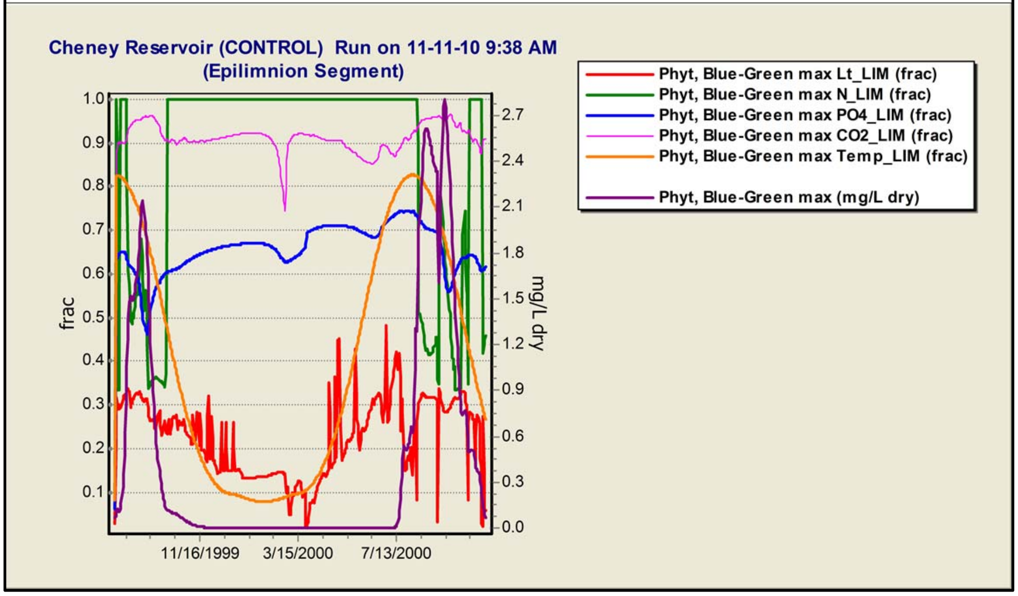
Time-varying limitations to photosynthesis also can be analyzed



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 cyanobaceria 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 cyanobaceria 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.

When nitrogen is highly limiting, nitrogen-fixation is assumed to occur in the cyanobaceria, removing the limitation in the simulation.

Calibration of Plants

- algae are differentiated on basis of:
  - nutrient half-saturation values
  - light saturation values
  - maximum photosynthesis
- Minnesota stream project has developed new parameter sets that span nutrient, light, and Pmax
  - See AQUATOX Technical Note 1: *A Calibrated Parameter Set for Simulation of Algae in Shallow Rivers*
- phytoplankton sedimentation rates differ between running and standing water
- critical force for periphyton scour and TOpt may need to calibrated for other sites

Tech Note URL:
http://www.epa.gov/waterscience/models/aquatox/download.html#technotes

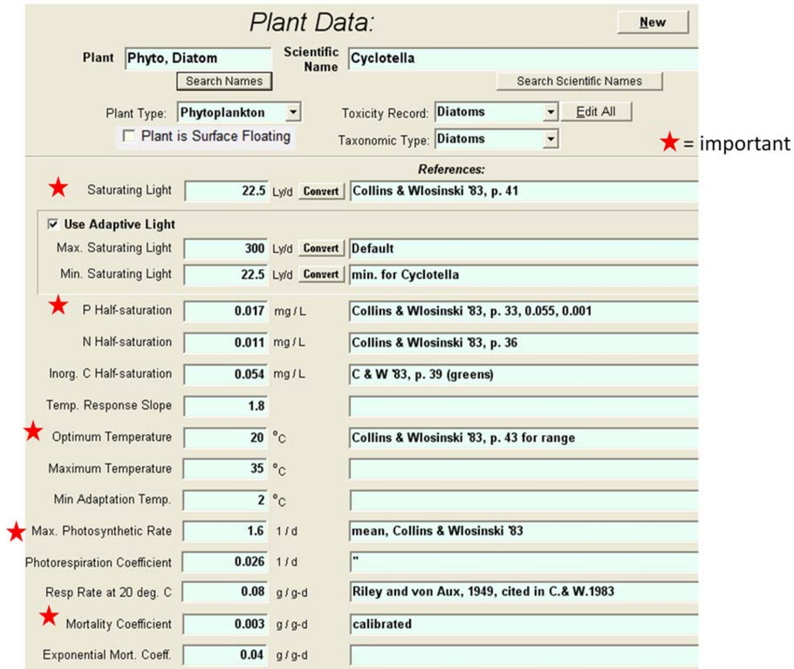
Global vs. Site-Specific Plant Parameters

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.

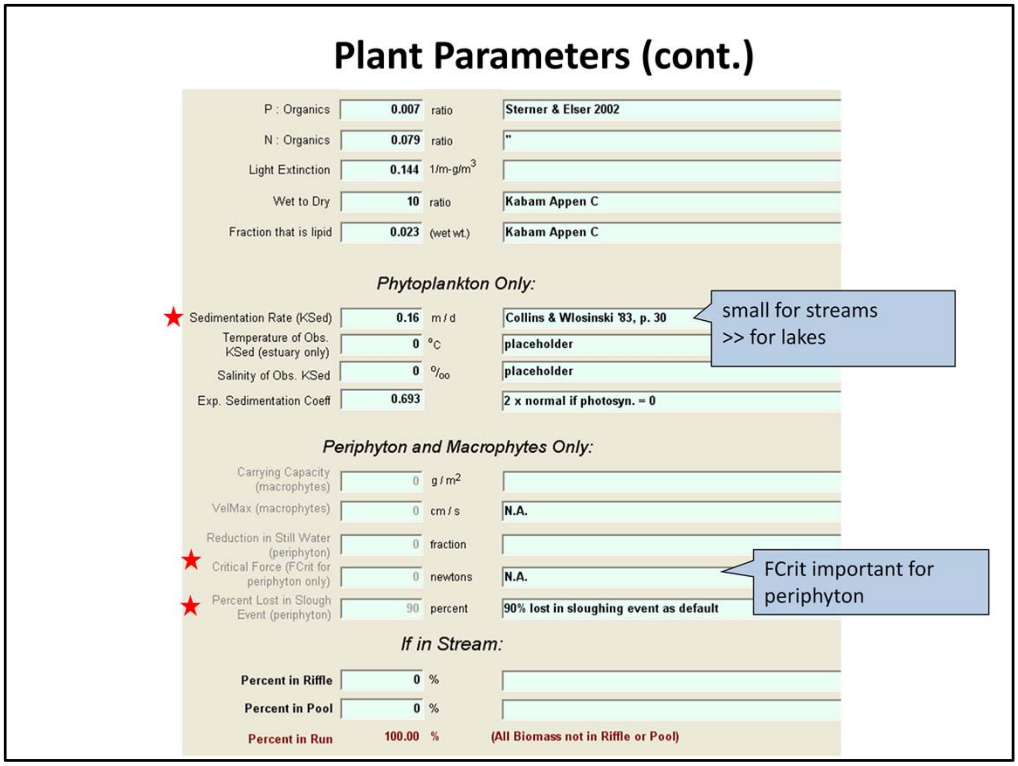
- Critical Force for Periphyton -- reflects site's substrate
- Carrying Capacity for Macrophytes -- reflects habitat
- Optimum Temperature -- reflects cold-/warm-water species
- Mortality Coefficients -- reflect quality of habitat

Plant Parameters



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.

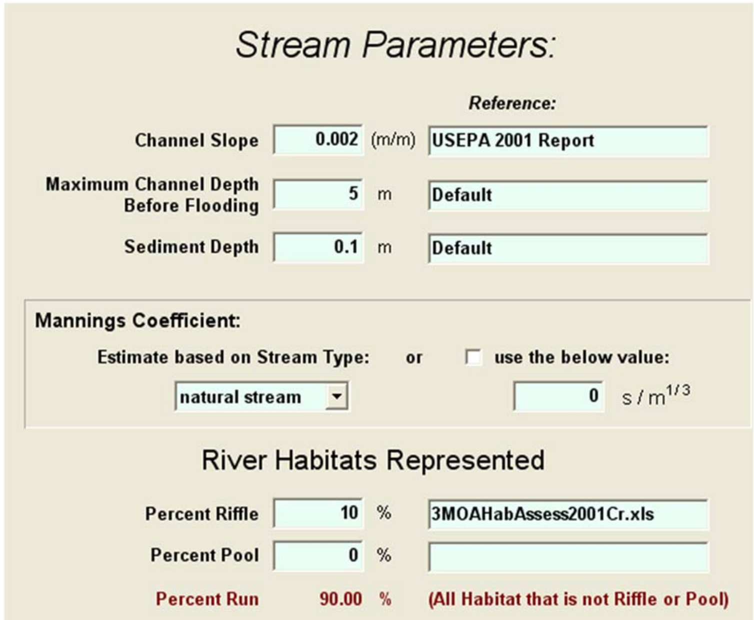
As an introduction to modeling plants, we will go fairly quickly through these parameters and will focus on the most important parameters for calibration.



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.

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.

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.

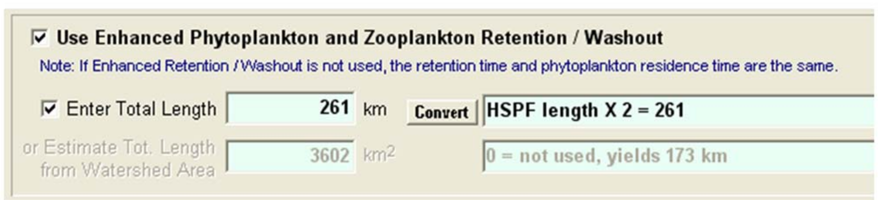
Difference Between Library Parameters and "Underlying Data"

- 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, cyanobacteria (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 Cyanobacteria/Surface-Floating Plants

- Phytoplankton may be specified as "surface floating"
  - assumed to be located in the top 0.1 m
  - if limited by lack of nutrients or sufficient wind occurs they are assumed located within the top 3 m
- The averaging depth for "surface floating" plants is 3 m to correspond to monitoring data.
- Cyanobacteria are assumed to be "surface floating"
- Cyanobacteria are not severely limited by nitrogen due to facultative nitrogen fixation (if N less than ½ KN)

Phytoplankton not specified as "surface floating" are assumed to be mixed throughout the well mixed layer, although subject to sinking. However, healthy cyanobacteria (and some other algal species) tend to float. Therefore, if the phytoplankton is specified as "surface floating" and the nutrient limitation is greater than 0.25 and the wind is less than 3 m/s then *DepthBottom* for surface floating algae is set to 0.1 m to account for buoyancy. Otherwise it is set to 3 m to represent downward transport by Langmuir circulation.

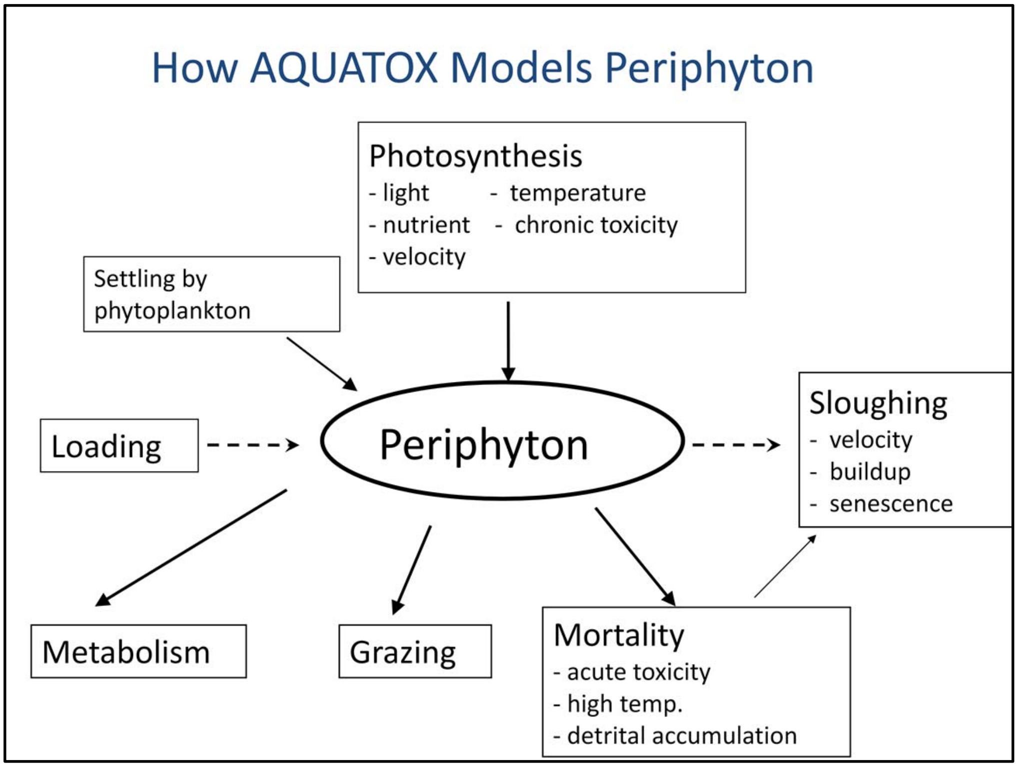
When calculating self-shading for surface-floating algae the model accounts for more intense self shading in the upper layer of the water column due to the floating concentration of algae there.

Rather than average the biomass of "surface floating" plants over the entire water column, the biomass is normalized to the top 3 m to more closely correspond with monitoring data.

