AQUATOX Short Course

SETAC Meeting, Portland Oregon
November 7, 2010

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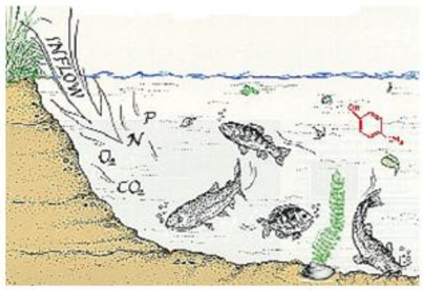


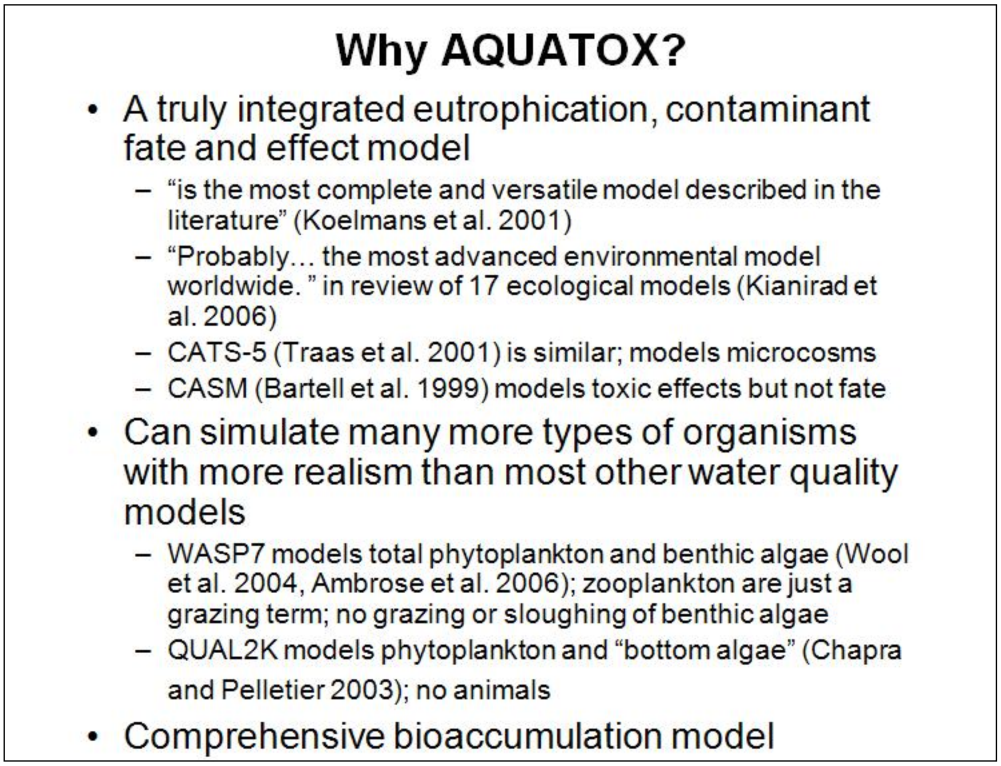
Introduction to Course, Organization

- Schedule and administrative details
- CD organization
  - Directory Setup
  - For those with laptops, files to look at during the day

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.



Ambrose, J., Robert B. , J. L. Martin, and T. A. Wool. 2006. WASP7 Benthic Algae - Model Theory and User's Guide, Supplement to Water Quality Analysis Simulation Program (WASP) User Documentation Pages 32. U.S. Environmental Protection Agency, Washington, DC

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.

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Kianirad, E., D. Bedoya, I. Ghosh, K. McGarvey, and V. Novotny. 2006. Technical Report No. 7, Review of Watershed Ecological Models. Pages 85. Center for Urban Environmental Studies, Northeastern University, Boston MA.

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.

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.

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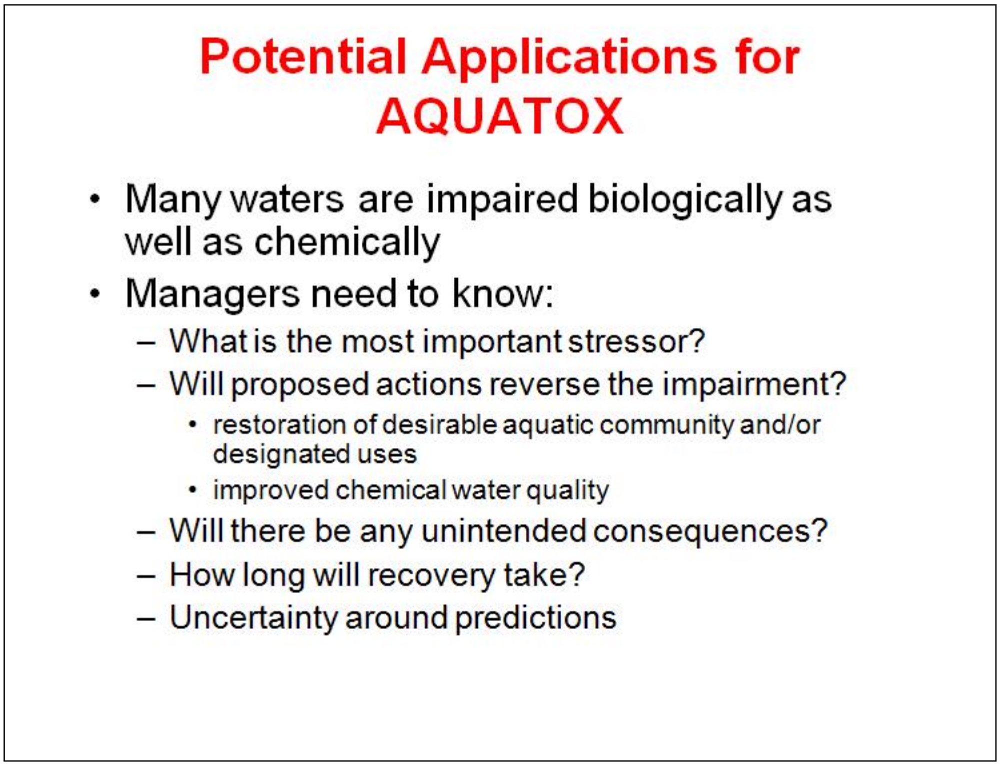
Lei, B., S. Huang, M. Qiao, T. Li, and Z. Wang. 2008. Prediction of the environmental fate and aquatic ecological impact of nitrobenzene in the Songhuajiang River using the modified AQUATOX model. *Journal of Environmental Sciences 20: 1-9.*



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.

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.

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.

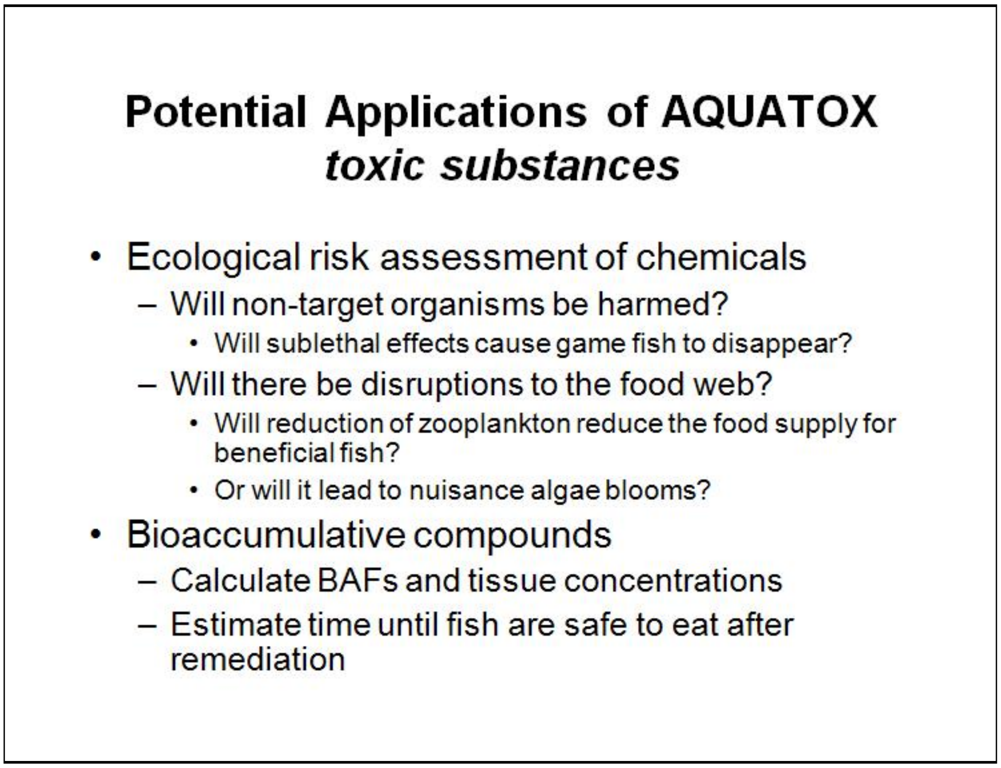
We'll discuss the different kinds of AQUATOX output in more detail a little later.

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, DeGray Lake Arkansas, three rivers in Minnesota, twenty streams in northern Florida, Venice Lagoon Italy, and Vitória Bay Brazil.



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
  - 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.

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

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

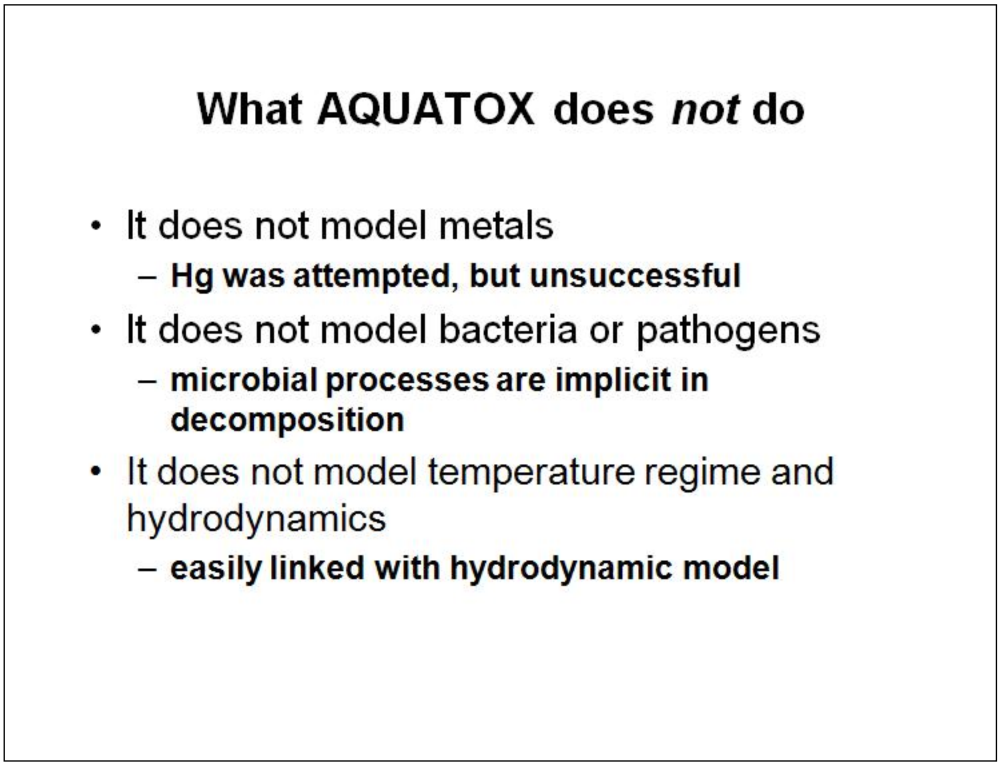
Table 3.2. Comparison of Bioaccumulation State Variables

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. 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.



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

Model has been used with flow field simulated by EFDC.

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

AQUATOX Structure

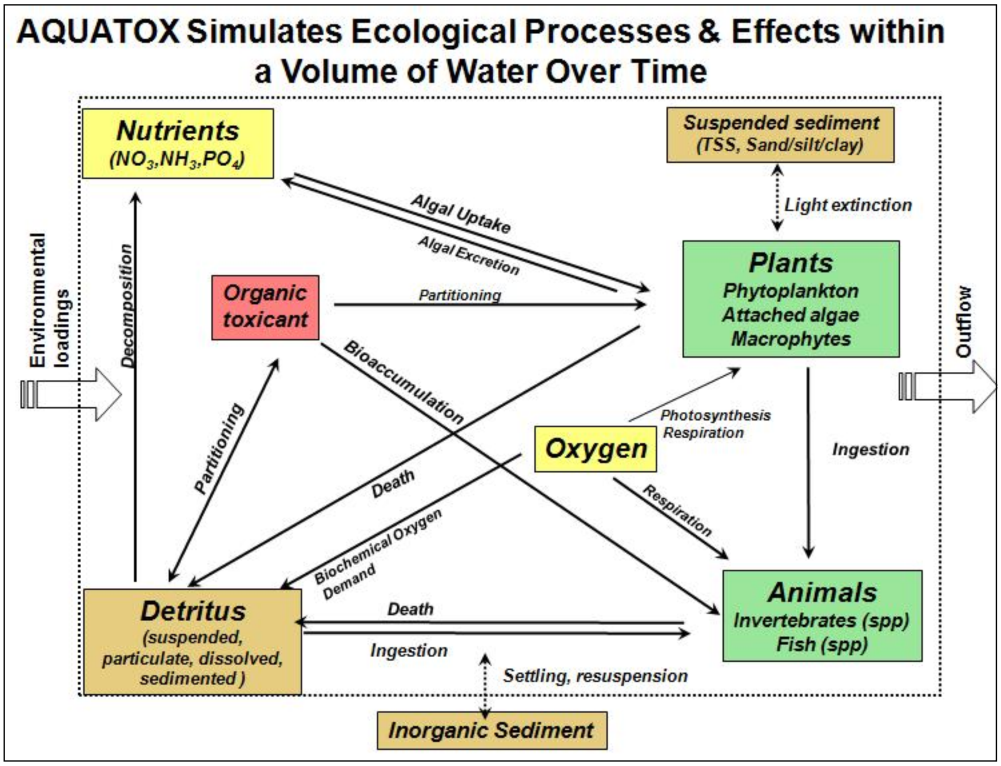
- Time-variable
  - variable-step 4th-5th order Runge-Kutta
    - usually daily reporting time step
    - can use hourly time-step and reporting
- Spatially simple unless linked to hydrodynamic model
  - thermal stratification
  - salinity stratification (based on salt balance)
- Modular and flexible
  - 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.

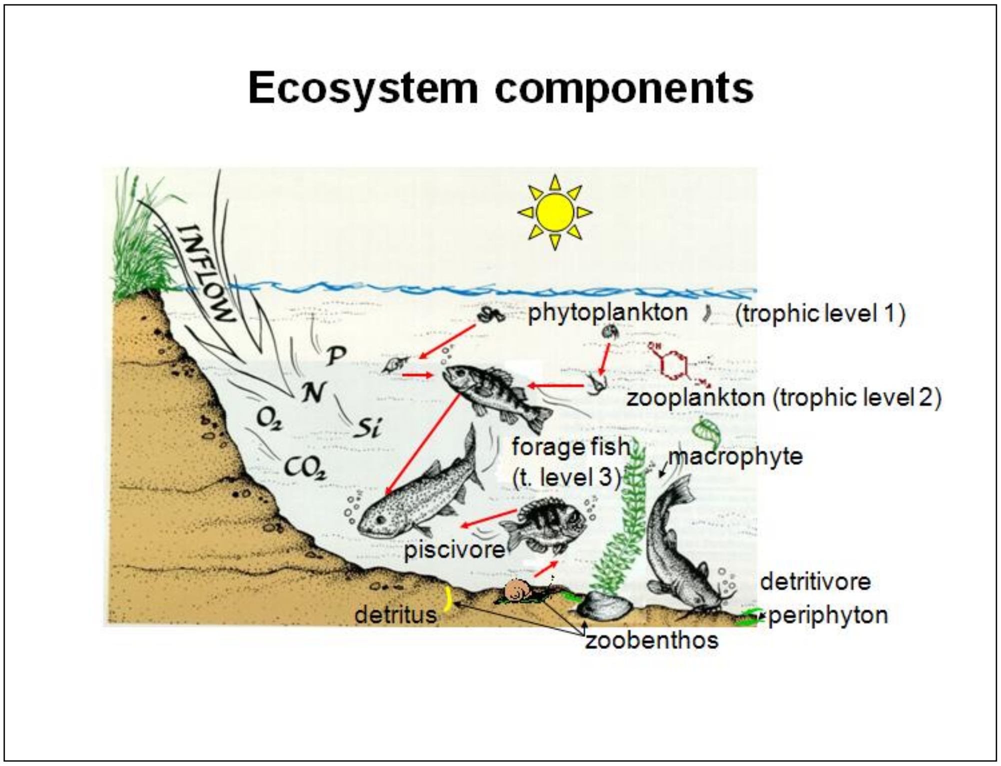
The model can simulate conditions with and without a perturbation in order to distinguish impacts. This means that a simulation doesn't have to be perfectly calibrated to evaluate an impact.


AQUATOX Simulates Ecological Processes & Effects within a Volume of Water Over Time
Nutrients
(NO_3,NH_3,PO_4)
Suspended sediment
(TSS, Sand/silt/clay)
Light extinction
Algal Uptake
Algal Excretion
Environmental loadings
Decomposition
Organic toxicant
Partitioning
Plants
Phytoplankton
Attached algae
Macrophytes
Outflow
Bioaccumulation
Partitioning
Photosynthesis
Respiration
Oxygen
Ingestion
Death
Respiration
Biochemical Oxygen Demand
Detritus
(suspended, particulate, dissolved, sedimented)
Death
Ingestion
Animals
Invertebrates (spp)
Fish (spp)
Settling, resuspension
Inorganic Sediment

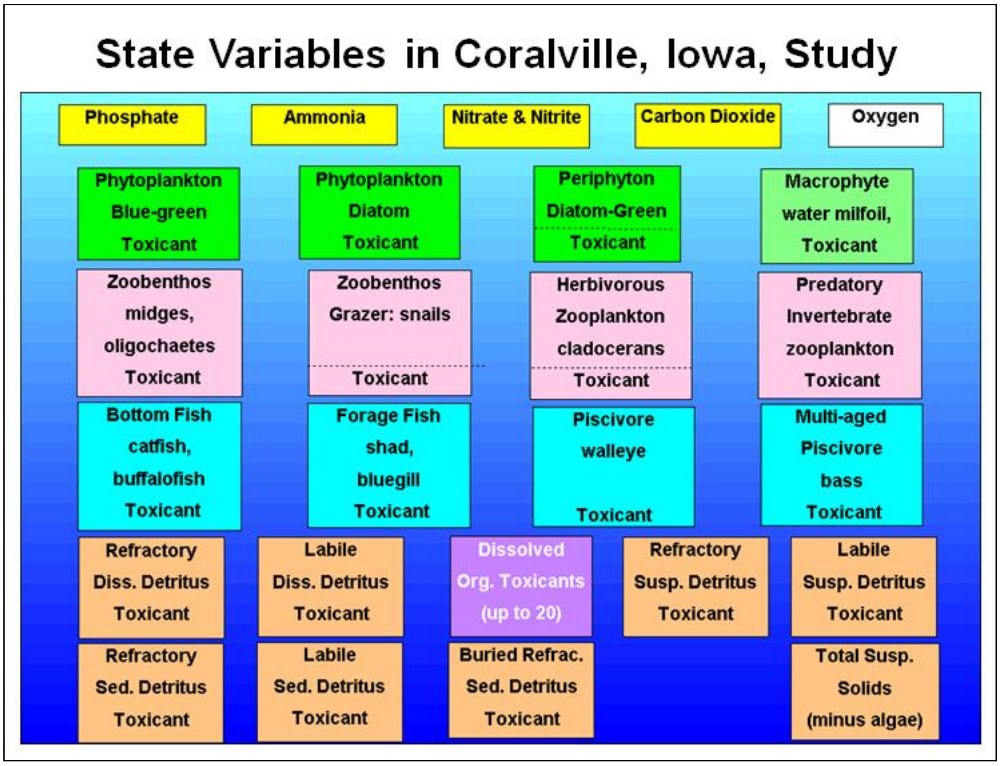
Processes Simulated

- 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.

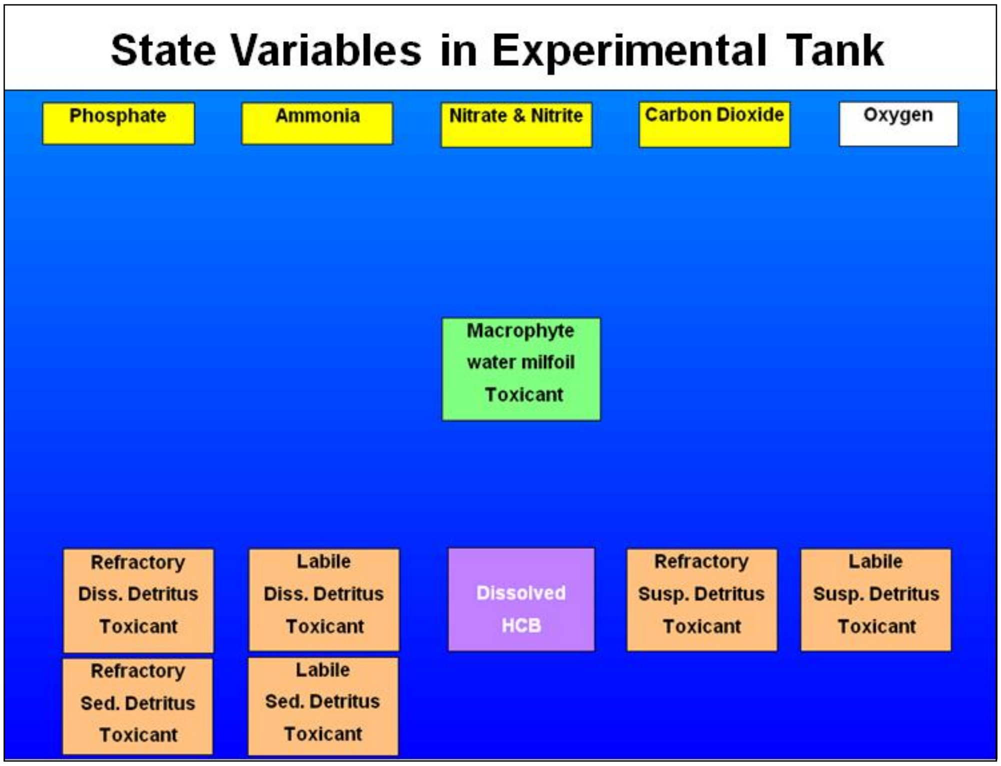


The ecosystem consists of abiotic and biotic components. Phytoplankton, periphyton, and macrophytes are the primary producers, fixing organic matter from nutrients and sunlight. As such they are the first trophic level. Zooplankton and many zoobenthos are primarily herbivores, thus they are the second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

AQUATOX Capabilities

(*Release 3 in red*)

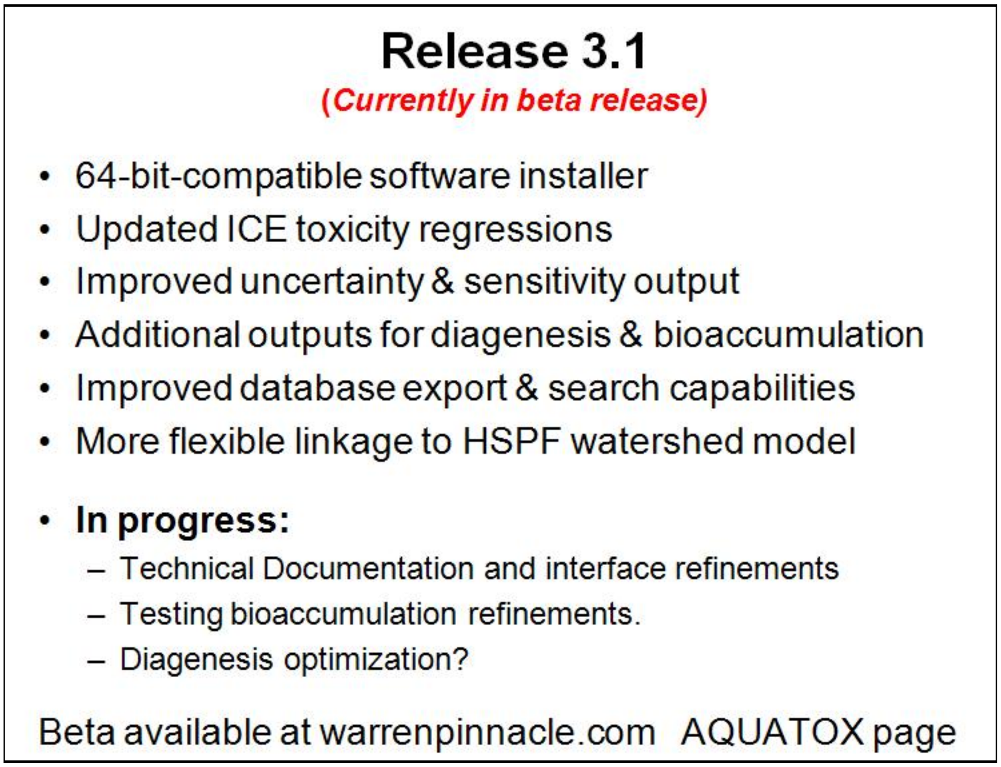
- Ponds, lakes, reservoirs, streams, rivers, estuaries
- Riffle, run, and pool habitats for streams
- Completely mixed, thermal stratification, or salinity stratification
- Linked segments, tributary inputs
- Multiple sediment layers with pore waters
- Sediment Diagenesis Model
- Diel oxygen and low 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.



Software Installer is 64-bit compatible

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

Added an "output to CSV" option for uncertainty runs so that complete results for every iteration may be examined. Also 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.

Demonstration 1

How is AQUATOX used? Overview of user-friendly graphical interface

- ❑ Installation Considerations
- ❑ The "APS" and "ALS" file units
- ❑ Looking at a few Parameters
- ❑ Libraries of Parameters
- ❑ Looking at Model Output vs. Observed
- ❑ Setup Screen
- ❑ Integrated Help-File and Users Manual

This demonstration 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.

Questions to answer on your own as we examine these 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?

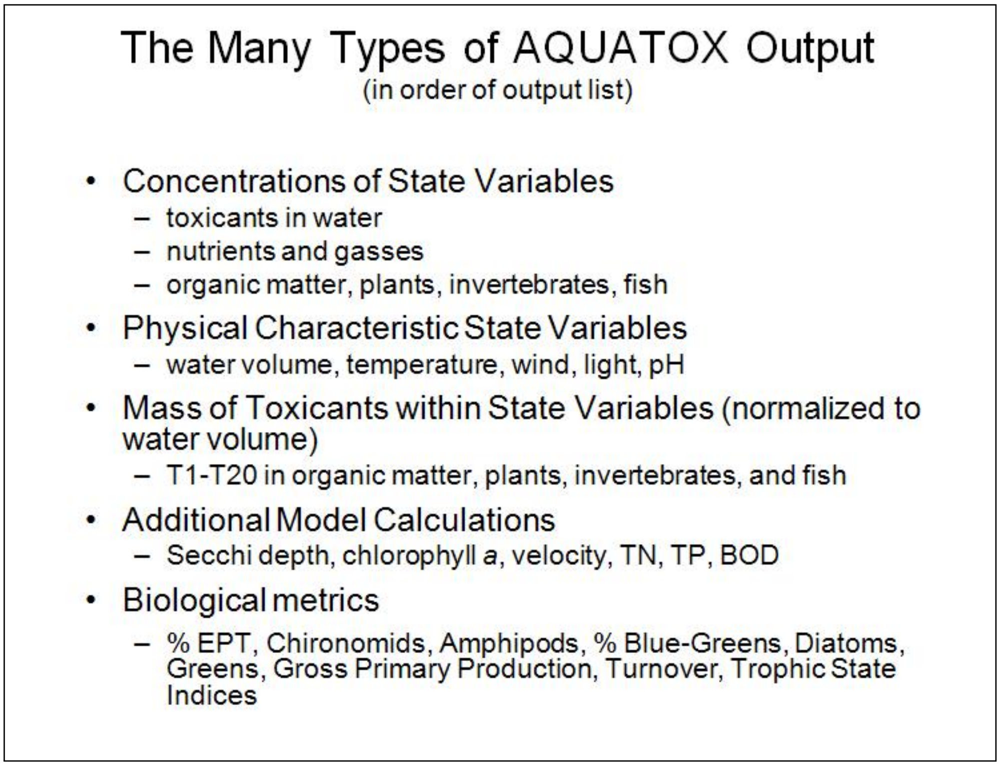
•What is the source of the esfenvalerate loadings?

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

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

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.



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.

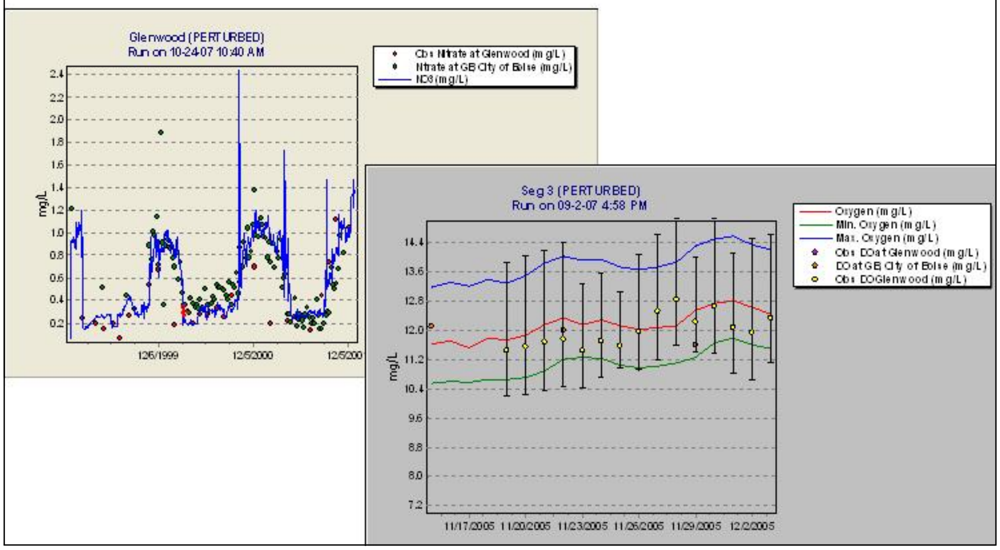
The Many Types of AQUATOX Output
(continued)

- Sediment diagenesis state variables
- Toxicant PPB
  - T1-T20 (PPB) in organic matter, plants, invertebrates, and fish
- Nitrogen and Phosphorus Mass Tracking Variables
- Bioaccumulation Factors
- Uptake, Depuration, and Bioconcentration Factors
- State Variable Rates
- Limitations to Photosynthesis
- Observed data imported by user

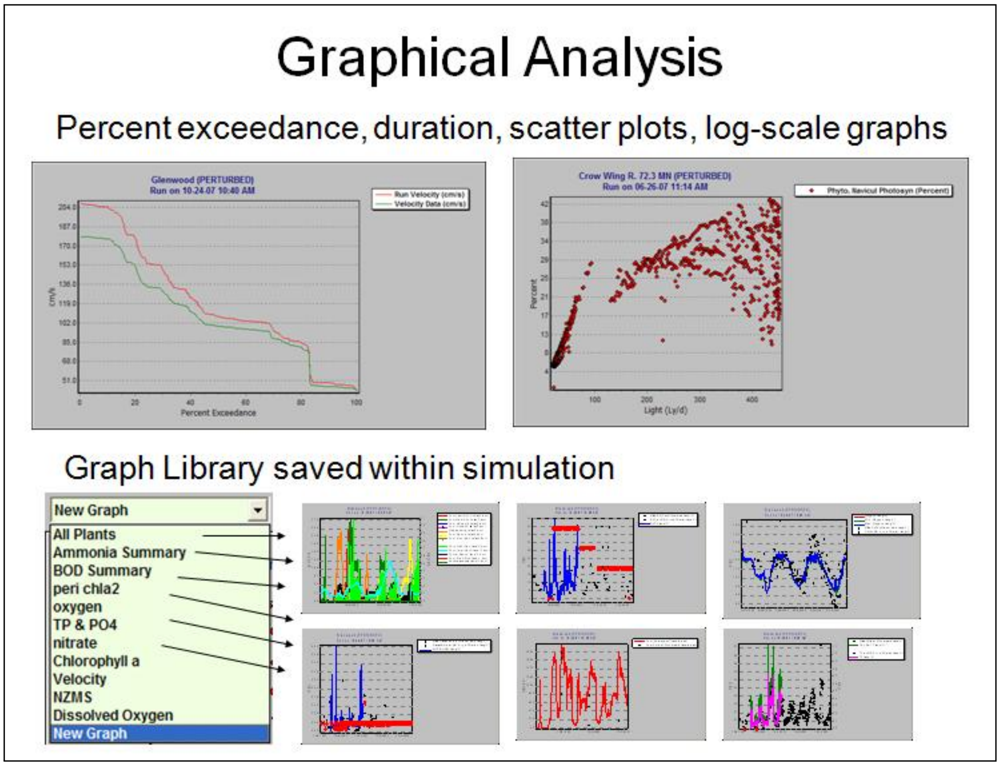
Output facilitates detailed analyses of simulated responses. Mass loadings and losses and mass balances are output for nutrients. K1, K2, and BCFs are output for toxicants. The ability to output in tabular and graphical form all the state-variable rates and the limitations to photosynthesis is especially powerful. Tabular data can also be easily exported to Excel.