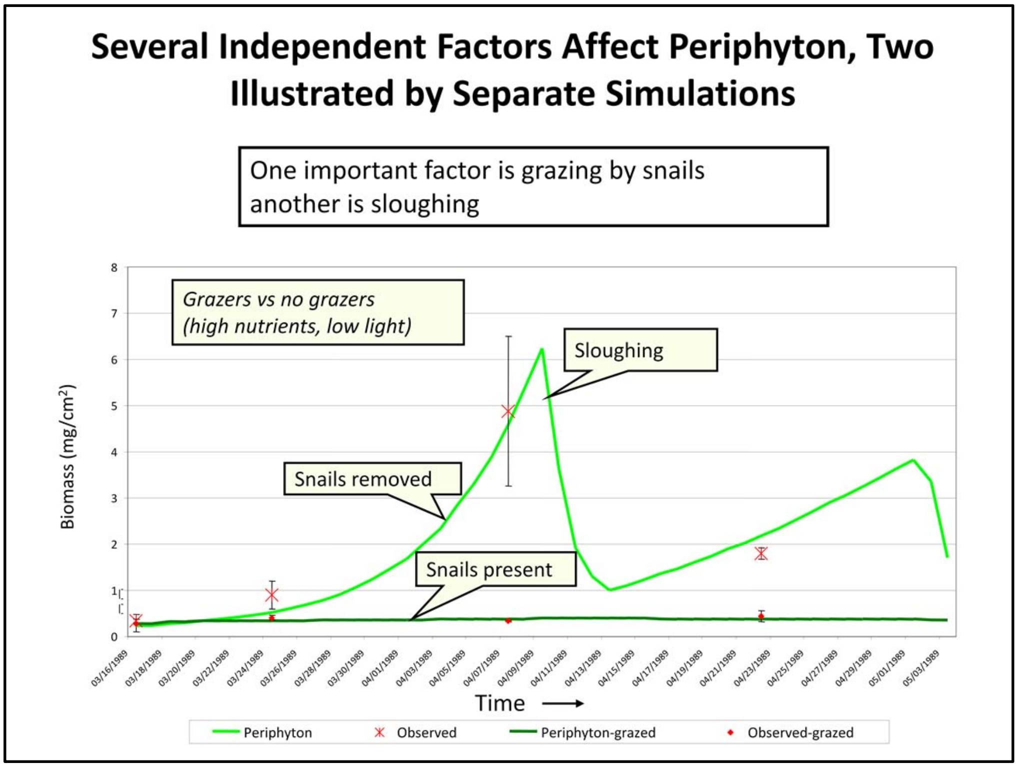
Modeling Periphyton

- 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

Periphyton are benthic algae and associated organic detritus that are attached to hard substrates and macrophytes and that carpet stabilized sands. They are an important constituent of the aquatic community, especially in shallow lakes, ponds, streams, and rivers. They also are an important link for bioaccumulation of organic contaminants. Periphyton have been shown to be sensitive to eutrophication of streams. Although they are nominally included in several ecosystem models, they have been difficult to model. AQUATOX includes processes such as grazing and sloughing that have been shown to be important but are ignored in some other models.



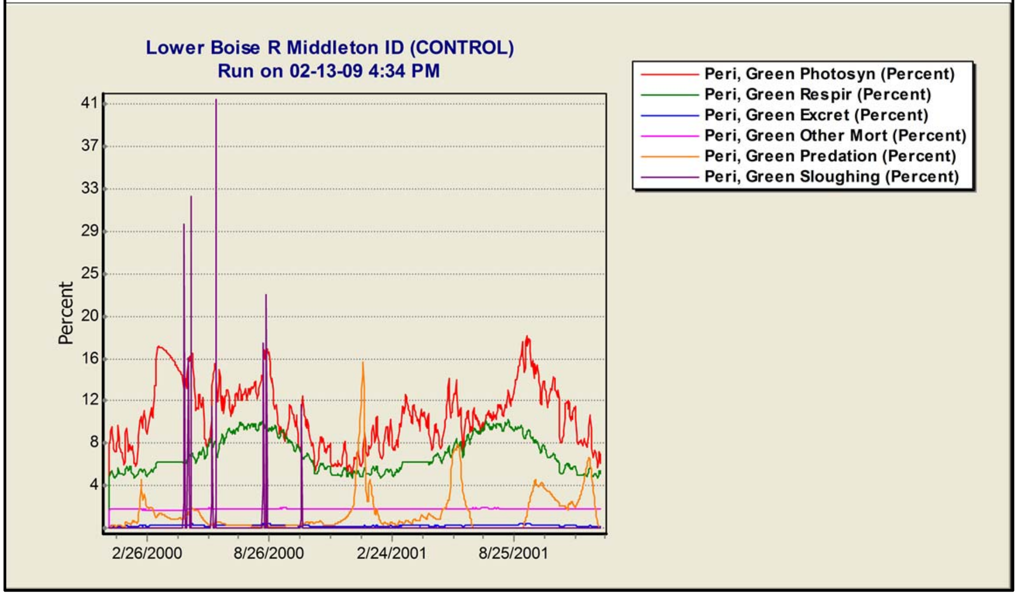
Note that periphyton and phytoplankton are linked, to better reflect reality, and to better correspond to monitoring data. This affects the chlorophyll *a* observed in the water column during a periphyton sloughing event. (This will be discussed in greater detail during Laboratory #3.)



This graph was 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. Two simulations illustrate the importance of grazing and sloughing.

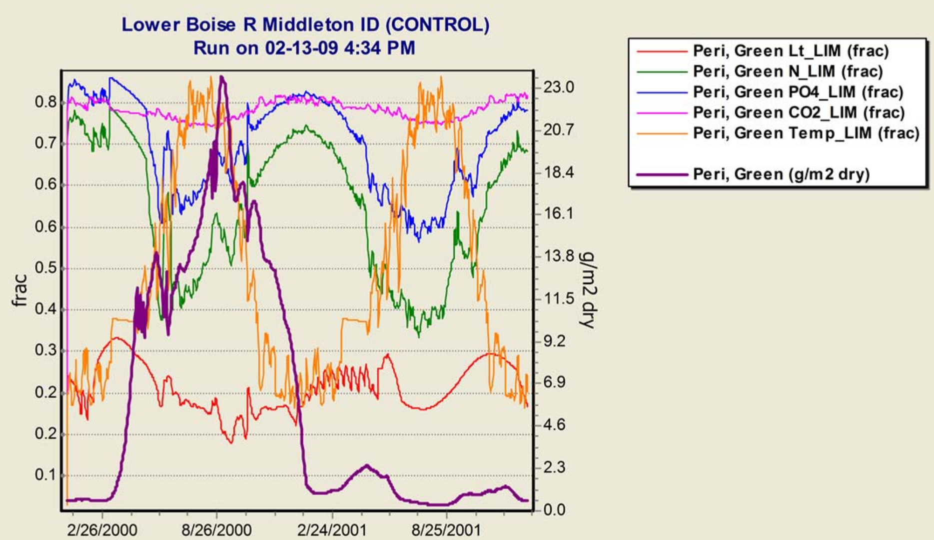
Rosemond, A. D. 1993. Seasonality and Control of Stream Periphyton: Effects of Nutrients, Light, and Herbivores. Pages 185. Vanderbilt University, Nashville, Tenn.

Sporadic Sloughing and Intense Grazing Characterize Periphyton



By plotting the rates we can see that in this simulation of Lower Boise River ID photosynthesis is offset by respiration and sporadic grazing and sloughing.

Nutrient limitation & self-shading are important, followed by winter temperature



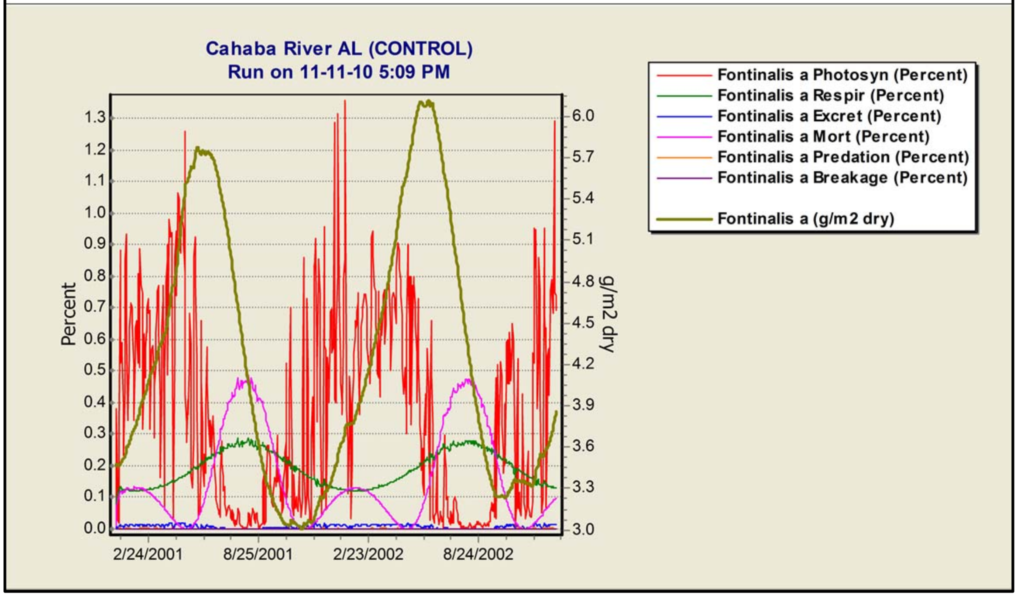
Limitations to photosynthesis are highly site-specific and vary during the year. This simulation is unusual in that nitrogen limitation is indicated. Light limitation is affected by the periphyton bloom; limitation in the second year is due to biomass of other periphytic groups. Low winter temperatures contribute to the decline of this warm-adapted periphyton.

Modeling Macrophytes

- Macrophytes may be specified as benthic, rooted-floating, or free-floating
- Macrophytes 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
- Leaves can provide significant surface area for periphyton growth
- Moss are a special category

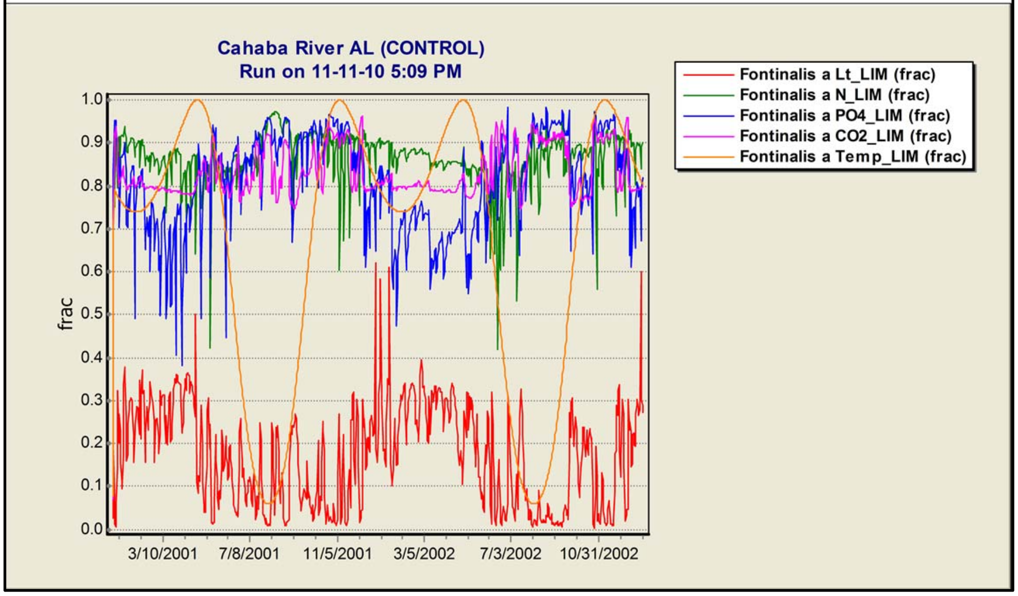
Submersed aquatic vegetation or macrophytes can be an important component of shallow aquatic ecosystems. It is not unusual for the majority of the biomass in a shallow ecosystem to be in the form of macrophytes during the growing season. Seasonal macrophyte growth, death, and decomposition can affect nutrient cycling, and detritus and oxygen concentrations. By forming dense cover, they can modify habitat and provide protection from predation for invertebrates and smaller fish; this function is represented in AQUATOX.

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, and when they die back in the summer or are scoured by storm events the detritus breaks down slowly. They are somewhat sensitive to nutrient 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; light limitation decreases when attached periphyton slough off. As parameterized, they are adapted to cold temperatures and exhibit summer die-back.

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.

Modeling Animals with AQUATOX

- Overview
- Equations
- Parameters
- Zooplankton
- Zoobenthos
- Fish
- Trophic Interaction Matrices

Animal Modeling Overview

- Animal biomasses calculated dynamically
  - **Gains** due to consumption and boundary-condition loadings
  - **Losses** due to defecation, respiration, excretion, mortality, predation, boundary condition losses
- Careful specification of feeding preferences required
- Allometric (weight) modeling for fish

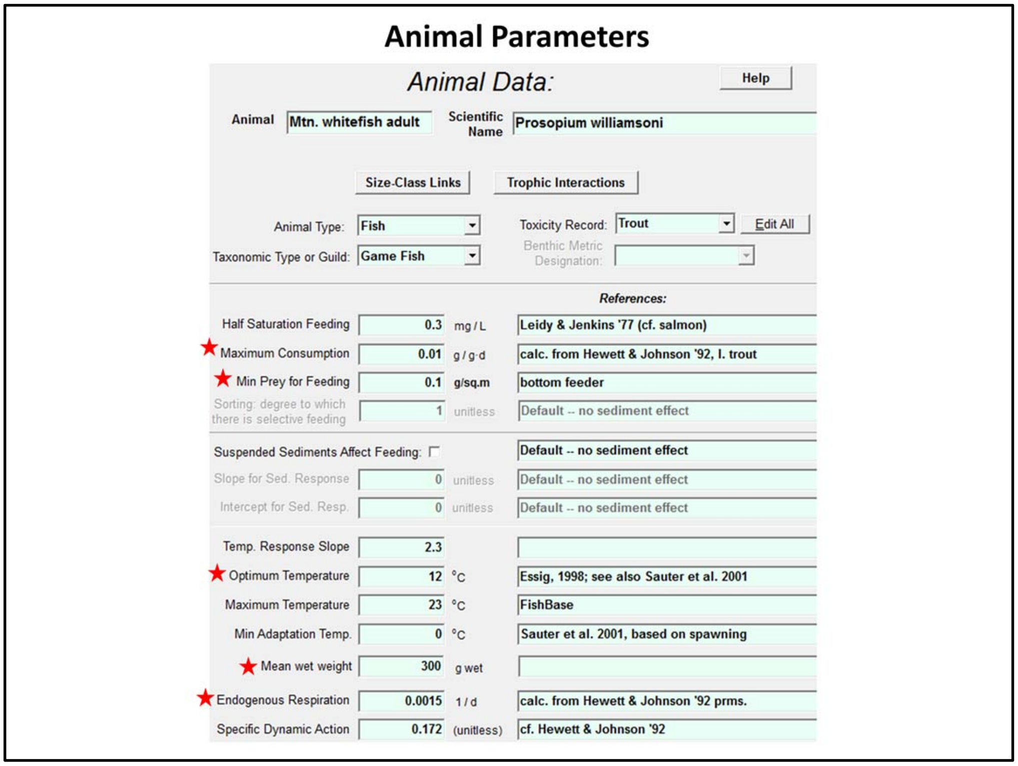
Zooplankton, benthic invertebrates, benthic insects, and fish are modeled, with only slight differences in formulations, with a generalized animal submodel that is parameterized to represent different groups.