Graphical Analysis

Compare observed data to model output



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

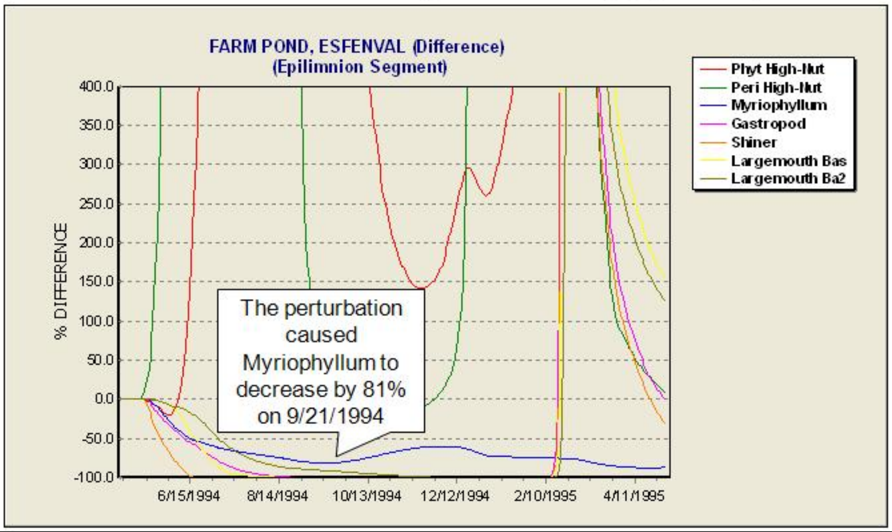


Fully integrated graphical output includes specialized graphs such as percent exceedance and duration graphs desired by decision makers.

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 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 biologically unimportant.

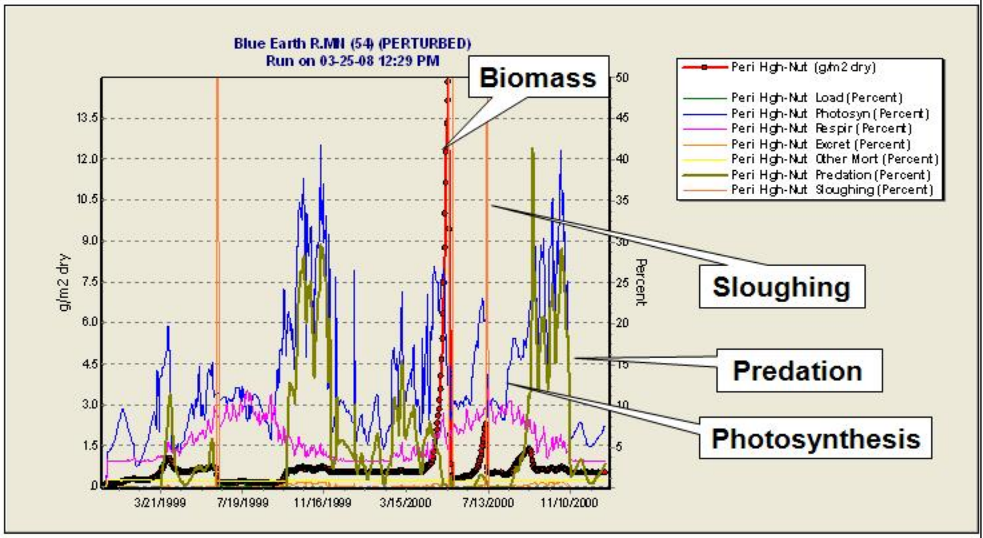
Process Rates

- 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

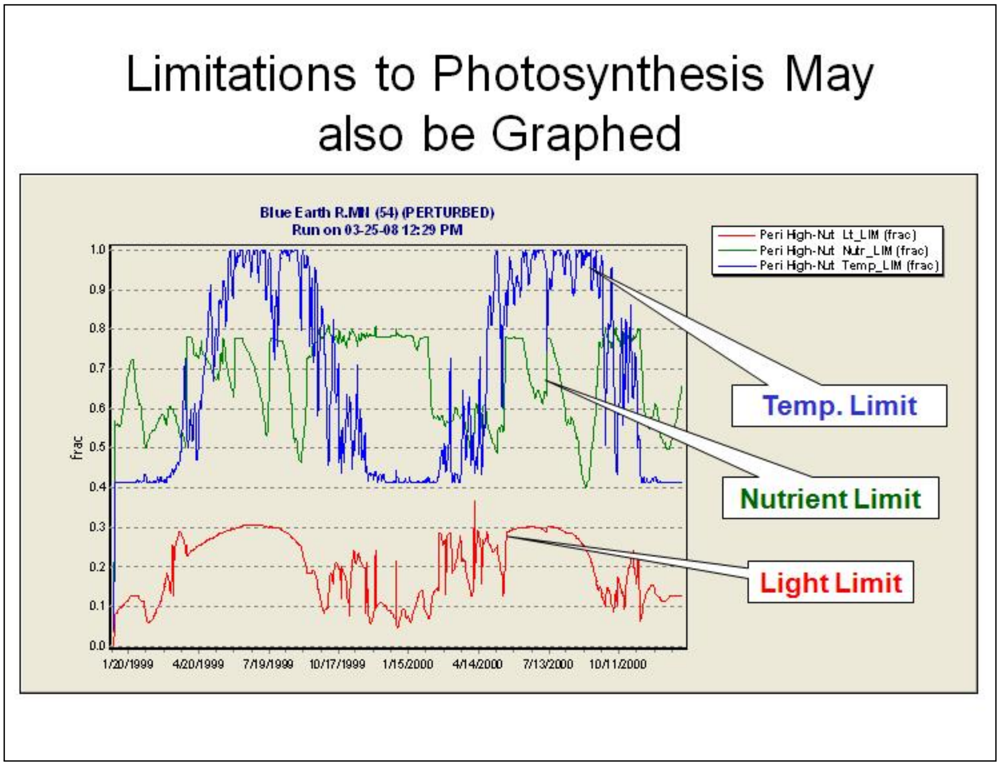


The red line with red circles represents the biomass. The user may wonder why there is such a large bloom of periphyton predicted in the second year. The answer maybe ascertained by examining the rates.

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 which drops down dramatically in the second year.

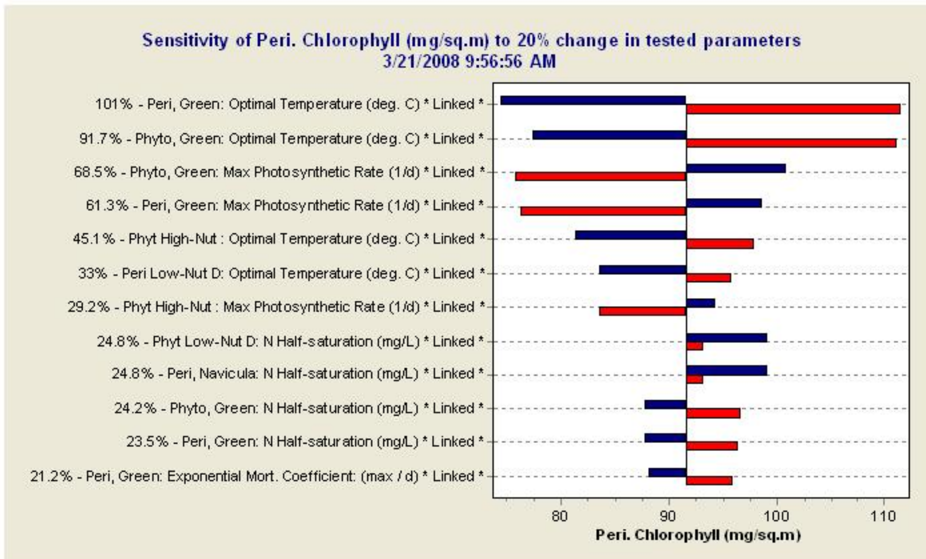
There are also three sloughing events worth noting in which periphyton is sloughed and transported downstream.



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

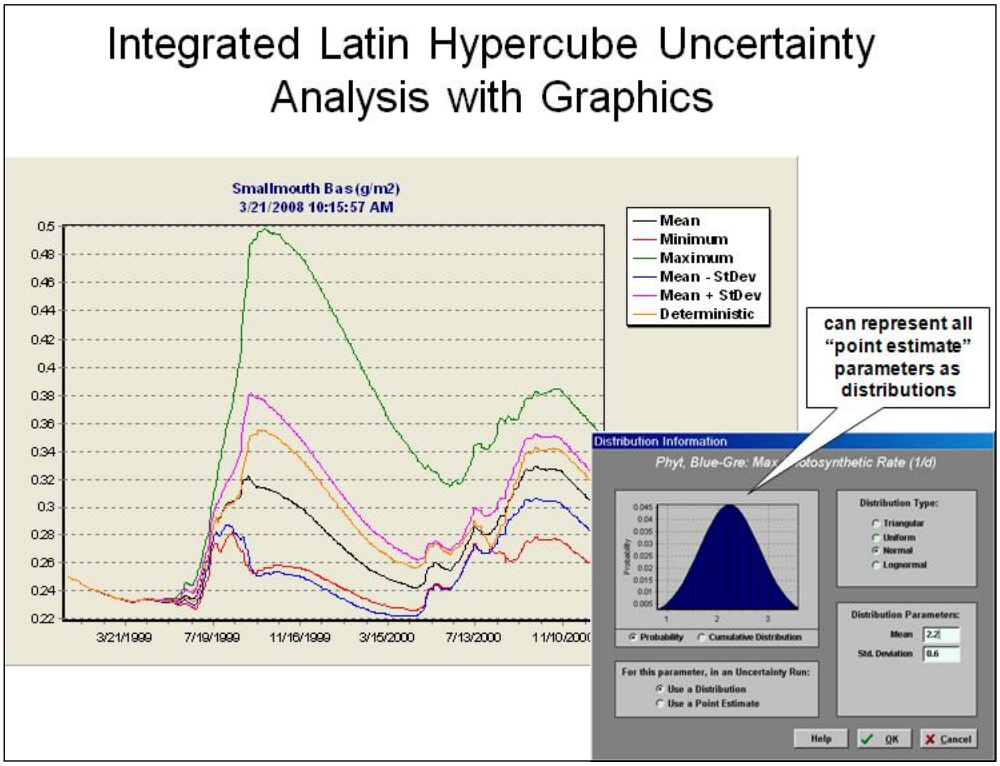
$$PProdLimit = LtLimit \cdot NutrLimit \cdot TCorr$$

Integrated Nominal Range Sensitivity Analysis with Graphics

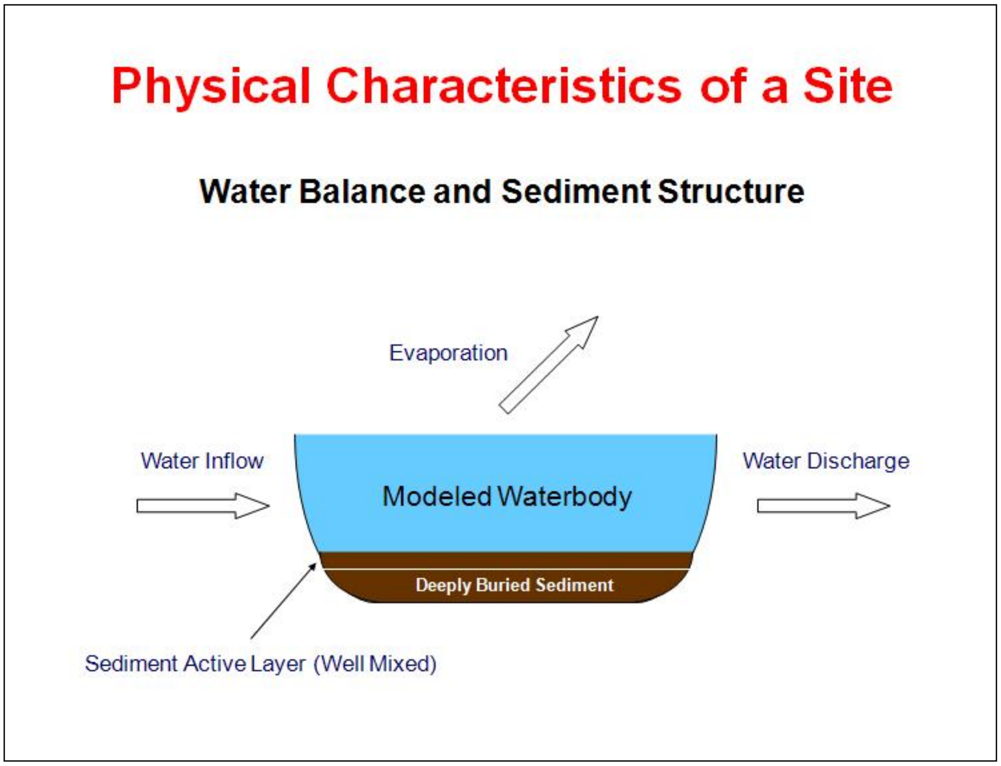


AQUATOX can automate a nominal range sensitivity analysis (also known as a "one-at-a-time" sensitivity analysis), in which multiple parameters are changed by a given percentage. The sensitivity of model output to the different perturbations can then be compared.

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.



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.

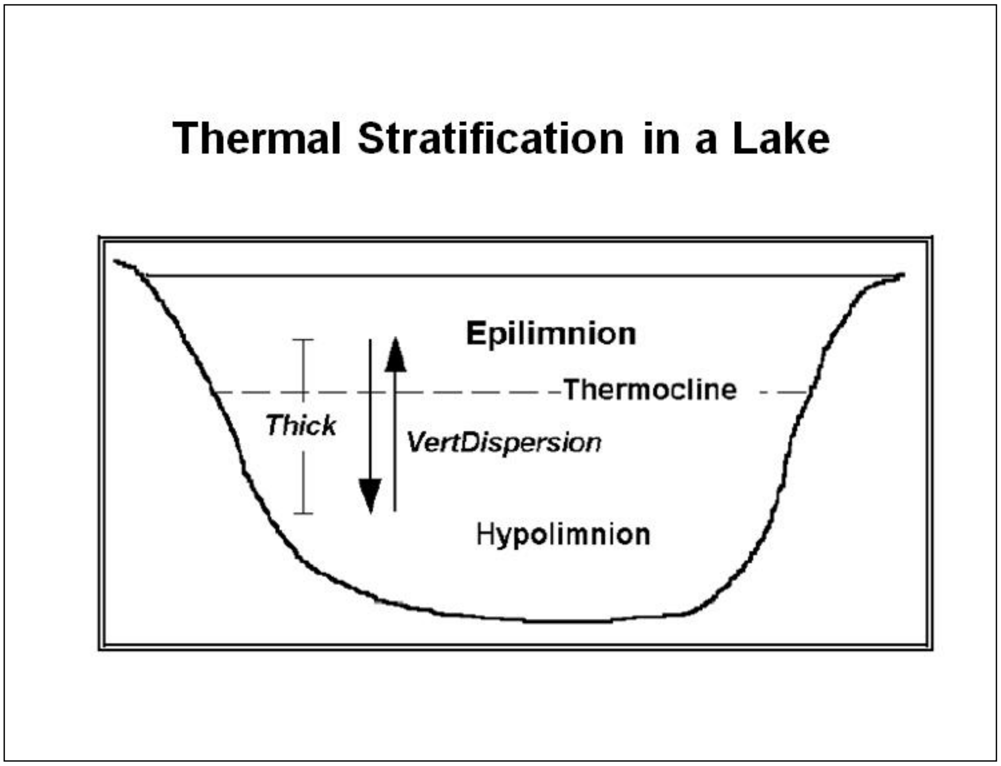


Water balance is defined as a function of inflow, evaporation, and discharge. We will discuss the various mechanisms for modeling water balance in a future slide. The modeled waterbody or river segment is assumed to be well mixed. Evaporation is a function of the site's surface area and the mean annual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

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

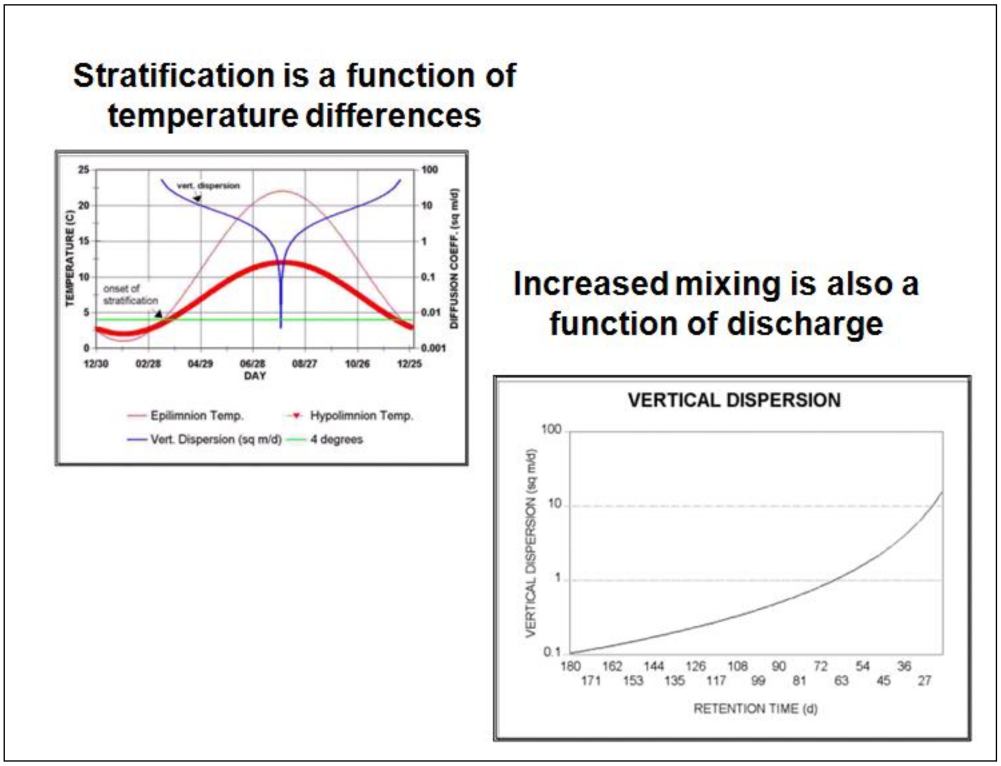
The bottom sediment includes an active layer and a deeply buried sediment layer that is not reactive with the overlying water unless scour reduces the active layer and the deeply buried sediment is exposed.

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



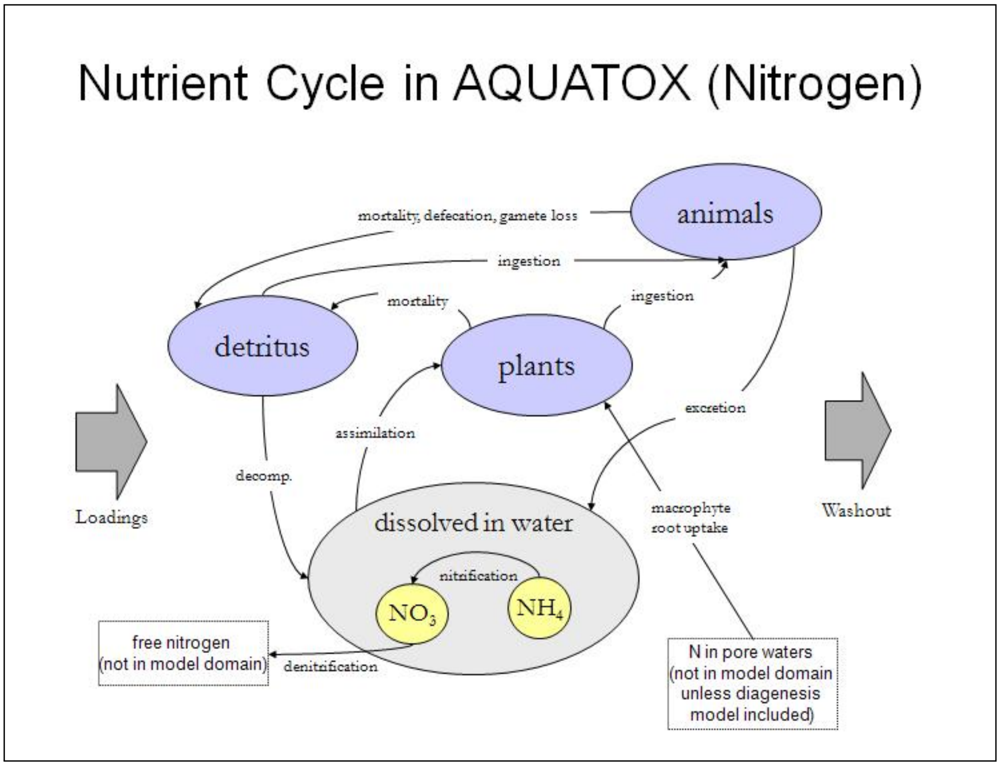
Thermal stratification is handled in the simplest form consistent with the goals of forecasting the effects of nutrients and toxicants. Lakes and reservoirs are considered in the model to have two vertical zones: epilimnion and hypolimnion; the metalimnion zone that separates these is ignored. Instead, 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). As a default, 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. However, stratification dates may also be specified by the user. Similarly, a temporally constant thermocline depth may be calculated or a time-series of thermocline depths may be specified by the user.



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.

High throughflow can also increase vertical mixing based on an empirical construct for Czech reservoirs (Straškraba 1973) .

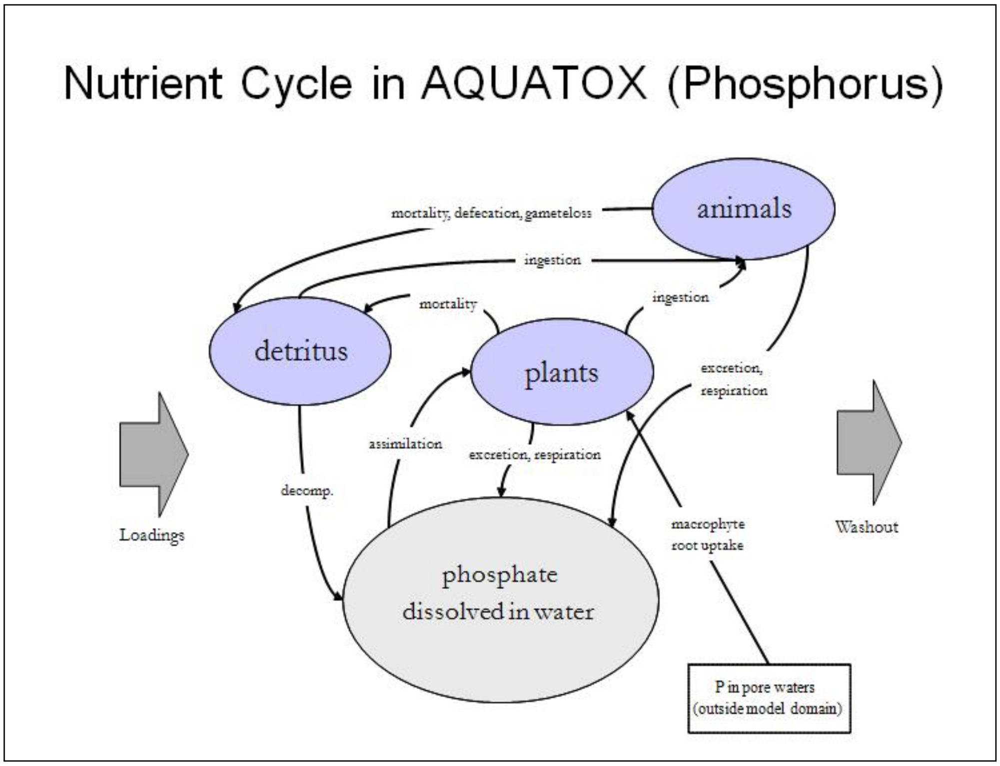


•While this graph looks complex, there is really a fairly straightforward cyclical nature to the movement of nutrients within AQUATOX. Nutrients are taken up into higher organisms through ingestion and assimilation , nutrients are released back into the water column through mortality, defecation, and gamete loss.

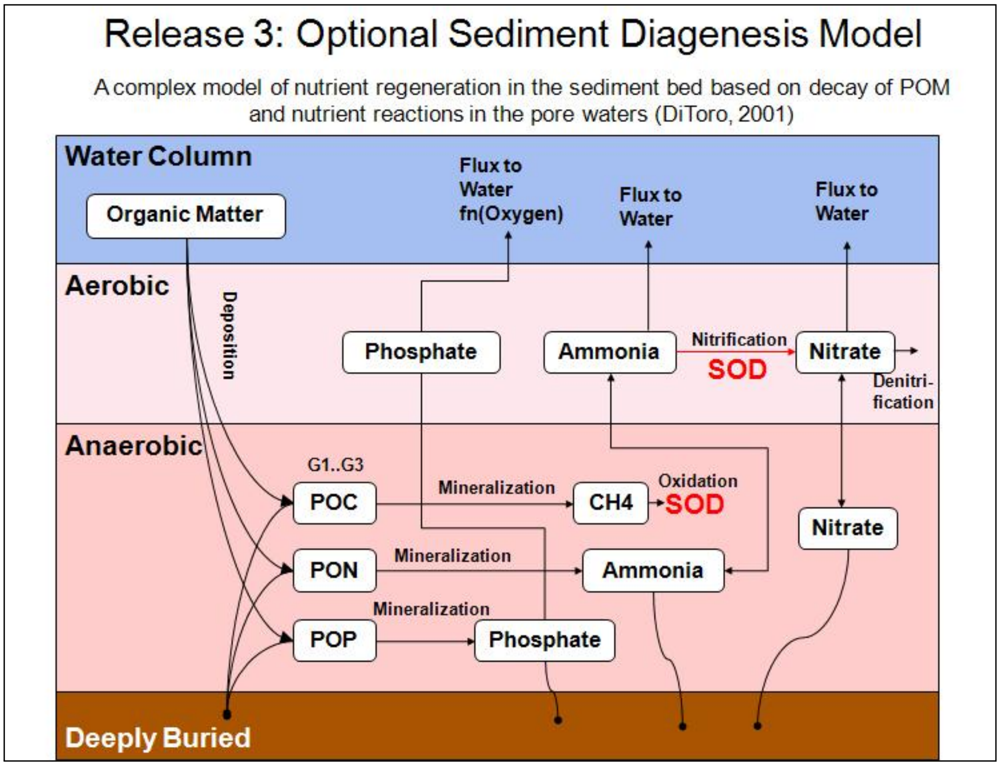
•Nutrients from animals and plants break down into various forms of detritus and then are returned to the water column through detrital decomposition.

•Un-ionized ammonia (NH3) is not modeled as a separate state variable but is estimated as a fraction of ammonia.

•The un-ionized form of ammonia is toxic to invertebrates and fish. Therefore, it is often singled out as a water quality criterion. Un-ionized ammonia is in equilibrium with the ammonium ion, NH4+, and the proportion is determined by pH and temperature



In addition to the pathways shown, Release 3 can simulated precipitation of $CaCO_3$ with sedimentation of sorbed P.



AQUATOX has been modified to include a representation of the sediment bed as presented in Di Toro's book on Sediment Flux Modeling (2001). This optional sediment submodel tracks the effects of organic matter decomposition on pore-water nutrients, and predicts the flux of nutrients from the pore waters to the overlying water column based on this decomposition. It is a more realistic representation of nutrient fluxes than the "classic" AQUATOX model. It includes silica, which will be modeled as a nutrient for diatoms in a later version.

The model assumes a small aerobic layer (L1) above a larger anaerobic layer (L2). For this reason, it is best to apply this optional submodel in eutrophic sites where anaerobic sediments are most likely to occur.

Key Points: Diagenesis Model

- Two sediment layers: thin aerobic and thicker anaerobic
- When oxygen is present, the diffusion of phosphorus from sediment pore waters is limited
  - Strong P sorption to oxidated ferrous iron in the aerobic layer (iron oxyhydroxide precipitate)
  - Under conditions of anoxia, phosphorus flux from sediments dramatically increases.
- Sediment oxygen demand (SOD) is a function of specific chemical reactions following the decomposition of organic matter
  - methane or sulfide production
  - nitrification of ammonia

Sediment Diagenesis Model: Simplifying Assumptions

- Model assumes a depositional environment (no scour is modeled).
- Two layers of sediment are modeled.
- Aerobic (top) layer is thin
- Model is best suited to represent predominantly anaerobic sediments.
- Deposition of particulate organic matter moves directly into Layer 2.
- The fraction of POP and PON within defecated or sedimented matter is assumed equal to the ratio of phosphate or nitrate to organic matter for given species.
- All methane is oxidized or lost.

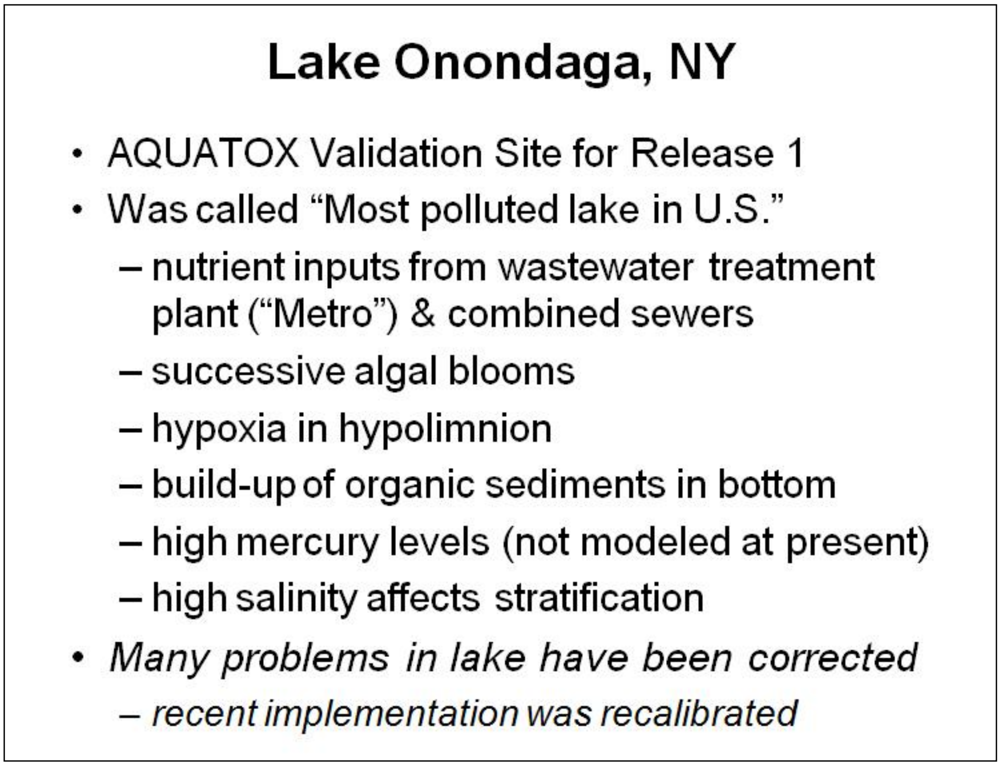
Nutrient Effects on Simulations

- Direct effects on algal growth rates
  - Maximum growth rates often limited by nutrients
  - Degree of limitation may be tracked and plotted
- Indirect repercussions throughout the foodweb due to bottom-up effects
- Light climate changes due to algal blooms
- Algal composition will be affected
- Decomposition of organic matter affects oxygen concentrations

Applications in Nutrient Analysis

- Lake Onondaga, NY
- Rum, Blue Earth, and Crow Wing Rivers, MN
- Cahaba River, AL
- Lower Boise River, ID
- Lake Tenkiller, OK
- Florida streams

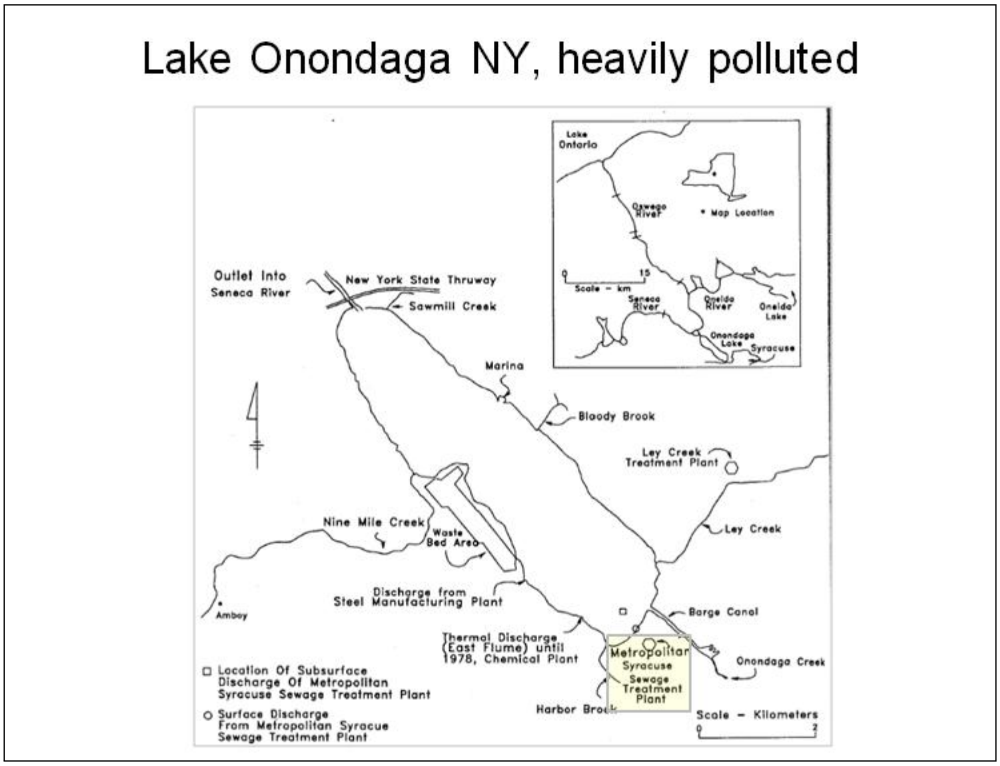
We will touch on several nutrient applications in the course of the next several sections.