Animal Derivatives

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

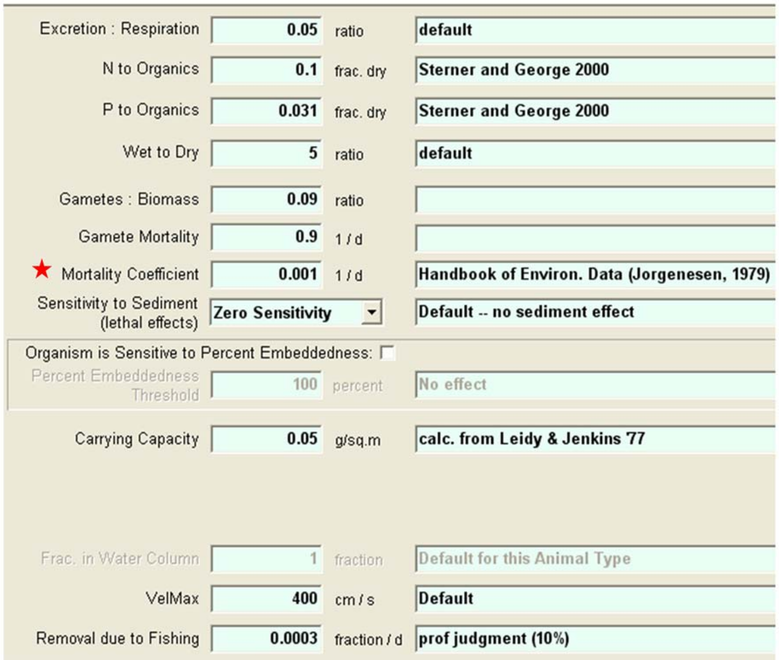
Note: *Promotion* includes emergence of aquatic insects

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.



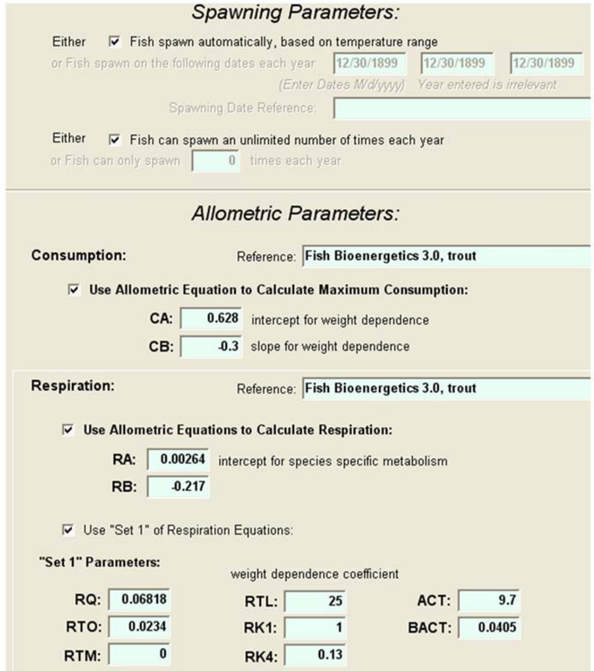
Sensitive parameters include maximum consumption rate and respiration rate, if not calculated based on weight (see slide below), and minimum biomass for feeding and optimum temperature.

Animal Parameters (cont.)



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

Animal Parameters (fish-specific allometric parameters)

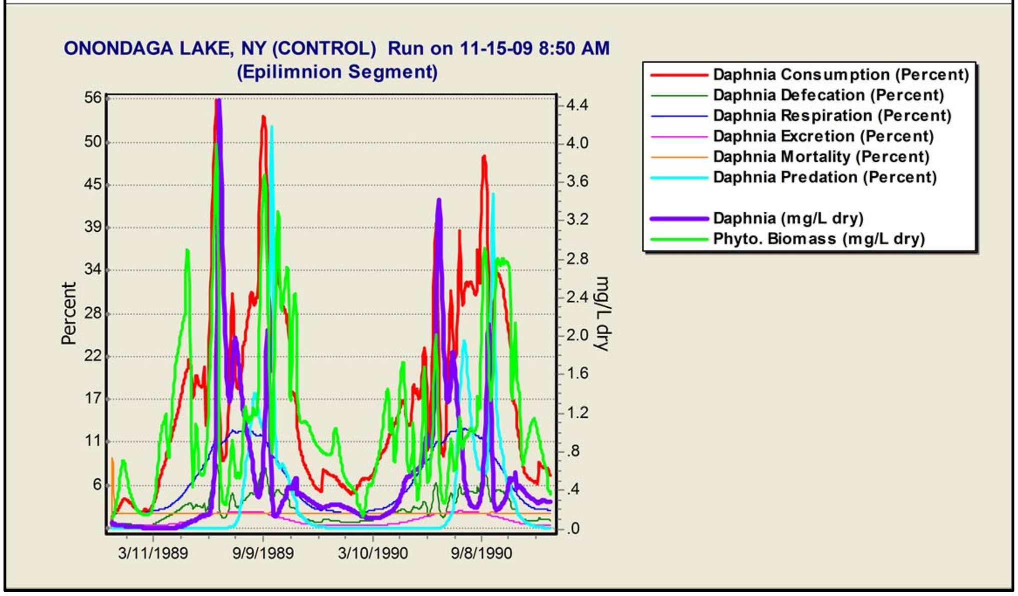


Allometric: change in metabolic rate in relation to the size of the organism.

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).

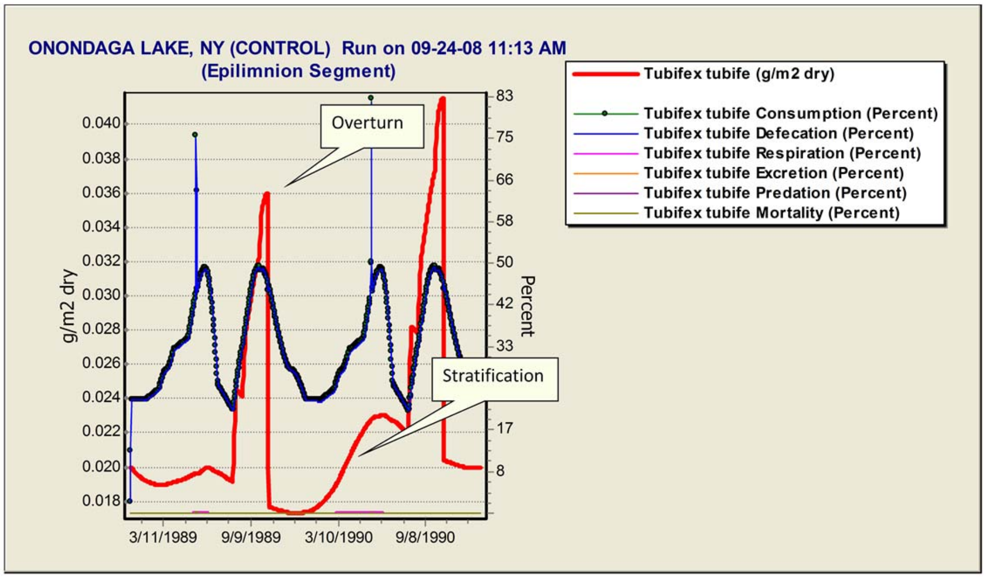
Hewett, S. W., and B. L. Johnson. 1992. Fish Bioenergetics 2 Model. Pages 79. University of Wisconsin Sea Grant Institute, Madison.
Hanson, Paul C., Timothy B. Johnson, Daniel E. Schindler, and James F. Kitchell. 1997. Fish Bioenergetics 3.0. Madison: Center for Limnology, University of Wisconsin.

Zooplankton consumption is often tied to phytoplankton productivity



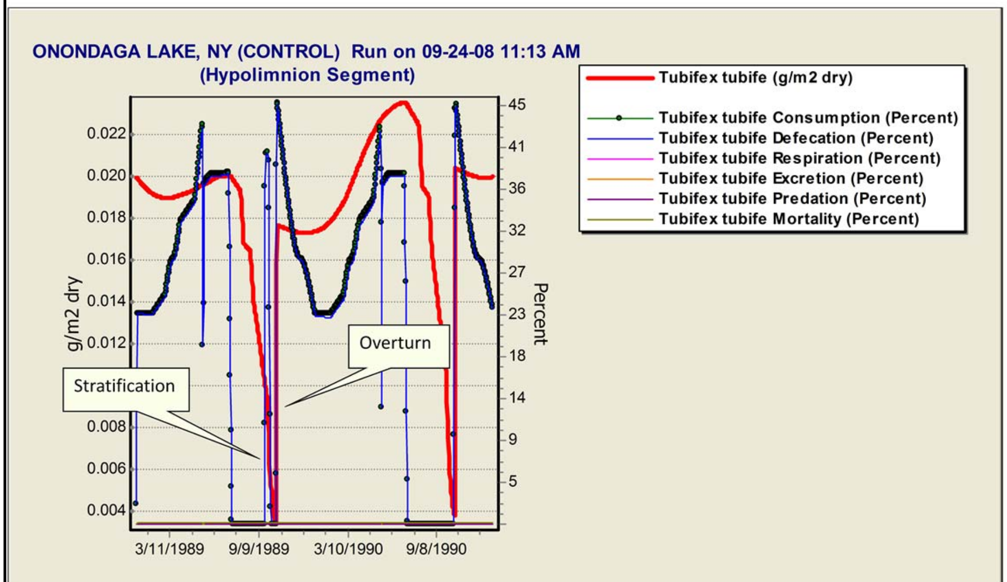
In Onondaga Lake consumption is heaviest during phytoplankton blooms, although detritus is a secondary source of food. (Without detritus as an alternate food source zooplankton would not be sustained.) Predation offsets high consumption in late summer.

Benthic invertebrates are also tied to phytoplankton productivity through detritus



High consumption occurs when algal blooms crash and detritus settles to the bottom. Note that this is a graph of one benthic invertebrate species in the epilimnion.

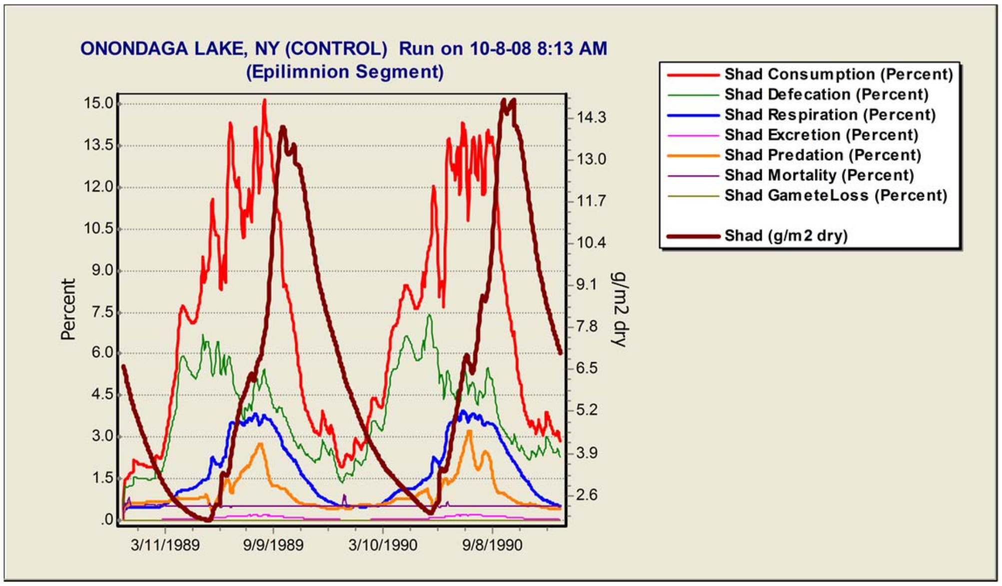
Tubifex in hypolimnion are tolerant of anoxia but stop feeding and slowly decline



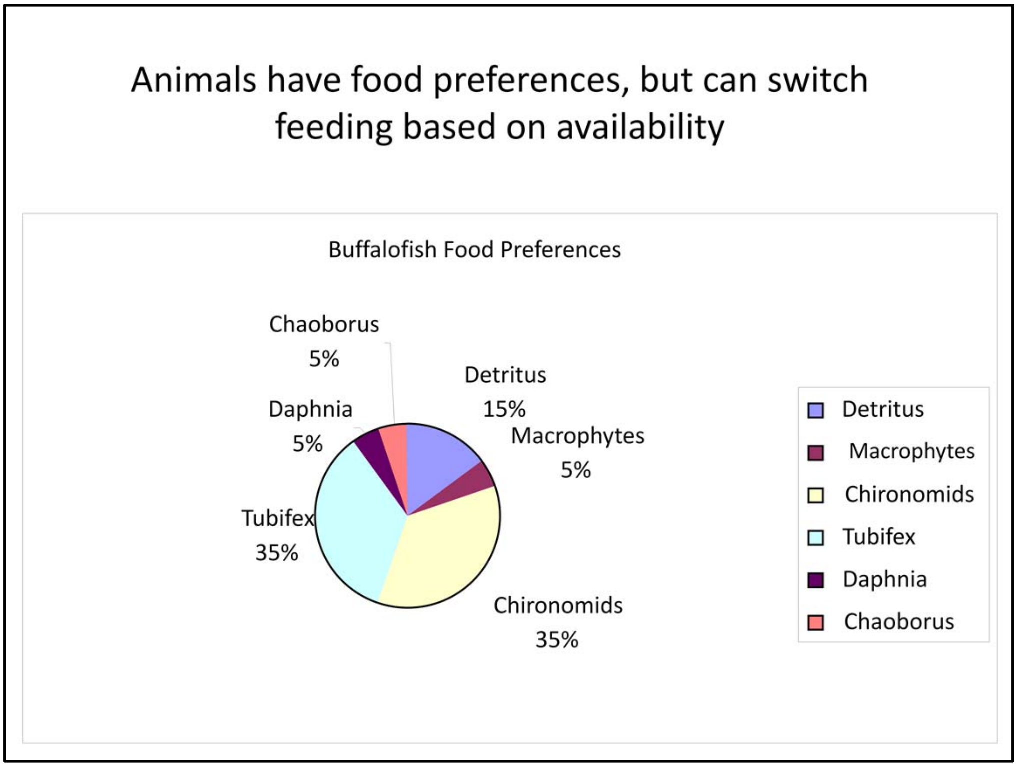
The pattern between the epilimnion (previous slide) and the hypolimnion is quite different. *Tubifex* stops feeding with anoxic conditions, and biomass is slowly lost. The rebound is actually the combination of biomasses when the epilimnion and hypolimnion are combined at overturn. However, as long as there is stratification, the zoobenthos are restricted to the two layers as separate populations.

The zooplankton, on the other hand, are able to migrate into the epilimnion when the hypolimnion becomes hypoxic.

Fish exhibit seasonal patterns based on food availability and temperature



Shad feed on plankton, so they too show a tightly-coupled, seasonal pattern of growth and decline.