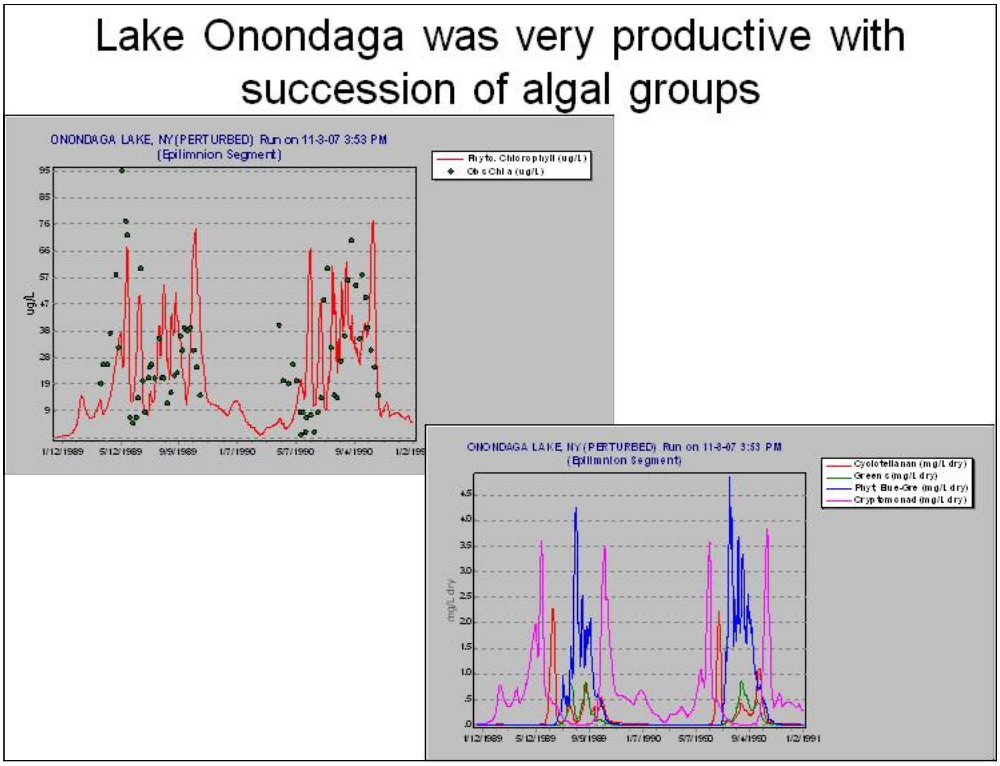
"Lake Onondaga is arguably the most polluted lake in the United States" according to Effler (1996) in the preface to his comprehensive book, which serves as the primary reference for the following information and data on the lake. The shore of this lake in central New York State was industrialized before 1800, and over the last hundred years at least thirty different chemicals were produced from nearby salt and limestone deposits. Unfortunately, the lake was a convenient dumping ground for waste products. Production of soda ash resulted in waste beds as much as 21 m deep and 8.1 km^2 in area along 30% of the lake shore; the wastes include NaCl and $CaCl_2$ that easily leach into the lake. The salinity of the lake was around 3‰ (parts per thousand) prior to closure of the soda ash plant in 1986; by 1990 the salinity had decreased to 1.3‰. Nevertheless, this salinity creates unusual density gradients and intense stratification of the lake. A chlor-alkali plant produced NaOH and Cl by electrolysis, using Hg as the cathode. From 1946 to 1970 as much as 75,000 kg of Hg were discharged into the lake. Aside from an advisory against eating fish from the lake, the high mercury levels may have adversely affected the functioning of the lake ecosystem.

Until recently, the lake was a receptacle for most of the domestic waste and urban runoff from Syracuse and the surrounding area. Prior to 1960 untreated and poorly treated sewage was discharged directly to the lake. In 1960 the Metropolitan Sewer District (METRO) primary treatment plant was completed; in 1979 it was upgraded to secondary treatment; and in 1981 tertiary treatment (removal of phosphorus) was instituted. By design, there was little reduction in ammonia in the sewage effluent. Most troubling were the combined sewer overflows (CSOs) that carried storm water and raw sewage into tributary creeks about 50 times a year. Nearly 20% of the annual inflow into the lake is from METRO, which complicates a proposed bypass to the Seneca River below the outlet.

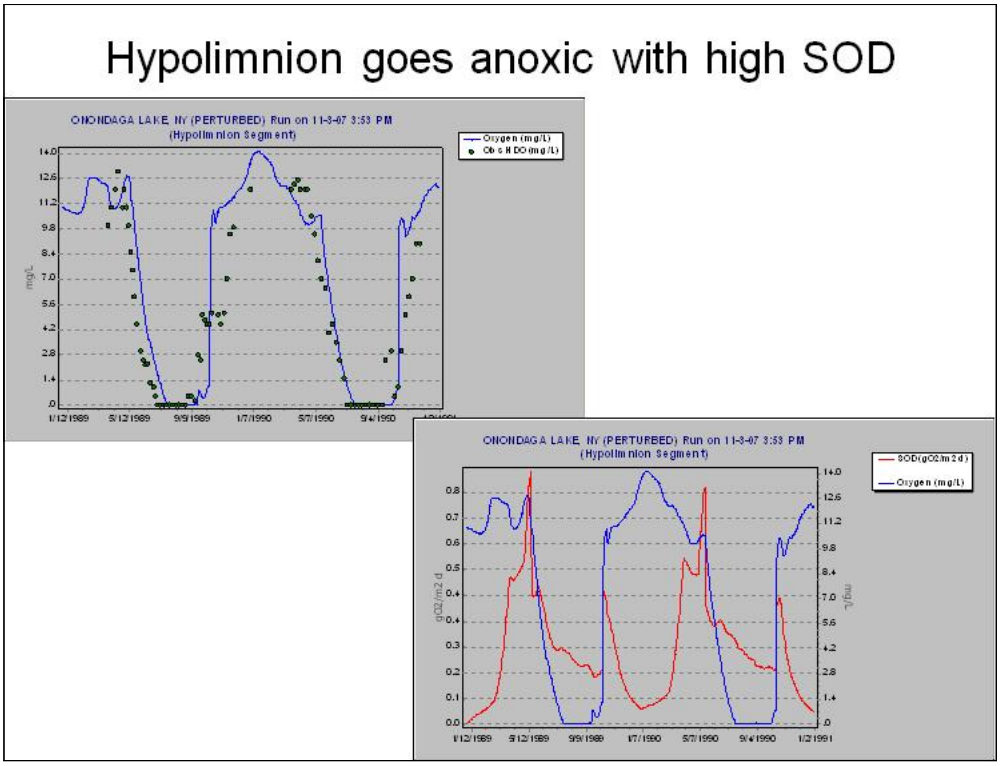
Recently AQUATOX was calibrated to current conditions, including invasive zebra mussels and significantly reduced pollutant loads. The examples given here are based on conditions that prevailed in 1989-1990.



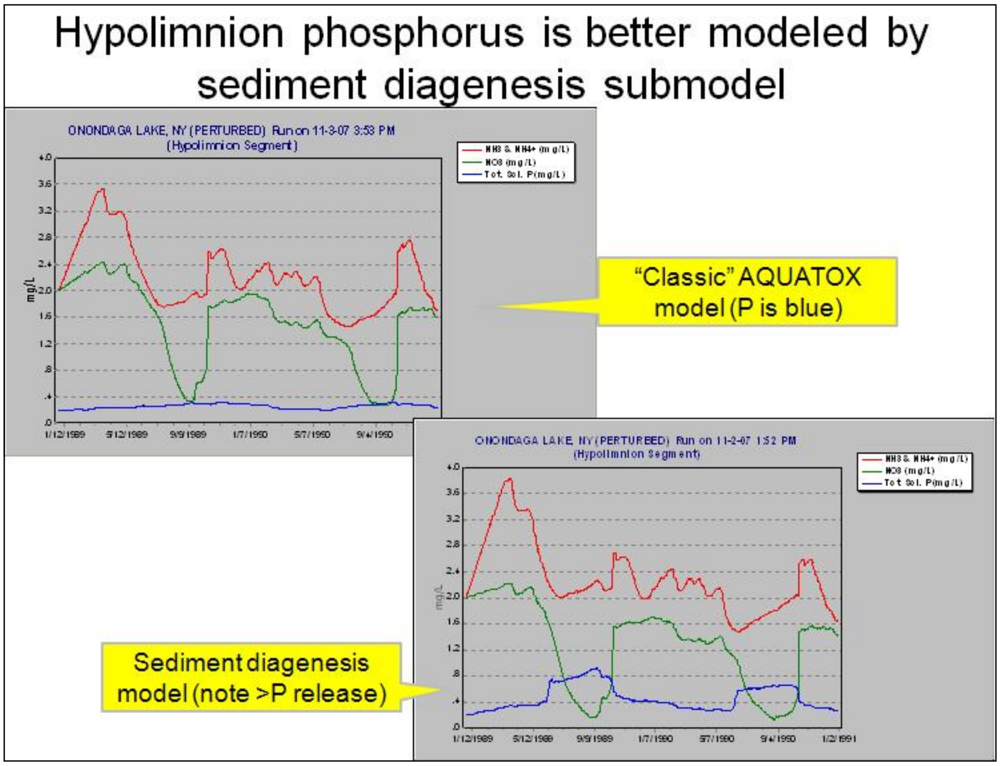
Historically, a number of non-point and point sources contributed to the pollution.



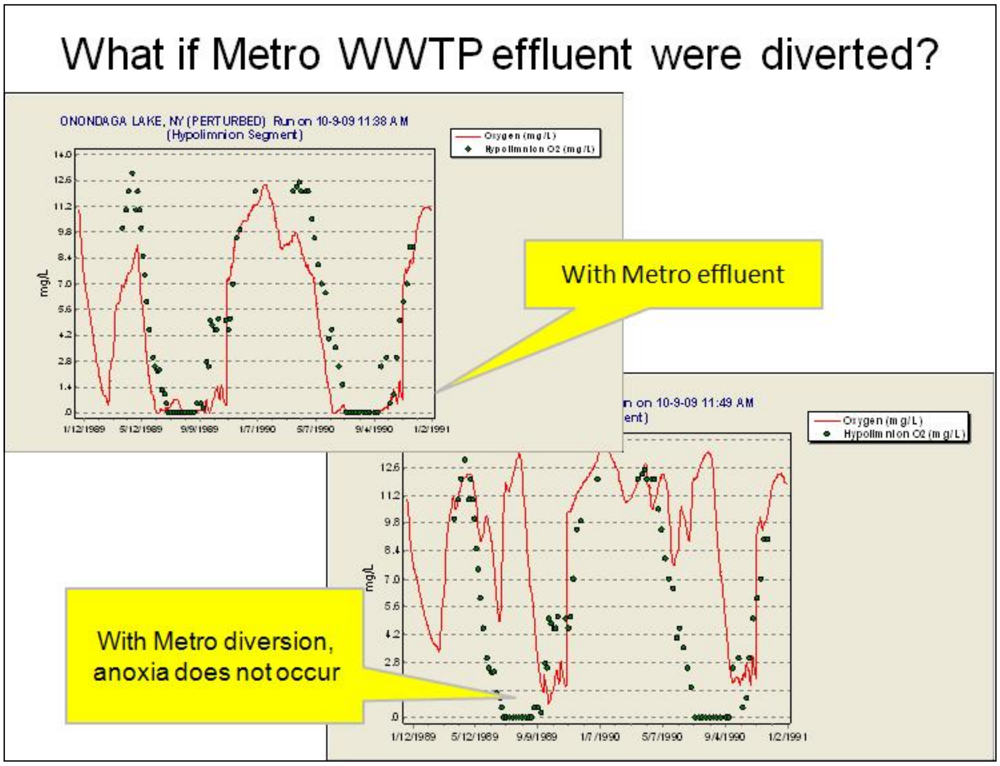
This has now changed with reductions in nutrient loadings and the invasion of zebra mussels.



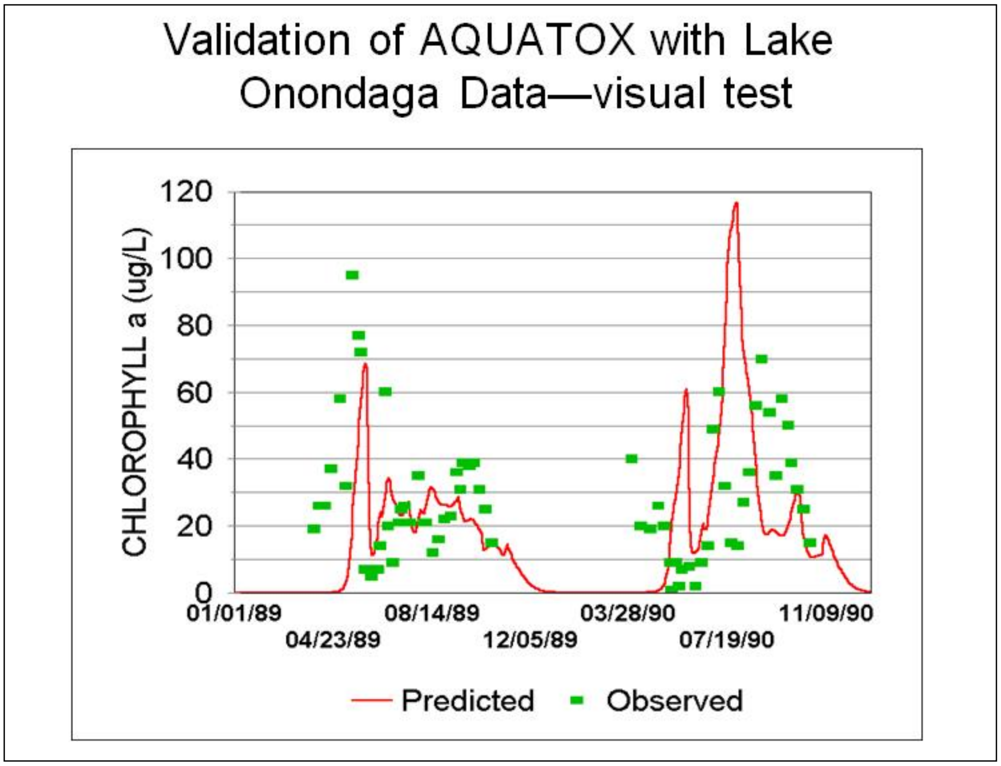
Observed data are shown as circles in the above graph while the AQUATOX simulation is the blue line. Simulated sediment oxygen demand is shown in red.



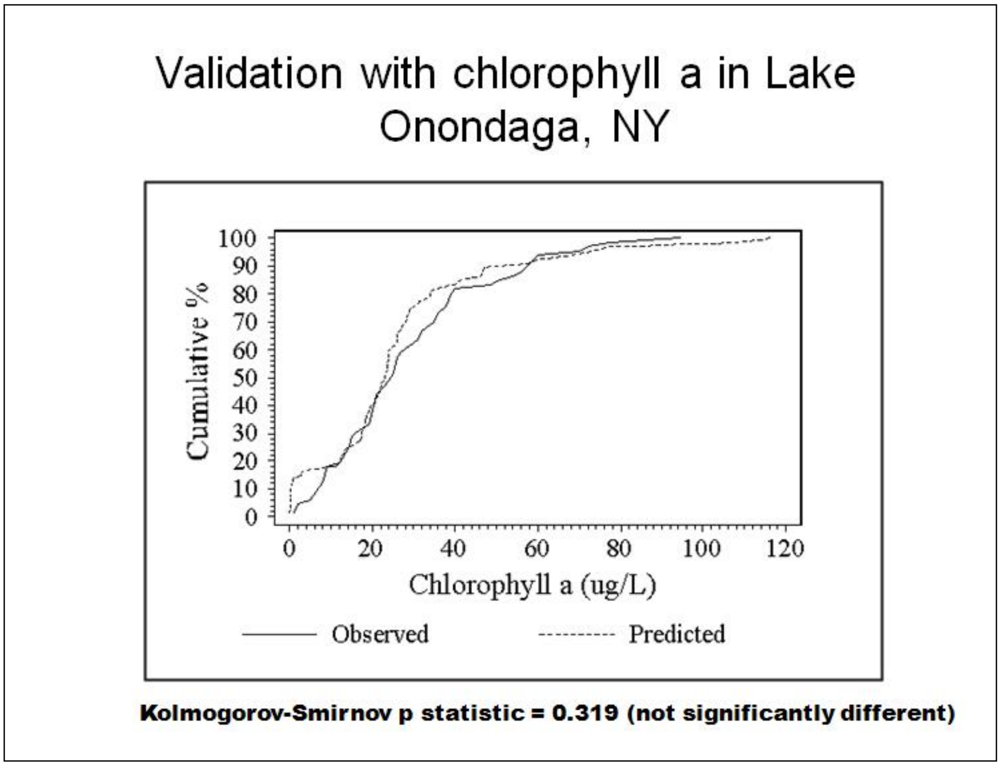
These images are for Onondaga Lake, NY. The diagenesis submodel also had a dramatic effect on the modeling of sediment oxygen demand from the Tenkiller Lake OK sediments. It was nearly impossible to calibrate dissolved oxygen in the Tenkiller hypolimnion without the diagenesis submodel , but with the submodel the simulation calibrated without much effort.



For example, what might be the effects on dissolved oxygen be if the highly nutrient-enriched WWTP discharge into Onondaga Lake were eliminated (one possible management option)? AQUATOX predicts a significant decrease in the magnitude and duration of the hypoxia.



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.

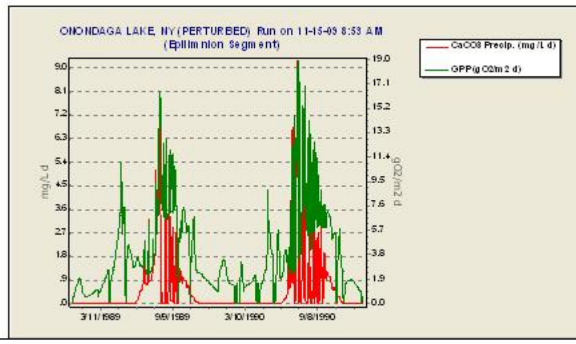


U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports. Washington, DC.

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.

Release 3 Addition: Calcium Carbonate Precipitation

- Predicted as a function of pH and algal type
  - When pH exceeds 7.5, precipitation is predicted
  - Precipitation rate is dependent on photosynthesis rate (gross primary production) in some, but not all, algae
- $CaCO_3$ sorbs phosphate from the water column



At high pH CaCO3 comes out of solution, precipitates, and takes PO4 along with it. This process is mediated by algae, so precipitation parallels photosynthesis (shown here as Gross Primary Production).

Modeling Phytoplankton

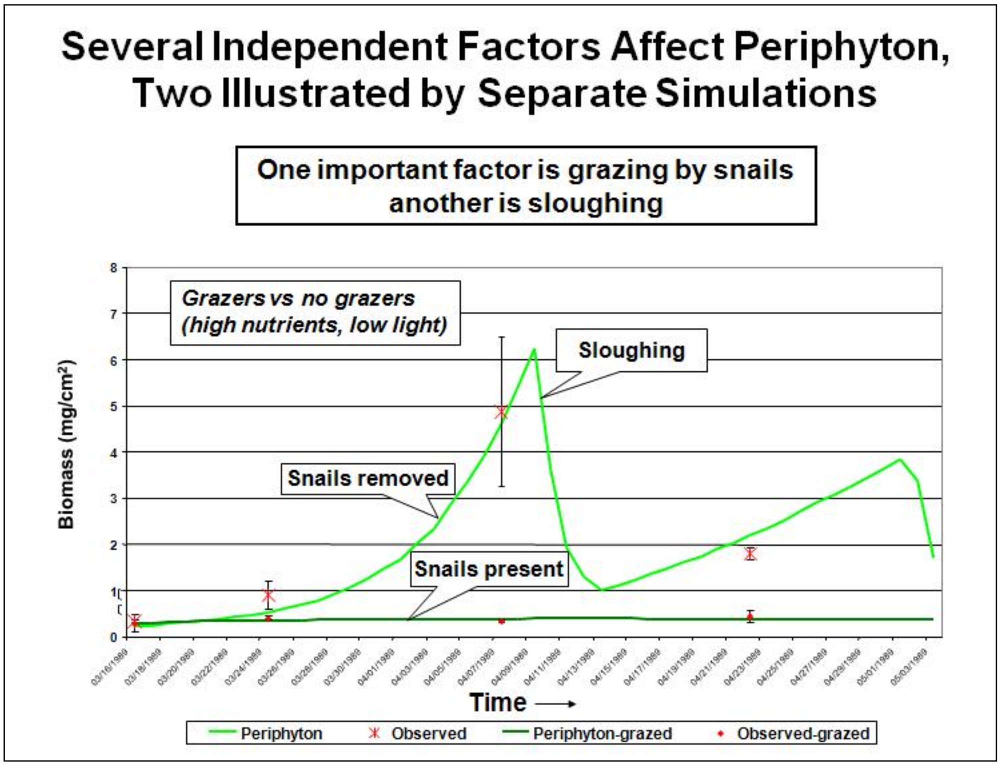
- Phytoplankton may be greens, blue-greens, diatoms or “other algae”
- Subject to sedimentation, washout, and turbulent diffusion
- In stream simulations, assumptions about flow and upstream production are important

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

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.



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.

Modeling Macrophytes

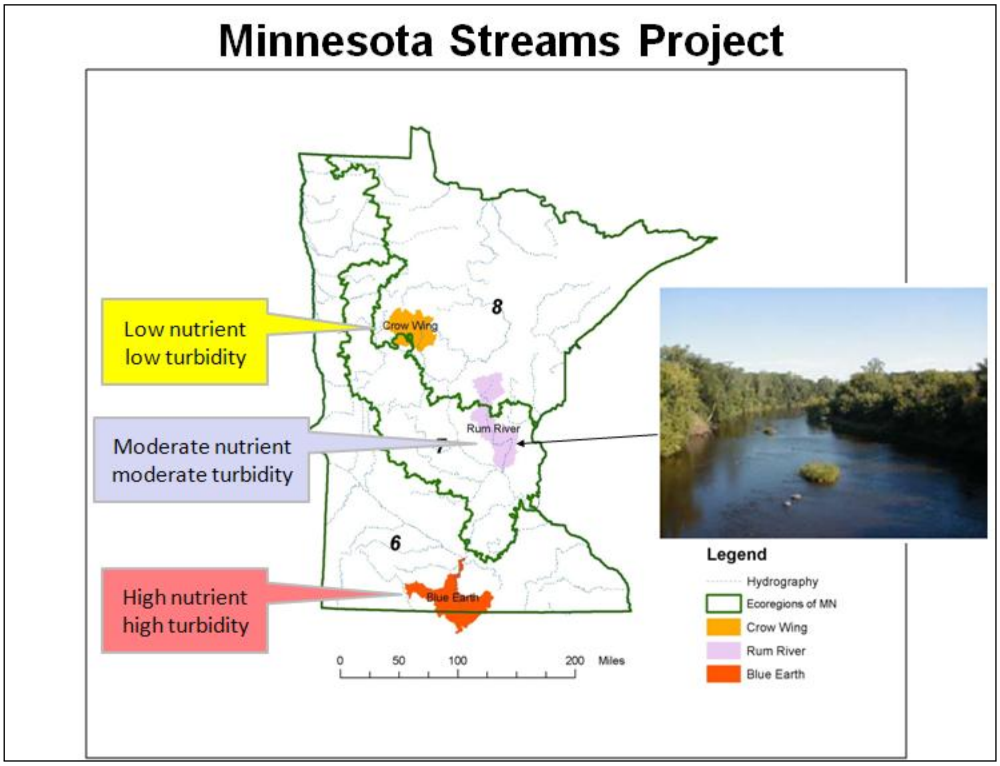
- Macrophytes may be specified as benthic, rooted-floating, or free-floating
- Macrophytes can have significant effect on light climate and other algae communities
- Root uptake of nutrients is assumed and mass balance tracked
- May act as refuge from predation for animals
- Leaves can provide significant 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.

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



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 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.

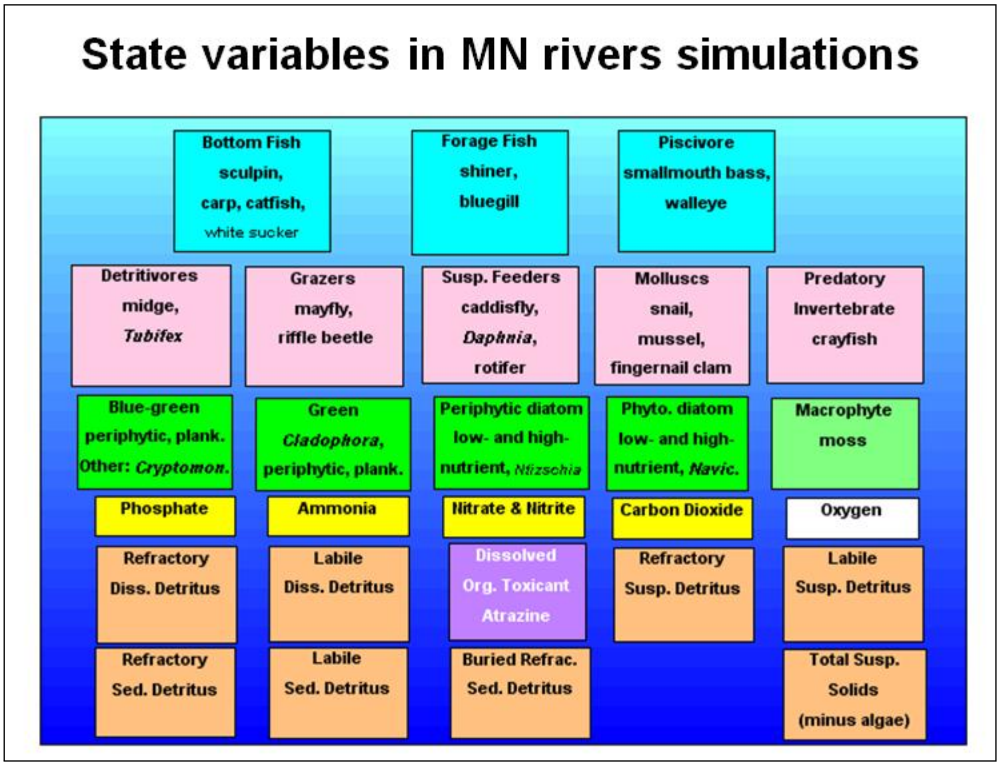
Calibration Strategy for Minnesota Rivers

- 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

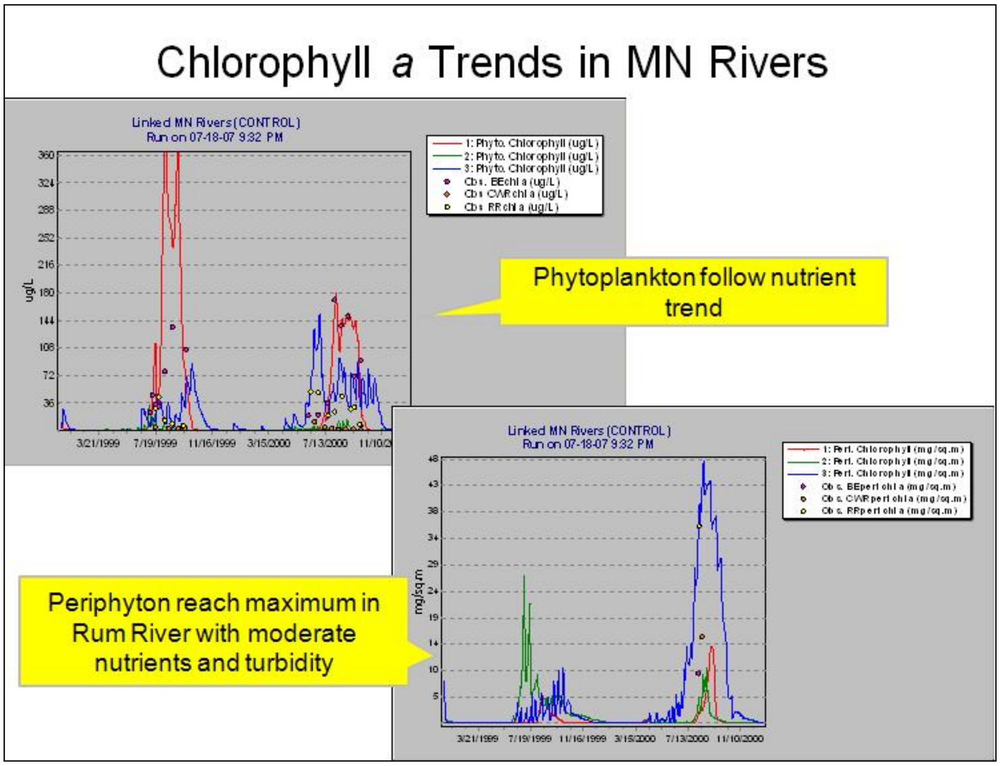
First the model was calibrated against observed data for the Blue Earth River, then the same parameter set was used to simulate the Crow Wing River. Adjustments were made to parameters, especially for the low-nutrient algae, until a suitable fit was obtained, and then the new values were used to simulate 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.



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.



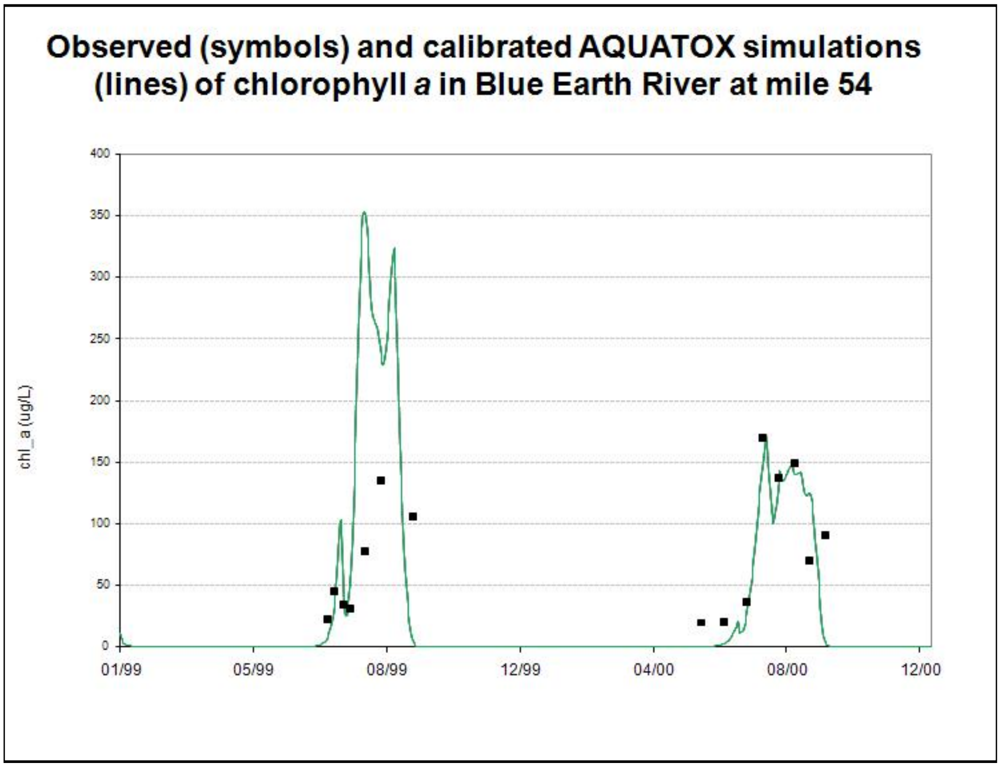
In general the phytoplankton biomass reflected the nutrient gradient.

In contrast, periphyton was affected by turbidity and flow as well nutrients.

Red lines: Blue Earth River

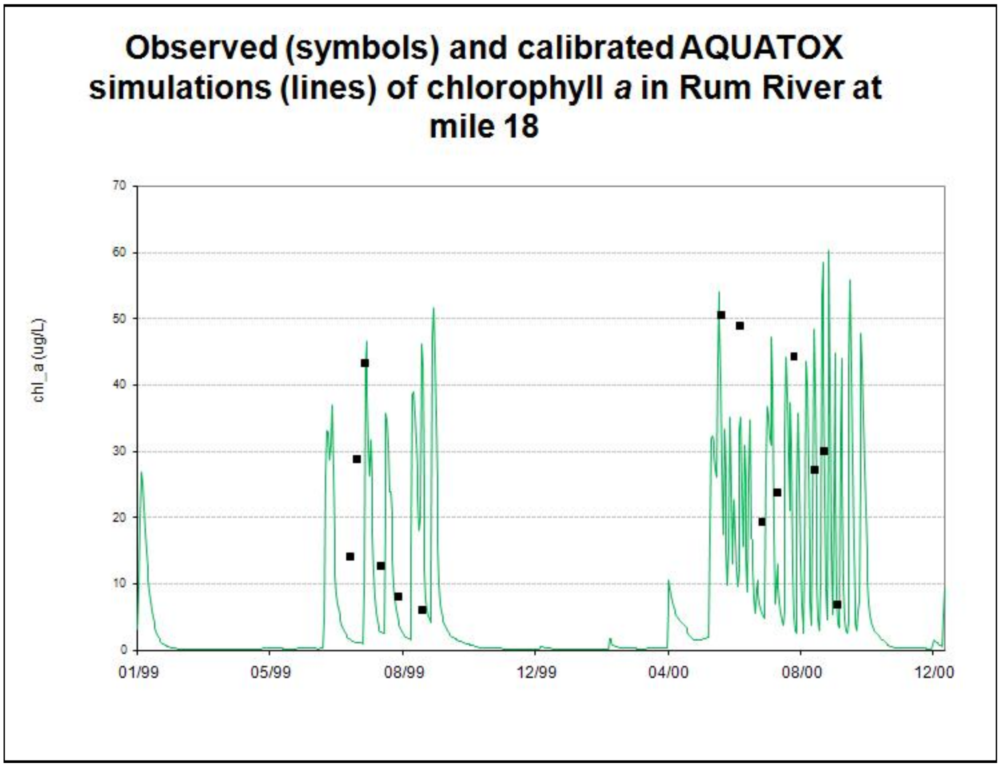
Blue lines: Rum River

Green lines: Crow Wing River

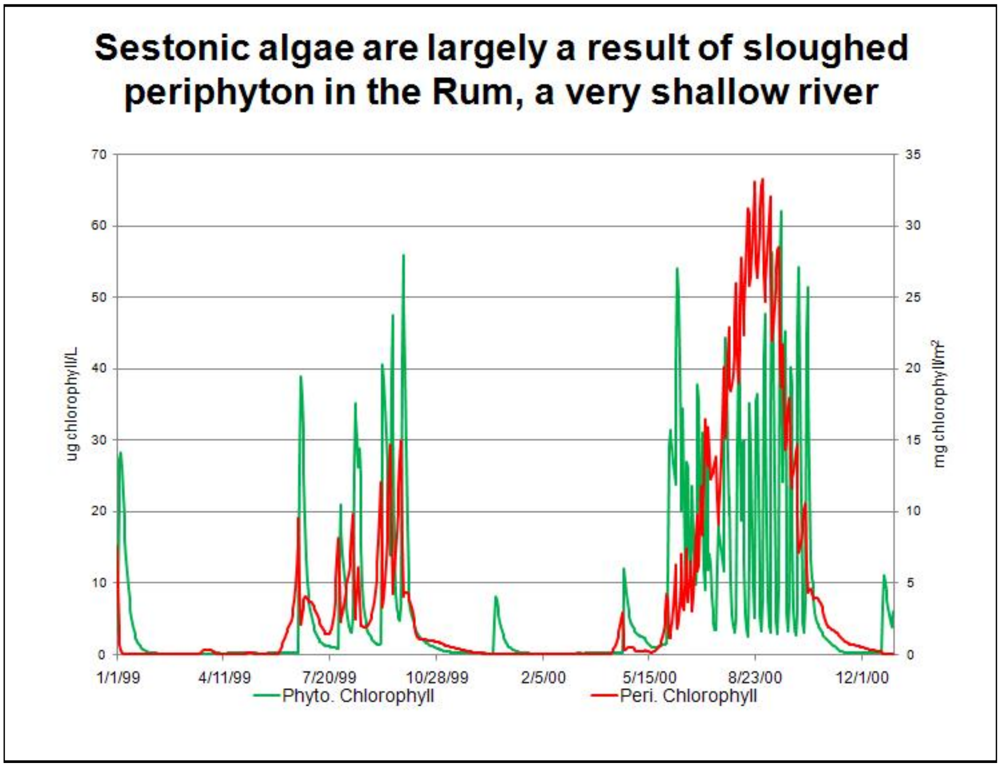


The Blue Earth River is in a highly cultivated agricultural watershed, with very high nutrient and sediment loads.

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

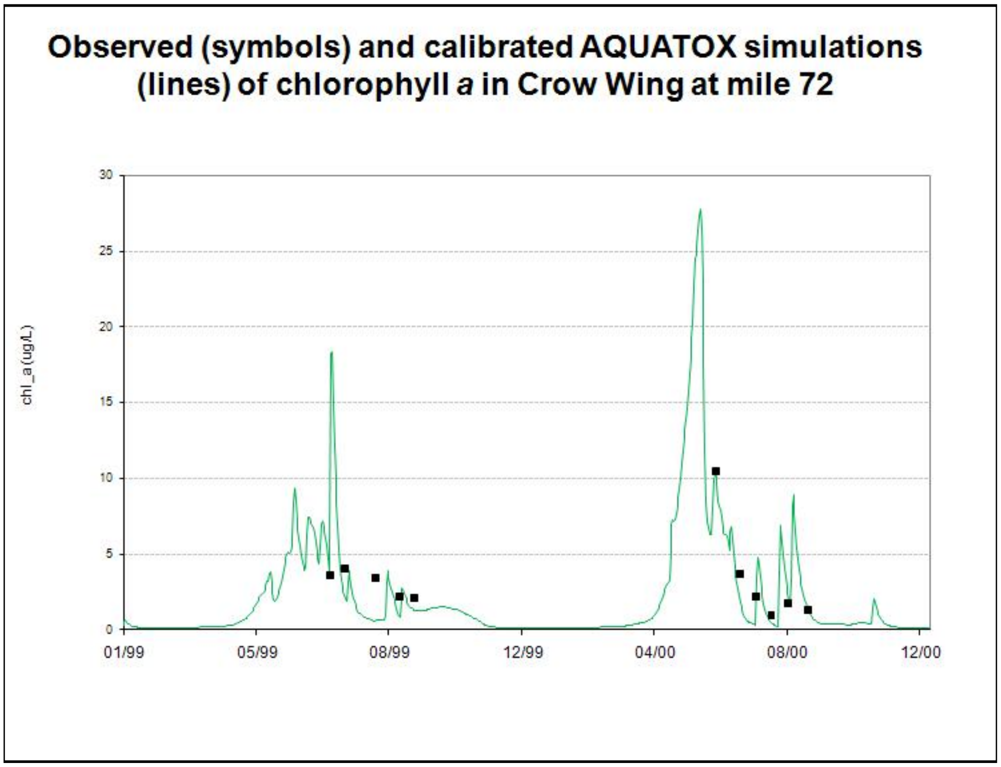


Rum River is moderately impacted by nutrients and turbidity, but is also very shallow and its flow is flashy.



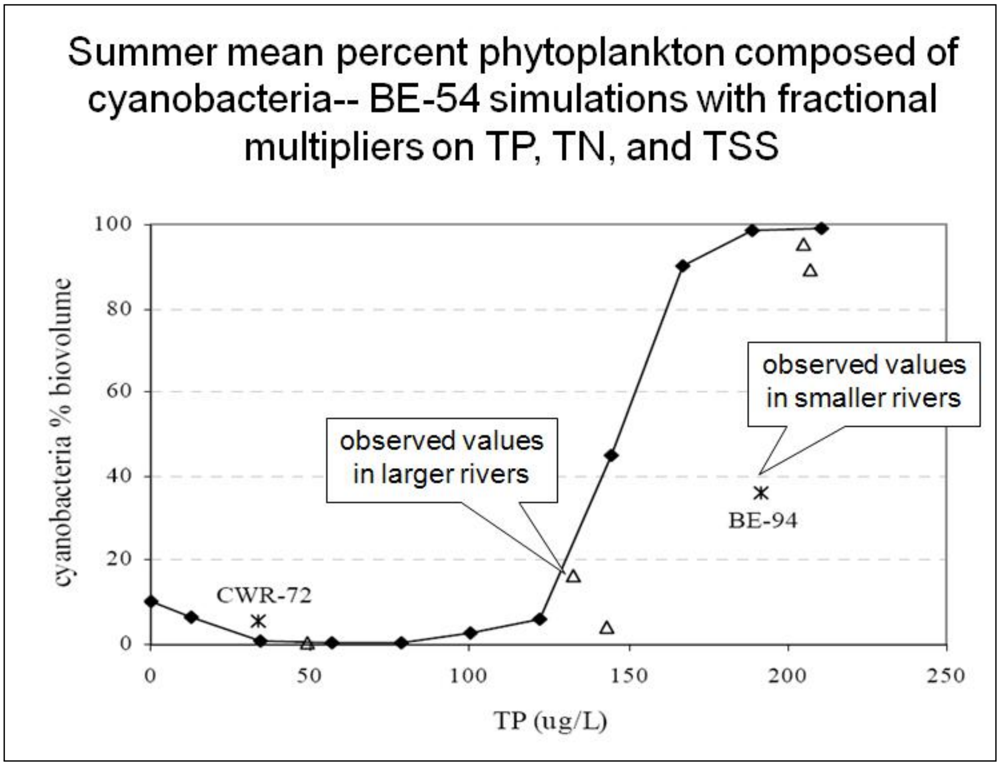
Periphyton may slough or be physically scoured, contributing to the suspended algae; this may be reflected in the chlorophyll *a* observed in the water column. Periphyton may be linked to a phytoplankton compartment so that sestonic chlorophyll *a* results reflect the results of periphyton sloughing. 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.

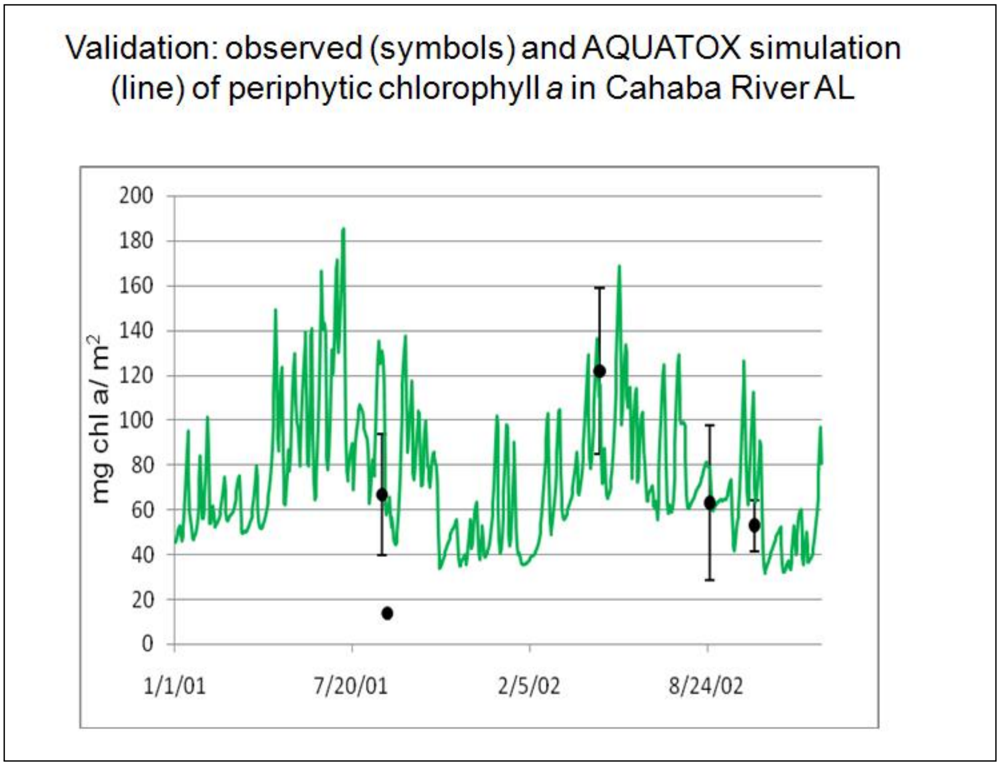


Crow Wing River is in a mostly forested watershed, and is low in both nutrients and sediments.

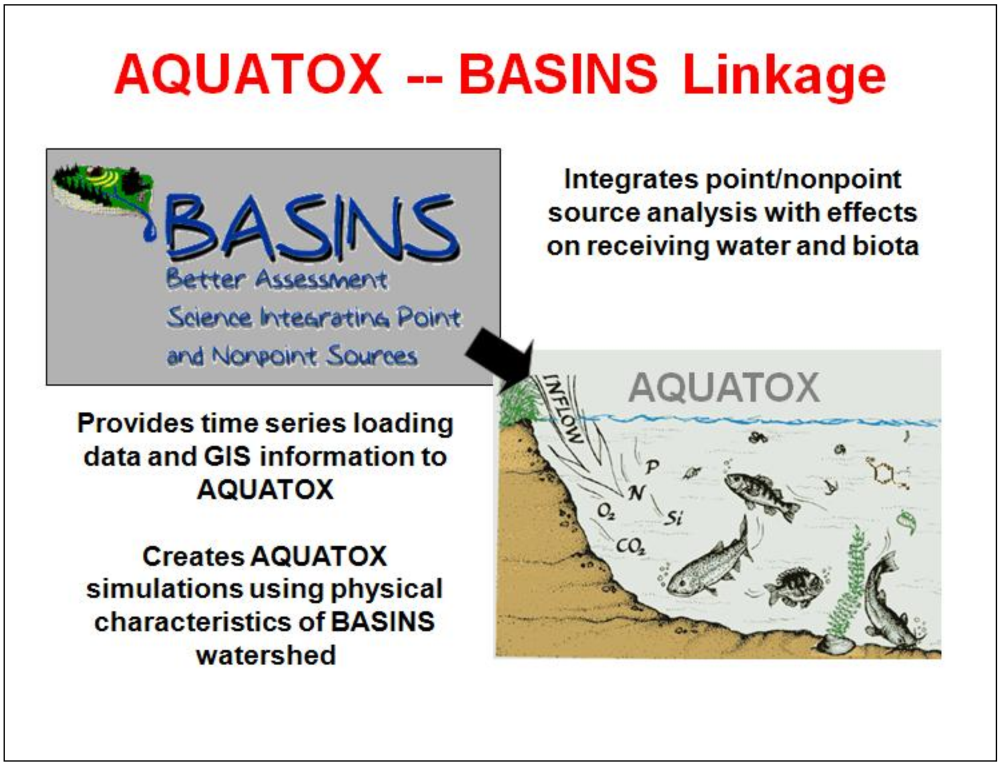
Note scale in comparison with earlier figures



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.

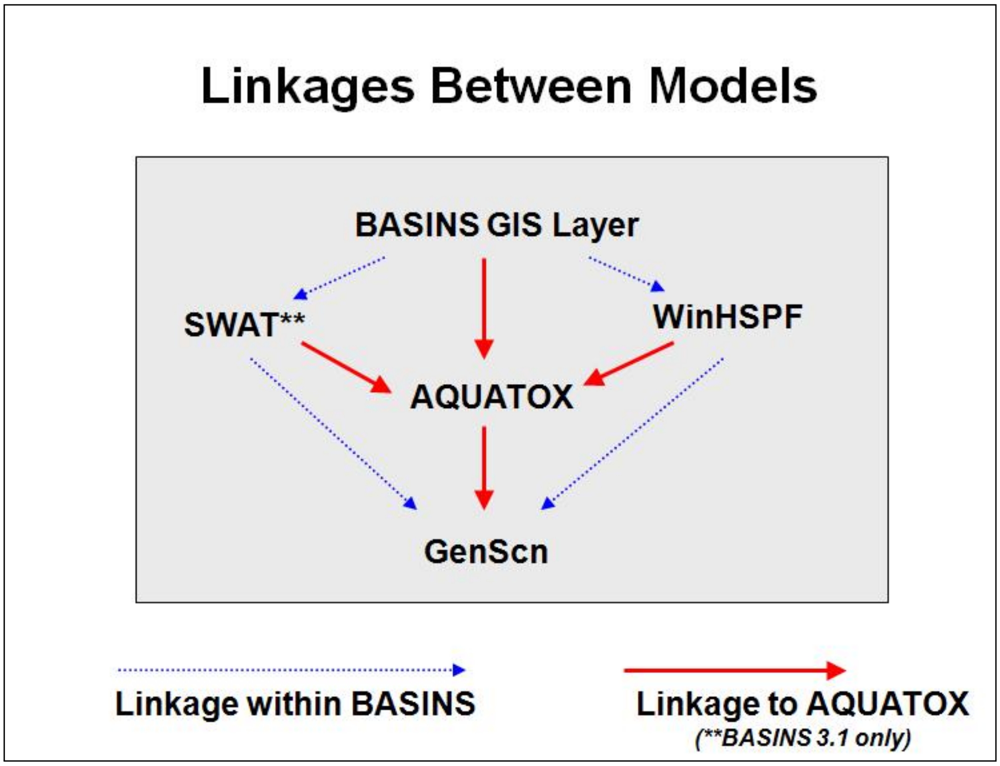


The MN parameter set was used with only a couple modifications. The critical force for periphyton scour was increased based on the bedrock riffles, and the optimum temperature was increased for two groups based on the difference in temperature between MN and AL. Therefore, this is considered a good partial validation.



BASINS is a multipurpose environmental analysis system for use by regional, state, and local agencies in performing watershed and water quality based studies. BASINS makes it possible to quickly assess large amounts of point source and nonpoint source data in a format that is easy to use and understand. BASINS combines GIS technology, environmental data, watershed and water quality models and other tools. More information can be found on the BASINS web site at
http://water.epa.gov/scitech/datait/models/basins/index.cfm

BASINS 3.1 and 4 are able to link with AQUATOX. The GIS–based data and watershed models provide input data (pollutant loads, flow, and water body or channel characteristics) to AQUATOX.



These are the specific data that are passed with the various AQUATOX/BASINS linkages:

• BASINS GIS to AQUATOX

Channel geometry (length, depth, slope)

• WinHSPF to AQUATOX

Geometry

Time series: flow, water quality (nutrients, BOD, temperature, sand/silt/clay)

• SWAT to AQUATOX *(a new version of SWAT has just been added to BASINS 4; due to changes in the SWAT output format, the link to AQUATOX will require modification)*

Geometry

Time series: flow, water quality (nutrients, BOD, pesticides, TSS)

• AQUATOX to GenScn

All time series output

Note that many of the graphing capabilities of GenScn are now available within AQUATOX

The linkage program takes the rather voluminous output from SWAT or HSPF and formats it correctly for AQUATOX, potentially a huge time savings for the user.

Use of AQUATOX in Water Quality Management Decisions

- 2008 peer review suggests AQUATOX is suited to support existing approaches used to develop water quality standards and criteria
  - One tool among many that should be used in a weight-of-evidence approach
- AQUATOX enables the evaluation of multiple stressor scenarios
  - What is the most important stressor driving algal response?
- Go beyond chlorophyll *a* to evaluate quality, not just quantity, of algal responses (e.g., reduction of blue-green algal blooms)

The application of AQUATOX in water quality management decisions is in its early stages, but has great potential, particularly with regard to linking chemical and physical water quality and the support of designated aquatic life uses.

As an example application, we will focus on water quality targets for nutrients, and discuss it in the context of the Minnesota rivers modeling.

Use analytical power of AQUATOX to analyze what factors are driving algal response:

Suspended sediments & light

Canopy and light

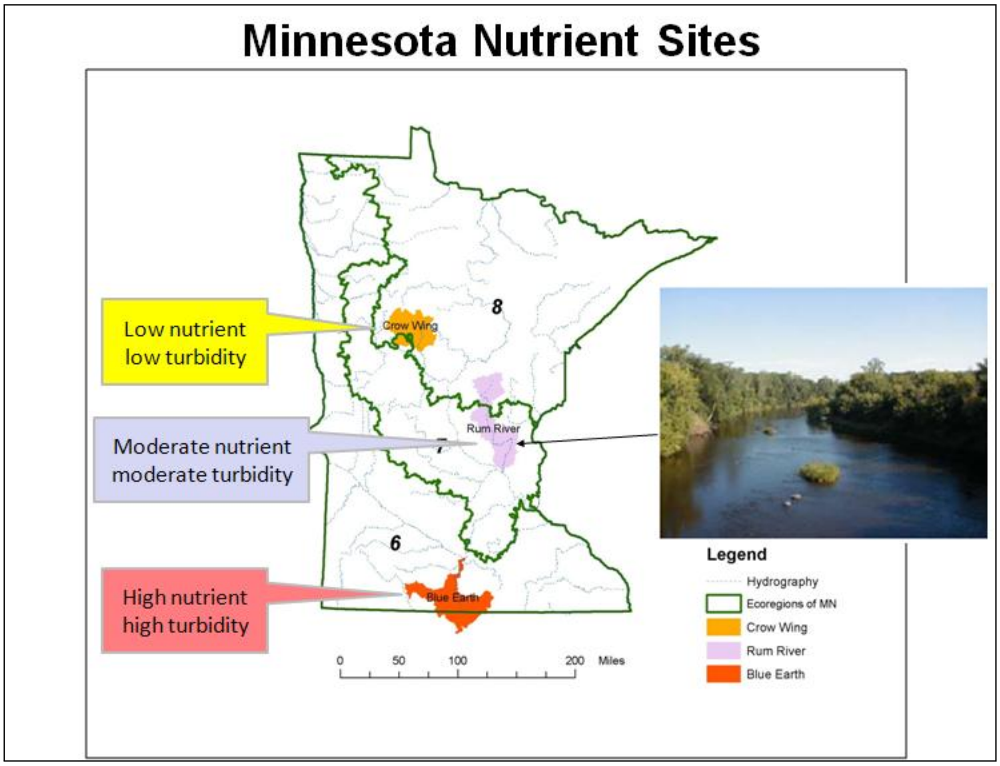
Nutrients

Organic loads

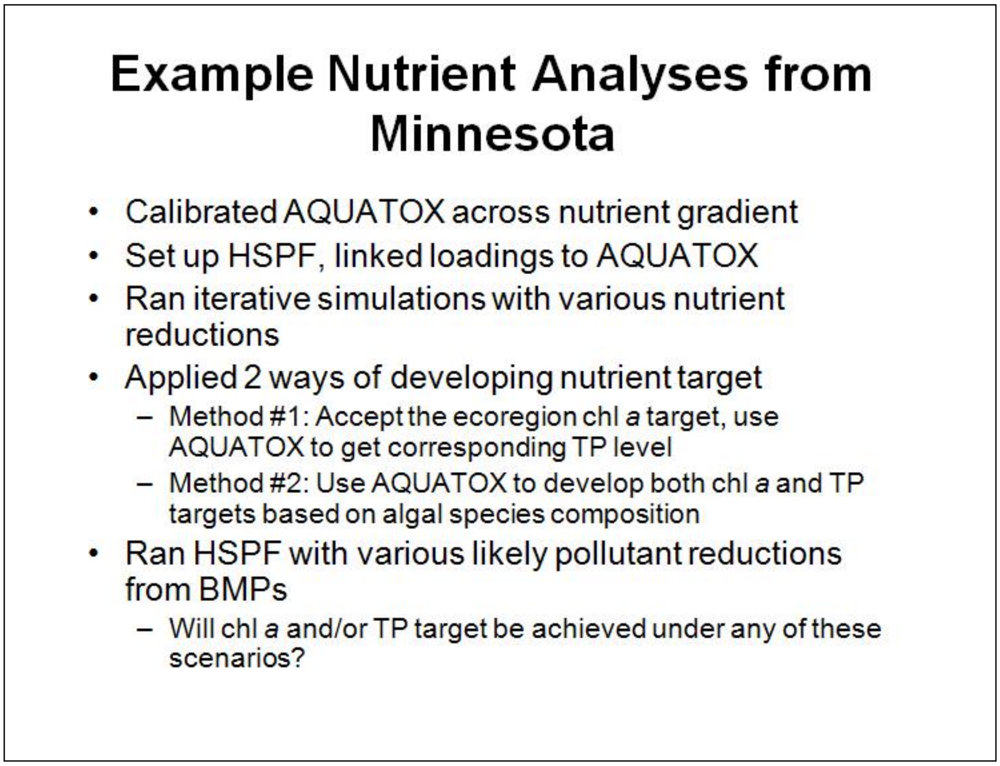
Flow regime

Herbicides

Combination of factors



We will return to the 3 MN sites.

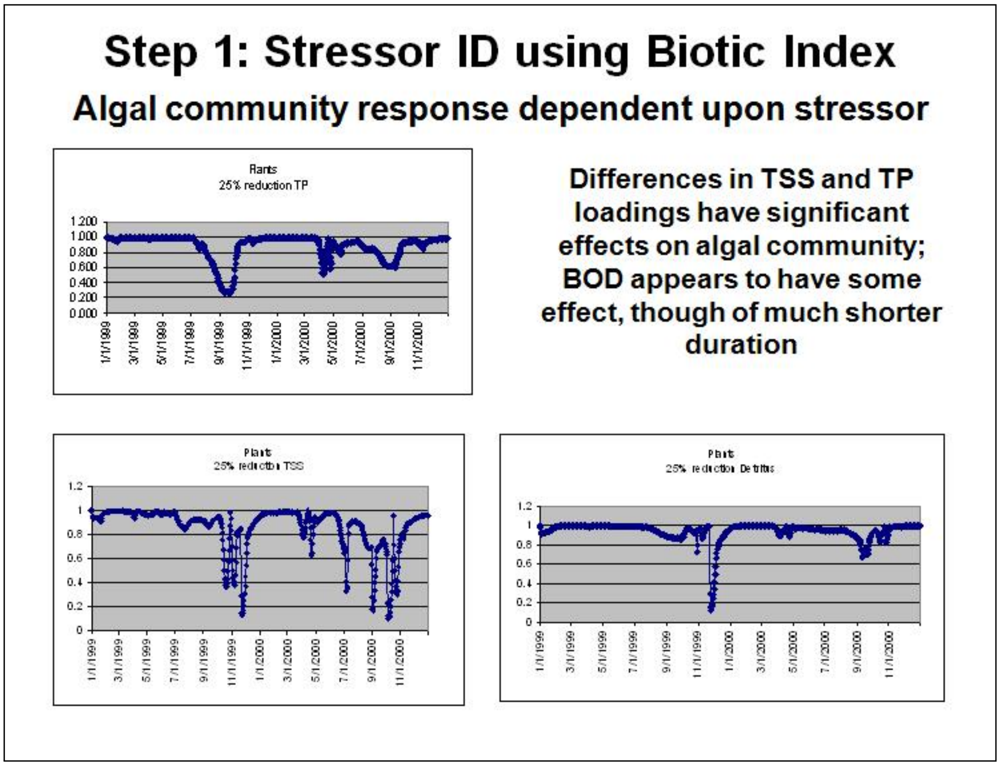


Although this discussion presents some alternatives to existing EPA recommendations for nutrients, our intent is NOT to undercut them, but rather to illustrate a technique to supplement and enhance the process of determining appropriate nutrient concentrations in our nation's waters.

This is a demonstration project designed to investigate how AQUATOX, coupled with the watershed modeling capabilities in BASINS, could be used as a tool in the analysis of potential WQC. The project also looked at whether reasonable management practices and load reductions could be expected to lead to attainment of the criteria.

The illustrations here were developed for the purposes of the workshop and were based on preliminary model simulations, and were not the same as presented in the final paper in Environmental Management. I hope also to provide illustrations of how several of the tools in AQUATOX can be used.

With AQUATOX calibrated across a gradient of nutrient concentrations in similarly sized rivers, we have reasonable confidence in our ability to predict mean responses to hypothetical reductions in nutrient concentrations in the high nutrient system. This exercise focused on the Blue Earth river as an example of a water body in which nutrient reductions might be desired. We asked the question what sort of nutrient reductions might be needed to bring chlorophyll *a* in that river down to some predefined acceptable level, i.e. possible response variable criterion.



First we used one of the biological metrics calculated by AQUATOX to reduce the number of stressors considered in the analysis.

Steinhaus community similarity indices can be calculated easily by AQUATOX; the model calculates the similarity between the control and perturbed runs for plants, invertebrates, fish, and all animals. A Steinhaus index of 1.0 indicates that all species have identical biomass in both simulations (i.e., the perturbed and control simulations); an index of 0.0 indicates a complete dissimilarity between the two simulations. See Sec 4.5 of the Release 3 Technical Documentation for more information.

First I changed the loadings for TSS, TP, BOD, NH3 and NO3 individually to see which made the greatest difference in the plant community (in this instance, the algae). TSS and TP had significant effects on the Steinhaus values; BOD had only transitory effects, and NH3 and NO3 had almost no effect (not shown). For purposes of the exercise, we eliminated NH3, NO3 and BOD as significant stressors, and focused on TP and TSS reductions.

Step 2: Run AQUATOX with multiple load reduction scenarios.

Compare Mean TP and Chl a

TP/TSS multiplier	Mean TP (ug/L)	Mean chl_*a* (ug/L)
1.0	268	18.3
0.8	214	11.0
0.6	161	9.5
0.4	107	8.2
0.2	54	8.0
0.0	0*	0.2
Ecoregional criterion	***118.13***	***7.85***

We ran Blue Earth River AQUATOX model simulations with fractional multipliers applied to the influent TP loadings from the linked HSPF simulation. This table shows the resulting mean chlorophyll *a* concentrations from these runs.

These results suggest that >80 percent reduction in TP would be required to bring the mean chlorophyll *a* in the Blue Earth River down to 7.85 ug/L. By contrast, the 304a TP value (118.13 ug/L) corresponds with only a 56 percent reduction.

We used reductions of TSS as well as TP because most of the management measures that control P would also reduce TSS, though not necessarily 1:1, as we have assumed here.

Step 3a: Water Quality Target Development
Method #1

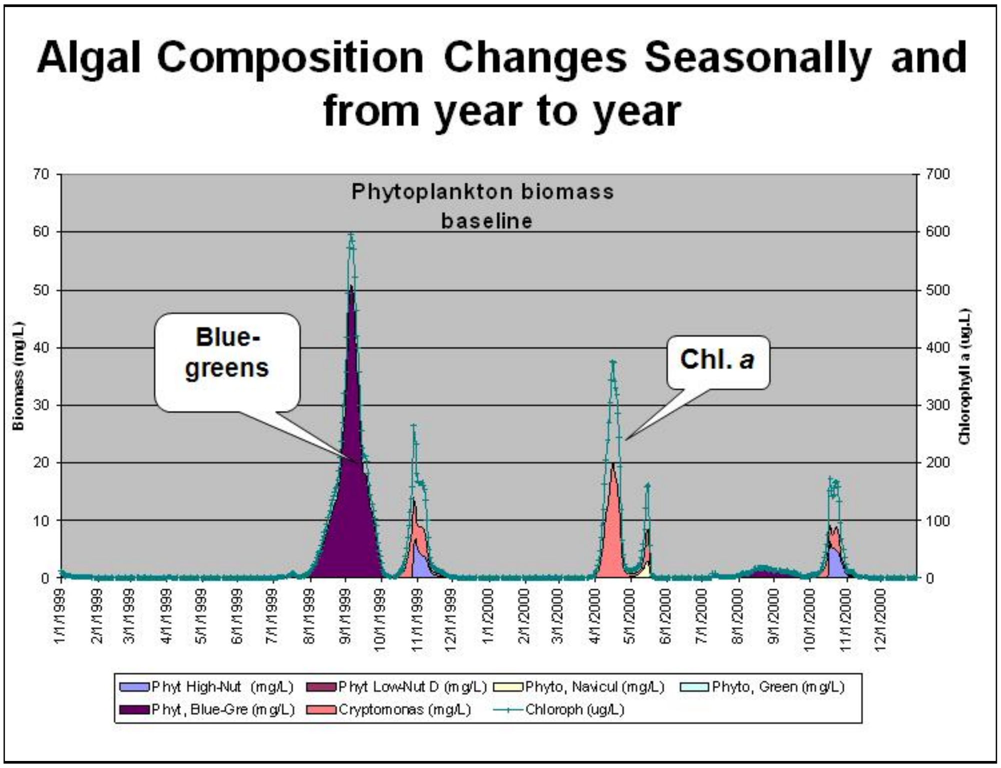
- Focus on TP and chl *a* only
- according to model: 80% TP reduction required to meet 7.85 ug/L chl *a*
- according to 304(a) recommendation: 56% TP reduction required to meet same chl *a* level

Step 3b: Water Quality Target Development
Method #2

- Focus on algal community, not total chl *a*
  - Blooms of blue-green algae (cyanobacteria) can be noxious and cause taste and odor problems
  - At what levels of total chl *a* do blue-greens reach an "acceptable" proportion of total algae? What is the corresponding TP?
- Where might there be shifts in species composition?

If the State wishes to consider the composition of the algal community as well as the total chlorophyll *a* value, AQUATOX provides a way to do so.

Obviously, what percentage of blue-green is "acceptable" is subject to debate. There is some work being done on developing this kind of metric, but to our knowledge, no one has adopted one into WQS.