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

Foodweb Model specified as Trophic Matrix

Interactions are normalized to 100%

AQUATOX-- Trophic Interaction Matrix

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

Show Preferences   Show Egestion Coefficients   Show Comments

	Tubifex tubi	Daphnia	Rotifer, Brac	Predatory Z	Shad	Bluegill	White Perc	Catfish	Largemouth	Largemouth	Walleye
R detr sed	50.0							1.2			
L detr sed	50.0							4.7			
R detr part					12.5				2.1		
L detr part		30.0	40.0		12.5	3.9	0.5		2.1		
Cyclotella nan		35.0	5.0		12.5						
Greens		30.0	5.0		12.5						
Phyt, Blue-Gre					12.5						
Cryptomonad		5.0	50.0								
Tubifex tubife						9.5	29.8	46.5	40.4	0.3	1.0
Daphnia				50.0	12.5	15.7	29.9	2.9	27.7	0.3	
Rotifer, Brach				50.0	12.4	15.7					
Predatory Zoop					12.5	7.9	29.9	2.9	27.7	38.2	1.6
Shad						15.8		20.9		44.3	23.1
Bluegill										2.9	
White Perch						15.7	10.0	20.9		10.1	24.8
Catfish											24.8
Largemouth Bas						15.7					24.8
Largemouth Ba2											
Walleye										3.9	

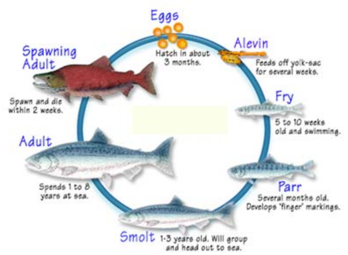
AQUATOX models **prey switching** based on prey biomasses: during each time-step of the simulation, prey species are assessed to see if they exceed the minimum prey threshold (BMIN). If there is insufficient prey for feeding, that compartment is zeroed out and the normalization to 100% continues with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

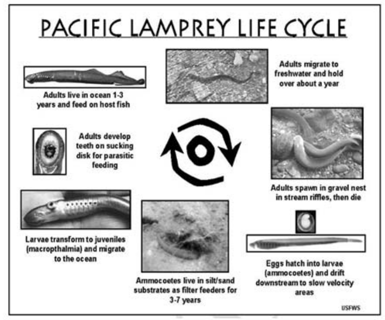
It is not only good modeling practice, it is imperative that you examine the trophic matrix and the associated matrix of egestion coefficients for anomalies. These may be caused by changing the selection of animals and adding prey preferences without accounting for the quality of the newly added food.

This matrix can be exported to Excel (button is at lower left corner of screen) and printed.

Anadromous fish considerations

- Chinook Salmon and Pacific Lamprey Life Cycles





- Model Predictions:
  - Chemical bioaccumulation, onsite and off
    - Safe for consumption?
  - Nutrient effects on stream ecosystem
  - Toxicant effects on food web

A new option in AQUATOX Release 3.1 is to model the migration of fish into and out of the main study area in order to approximate anadromous migration behavior. Anadromous fish live most of their adult life in saltwater, but they return to freshwater to spawn, and juveniles grow for a few months to a few years before going to saltwater; during their time in freshwater they may be exposed to and bioaccumulate organic toxicants. Chinook salmon and Pacific lamprey are two species in the animal database that can be used with this model. The anadromous migration component is a fairly simple model that holds off-site fish in what is assumed to be a clean “holding tank.” No additional exposure of the fish to the toxicant is predicted to occur while off-site, but growth dilution and depuration of toxicant is assumed to occur.

Three Options for Anadromous Fish in AQUATOX

1. Migration into and out of system using loadings
   - Nutrient effects considered
   - Biomass coming and going must be specified
   - Toxicant loadings in returning fish must be specified
2. New Anadromous Fish model for Release 3.1
   - Size-class fish (juveniles and adults)
   - Off-site fish modeled in clean "holding tank"
   - Off-site location fairly simple (no toxic exposure)
3. Model all migration sites explicitly
   - Linked mode implementation, data requirements
   - Off-site toxicant uptake and loss explicitly modeled

A spreadsheet version of the sub-model discussed above ("2.") is available in "Anadromous_Model.xlsx" and is installed in the STUDIES directory when Release 3.1 is installed.

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
- Discussion of model calibration goals

Model Performance

Sources of Parameter Values

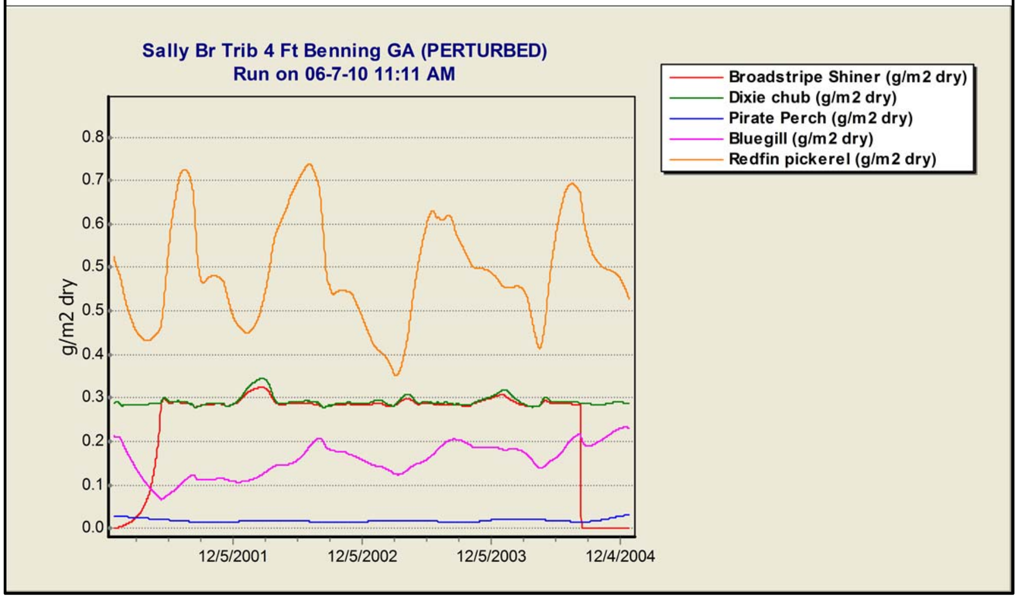
Calibration Strategy for Minnesota Rivers

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

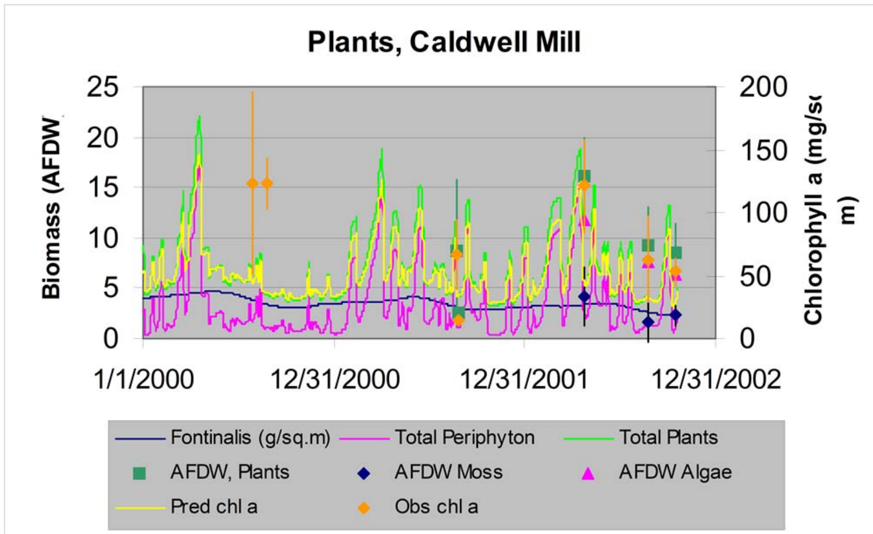
Reasonable ecosystem behavior test



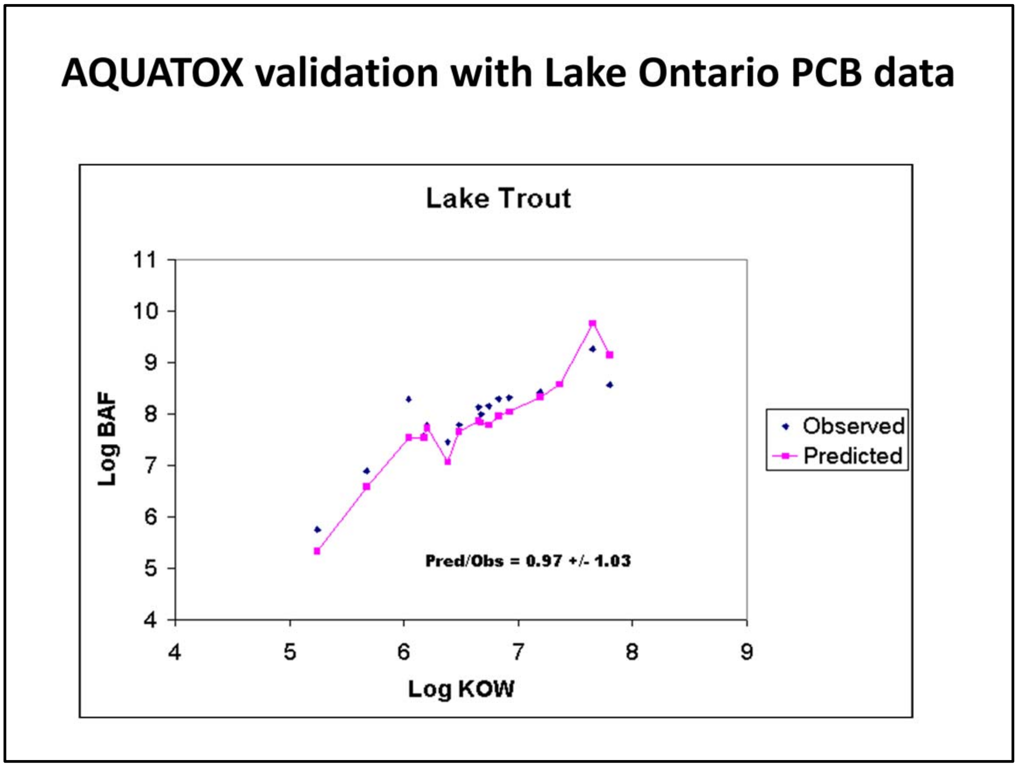
In the absence of data, we can run a multiple-year simulation and look for stability and reasonableness of biomass values. (Note: the broadstripe shiner is sensitive to sedimentation and disappears near the end of the simulation.)

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

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

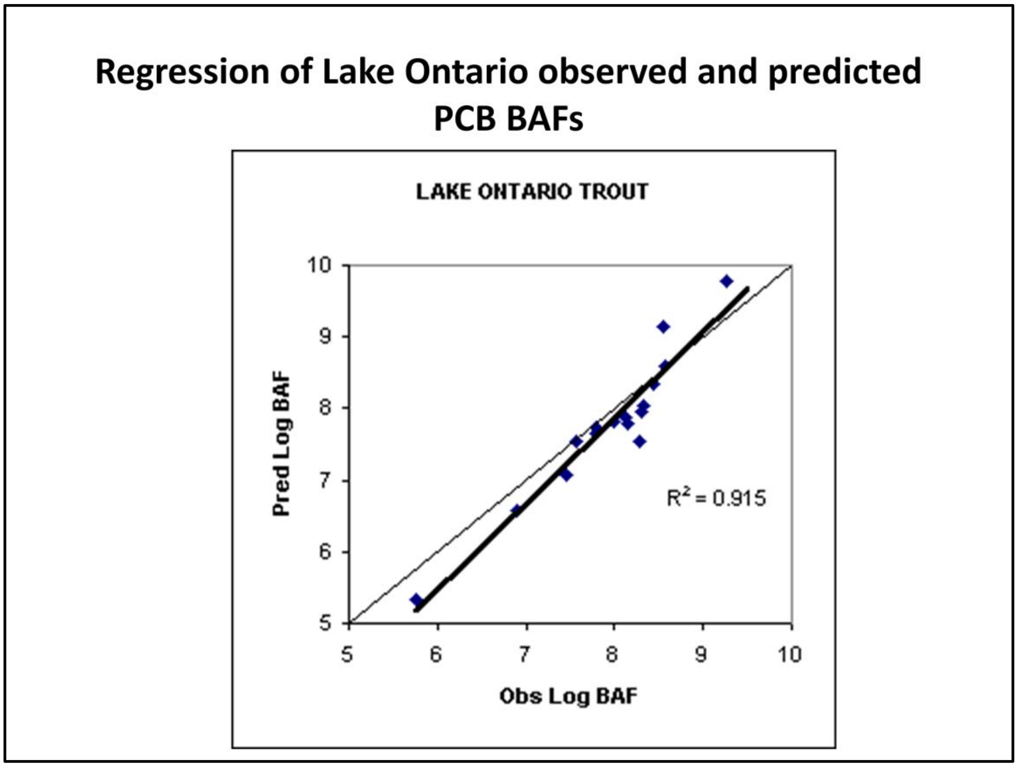


Visual inspections of fits of predictions to observed data are useful in evaluating how well patterns are represented, with allowance for the vagaries of widely spaced data points. Although not quantitative, they contribute considerably to the weight of evidence that the model is representing the periphyton 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).



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.



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

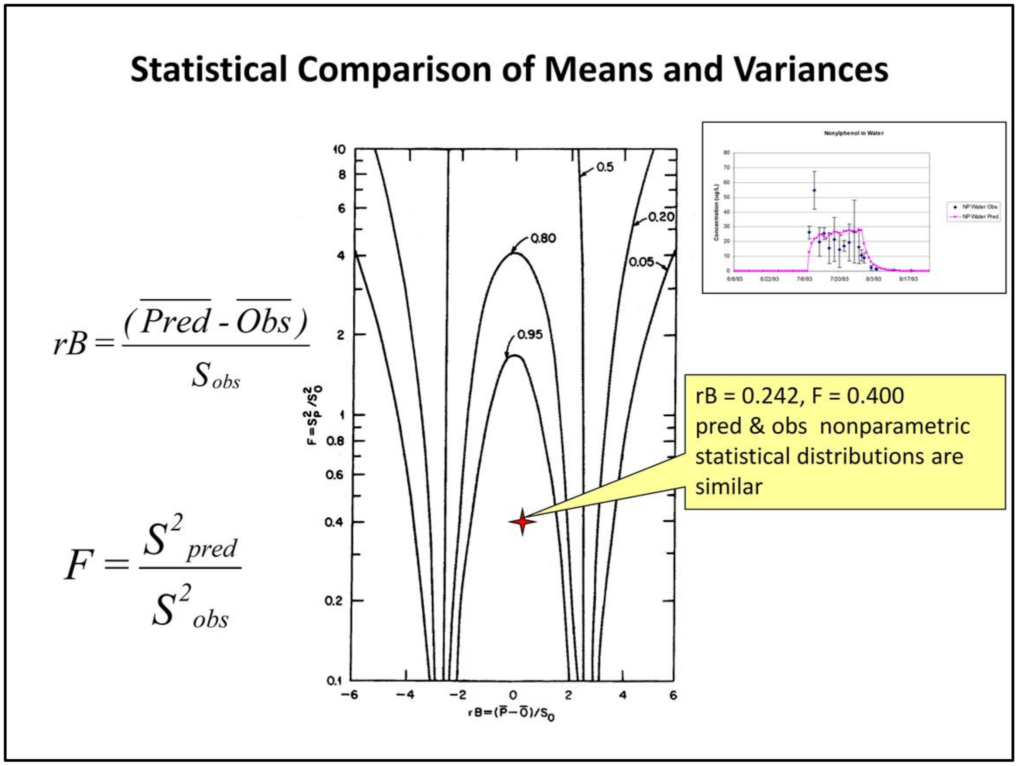
Gobas, 1993, model (results, Burkhard, 1998)

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).