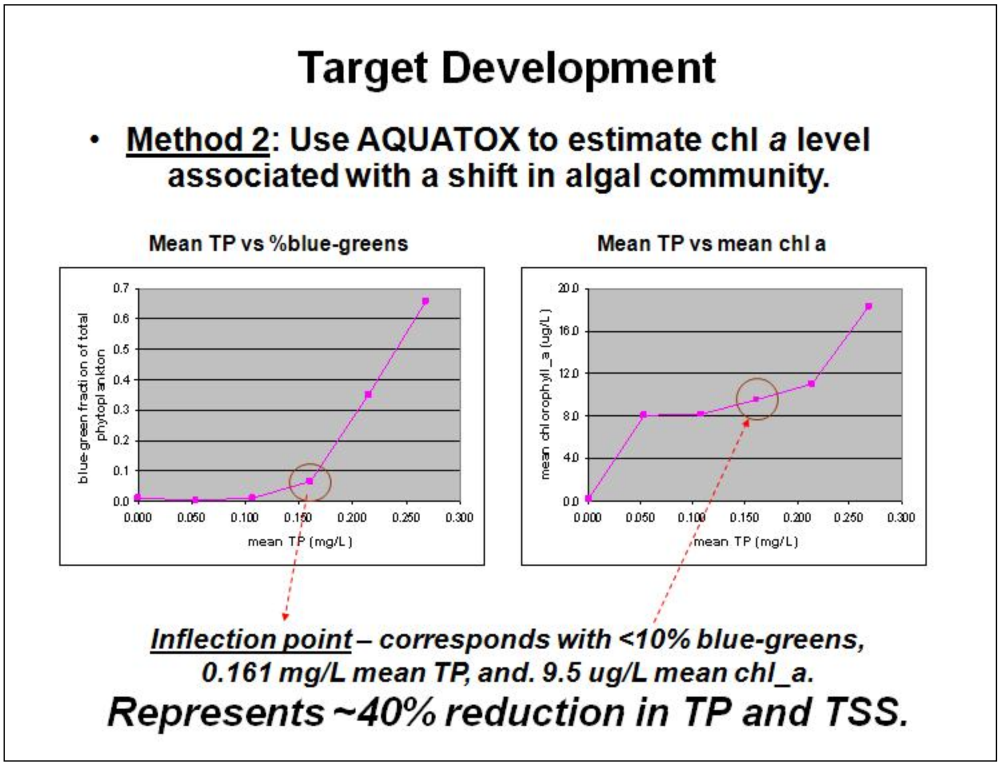


Use the Export function to export results to EXCEL; and graph them to get visual representation of algal composition changes over time

Blue Earth River had reports of severe blooms of blue-green algae in some years.

The model simulated very high chl a peaks (almost 600 ug/L) for 1999. Largest bloom (in the fall) is dominated by blue-greens, and lasts almost 2 months; later bloom by cryptomonads, plus a high-nutrient diatom.

Note that there is no spring bloom in 1999, probably due to light limitation or washout; it was a very high flow year.



In the second example, we used the AQUATOX runs to estimate a chl *a* concentration that corresponds with the point where a shift between dominance of blue-greens and more desirable algal species occurs. The left figure shows blue-greens as a fraction of total water column phytoplankton, and the right shows mean chl *a* concentrations. Both are plotted as functions of mean TP, in increments of 20% reduction on the horizontal axis.

The left figure shows an inflection point at a approximately 0.161 mg/L, a 40 percent decrease in TP below existing concentrations. The inflection point occurs at a blue-green fraction of slightly less than 10% total phytoplankton; it also corresponds with mean chl *a* of 9.5 ug/L (on the right). The chl *a* value is slightly higher than the 304(a) number, and the TP value is substantially higher than the 304a value. So if the management goal focuses on the % blue-greens rather than chl *a* per se, and if "less than 10% blue-greens" is an acceptable target, 9.5 ug/L would be as our second hypothetical chlorophyll *a* criterion.

So we had two different hypothetical criteria values for chl*a*: the reference condition 304a number itself, and a slightly higher number corresponding with the inflection point in the left figure. The corresponding TP values are rather different between the 2 methods using AQUATOX, and between them and the 304(a) recommendations.

Summary of Minnesota Analysis

- Stressor-identification: Algal responses linked quantitatively with TP and TSS levels.
- Pollutant reduction scenarios: derived algal response to hypothetical reduction scenarios
- Target development: Derived alternative hypothetical criteria, one based on ecologically meaningful endpoint (%blue-greens).
- Attainability: Link to watershed loading model. Results suggest both 304(a) and hypothetical criteria may be very difficult to achieve in Blue Earth river, even with heavy use of BMPs.

So to summarize, we used mechanistic modeling to quantitatively link nutrient stressor and response variables in three Minnesota rivers. We identified TP and TSS as the most important stressors controlling instream phytoplankton concentrations, though not necessarily downstream conditions. Using these model results we derived an example of a hypothetical chl *a* criterion based on a biological metric that we came up purely with for illustrative purposes.

In a next step, though not shown here, we used a linked watershed model to assess the attainability of this hypothetical criterion, as well the ecoregion 304a criteria, by adding BMPs at various densities into the watershed model and simulating their impact on water quality. These model runs suggested that even extensive use of BMPs might not lead to attainment of the criteria.

Other Possible Analyses to Support Development of Water Quality Targets

- For different target concentrations you could compare differences in:
  - Duration of hypoxia or anoxia in hypolimnion
  - Duration of algal blooms
  - Trophic State Indices (TSIs)
  - Secchi depth
  - Fish and invertebrate species composition

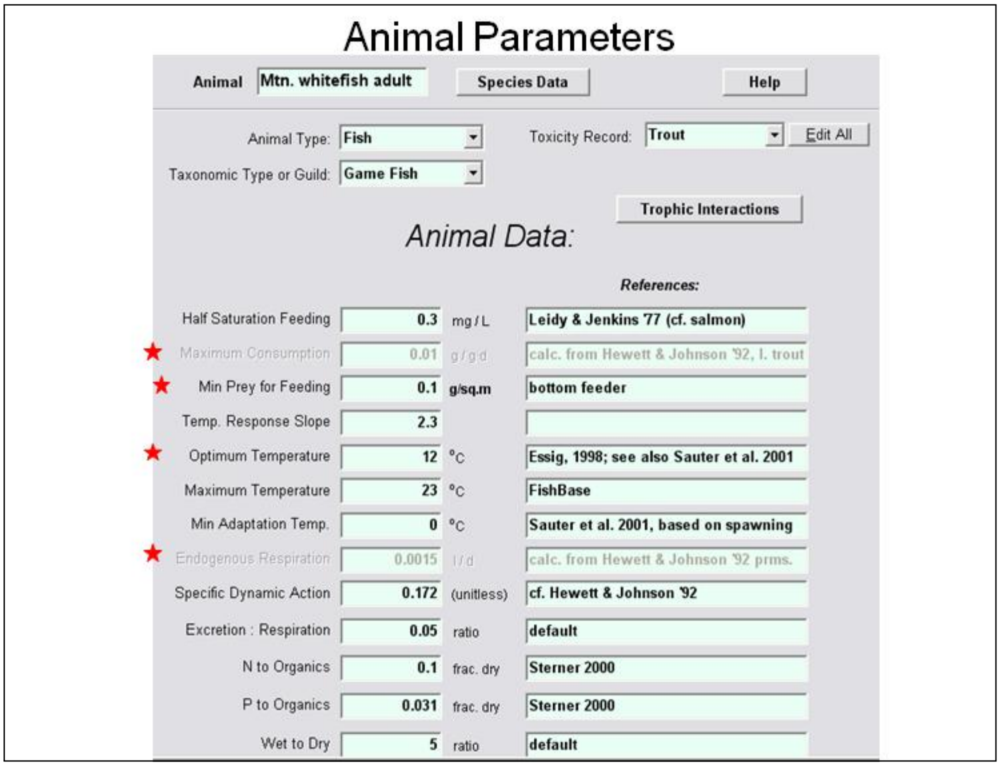
Modeling Animals with AQUATOX

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

Animal Modeling Overview

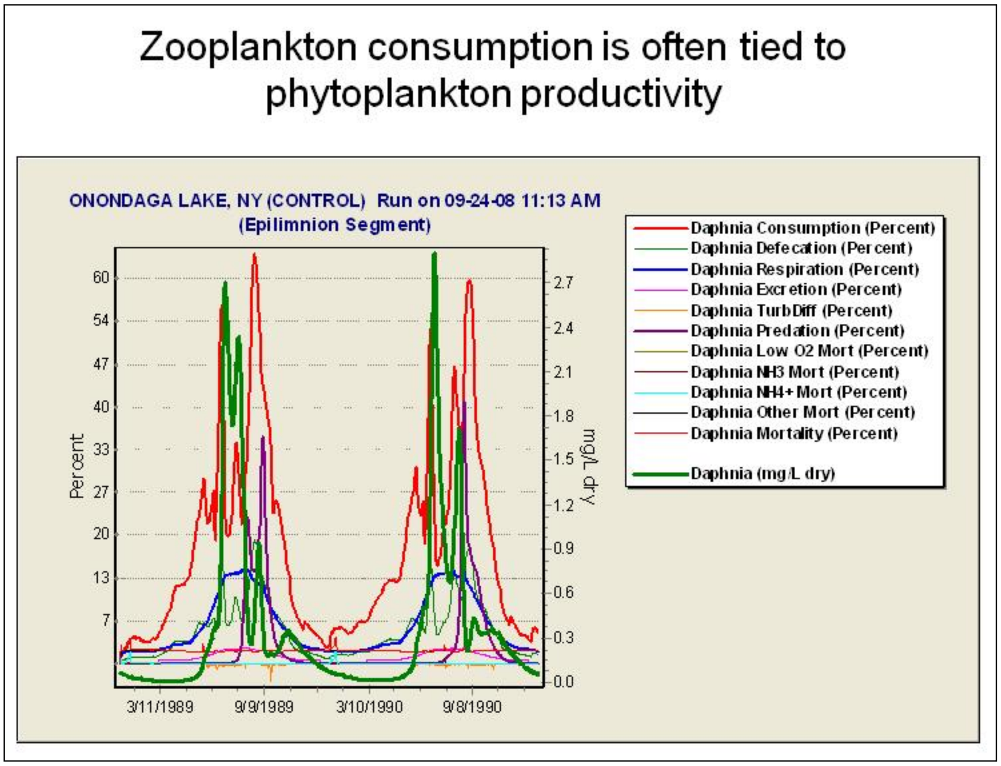
- Animal biomasses calculated dynamically
  - **Gains** due to consumption and boundary-condition loadings
  - **Losses** due to defecation, respiration, excretion, mortality, predation, boundary condition losses
- Careful specification of feeding preferences required
- Bioenergetic modeling for fish

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.

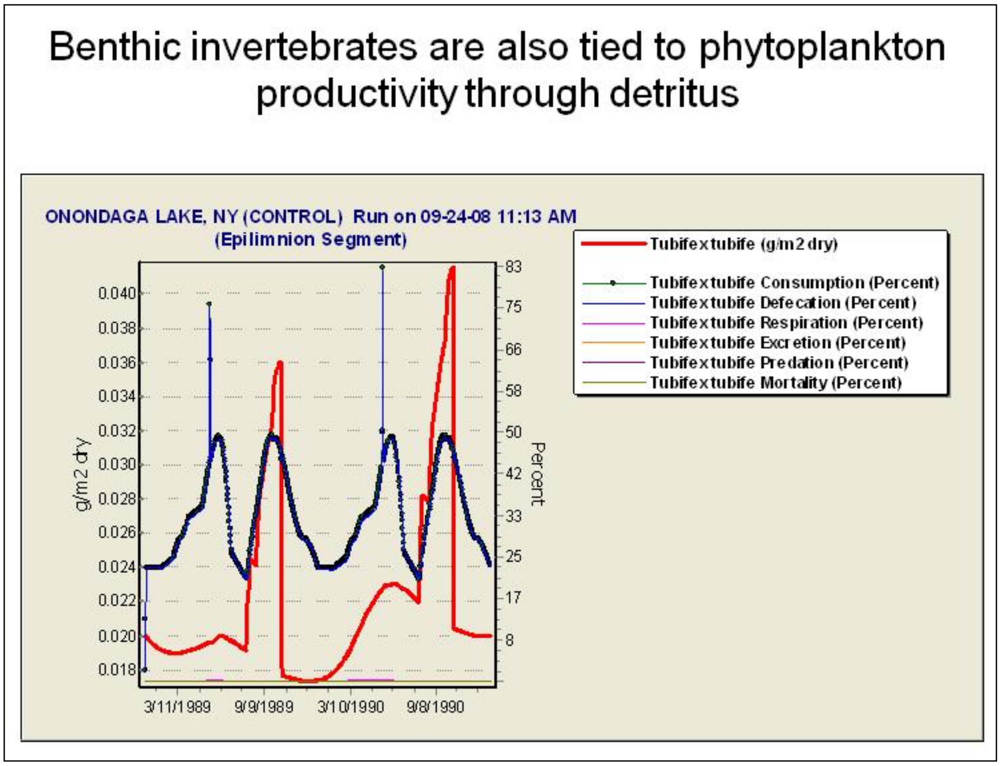


Sensitive parameters include maximum consumption rate and respiration rate if not calculated based on weight using the Wisconsin bioenergetic parameters (Hanson et al. 1997).

Hanson, P. C., T. B. Johnson, D. E. Schindler, and J. F. Kitchell. 1997. Fish Bioenergetics 3.0. Center for Limnology, University of Wisconsin, Madison.

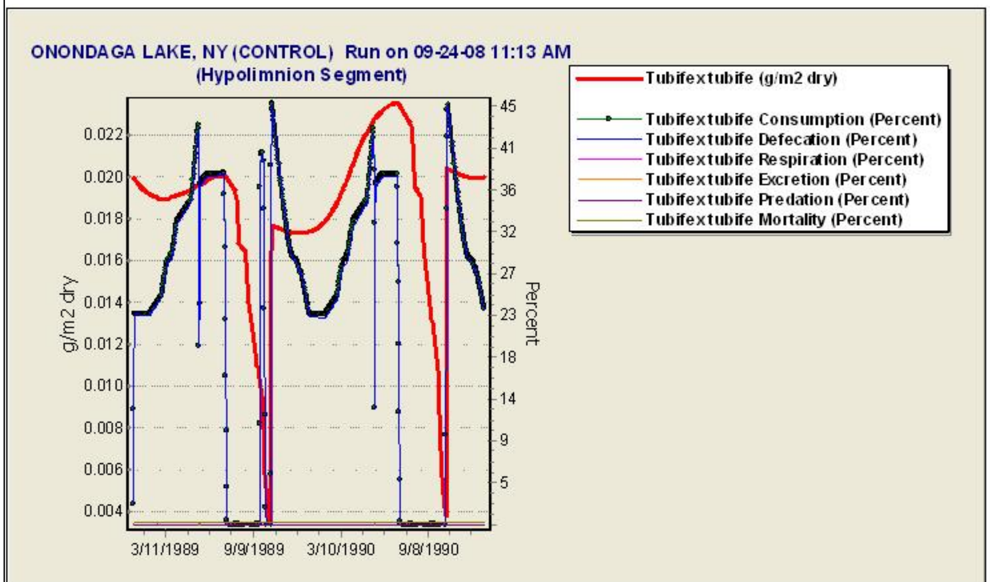


In Onondaga Lake consumption is heaviest during phytoplankton blooms, although detritus is a secondary source of food. (Without detritus as an alternate food source zooplankton would not be sustained.) Predation offsets high consumption in late summer.

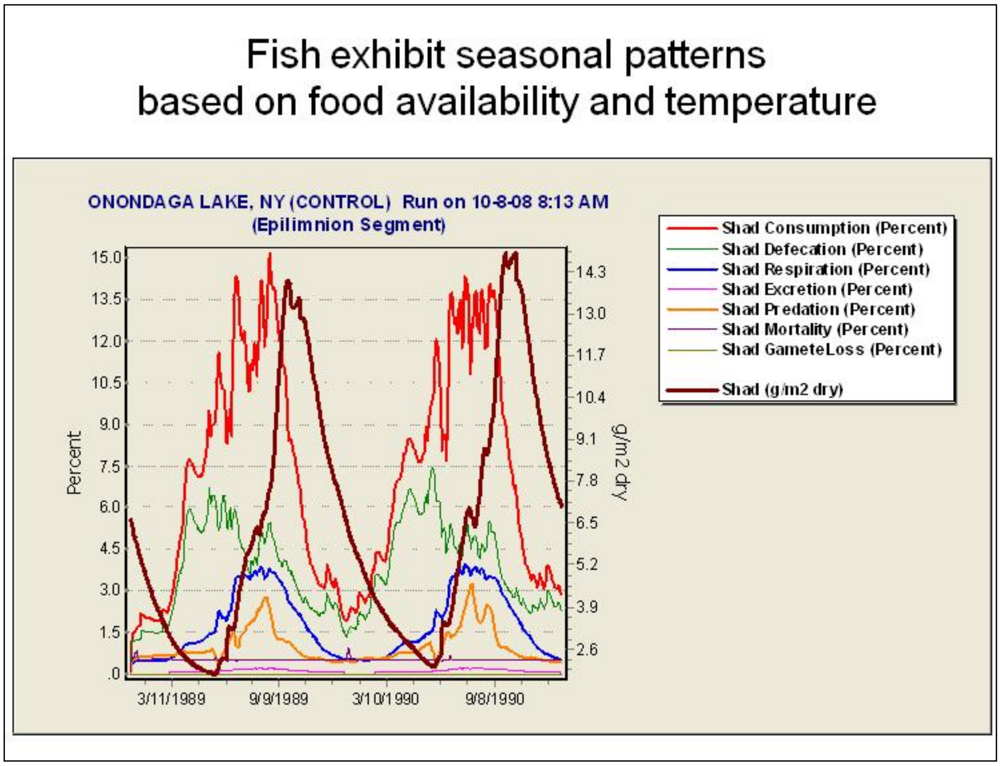


High consumption occurs when algal blooms crash and detritus settles to the bottom.

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. The rebound is actually the combination of biomasses when the epilimnion and hypolimnion are combined at overturn.



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

Foodweb Model specified as Trophic Matrix

Interactions are normalized to 100%

AQUATOX-- Trophic Interaction Matrix

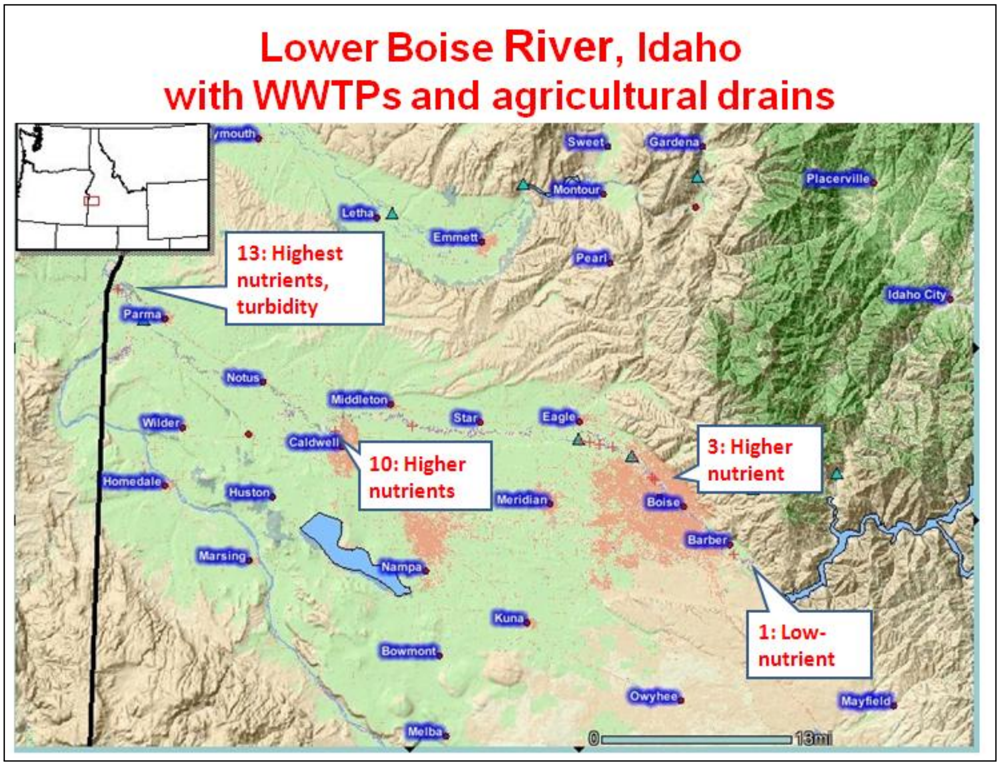
Preference percentages are initially normalized to 100% based on species in the simulation. Renormalize

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.



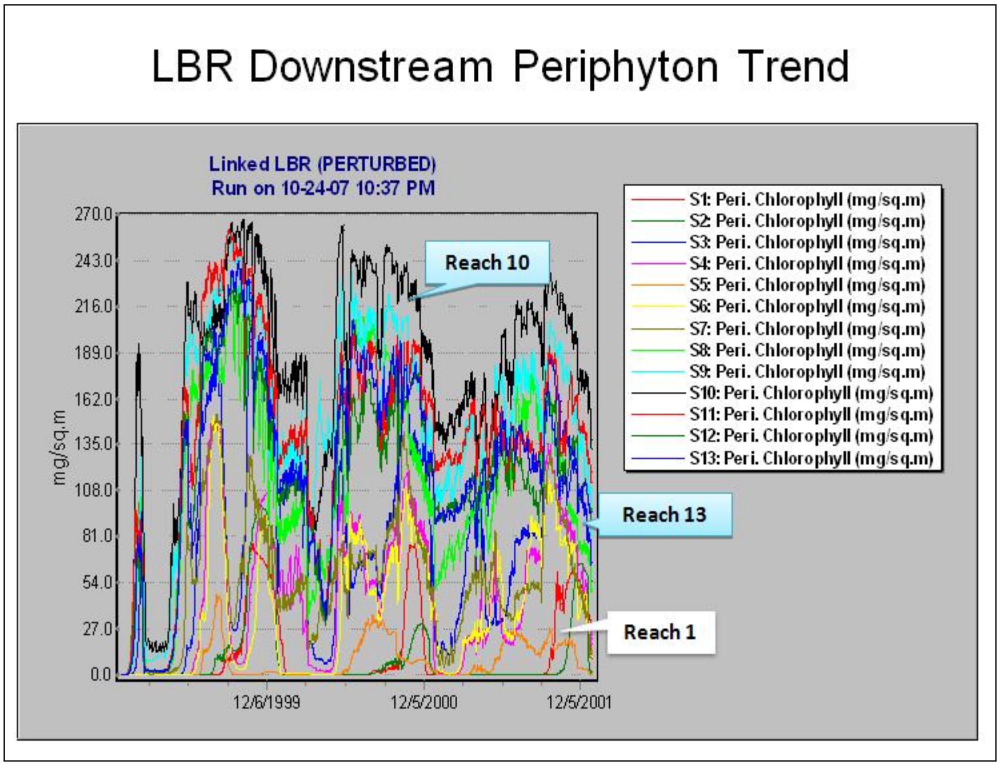
The Lower Boise River is a shallow river that is heavily managed for irrigation. In fact, the downstream segment 10 has the lowest flow because of diversions; below that reach, drains bring in nutrient- and sediment-laden return flow.

Lower Boise River in Boise, Idaho

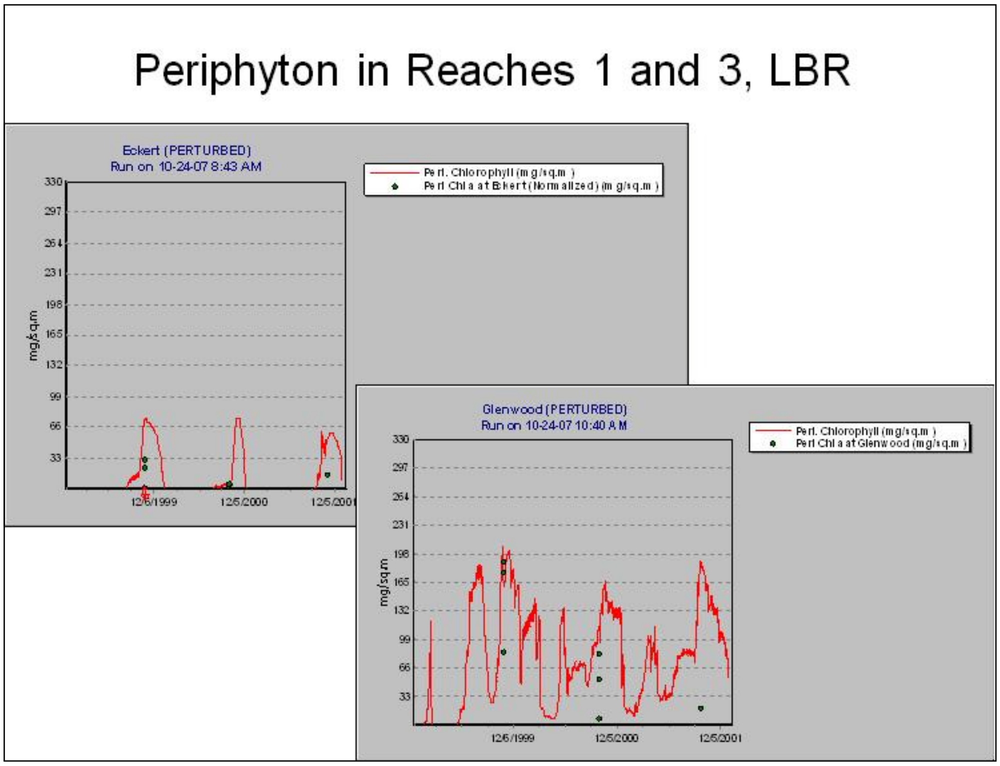
Note how shallow the river is.

Complex Linked Model

- 13 main-stem segments modeled
- 26 “tributary inputs”
  - Groundwater inputs
  - Waste Water Treatment Facilities
  - Input drains and tributaries
- Extensive water withdrawals
- Complex water-balance model
- Nutrients are integrated within main-stem

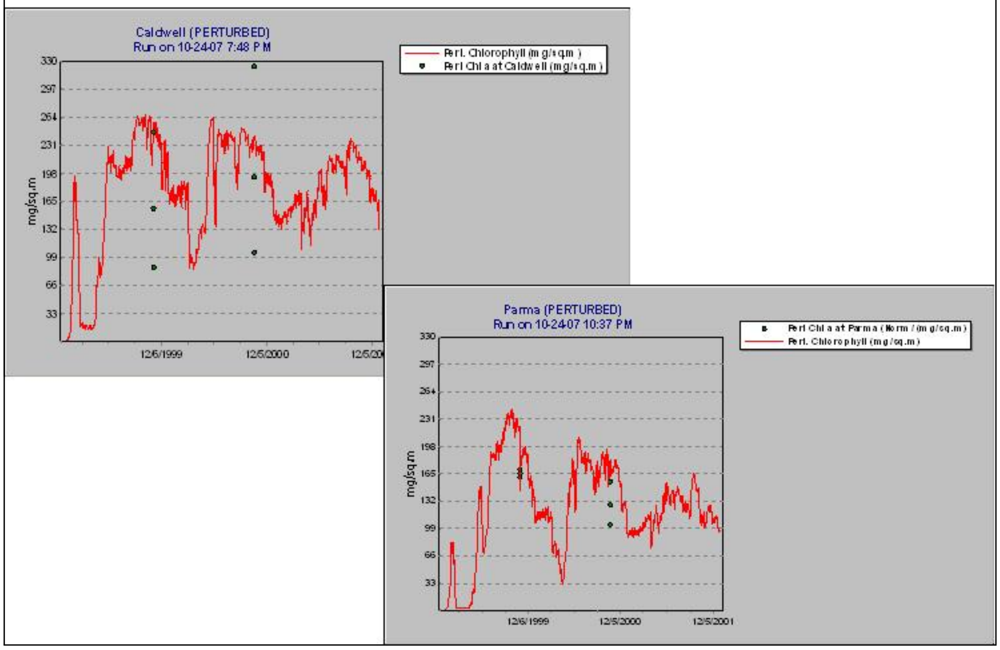


Nutrient-poor Reach 1 has the lowest periphyton biomass. Reach 10 with nutrient-rich clear water has the highest periphyton.

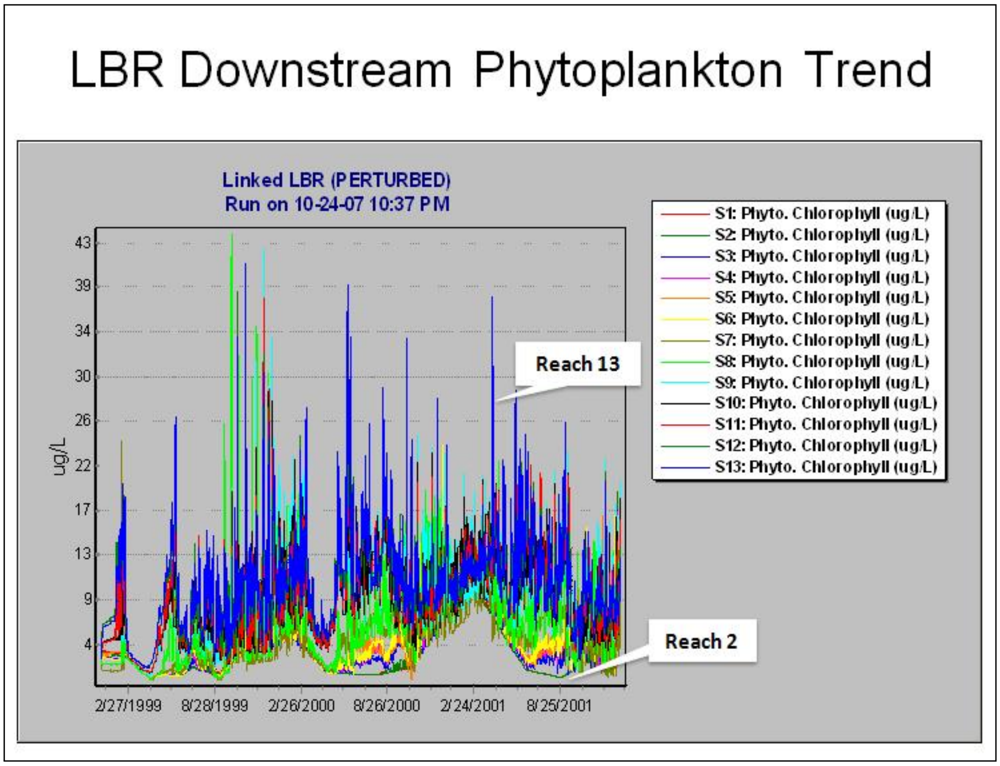


All four graphs have the same scale – note the large differences in biomass at the different sites.
As is often the case, the available periphyton data are very sparse, and are often highly variable within a sampling episode.

Periphyton in Reaches 10 and 13, LBR

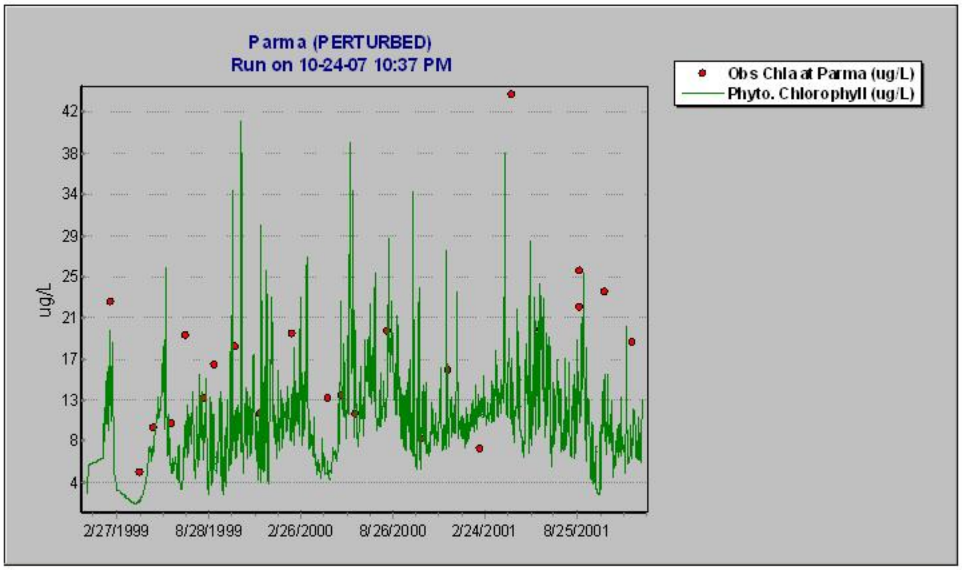


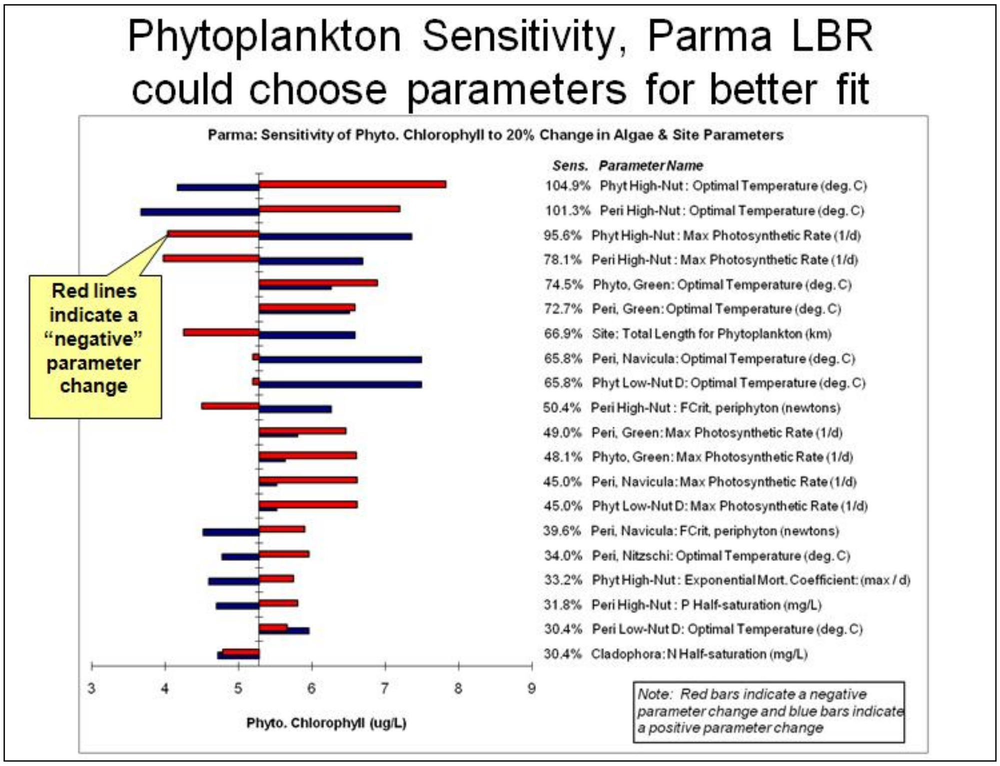
All four graphs have the same scale.