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

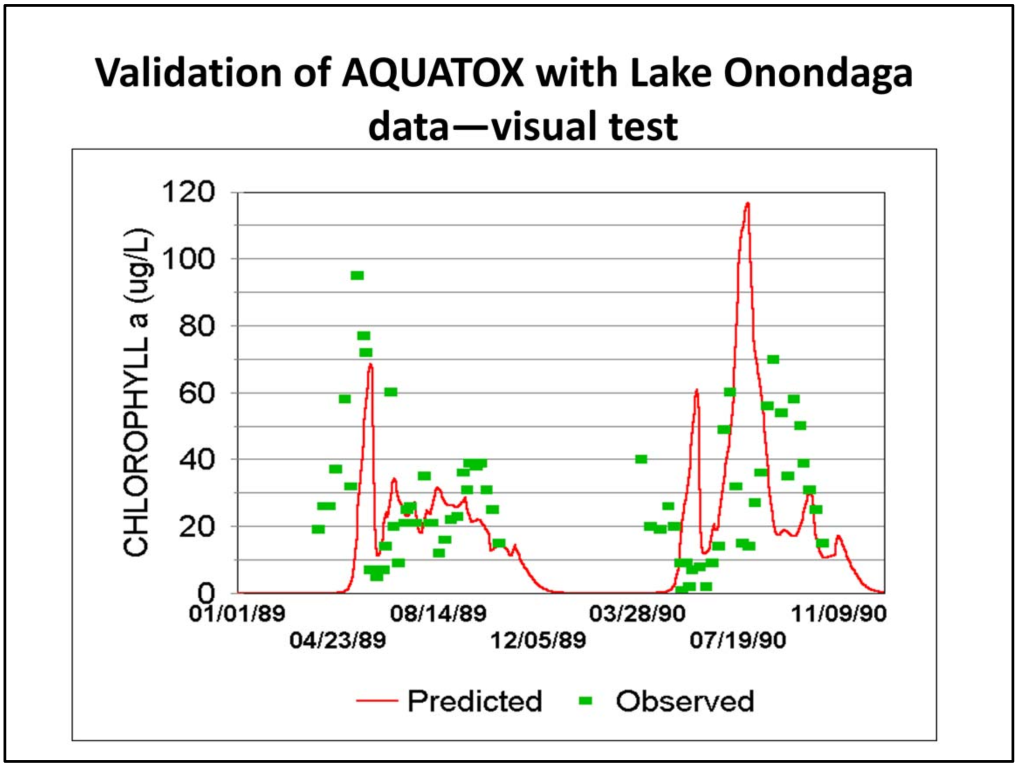
where:

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

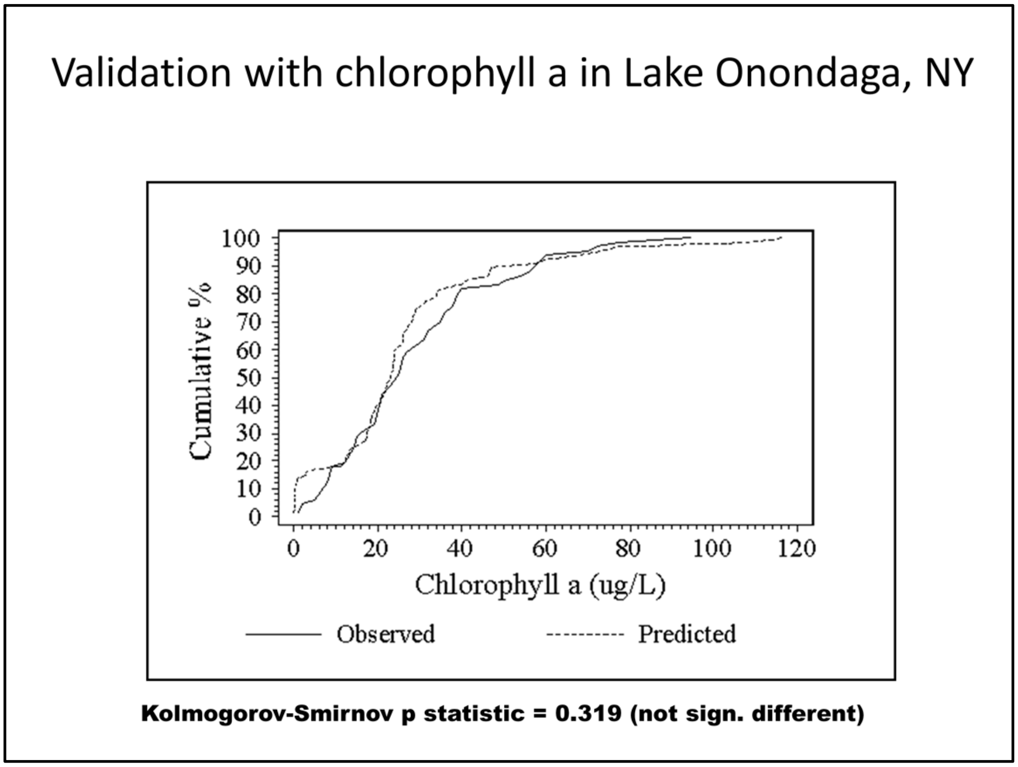
Very small F values suggest that the observed data may be too variable to determine the goodness of fit; very large F values indicate that the predictions are imprecise (Bartell et al., 1992). Large F values also may indicate that the model is predicting greater fluctuations than can be supported by 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.



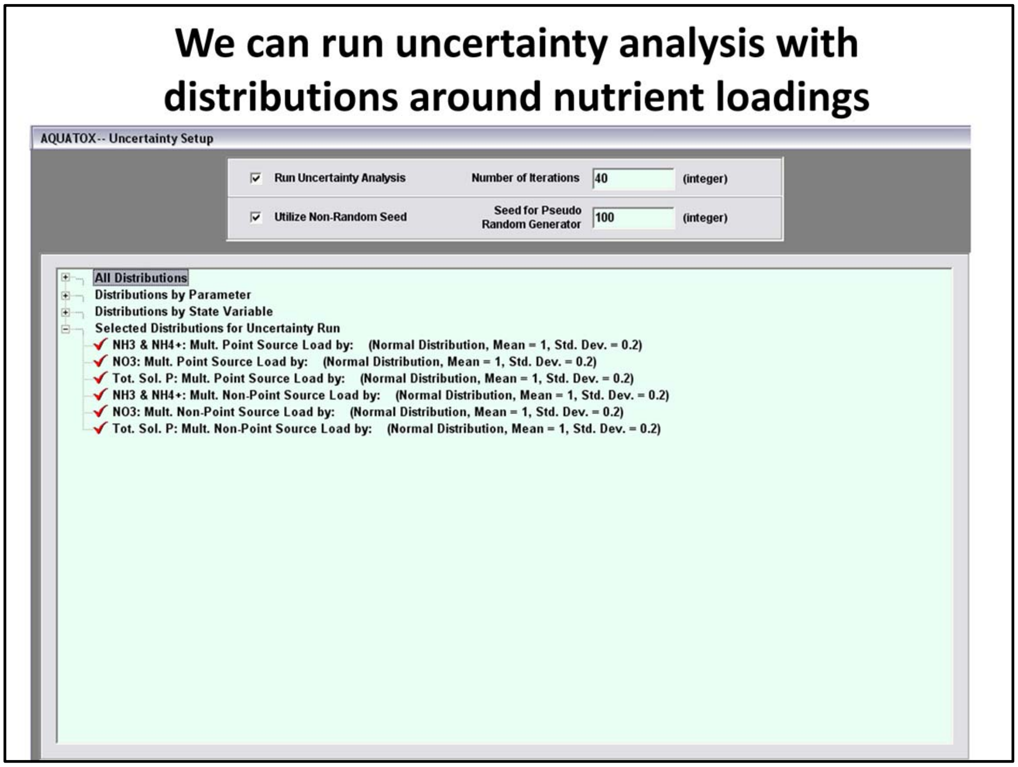
U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports. Washington, DC.

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



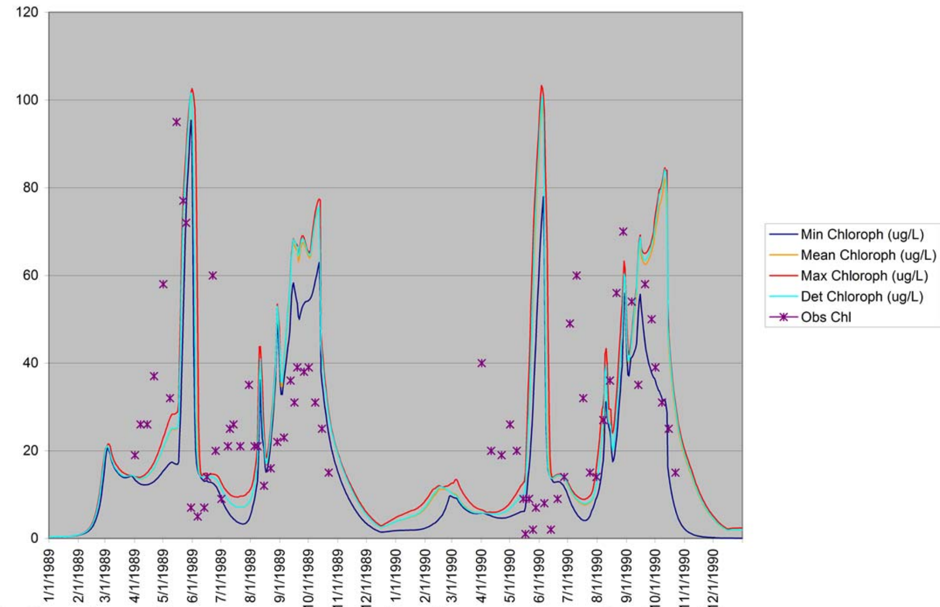
U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports. Washington, DC.

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.

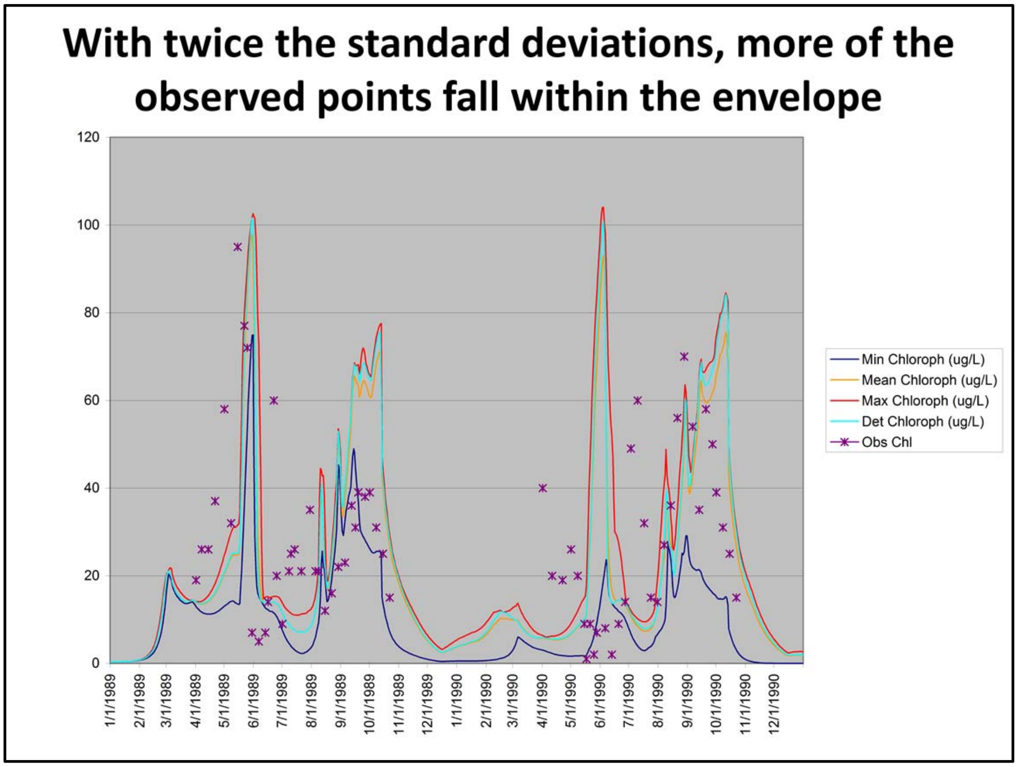


Uncertainty analysis is available to compare envelope of predictions with observed data. For example, still using the Lake Onondaga study, we can provide distributions of values for the nutrient loadings.

Plotting observed points with uncertainty bands for simulation suggests imperfect fit

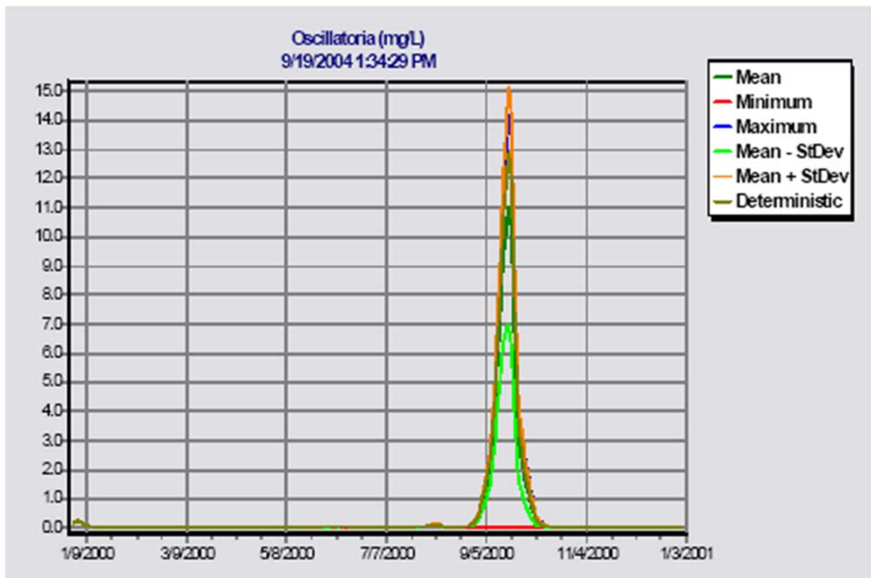


Lake Onondaga with more recent simulation than previous validation slide

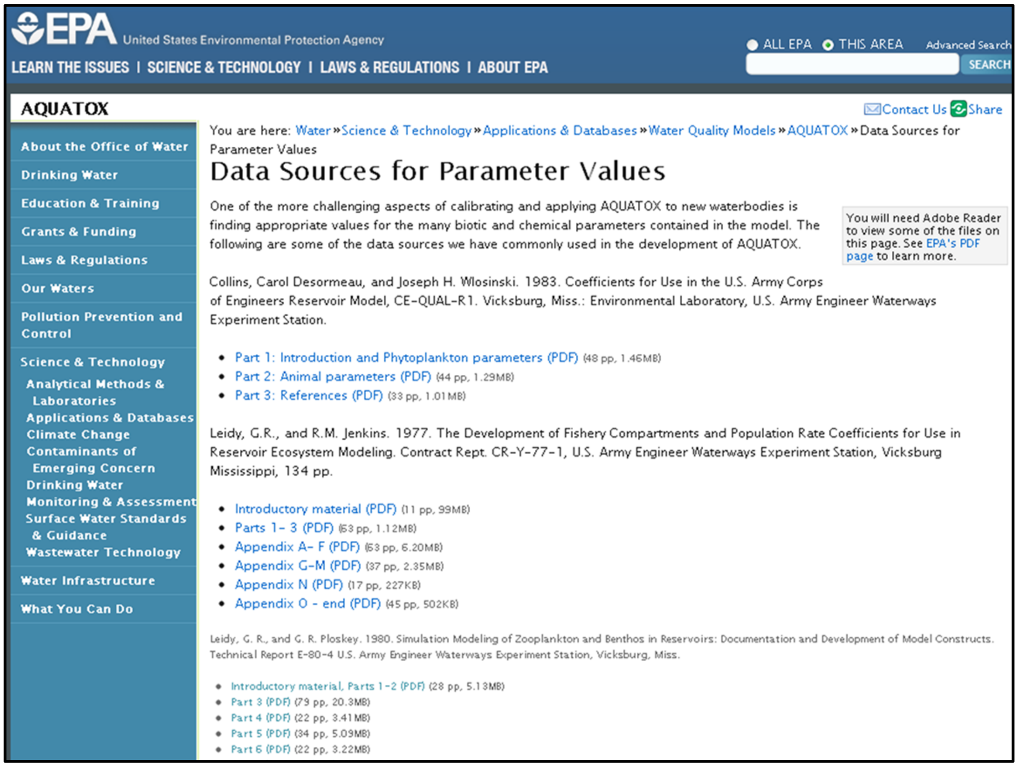


If we double the standard deviations for each of the nutrient loading distributions we can compare the increased envelope of uncertainty with the observed data. Most of the observed values are contained within the envelope of uncertainty.

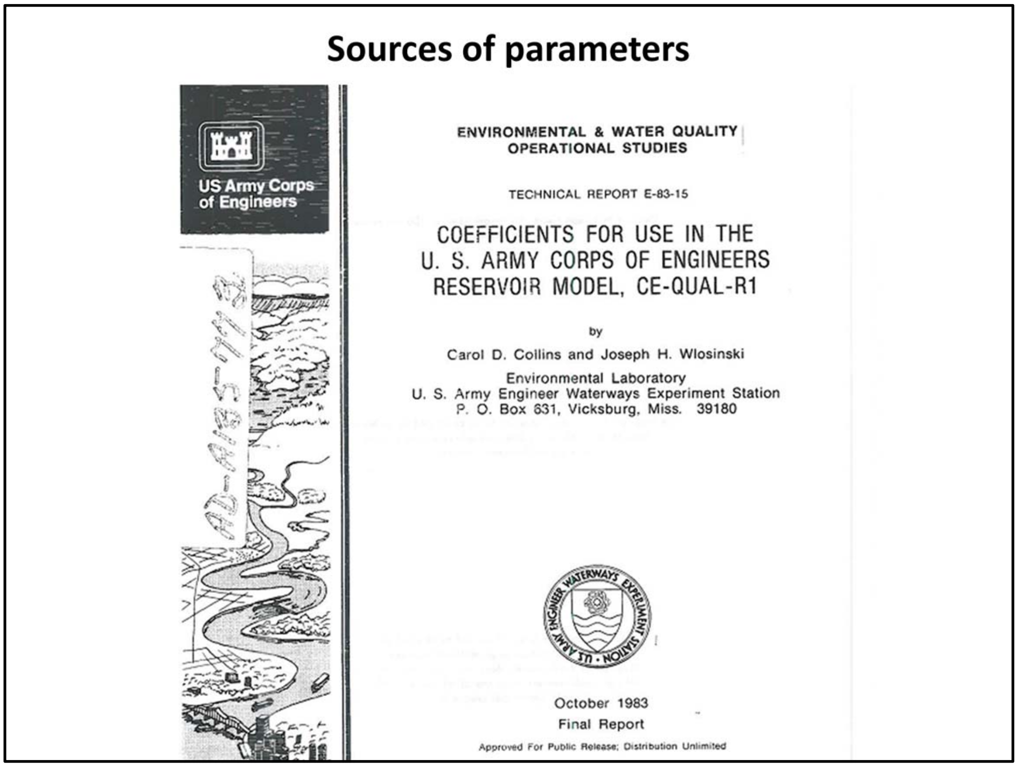
Statistical sensitivity analysis of blue-green to saturated light parameter (74+-30)



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.



Three sources of parameter values used in AQUATOX are provided on the Web site for download. Although compiled in the 1970s and 1980s, these are still excellent sources. Examples are shown in the following slides.



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.

This is available for download from the AQUATOX Web site.

Data Sources for Parameter Values

available for download from AQUATOX Web site

http://water.epa.gov/scitech/datait/models/aquatox/data.cfm

Table 7

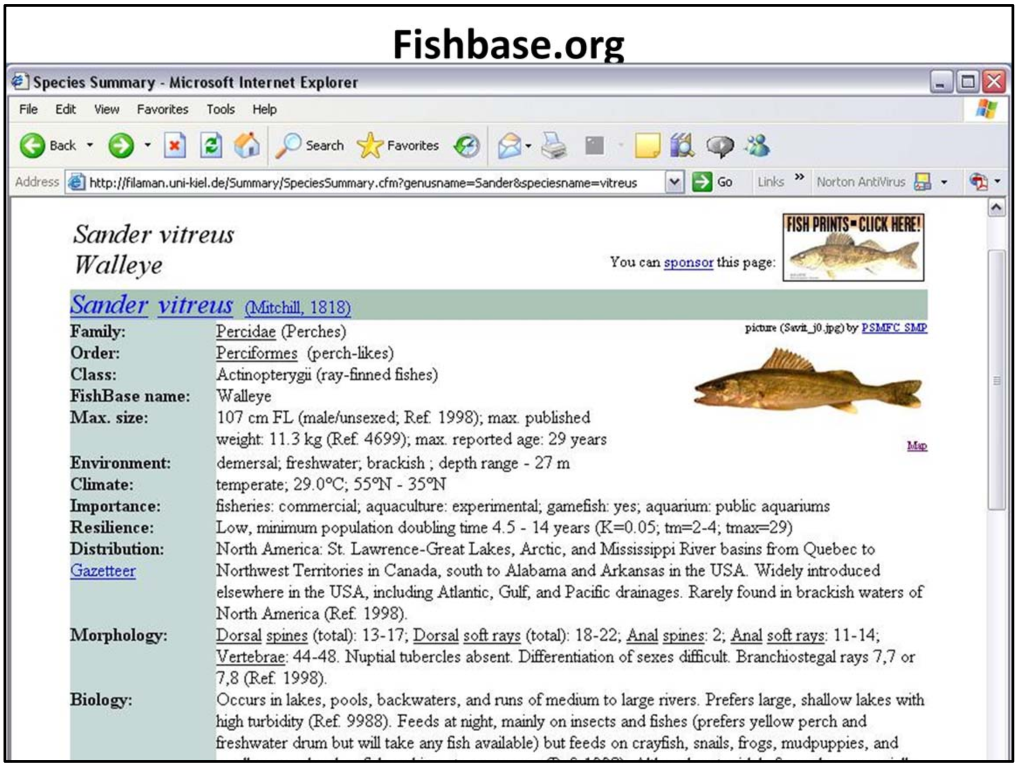
Phytoplankton half-saturation coefficients for P limitation (mg/L)

SPECIES	PS2PO4	REFERENCE
Asterionella formosa	0.002	Holm and Armstrong 1981
Asterionella japonica	0.014	Thomas and Dodson 1968
Biddulphia sinensis	0.016	Quasim et al. 1973
Cerataulina bergonii	0.003	Finenko and Krupatikina 1974
Chaetoceros curvisetus	0.074-.105	Finenko and Krupatikina 1974
Chaetoceros socialis	0.001	Finenko and Krupatikina 1974
Chlorella pyrenoidosa	0.38-.475	Jeanjean 1969
Cyclotella nana	0.055	Fuhs et al. 1972
Cyclotella nana	0.001	Fogg 1973
Dinobryon cylindricum	0.076	Lehman (unpubl. data)
Dinobryon sociale var. americanum	0.047	Lehman (unpubl. data)
Euglena gracilis	1.52	Blum 1966
Freshwater phytoplankton	0.02-.075	Halmann and Stiller 1974
Microcystis aeruginosa	0.006	Holm and Armstrong 1981
Nitzschia actinastreoides	0.095	von Muller 1972
Pediastrum duplex	0.105	Lehman (unpubl. data)
Pithophora oedogonia	0.098	Spencer and Lembi 1981
Scenedesmus obliquus	0.002	Fogg 1973
Scenedesmus sp.	0.002-.05	Rhee 1973
Thalassiosira fluviatilis	0.163	Fogg 1973

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.

Leidy, G.R., and R.M. Jenkins. 1977. The Development of Fishery Compartments and Population Rate Coefficients for Use in Reservoir Ecosystem Modeling. Contract Rept. CR-Y-77-1, U.S. Army Engineer Waterways Experiment Station, Vicksburg Mississippi, 134 pp.

Leidy, G. R., and G. R. Ploskey. 1980. Simulation Modeling of Zooplankton and Benthos in Reservoirs: Documentation and Development of Model Constructs. Technical Report E-80-4 U.S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

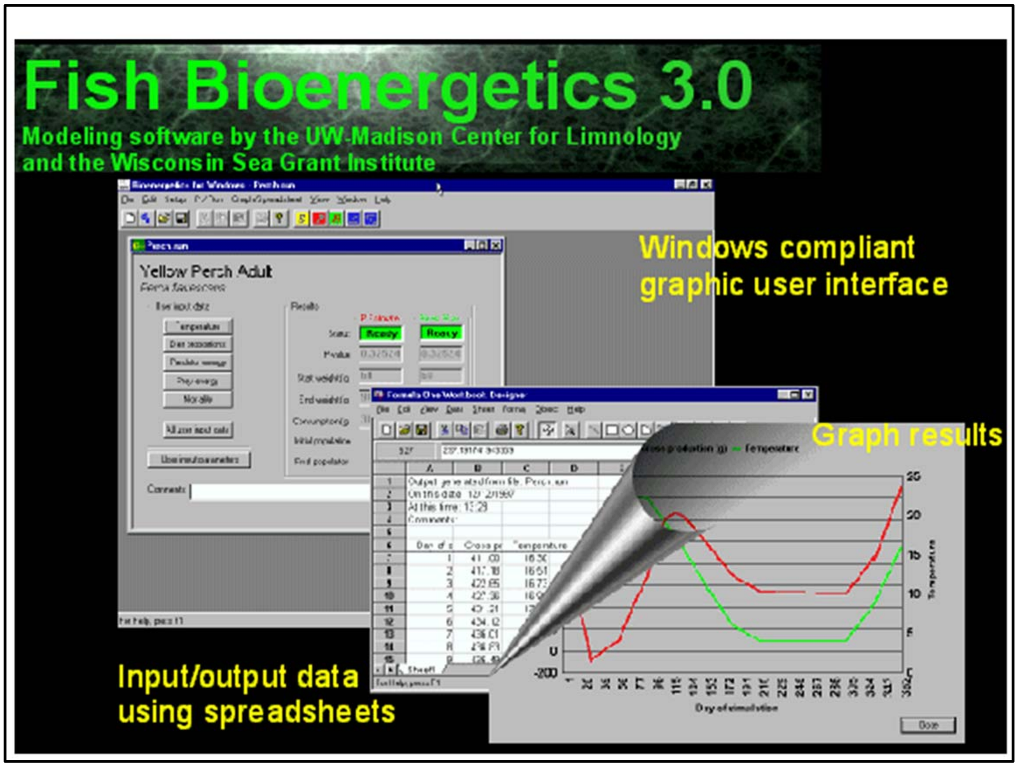


The German mirror Web site is often faster than the primary Web site, especially in the afternoon:
http://filaman.uni-kiel.de/Summary/SpeciesSummary.cfm?genusname=Sander&speciesname=vitreus

This and other links may be broken, in which case search for key words (“FishBase”) to obtain a current link.