Sestonic algae include sloughed periphyton upstream and true phytoplankton downstream.

Sestonic algae at Parma (Reach 13), both upstream loadings and periphyton sloughing





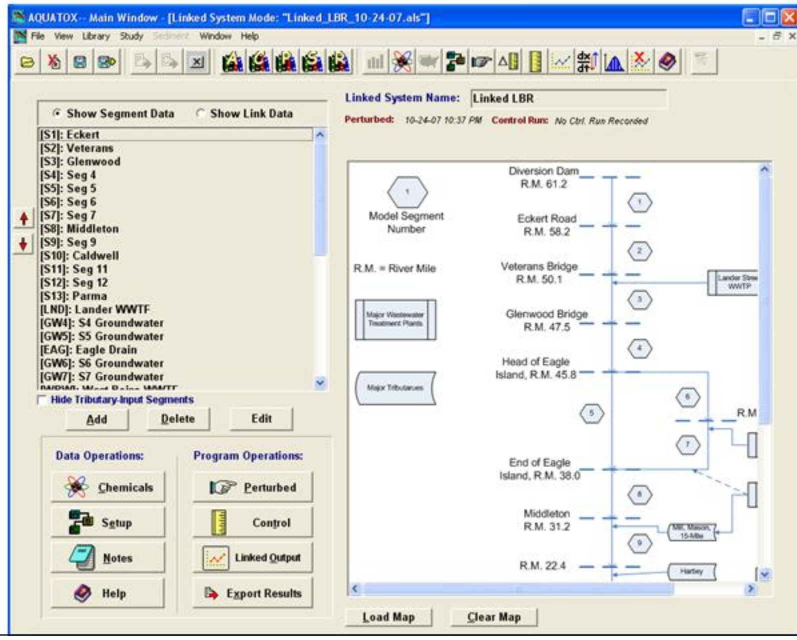
Nominal range sensitivity analysis can be performed easily with AQUATOX. With it you can identify those parameters that make the specific model output most sensitive; this indicates a need for the best data possible for those parameters.

Demonstration 2: Linked Segment Version

- Developed as part of a Superfund project; now part of Release 3
- Allows the capability to model multiple linked segments--converting AQUATOX into a two dimensional model
- State variables move from one linked segment to the next through water flow, diffusion, bed-load, and migration.

Migration of fish into and out of the model's spatial domain (e.g. spawning runs) is not modeled.

Segmented Version can Represent Dynamically Linked Multiple Segments



In this example main-stem reaches, tributary agricultural drains, groundwater, and waste water treatment effluents are linked in simulating 61 miles of the Lower Boise River, Idaho.

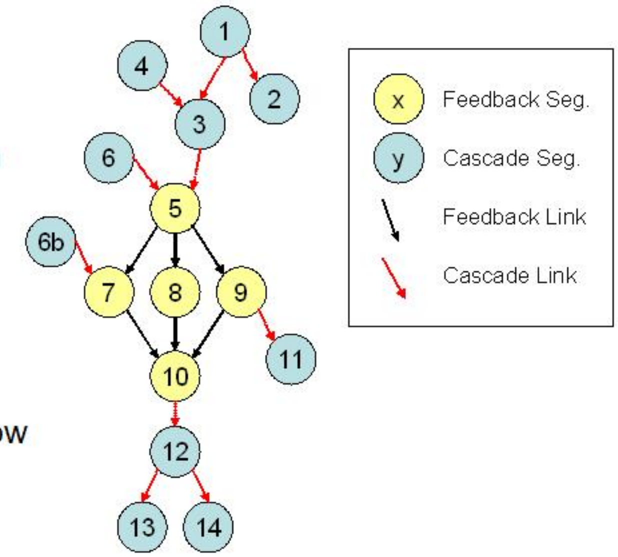
Cascade & Feedback Linkages

Cascade Linkages:

One-way linkages with no backwards flow or diffusion across segment boundaries

Feedback Linkages:

Two-way linkages that allow for backwards flow and diffusion

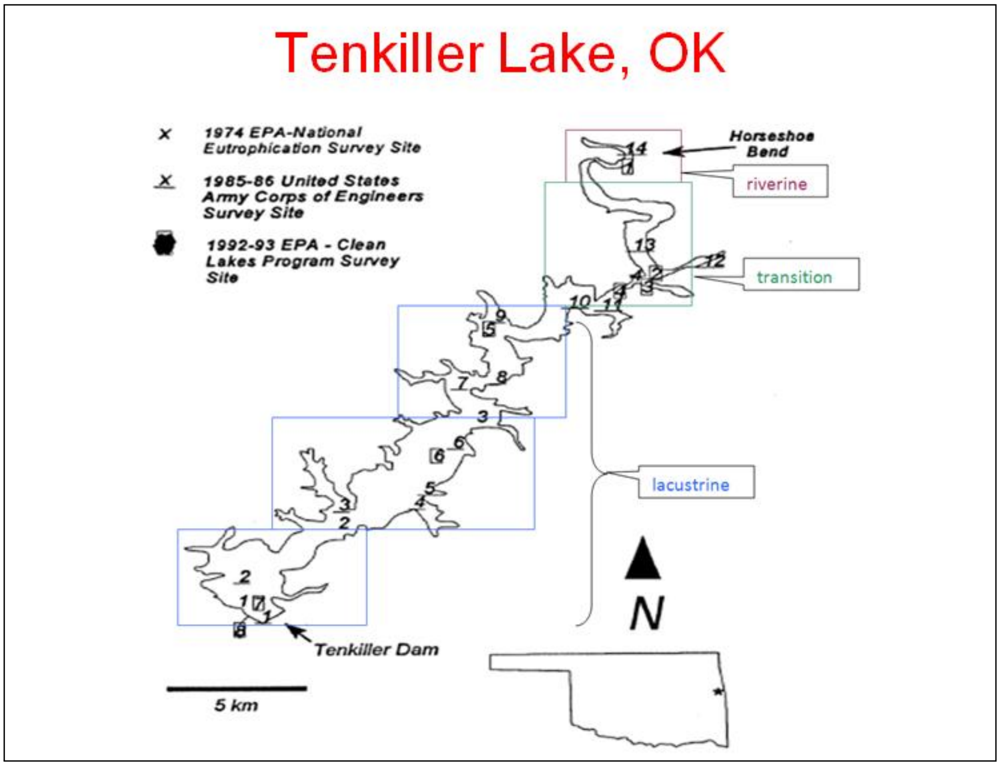


- After cascade and feedback linkages are defined, note that the purpose of this is to allow for slower running segments (i.e. segments with rapid water flow) to solve independently of other segments.
- In the diagram shown AQUATOX would first run the "upper cascade" segments. Those being 1, 2, 3, 4, 6, and 6b.
- AQUATOX would use the loadings from the "upper cascade" run to run the "feedback" segments. Those being 5, 7, 8, 9, and 10.
- Finally, AQUATOX would use the loadings from the feedback run to run the "lower cascade" segments. Those being 11, 12, 13, and 14.
- Mass balance of water, toxicants, nutrients, organisms is maintained through a complex system such as this one.

Linked Segment Model Data Requirements

- Water flows between segments
- Initial conditions for all state variables for each segment modeled
  - All segments must have the same state variables
- Inflows, point-sources and non-point-source loadings for each segment
- Tributary or groundwater inputs and/or any withdrawals

Interface Demonstration to follow



Based on availability of sampling stations, Tenkiller Lake was divided into five horizontal epilimnetic segments and four hypolimnetic segments (the riverine zone was considered to be well mixed).

Tenkiller Lake Background

- Reservoir in eastern Oklahoma formed by the damming of the Illinois River (1947-1952)
- Identified on Oklahoma's 1998 303(d) list as impaired (nutrients)
- High-priority target for TMDL development
- 1996 Clean Lakes Study: nutrient concentrations and water clarity are indicative of eutrophic conditions

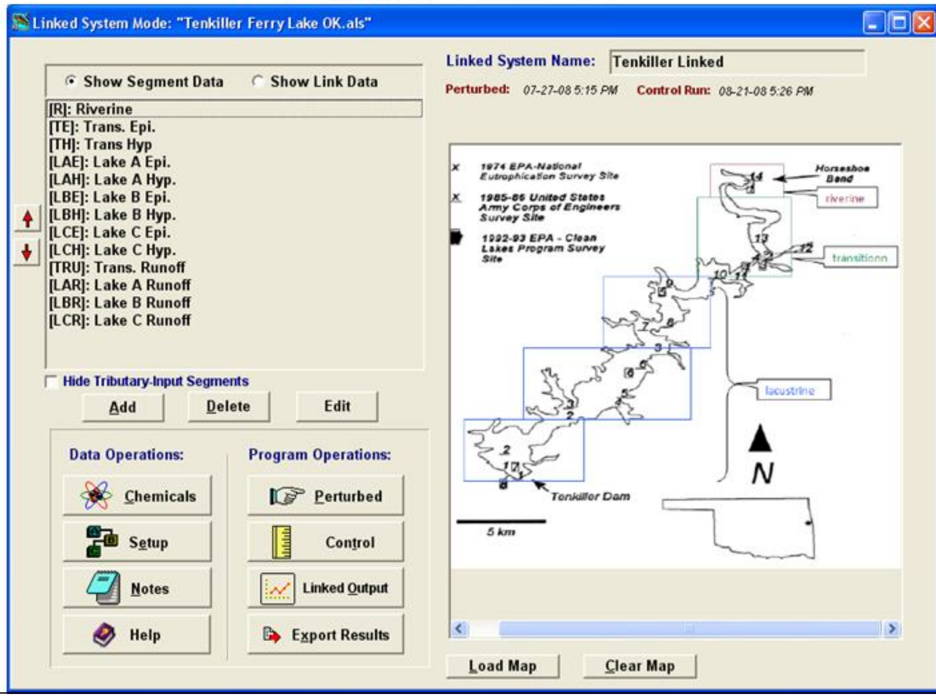
Tenkiller Ferry Lake was selected as the location for a nutrient criteria modeling case study due to its current nutrient problems, and because the State of Oklahoma had expressed interest in a collaborative working relationship with EPA. In addition, some water monitoring data needed to support this modeling project was available.

Tenkiller Lake Application

- Linked Model application includes nine segments
  - Riverine segment
  - Vertically stratified transitional segment
  - Three vertically stratified lacustrine segments
- Model linkage to HSPF (watershed) and EFDC (in-lake hydrology) models
- Model can predict chlorophyll *a* levels based on nutrient loadings (BMPs)

An existing HSPF watershed model of the Illinois River and its watershed was available, with a recent re-calibration effort for water quantity and quality. Output from this model was linked to AQUATOX simulations of Tenkiller Ferry Lake, and used to provide daily influent hydrologic and nutrient loadings for the simulated time period. Furthermore, the EFDC model had been calibrated for Tenkiller Ferry Lake for 1992-1993, and those simulations provided the flow field for linking segments in AQUATOX.

Tenkiller Lake OK

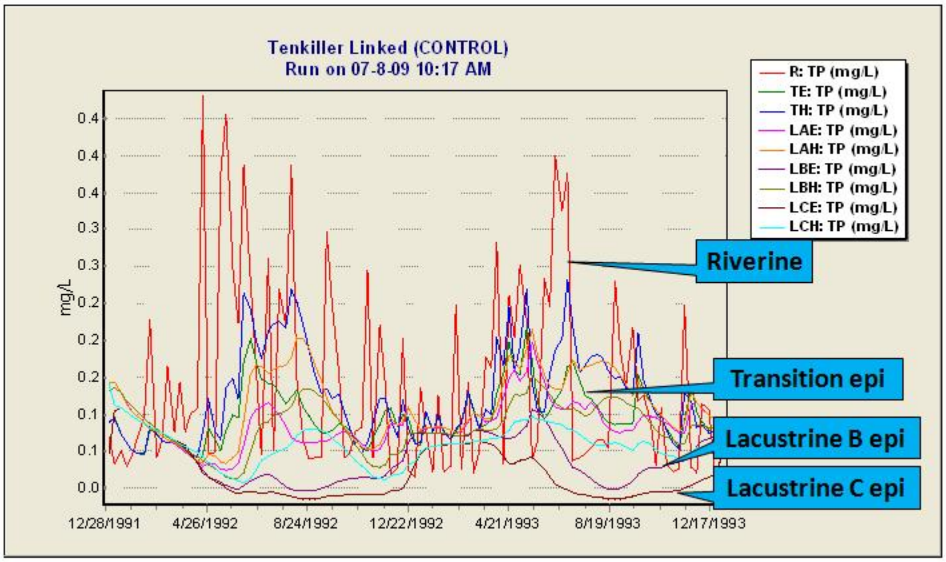


Storm-water plume, algae-rich riverine segment

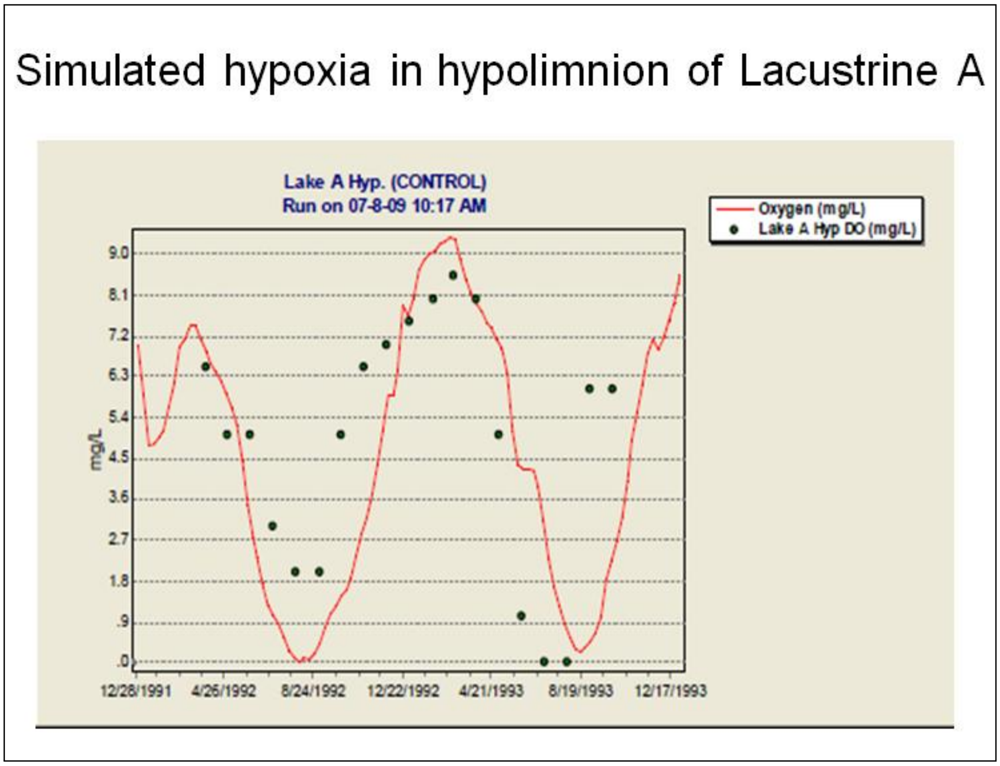
duckweed (*Lemna* sp.) forms surface scum at the interface

A site visit happened to follow a storm event, and the storm-water plunge zone was an obvious boundary between the riverine and transition zones. Duckweed, a small floating macrophyte, formed a surface concentration in the plunge zone.

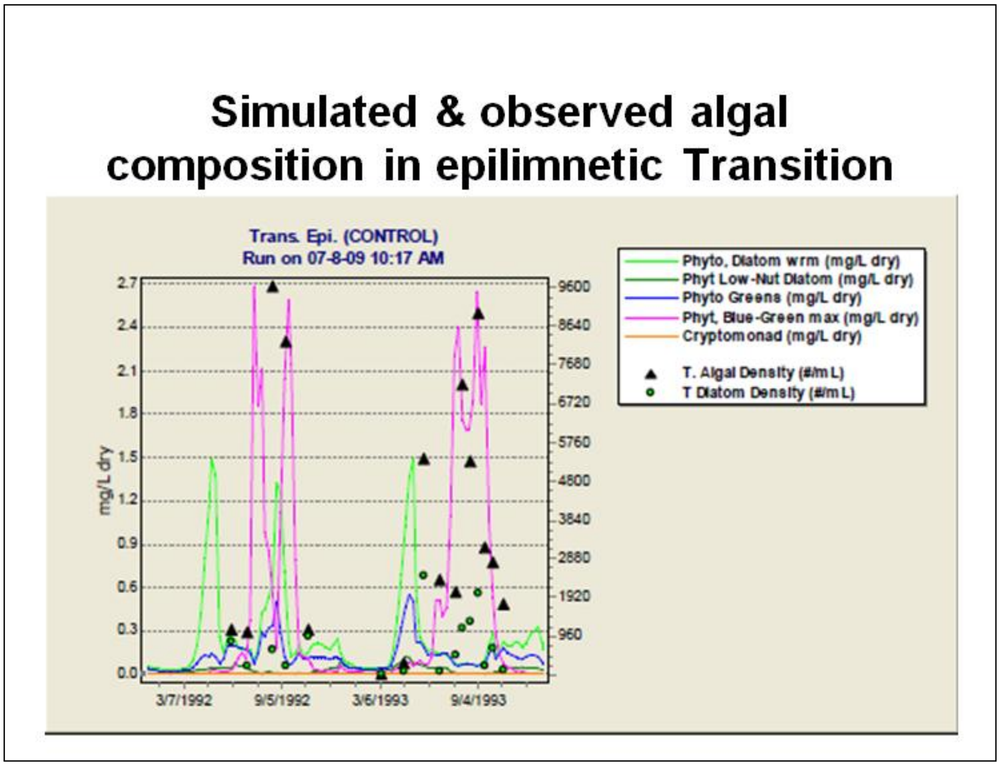
Total phosphorus in water column decreases toward dam; loss to sediments is simulated



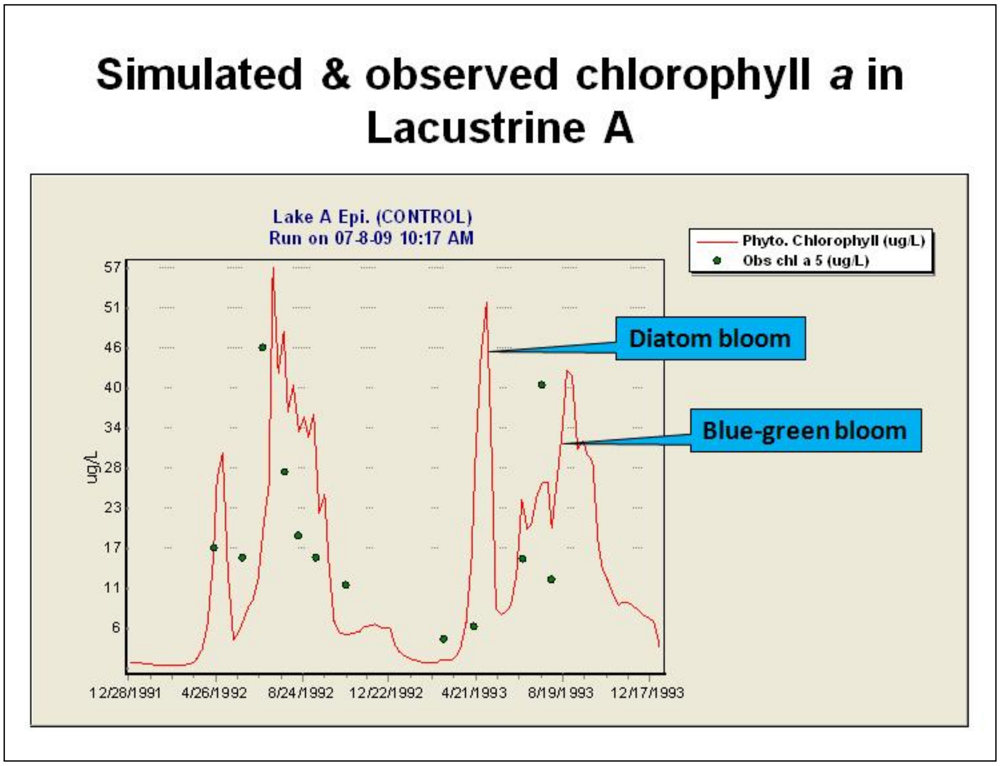
Precipitation of PO4 with CaCO3 was an important loss process.



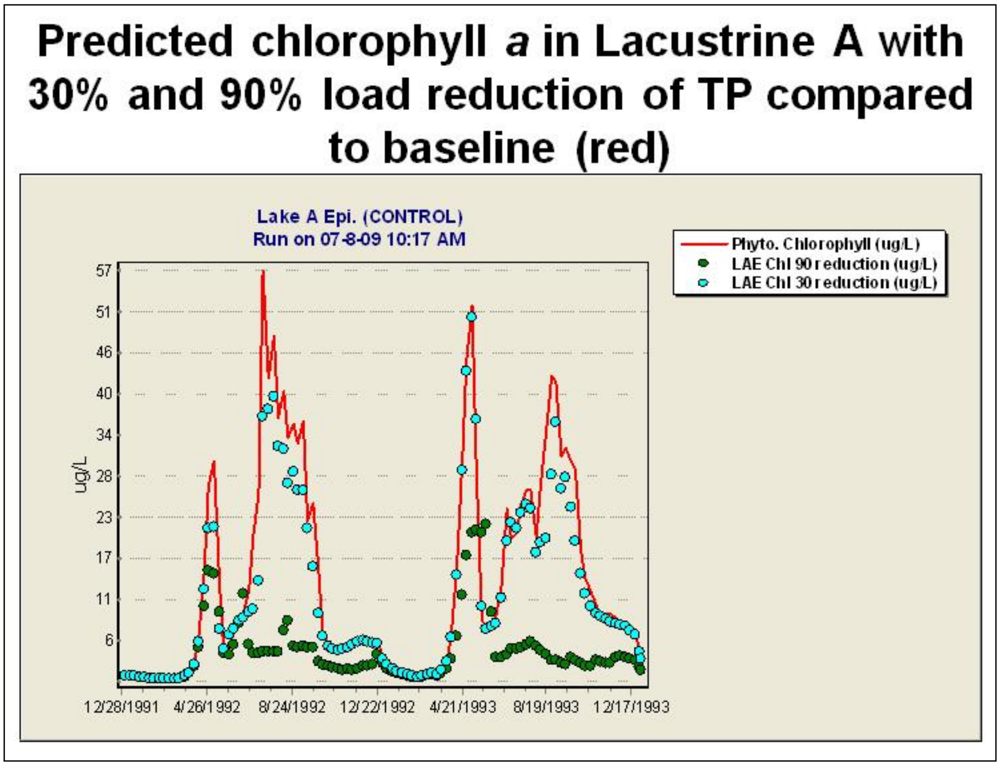
The sediment diagenesis submodel was necessary to represent the influence of bottom sediments on hypoxia.



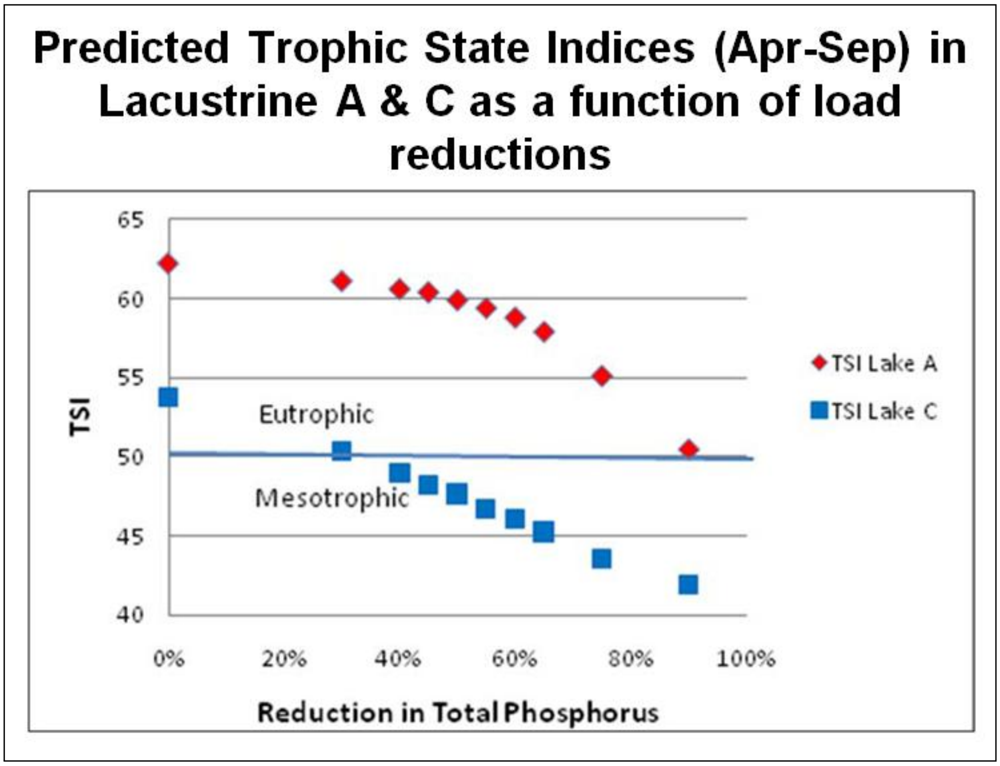
The model fit the available algal data reasonably well based on visual inspection.



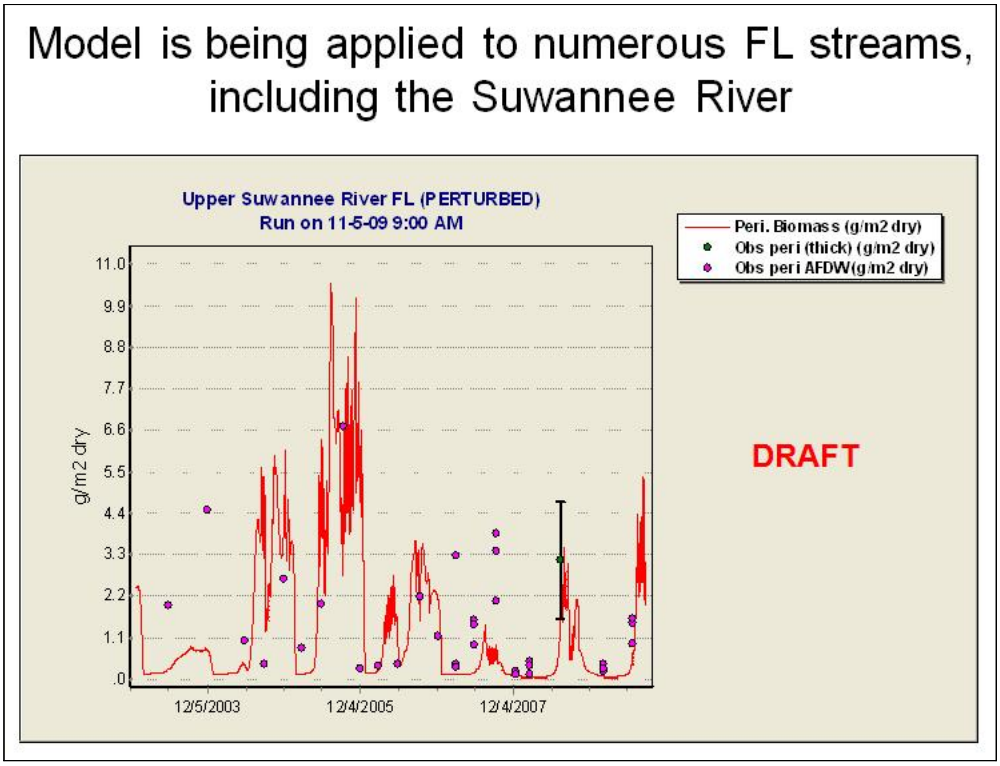
A common problem in evaluating goodness of fit is in comparing short-lived phenomena, such as the simulated diatom bloom, with sporadic observed data.



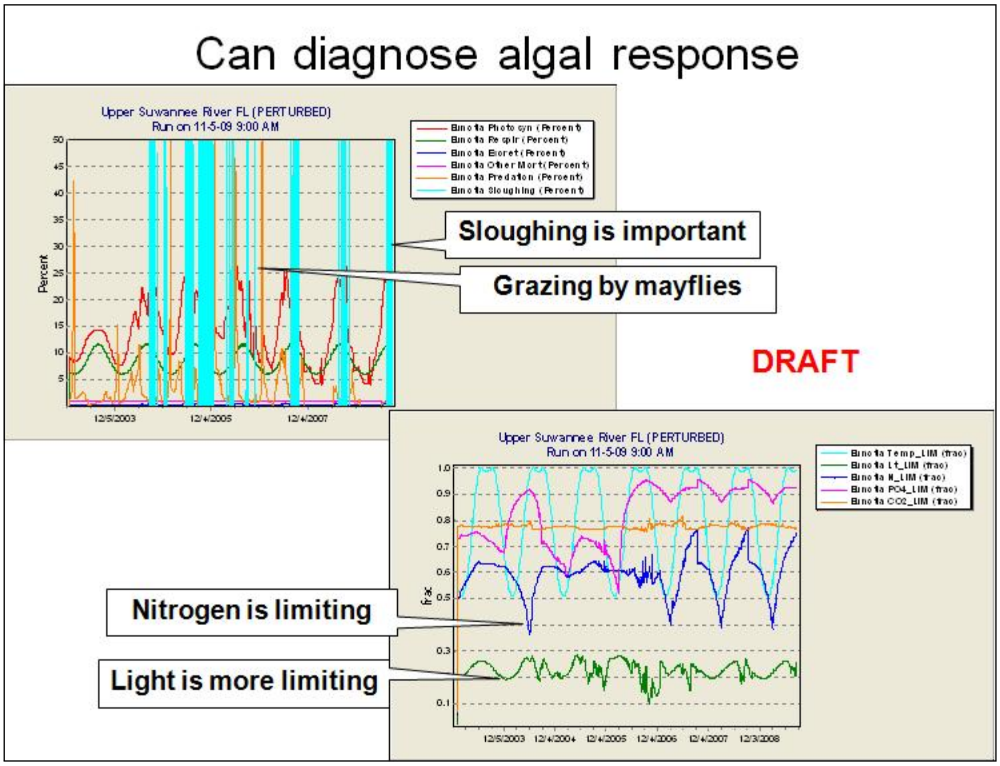
Load reduction factors were assigned to represent overall load reductions to the lake by a mixture of best management practices (BMP) and point-source reduction scenarios. Influent TP, TN, and BOD concentrations were modified concurrently, in a manner representative of their correlated susceptibility to management practices. Any percent TP decrease would be accompanied by percent decreases in the other pollutants.