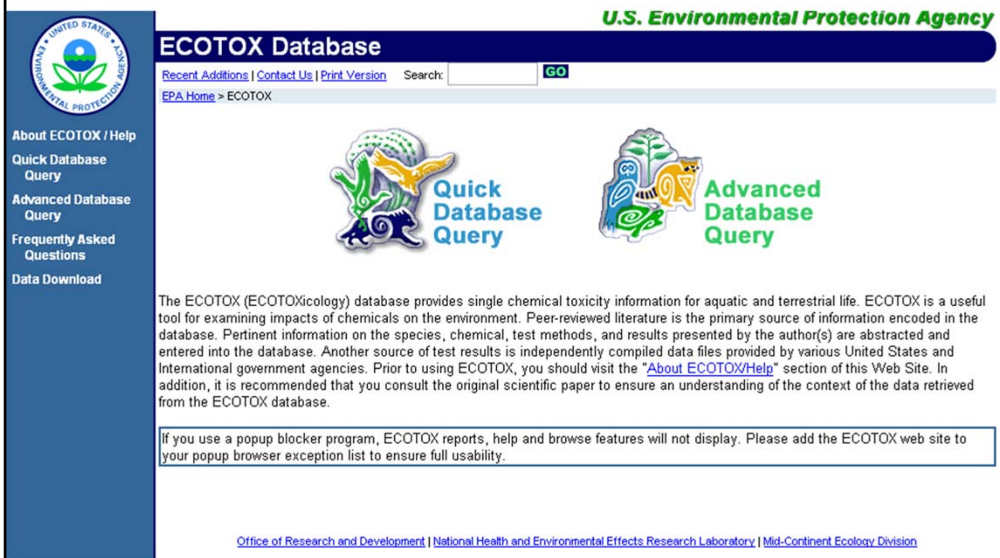
Useful information available for AQUATOX from Fishbase.org:

- Food preferences
- Habitat type
- Sediment tolerance
- Weight
- Respiration (O_2 consumption)
- Spawning details



http://limnology.wisc.edu/research/bioenergetics/bioenergetics.html

ECOTOX (EPA Toxicity Database)

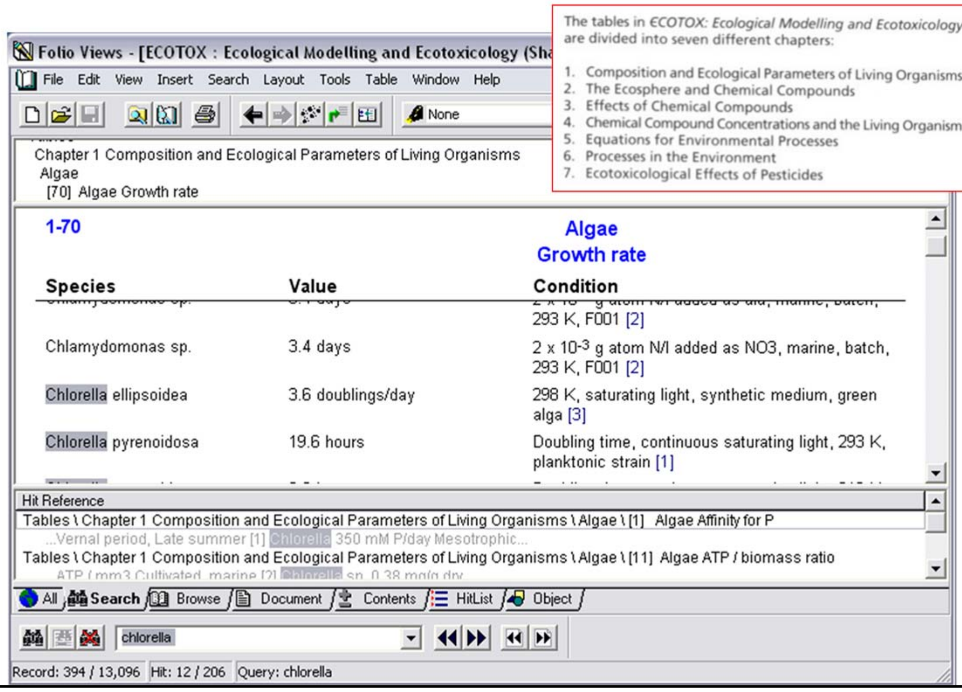


This is a comprehensive database of toxicity parameters that is constantly updated.

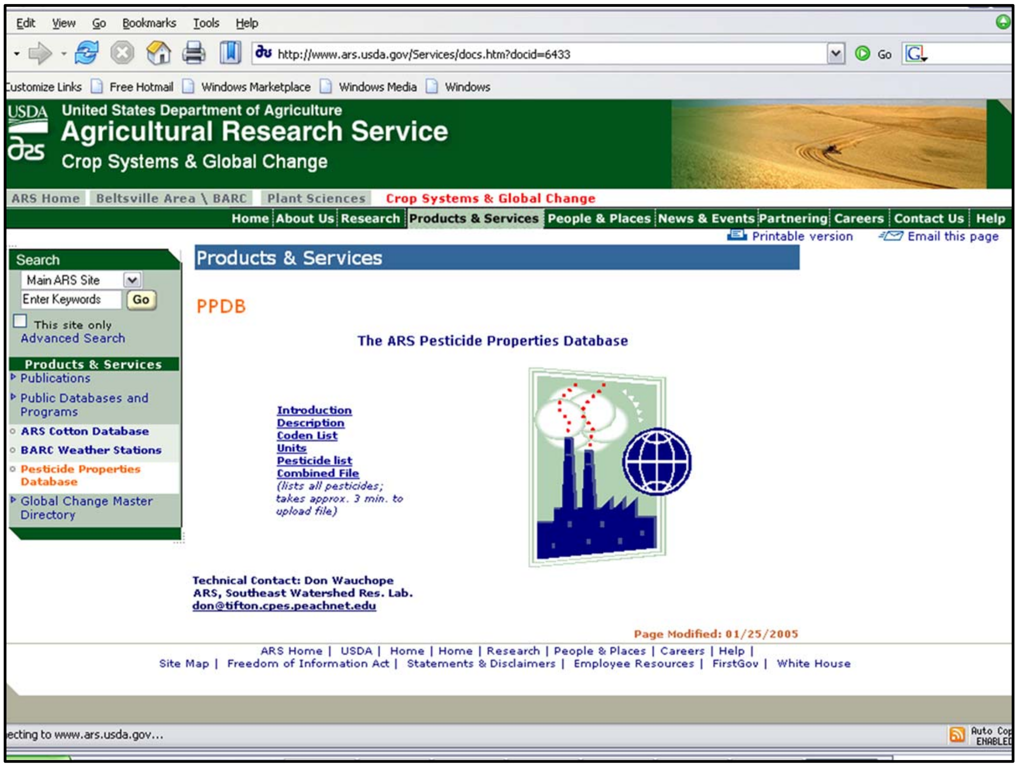
Provides different endpoint values (LC50 , EC50, non-mortal effects, etc.) for plants and animals for various chemicals along with full citations of the references where these values were determined.

http://cfpub.epa.gov/ecotox/

ECOTOX (Elsevier product)



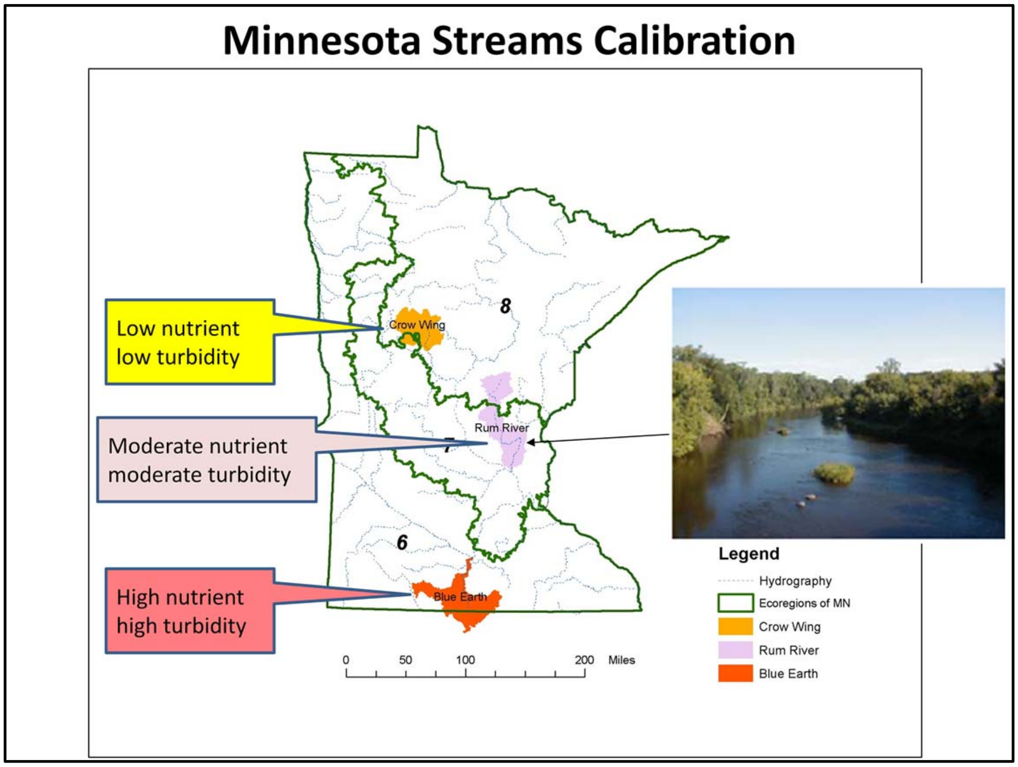
This is an expensive database (Amazon lists a used copy for $399), but it provides an extensive survey of parameter values. However, be careful of calibrated values mixed in with values observed from experiments. Also, it has not been updated since 2000 and appears to be out of print.



The ARS Pesticide Properties Database is quite useful for finding properties of pesticides:

http://www.ars.usda.gov/Services/docs.htm?docid=14199

However, the URL changes occasionally, so if the link is broken then use a search engine to find the portal.



For this exercise, we made use of some chemical and biological data that Minnesota Pollution Control Agency had collected from medium-sized rivers. These watersheds are in different ecoregions and have different mixes of land uses. 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.

The nutrient concentrations in these rivers span roughly an order of magnitude, increasing generally in a N-S direction from the Crow Wing to the Blue Earth, as the land becomes increasingly dominated by agriculture.

Three sites, representing a wide range of nutrient conditions, were modeled.

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
  - Used linked version for simultaneous calibration across sites
- When goodness-of-fit is acceptable for both sites, apply to an intermediate site (Rum River) and reiterate calibration across all three sites
- Parameter set was validated with Cahaba River AL data

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. 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. 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. The procedure is not only efficient, it facilitates comparisons among the three sites.

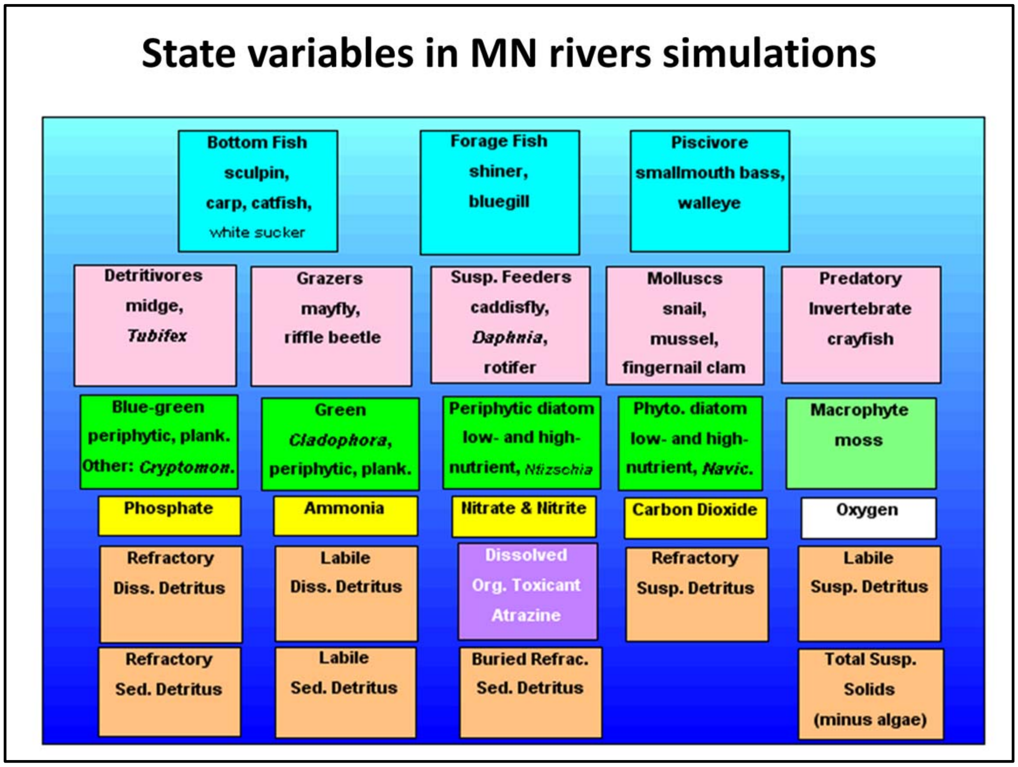
Park, R. A., J. N. Carleton, J. S. Clough, and M. C. Wellman. 2009. AQUATOX Technical Note 1: A Calibrated Parameter Set for Simulation of Algae in Shallow Rivers. Pages 19. U.S. Environmental Protection Agency, Washington D.C.

Rum River, Minnesota

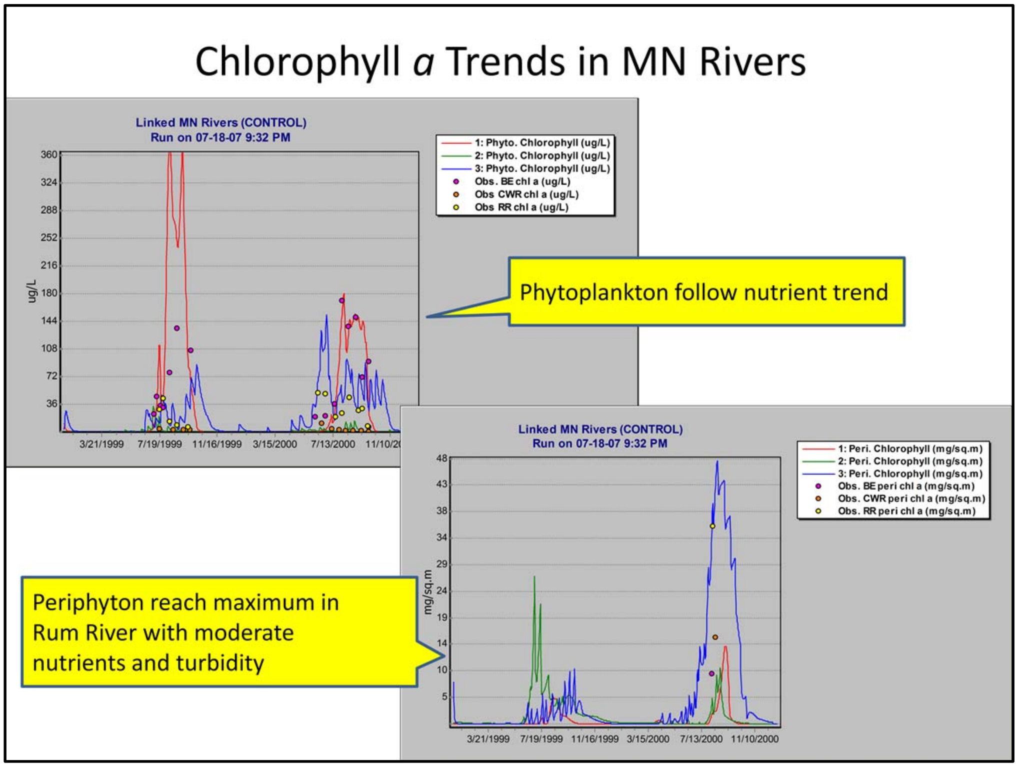
(Heiskary & Markus, 2003)

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.

Heiskary S, Markus H (2003) Establishing relationships among instream nutrient concentrations, sestonic algae abundance and composition, fish IBI and biochemical oxygen demand in
Minnesota USA rivers. Minnesota Pollution Control Agency, St. Paul
http://www.pca.state.mn.us/index.php/view-document.html?gid=12867



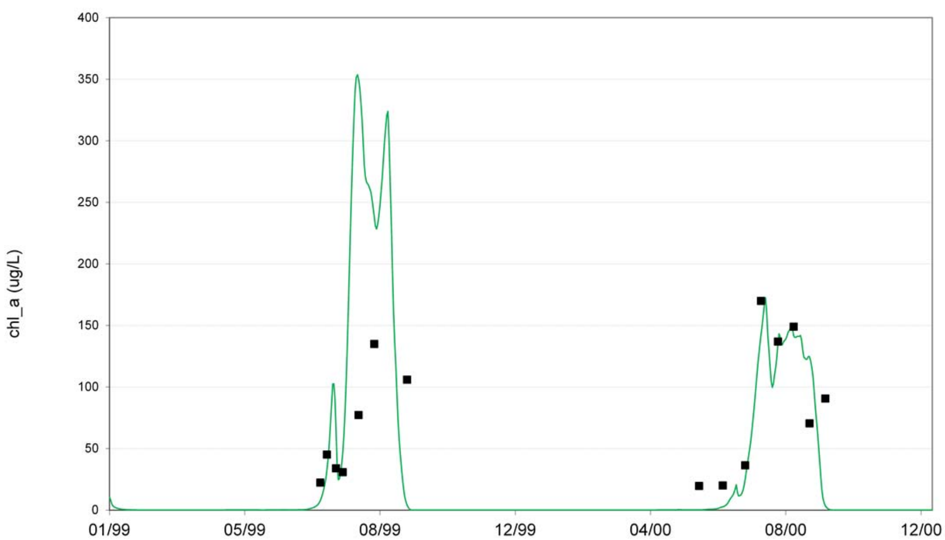
State variables were chosen to represent both the nutrient-poor, clear-water Crow Wing River and the nutrient-enriched, turbid Blue Earth River. Sculpin, a cold-water fish, was included although conditions in the Blue Earth River are too warm for its continued survival. Because the objective was to obtain 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.



In general the phytoplankton biomass reflected the nutrient gradient.
In contrast, periphyton was affected by turbidity and flow as well nutrients.

Red lines: Blue Earth River
Blue lines: Rum River
Green lines: Crow Wing River

Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Blue Earth River at mile 54



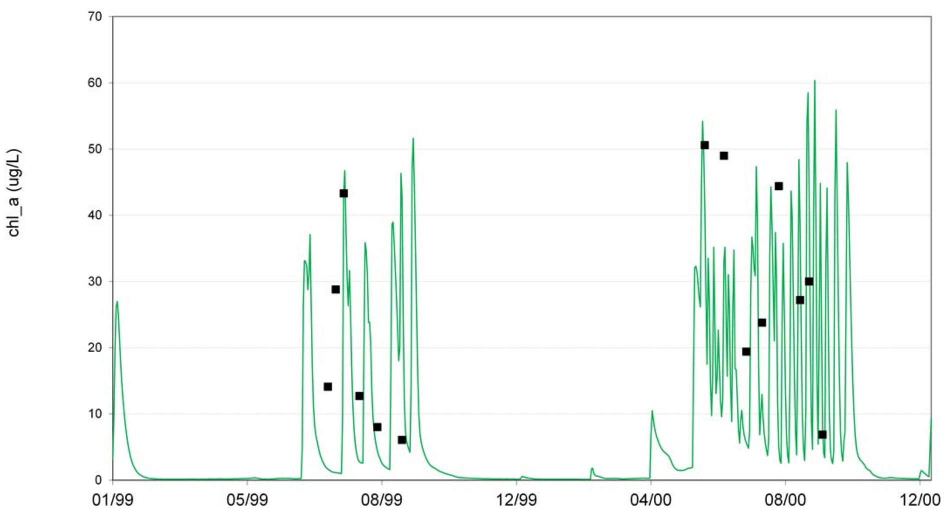
The Blue Earth River is in a highly cultivated agricultural watershed, with very high nutrient and sediment loads.

Note the order-of-magnitude range in scale between this and the following figure.

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.

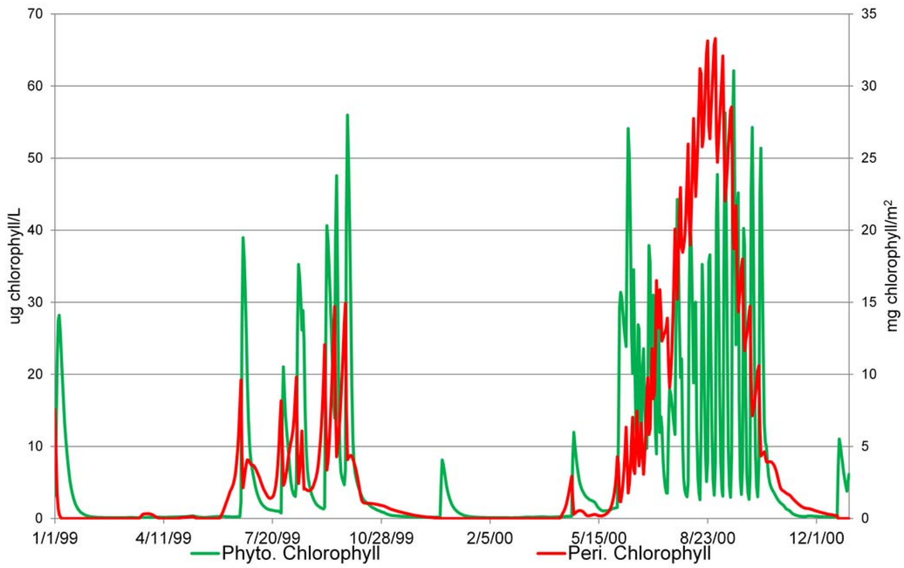
Predicted Blue Earth River phytoplankton are dominated by cyanobaceria, similar to what was observed, and cryptomonads. The latter are not as well supported by the observed data, but the samples do not cover the spring and late fall periods. Diatoms are not as important in the simulation as observed.

Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Rum River at mile 18



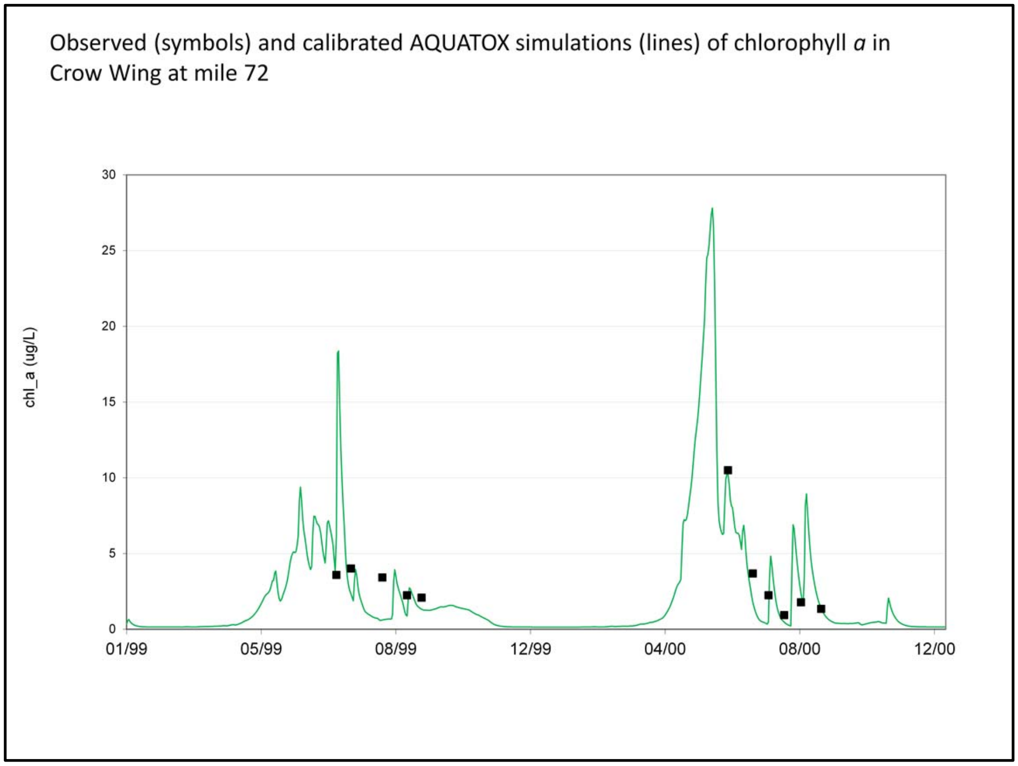
Rum River is moderately impacted by nutrients and turbidity, but is also very shallow and its flow is flashy.

Sestonic algae are largely a result of sloughed periphyton in the Rum, a very shallow river



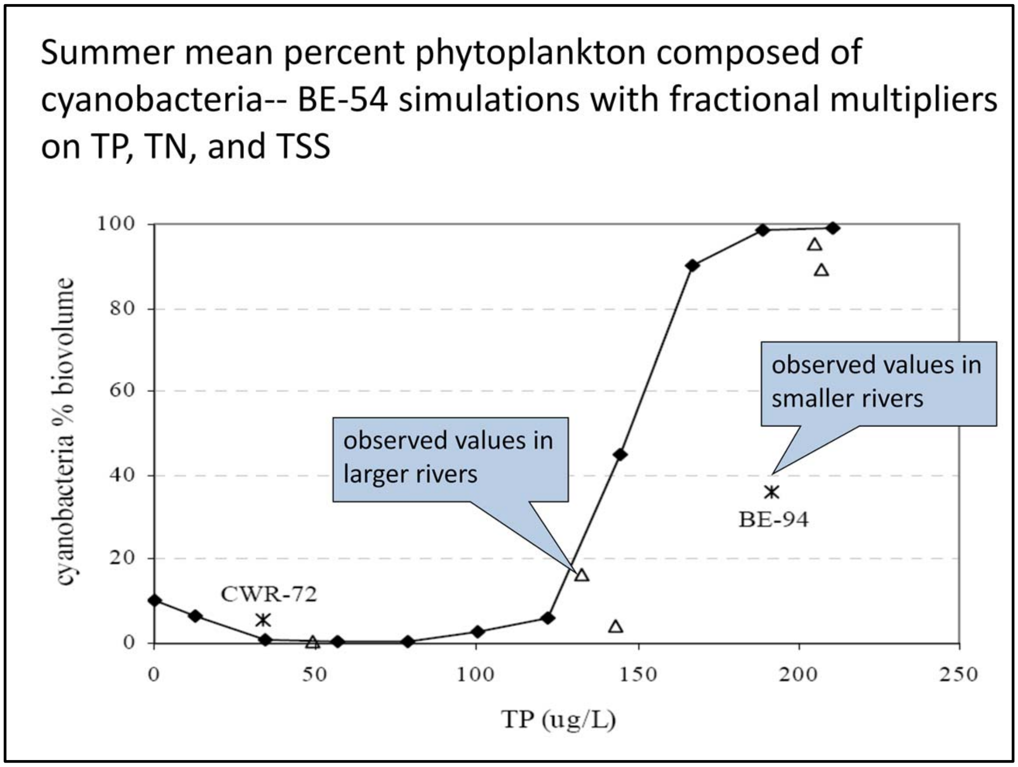
Periphyton may slough or be physically scoured, contributing to the suspended algae; this may be reflected in the chlorophyll *a* observed in the water column. Periphyton may be linked to a phytoplankton compartment so that sestonic chlorophyll *a* results reflect the results of periphyton sloughing. One-third of periphyton is assumed to become phytoplankton and two thirds is assumed to become suspended detritus in a sloughing event.

Additionally, when phytoplankton undergoes sedimentation it will now be incorporated into the linked periphyton layer if such a linkage exists.



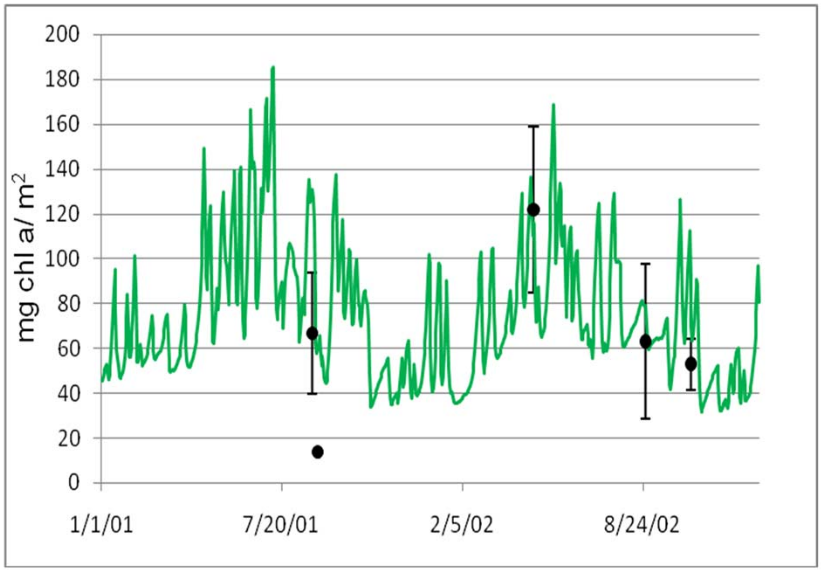
Crow Wing River is in a mostly forested watershed, and is low in both nutrients and sediments.

Note scale in comparison with earlier figures



One biotic metric sometimes used to evaluate nutrient status of waterbodies is % cyanobacteria (aka blue-green algae). Because it can form noxious, and sometime toxic, blooms, high proportions of cyanobacteria are generally considered undesirable.

Validation: observed (symbols) and AQUATOX simulation (line) of periphytic chlorophyll *a* in Cahaba River AL



The MN parameter set was used with only a couple modifications and no calibration. The critical force for periphyton scour was increased based on the bedrock riffles, and the optimum temperature was increased for two groups based on the difference in temperature between MN and AL. Therefore, this is considered a good partial validation.