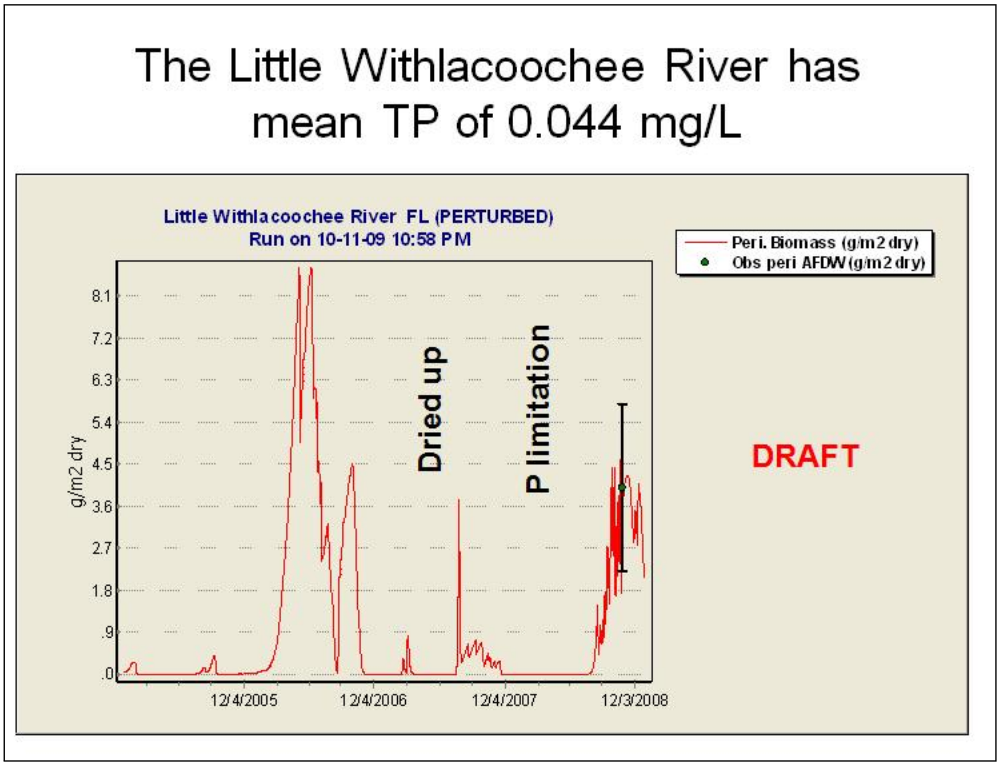
The Trophic State Index,TSI, based on chlorophyll is a useful way of presenting the results in the context of a eutrophication gradient. The simulated TSI values exhibit a gradient toward the dam during the 1992-93 period. This slide shows the predicted responses of both Lacustrine A and C to load reductions. A 30% reduction in TP loads places Lacustrine C on the borderline between eutrophic and mesotrophic, whereas a 90% reduction would be required for Lacustrine A based on the growing season.



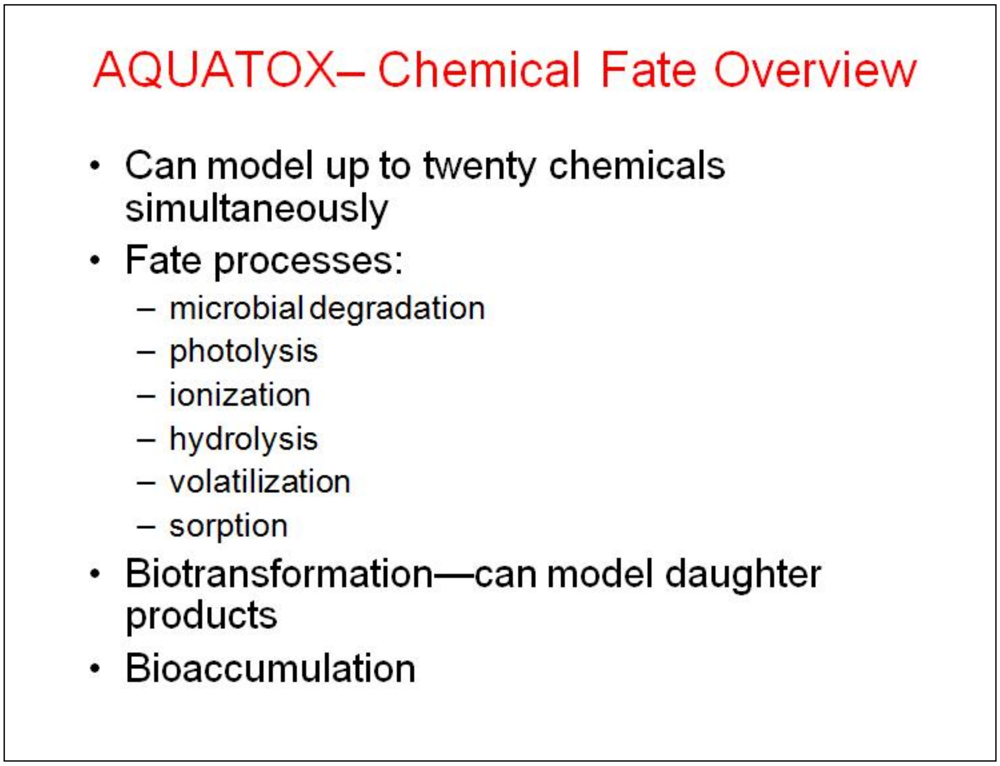
The Upper Suwannee River is a blackwater stream that drains the Okefenokee Swamp.



The pH in the Upper Suwannee is low enough that gastropods are excluded, decreasing the herbivory on periphyton. Sloughing, especially when biomass builds up and algae are stressed, is predicted to be an important loss term for this diatom. Total nitrogen (TN) averages 1.48 mg/L; however, much of it is tied up in refractory dissolved organic matter so that N is severely limiting, as is light.



AQUATOX successfully stepped through a period in which the river went dry. Severe phosphorus limitation is predicted to exclude periphyton at times.



The chemical fate module of AQUATOX predicts the partitioning of a compound between water, sediment, and biota, and estimates the rate of degradation and loss of the compound. Microbial degradation, photolysis, hydrolysis, volatilization, and biotransformation are modeled in AQUATOX.

• Microbial degradation is modeled by entering a maximum biodegradation rate for a particular organic toxicant, which is subsequently reduced to account for suboptimal temperature, pH, and dissolved oxygen.

• Photolysis is modeled by using a light screening factor (Schwarzenbach et al., 1993) and the near-surface, direct photolysis first-order rate constant for each pollutant. The light screening factor is a function of both the diffuse attenuation coefficient near the surface and the average diffuse attenuation coefficient for the whole water column.

• For those organic chemicals that undergo hydrolysis, neutral, acid-, and base-catalyzed reaction rates are entered into AQUATOX as applicable.

• Volatilization is modeled using a stagnant two-film model, with the air and water transfer velocities approximated by empirical equations based on reaeration of oxygen (Schwarzenbach et al., 1993).

• Sorption and desorption are modeled separately as kinetic processes.

• Biotransformation is represented by user-supplied first-order rate constants with the option of also modeling multiple daughter products.

• Bioaccumulation will be discussed later

Chemical fate clarified using half-Lives and DT95

Time-to-loss Estimated Using Loss Rates at a given time

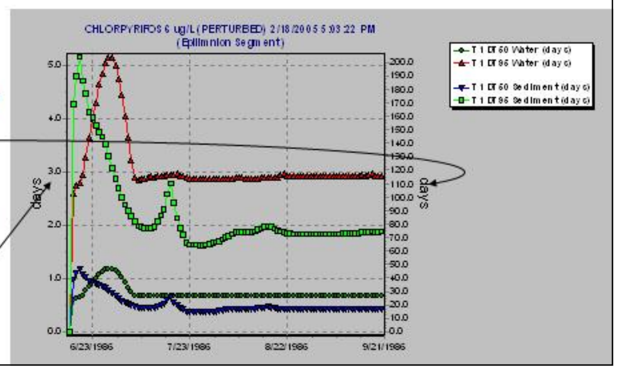
$$Loss_{Water} = \frac{Hydrolysis_{Water} + Photolysis + Microbial_{Water} + Washout + Volat. + Sorption}{Mass_{Water}}$$

$$Loss_{Sed} = \frac{Microbial_{Sed} + Hydrolysis_{Sed} + Desorption}{Mass_{Sed}}$$

For this Chlorpyrifos Study:

Half-life in Sediment of roughly 20 days
DT95 of roughly 75 days

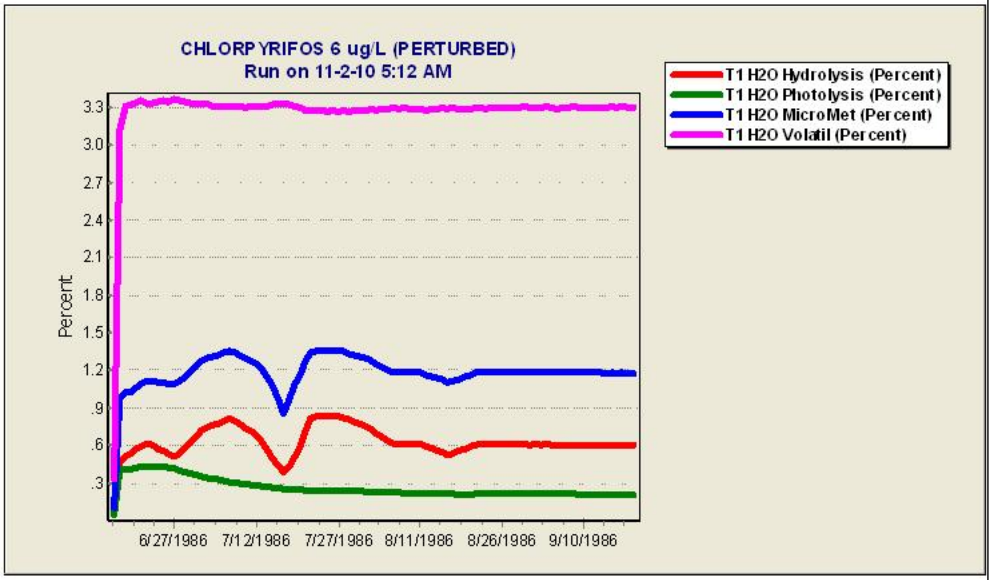
Half-life in water of roughly 16 hours, DT95 in water is roughly 3 days



AQUATOX estimates half-lives (DT50s) and time to 95% chemical loss (DT95s) independently in bottom sediment and in the water column. Estimates are produced at each output time-step depending on the average loss rate during that time-step in that medium.

Chemical rates may be tracked

Predicted In-situ Degradation Rates for Chlorpyrifos in Pond



From Wikipedia:

Chlorpyrifos is a crystalline organophosphate insecticide that inhibits acetylcholinesterase and is used to control insect pests. Trade names include Brodan, Detmol UA, Dowco 179, Dursban, Empire, Eradex, Lorsban, Paqeant, Piridane, Scout, and Stipend. Chlorpyrifos is moderately toxic and chronic exposure has been linked to neurological effects, developmental disorders, and autoimmune disorders.

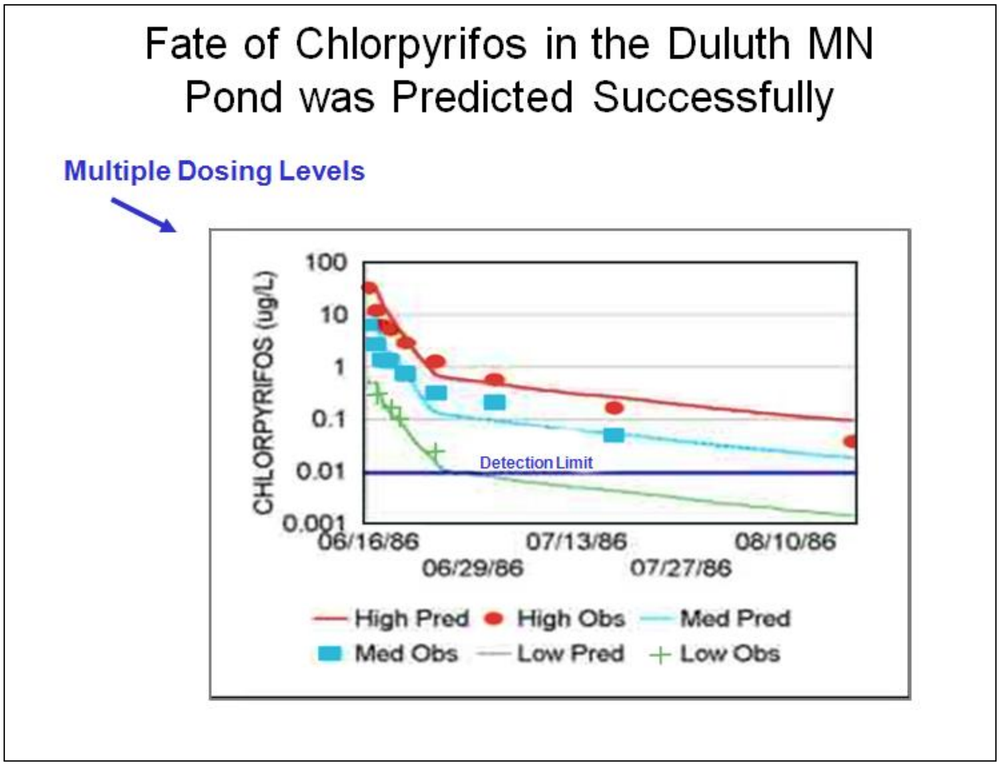
In the US, chlorpyrifos is registered only for agricultural use, where it is "one of the most widely used organophosphate insecticides," according to the United States Environmental Protection Agency (EPA). The crops with the most intense chlorpyrifos use are cotton, corn, almonds, and fruit trees including oranges and apples.

Chlorpyrifos is moderately persistent; however, according to the simulation about 3% per day is lost due to volatilization, about 1% due to microbial degradation, and another 1% due to hydrolysis and photolysis.

Toxicant mass balance tracking

- Extensive set of model outputs
- Provides mass accounting of total toxicant loadings to and total toxicant losses from the system
- Provides accounting of toxicants within the system at a given time
- Provides assurance of model mass balance throughout the complex cycling processes

Because the model is subject to use in a regulatory context, it is important to have accountability of simulated processes and assurance that mass balance is maintained. This is true for nutrients as well as for organic toxicants.



In a validation study several years ago, three levels of chlorpyrifos in a pond were predicted and compared to observed data.

HCB in tank

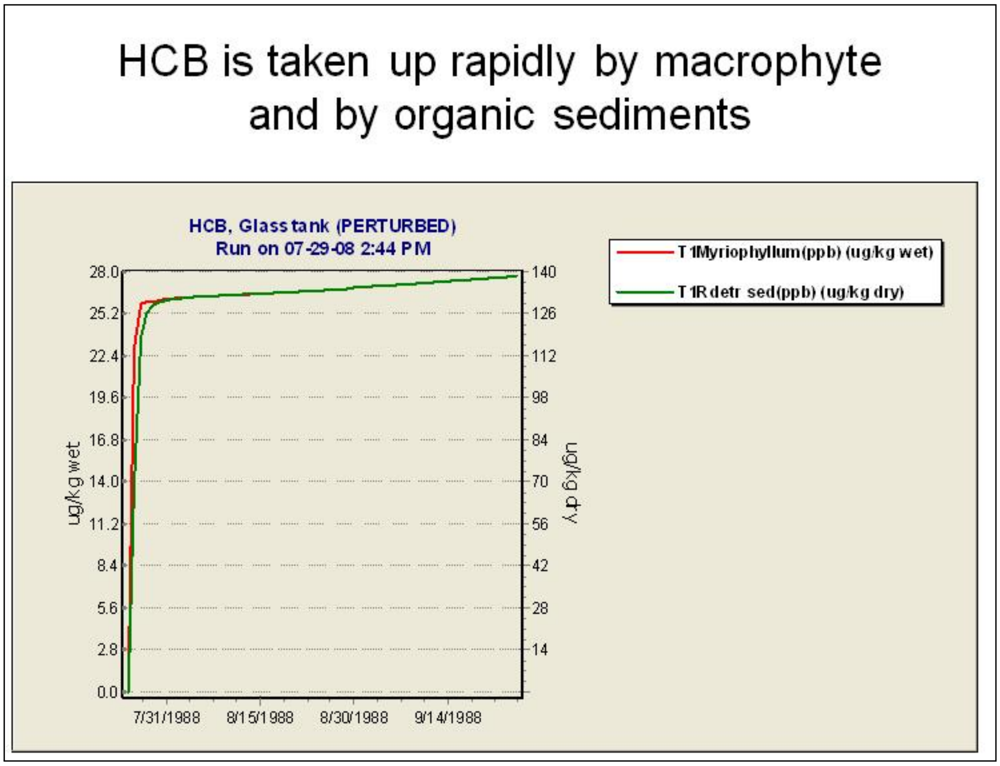
- Reproduces experimental results (Gobas) in which macrophytes are enclosed in an aquarium tank
- A single dose of hexachlorobenzene is applied at the beginning of the simulation
- Simplest type of AQUATOX model setup

From Wikipedia:

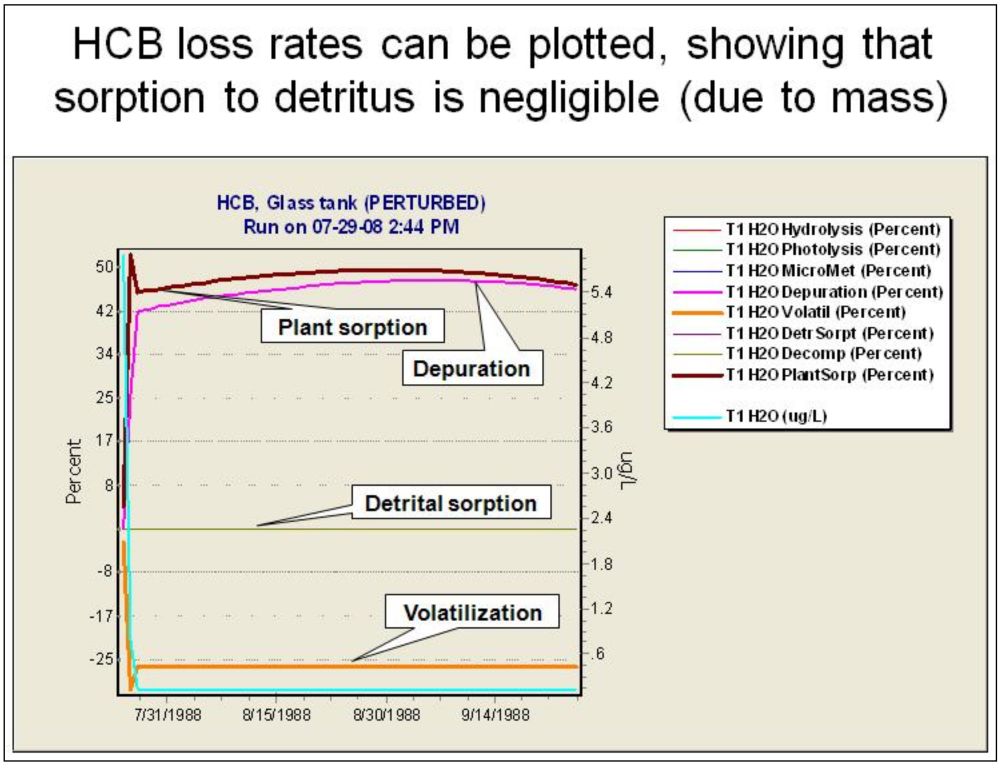
"**Hexachlorobenzene**, or **perchlorobenzene**, is a chlorocarbon with the molecular formula C_6Cl_6. It is a fungicide formerly used as a seed treatment, especially on wheat to control the fungal disease bunt. It has been banned globally under theStockholm Convention on persistent organic pollutants."

Replication of an experiment conducted by Gobas and others (1991) provides the simplest representation of the model. See slide 19 for the compartments.

Gobas, F. A. P. C., E. J. McNeil, L. Lovett-Doust, and G. D. Haffner. 1991. Bioconcentration of Chlorinated Aromatic Hydrocarbons in Aquatic Macrophytes (*Myriophyllum spicatum). Environmental Science & Technology 25: 924-929.*



Given the differences in scales, hexachlorobenzene is taken up similarly by the macrophyte *Myriophyllum* and by sediments. In fact, with a wet:dry ratio of 5, the scales are comparable. Also note that the macrophytes are the source of detritus.



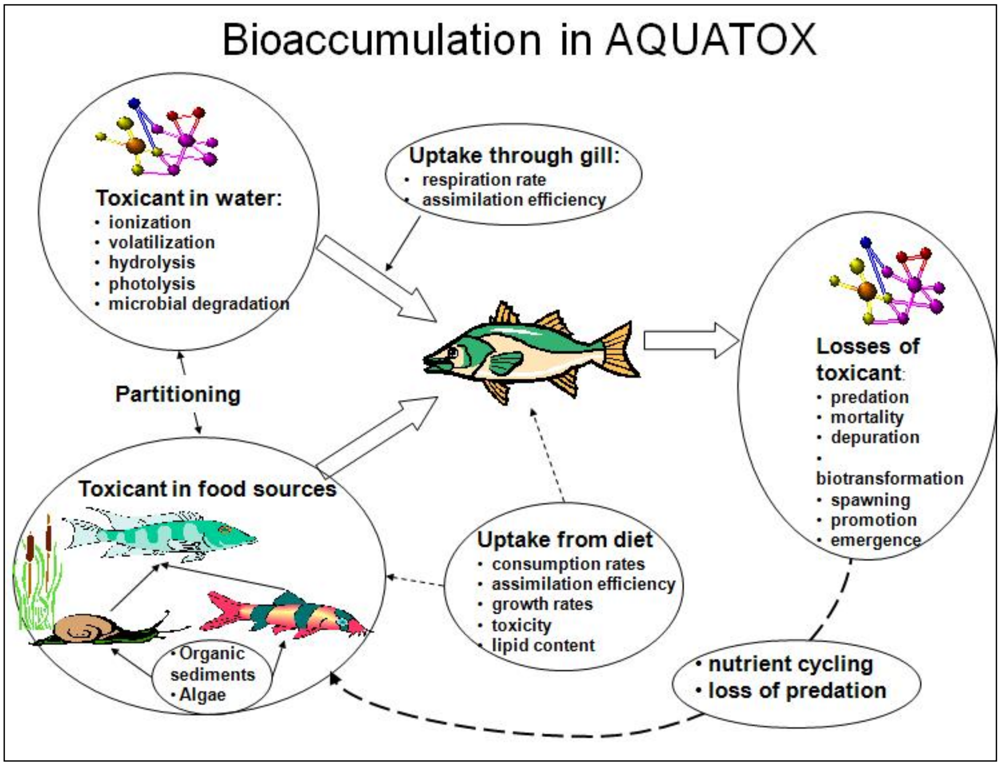
The rates plot indicate that the only significant processes in the tank are sorption by plants and volatilization. As we saw on the previous slide, the rate of sorption by detritus is almost the same as for plants; however the amount of detritus is so small that it accounts for only a fraction of a percent of the HCB in the water. The macrophytes, on the other hand, have a very large biomass in the tank, so much of the mass of HCB is taken up by the plants.

Note that volatilization is a negative when there is loss from the water into air (transfer through the water-air interface can be in either direction); this has recently been changed to plot as a positive rate to avoid confusion.

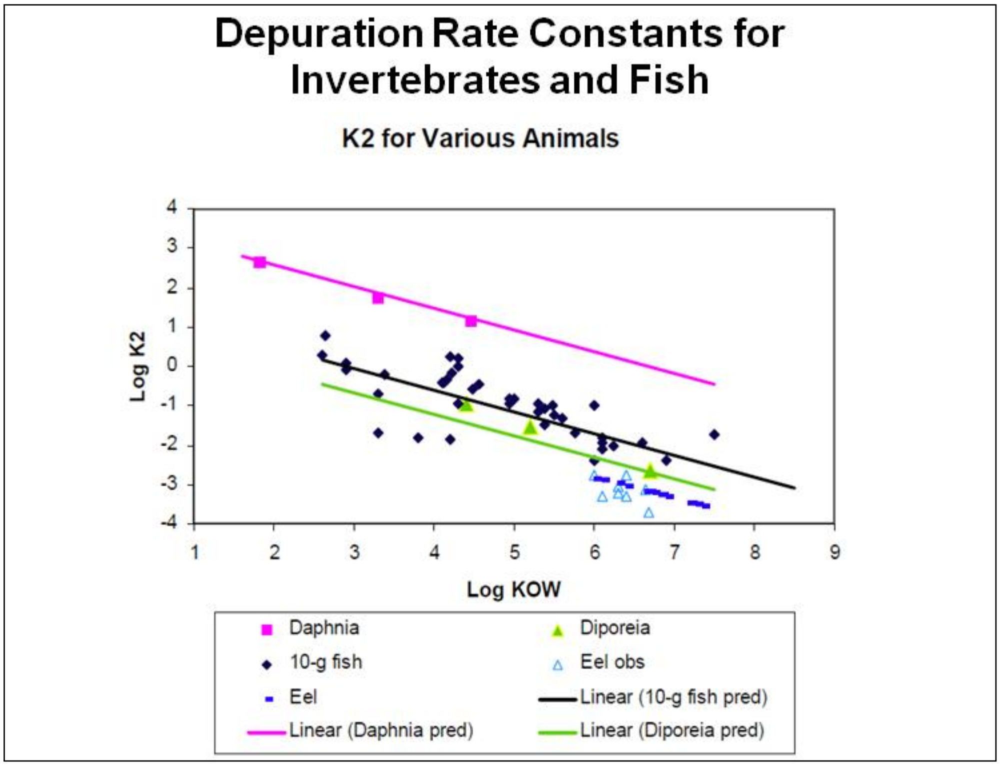
Chemical Bioaccumulation Overview

- Kinetic model of uptake and depuration
  - Uptake through gill
  - Uptake through diet
    - Consumption rate
    - Assimilation efficiency
  - Loss through depuration, biotransformation, growth dilution (implicit)
- Alternative (simple) BCF model available

Having reviewed the chemical fate processes represented by AQUATOX, we will now consider the simulated fate processes involving the biota.



Nonequilibrium concentrations, as represented by kinetic equations, depend on sorption, desorption, and elimination as functions of the chemical and exposure through water and food as a function of bioenergetics of the organism.



K2 can be estimated based on size, lipid content, and the LogKow of the chemical being modeled.

Alternative Chemical Uptake Model

The user may enter two of the three factors defining uptake (BCF, K1, K2) and the third factor is calculated:

$$BCF \ (\mathrm{L/kg}) = \frac{K1 \ (\mathrm{L/kg \cdot d})}{K2 \ (\mathrm{1/d})}$$

Given these parameters, AQUATOX calculates uptake and depuration in plants and animals as kinetic processes.

Dietary uptake of chemicals by animals is not affected by this alternative parameterization.

When performing bioaccumulation calculations, the default behavior of the AQUATOX model is to allow the user to enter elimination rate constants (K2) for all plants and animals for a particular organic chemical. K2 values may also be estimated based on the Log K_{OW} of the chemical, as shown earlier. Uptake in plants and gill uptake in animals is a function of K_{OW} in plants and respiration to chemical uptake efficiency in animals.

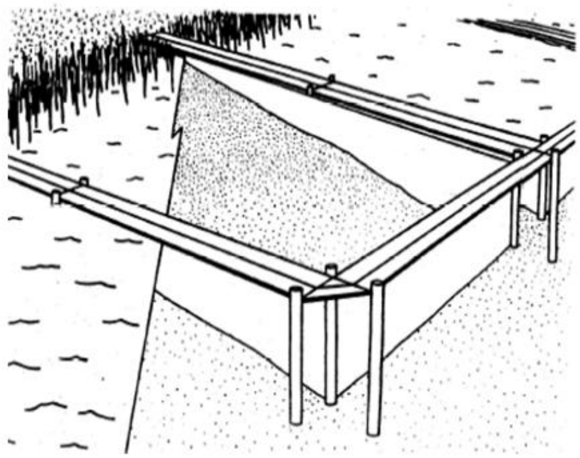
While the AQUATOX default model works well for a wide variety of organic chemicals, some chemicals with different physical characteristics are not effectively modeled using these relationships. For example, chemicals that are taken up very rapidly and those that have an external mode of toxicity, such as affecting the gills directly, are best simulated with an external toxicity construct. For this reason, an alternative uptake model based on equilibrium relationships among K1, K2, and BCF is provided to the user.

Chlorpyrifos in Pond

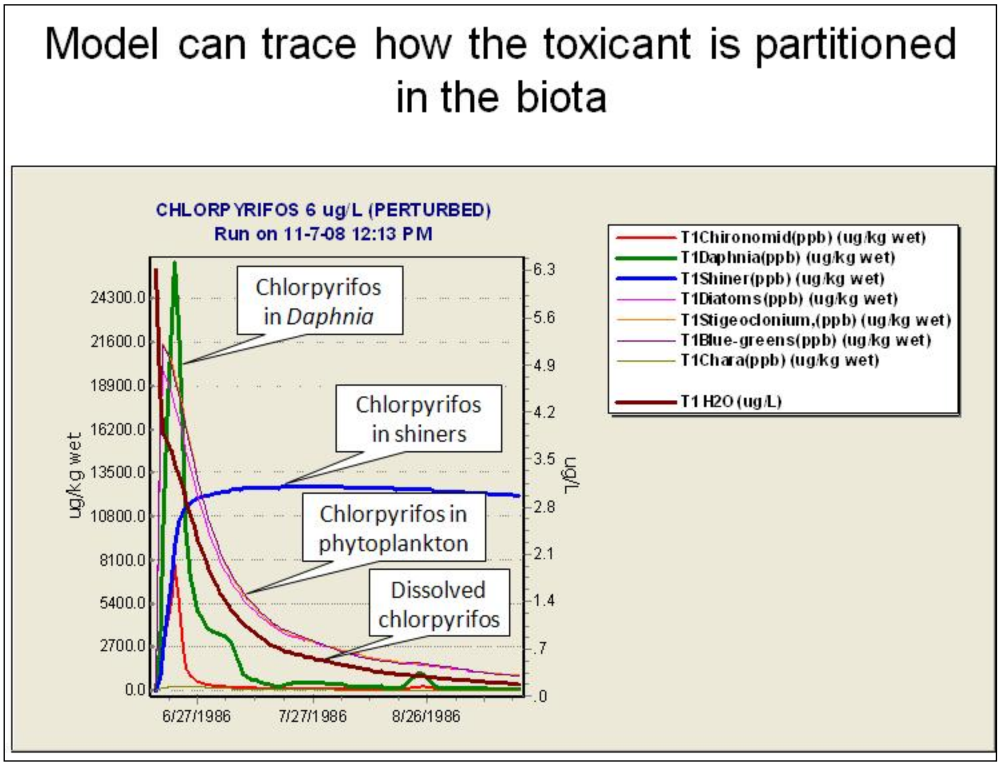
- Pond enclosure dosed with chlorpyrifos at EPA Duluth lab
- A single dose of chlorpyrifos is applied at the beginning of the simulation
- Additional biotic compartments
  - diatoms, greens, invertebrates,
  - sunfish, shiner

A series of experiments conducted at the US EPA Laboratory at Duluth MN provided data for testing how well AQUATOX represents chemical fate (slides 116, 117, 119), bioaccumulation (127-129), and toxicity (slides 153-158).

Chlorpyrifos-dosed pond enclosures at Duluth MN used to validate fate and effects model



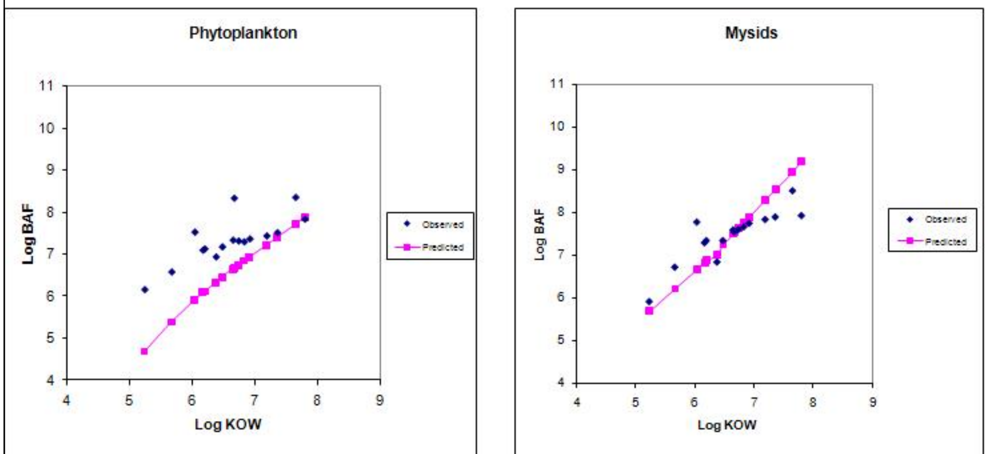
AQUATOX has the capability of representing enclosures, including accounting for the extra surface area of the enclosure walls, which is important as substrate for periphyton.



The fate depends in part on the effects: shiners (minnows) are tolerant of chlorpyrifos but *Daphnia* and chironomids aren't.

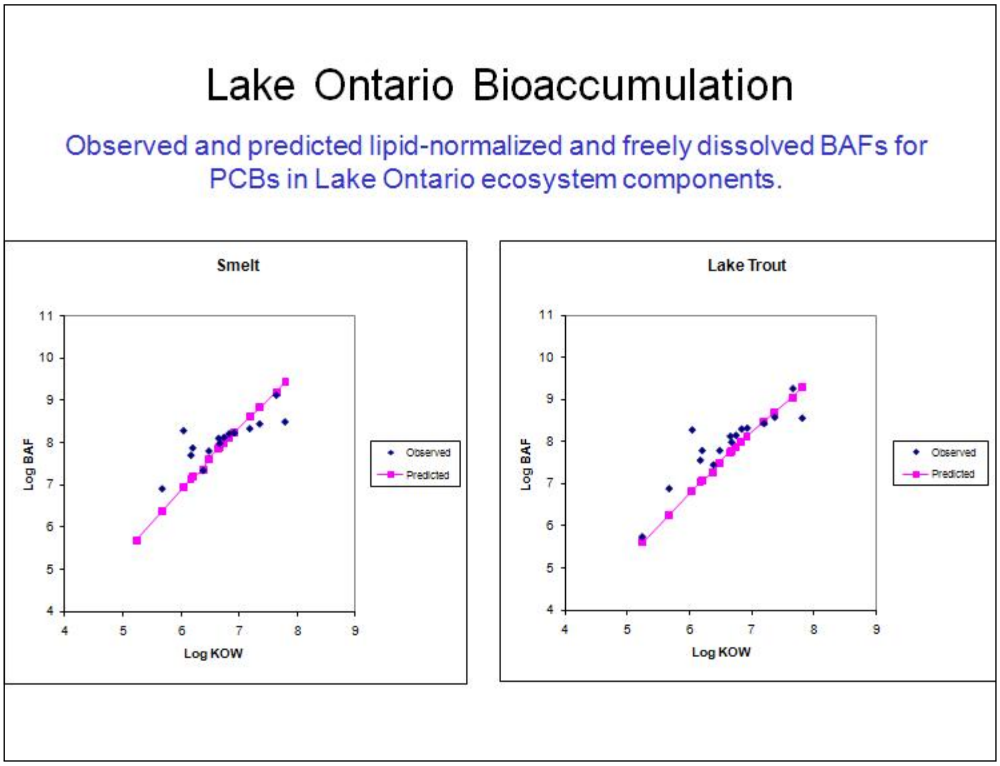
Lake Ontario Bioaccumulation

Observed and predicted lipid-normalized and freely dissolved BAFs for PCBs in Lake Ontario ecosystem components.

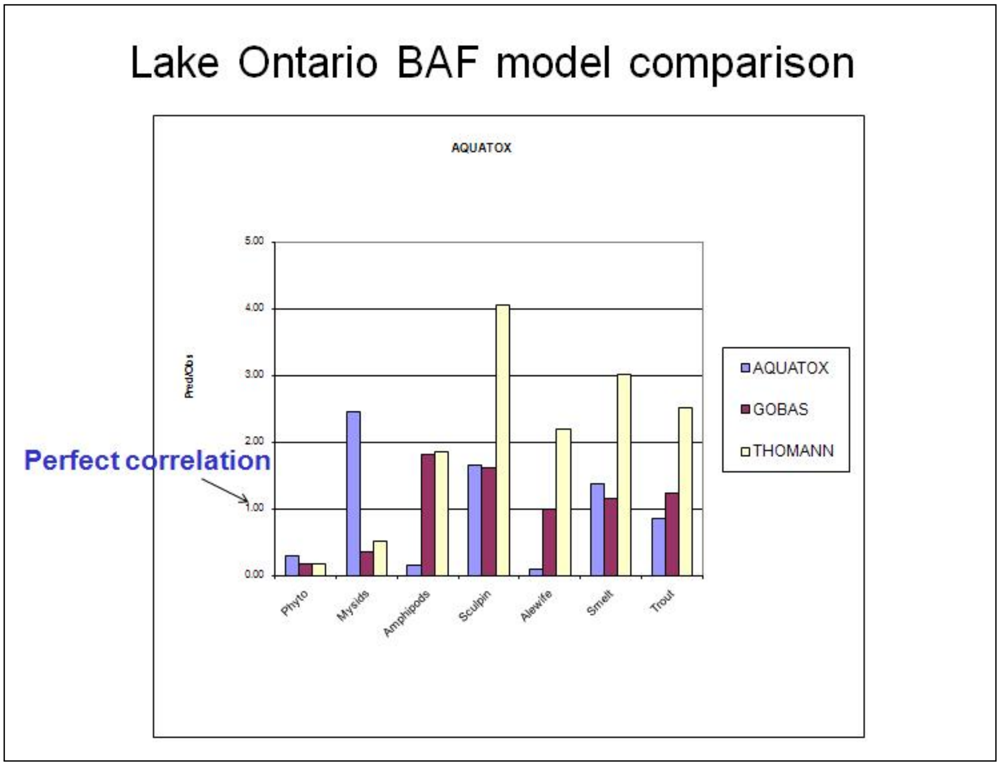


These are graphs from the validation studies done for Release 1.

Phytoplankton BAFs are under-predicted, but observed values include zooplankton.



These are the best fits to observed data.



AQUATOX under-predicts amphipod and alewife BAFs, for reasons that we are still investigating; phytoplankton BAFs are also under-predicted, but that is in comparison to combined phytoplankton and zooplankton BAFs. Mysids are over-predicted. The model compares favorably with the Gobas and Thomann models as applied by Burkhard (1998).

Burkhard, L. P. 1998. Comparison of Two Models for Predicting Bioaccumulation of Hydrophobic Organic Chemicals in a Great Lakes Food Web. Environmental Toxicology and Chemistry **17:383-393.**

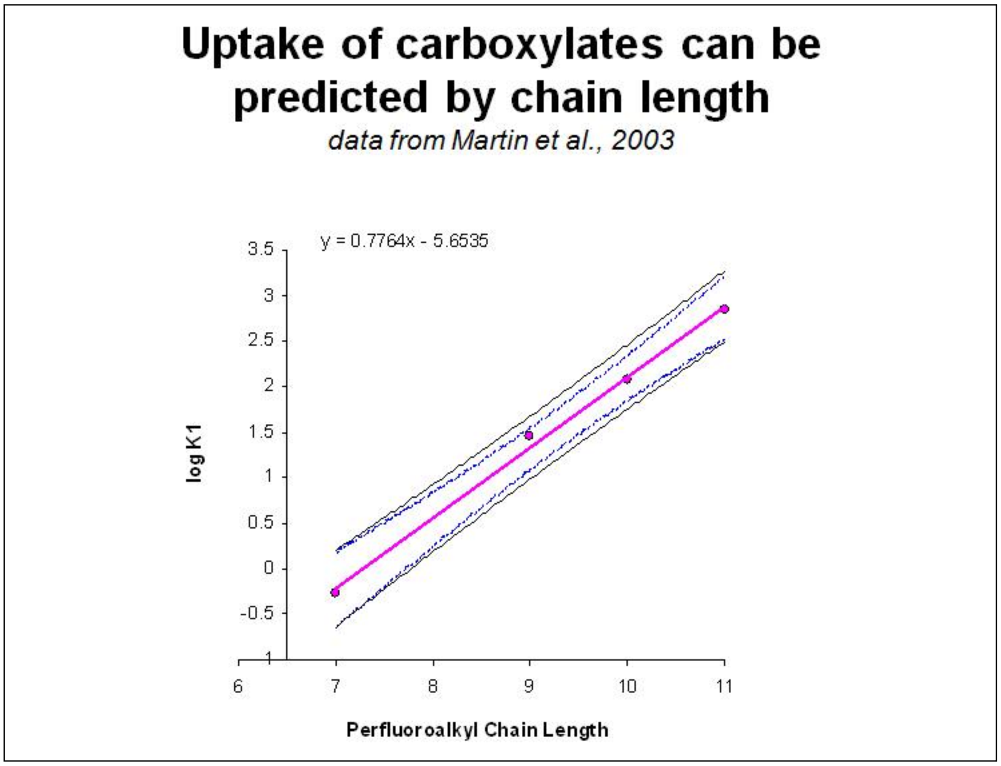
Perfluorinated Surfactants (PFAs)

- Originally developed as part of estuarine model
  - Sorption modeled using empirical approach
  - Animal Uptake/Depuration a function of chain length and PFA type (sulfonate/ carboxylate)
  - Biotransformation can be modeled

The addition of code specifically developed for perfluorinated surfactants is an example of how AQUATOX can be modified to evaluate unusual chemicals.

Several years ago EPA evaluated the bioaccumulation and effects of a group of chemicals known as perfluorinated surfactants. There are two major types of perfluorinated surfactants: perfluoroalkanesulfonates and perfluorocarboxylates. Perfluoroctane sulfonate (PFOS) belongs to the perfluoroalkanesulfonate group and Perfluorooctanoic acid (PFOA) belongs to the perfluorocarboxylate group. These persistent chemicals have been found in humans, fish, birds, marine and terrestrial animals throughout the world. PFOS has an especially high bioconcentration factor in fish. At present there is increasing public concern about PFOA, which is associated with the manufacture of Teflon (see, for example, an article in the August 8, 2004, NY Times).

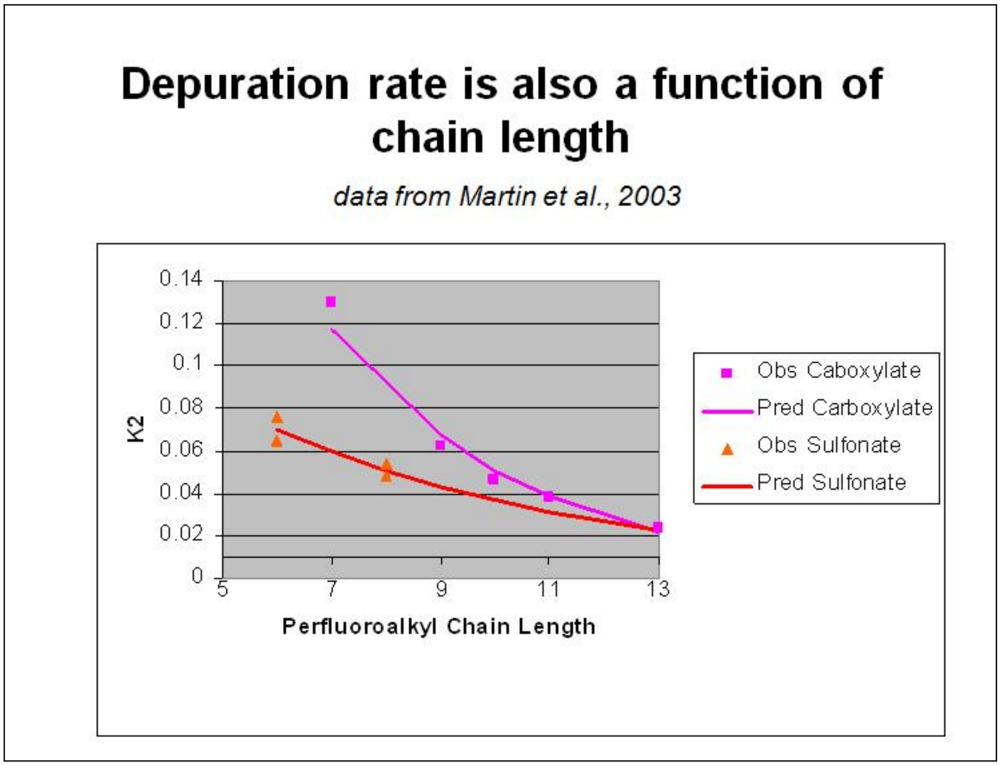
Park, R. A., and J. S. Clough. 2003. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems: Perfluoroalkylated Surfactant and Estuarine Versions, Addendum to Release 2 Technical Documentation (Unpublished report). U.S. Environmental Protection Agency, Washington, D.C.



Because PFAs behave differently from most bioaccumulative compounds it was necessary to program estimation procedures for uptake and depuration specific to them. Fortunately, papers documenting such estimation procedures appeared just as we embarked on this project:

Martin, Jonathan W., Scott A. Mabury, Keith R. Solomon, and Derek C.G. Muir. 2003. Bioconcentration and Tissue Distribution of Perfluorinated Acids in Rainbow Trout (*Oncorhyncus mykiss*). *Environmental Toxicology and Chemistry* 22 (1):196-204.

Martin, Jonathan W., Scott A. Mabury, Keith R. Solomon, and Derek C.G. Muir. 2003. Dietary Accumulation of Perfluorinated Acids in Juvenile Rainbow Trout (*Oncorhynchus mykiss*). *Environmental Toxicology and Chemistry* 22 (1):189-195.



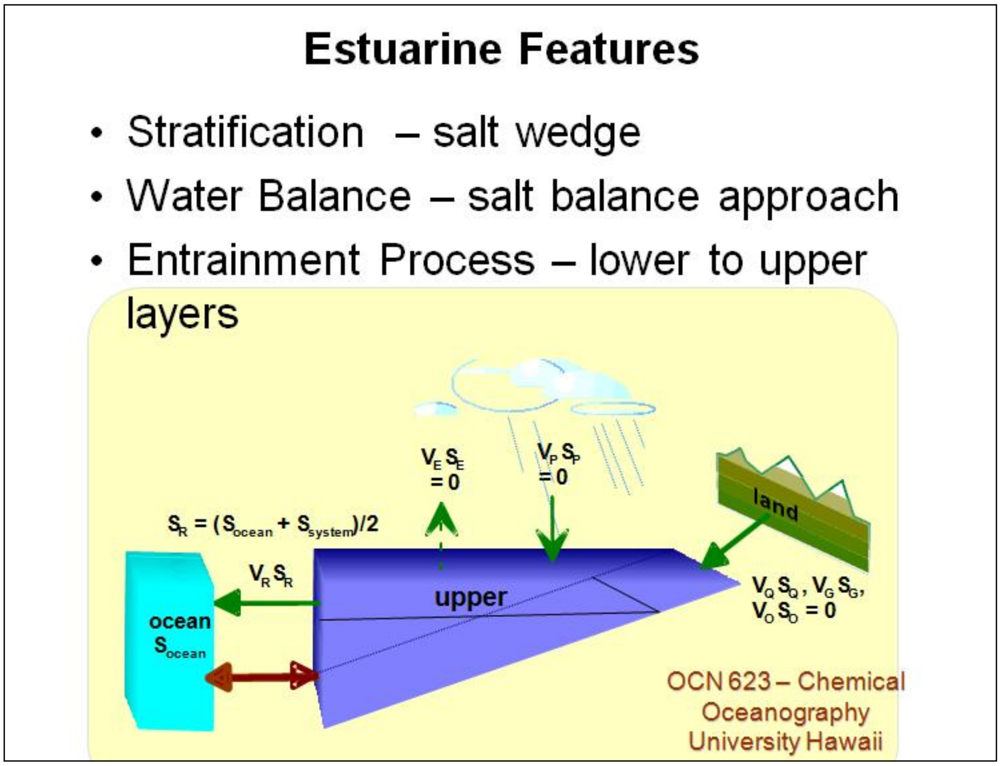
Martin, Jonathan W., Scott A. Mabury, Keith R. Solomon, and Derek C.G. Muir. 2003. Bioconcentration and Tissue Distribution of Perfluorinated Acids in Rainbow Trout (*Oncorhyncus mykiss*). *Environmental Toxicology and Chemistry* 22 (1):196-204.

Martin, Jonathan W., Scott A. Mabury, Keith R. Solomon, and Derek C.G. Muir. 2003. Dietary Accumulation of Perfluorinated Acids in Juvenile Rainbow Trout (*Oncorhynchus mykiss*). *Environmental Toxicology and Chemistry* 22 (1):189-195.

Estuarine version applied to Galveston Bay, Texas, to evaluate toxicants

Photo Courtesy NASA Johnson Space Center

AQUATOX Rincludes an estuarine module. It was calibrated and partially verified using Galveston Bay, Texas.



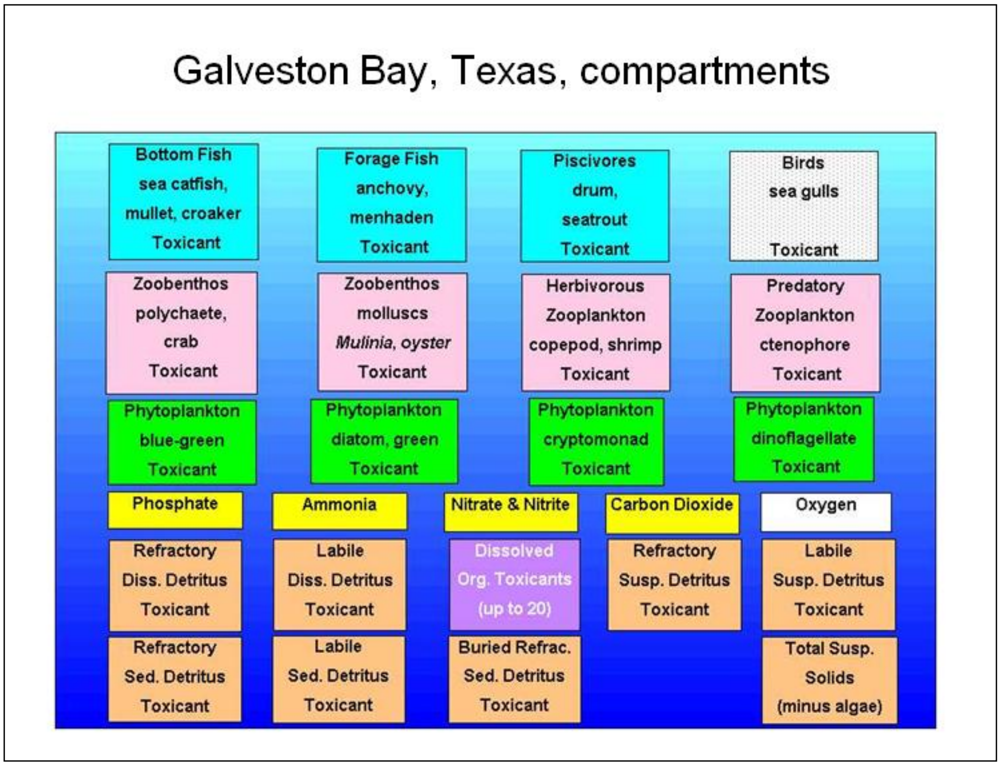
- Estuaries are considered to be permanently stratified, though at times the extent of turbulent diffusion will essentially mean that they are well mixed.
- Salt balance approach: salt water inflow and outflow at the estuary mouth is a function of salinity and residual flow.
- Entrainment (water movement from the lower level to the upper level) transports suspended and dissolved substances from one layer to the next.

Estuary Model Data Requirements

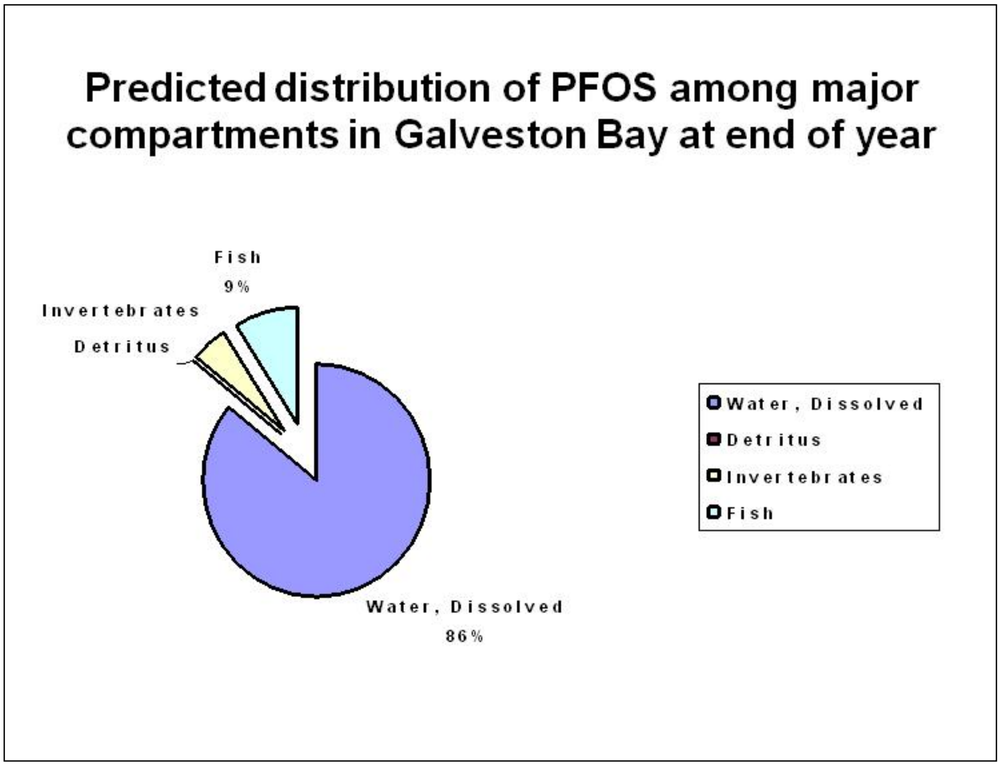
- Time series of “Upper Layer” and “Lower Layer” salinities at mouth for Salt Wedge Model
- Tidal range model parameters
  - “harmonic constants”, often available from NOAA website
- Estuary site width
- Loadings of freshwater inflow

The website to load tide prediction parameters (harmonic constants) within the United States is:

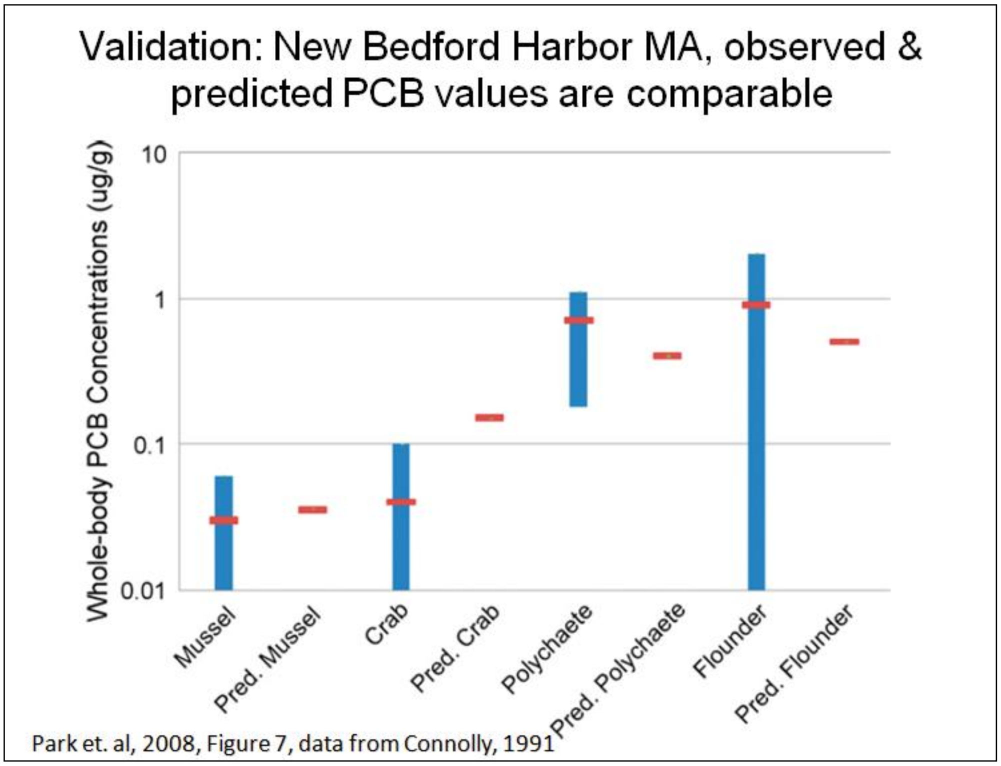
http://tidesandcurrents.noaa.gov/



Most commercial species are represented, as well as other critical food web components. Birds are a bioaccumulative endpoint (i.e. their biomass is not simulated, only the tissue concentrations of the toxicant). The concentration of chemical in their tissues is a function of given BAFs weighted by availability of preferred food .



The estuarine version was used to predict the fate and bioaccumulation of PFOS and other PFAs in the nearshore environment. Because of the volume of water, most of the mass resides in the dissolved phase.



In a partial validation, PCB concentrations in water and sediments in New Bedford Harbor, MA, were imported into Galveston Bay TX simulation. The results were comparable between observed and predicted mean whole-body concentrations.

The ranges and means are shown for observed whole-body concentrations (Connolly 1991).

Connolly, J. P. 1991. Application of a food chain model to polychlorinated biphenyl contamination of the lobster and winter flounder food chains in New Bedford Harbor. *Environ. Sci. Technol.* **25**: 760-770.

Modeling Toxicity of Chemicals

- Lethal and sublethal effects are represented
- Chronic and acute toxicity are both represented
- Effects based on total internal concentrations
- Uses the critical body residue approach (McCarty 1986, McCarty and Mackay 1993)
- Can also model external toxicity
  - Useful if uptake and depuration are very fast (as with herbicides)

Sublethal effects include reduction in photosynthesis, ingestion, and reproduction, and increased egestion, drift, and sloughing of periphyton.

From Wikipedia, the free encyclopedia:

Chronic toxicity is a property of a substance that has toxic effects on a living organism, when that organism is exposed to the substance continuously or repeatedly.

Acute Toxicity is a property of a substance that has toxic effects on a living organism, when that organism is exposed to a lethal dose of a substance once. In other words, basically a short-term version of chronic toxicity.

AQUATOX models time-varying toxicity—both chronic and acute.

McCarty, L.S., G.W. Ozburn, A.D. Smith, and D.G. Dixon. 1992. Toxicokinetic Modeling of Mixtures of Organic Chemicals. *Environmental Toxicology and Chemistry*, 11:1037-1047.

Mackay, D., H. Puig, and L.S. McCarty. 1992. An Equation Describing the Time Course and Variability in Uptake and Toxicity of Narcotic Chemicals to Fish. *Environmental Toxicology and Chemistry*, 11:941-951.

Toxicity Models within Bioaccumulation Models

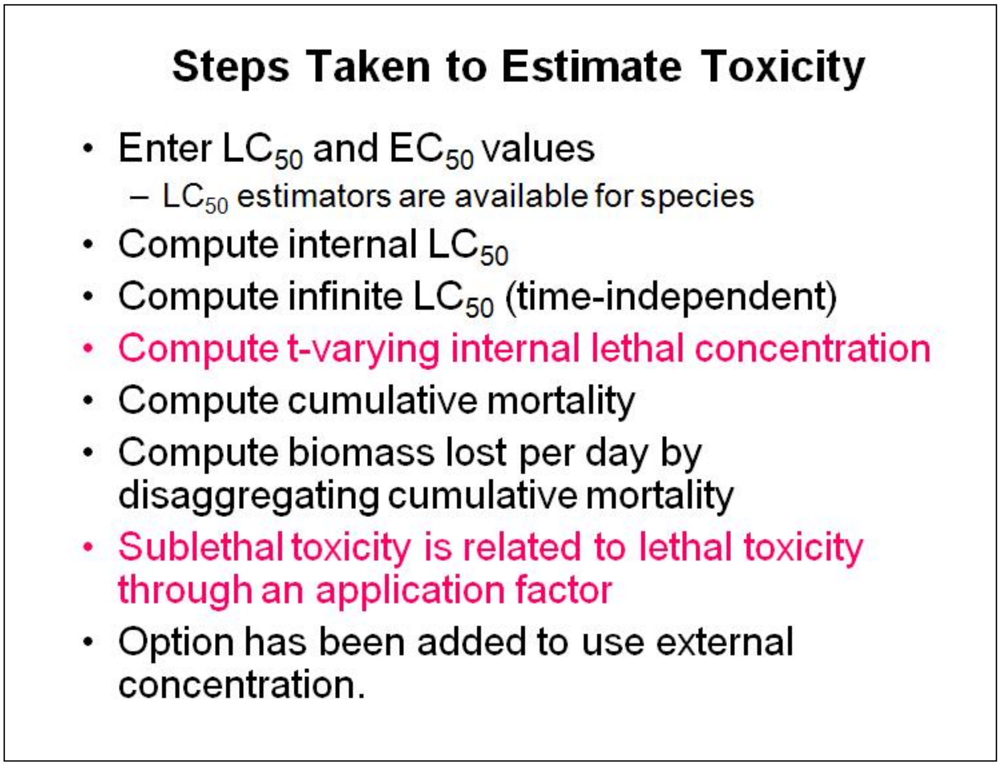
Table 3.5. Toxicity Models

	AQUATOX Release 2	BASS v 2.1	Biotic Ligand 1.0.0	RAMAS Ecosystem
Domain of Toxicity Models				
Acute Toxicity	★	★	★	★
Chronic Toxicity	★	★		★
Sub-Lethal Effects	★			
Toxicity Effects Feed Back to Bioconcentration Model	★	★		★
Toxicity Mechanisms				
Based on Total Internal Concentrations	★	★		★
Based on Concentrations in Organs			★	
User Input Required				
LC50 values	★	★		
EC50 values	★			★
Weibull Shape Parameter	★			★

Imhoff et al. 2004

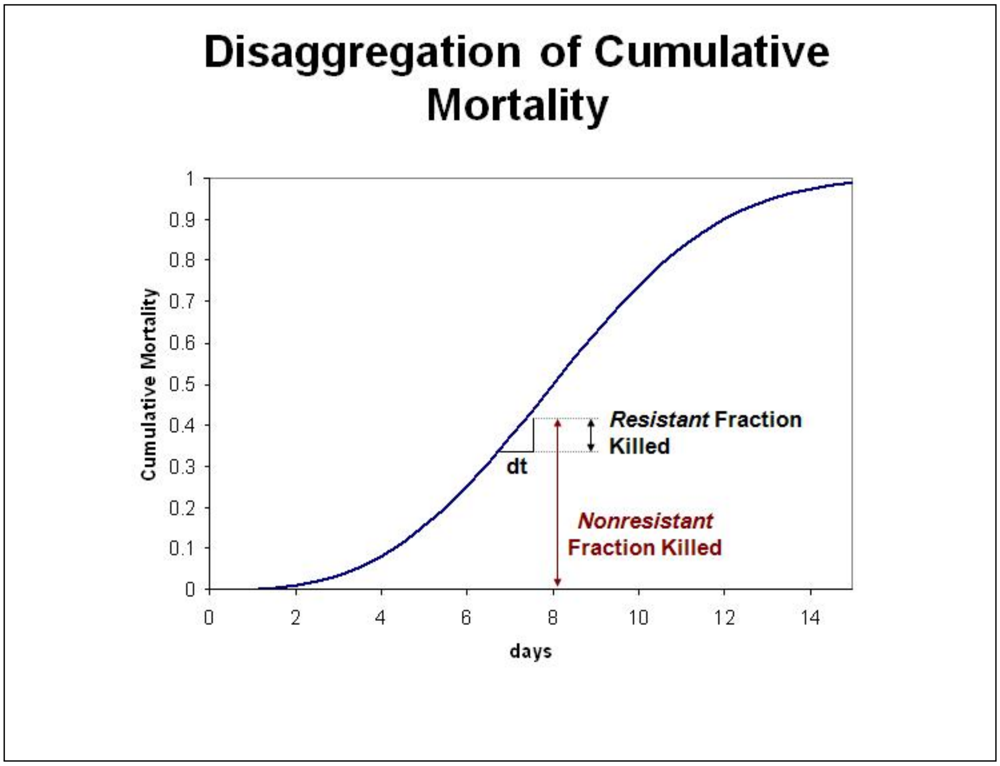
Many bioaccumulation models do not include toxicity, and of those, few include sub-lethal effects (such as toxicity-induced drift and periphyton sloughing).

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.



The modeling approach is complex; key elements are highlighted in red. The details are covered in Chapter 9 of the *Technical Documentation*.

By entering both LC_{50} and EC_{50} values for a species the application factor can be computed.



The biomass killed per day is computed by disaggregating the cumulative mortality. Think of the biomass at any given time as consisting of two types: biomass that has already been exposed to the toxicant previously, which is called *Resistant* because it represents the fraction that was not killed; and new biomass that has formed through growth, reproduction, and migration and has not been exposed to a given level of toxicant and therefore is referred to as *Nonresistant*.

Option to Model with External Concentrations

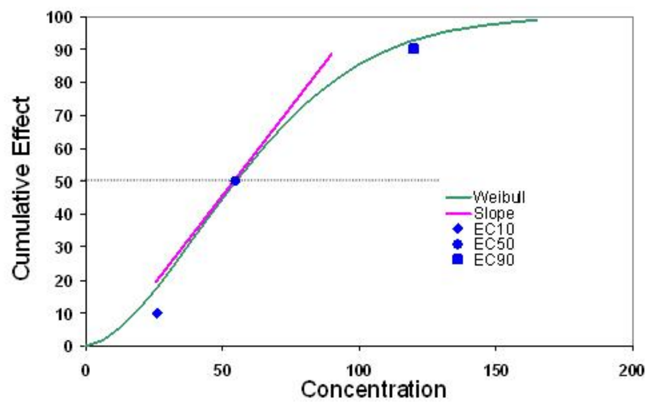
Two-parameter Weibull distribution as in Christiensen and Nyholm (1984)

$$CumFracKilled = 1 - \exp(-kz^{\eta})$$

Two Required Parameters:

LC50 (or EC50)

"Slope Factor" = Slope at LC50 multiplied by LC50



Chemicals that are taken up very rapidly and those that have an external mode of toxicity, such as affecting the gills directly, are best simulated with an external toxicity construct.

Rather than require the user to fit toxicological bioassay data to determine the parameters for ***k*** and η, these parameters are derived to fit the LC50 and the slope of the cumulative mortality curve at the LC50 (in the manner of the RAMAS Ecotoxicology model, Spencer and Ferson, 1997). (See section 9.3 in the *Technical Documentation*)

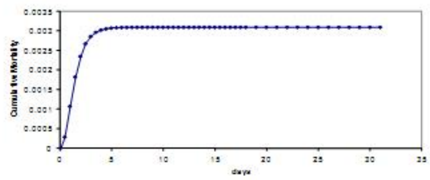
AQUATOX assumes that each chemical's dose response curve has a distinct shape, relevant to all organisms modeled. In this manner, a single parameter describing the shape of the Weibull parameter can be entered in the chemical record rather than requiring the user to derive slope parameters for each organism modeled. However, as shown in the slide above, the slope of the curve at the LC50 is both a function of the shape of the Weibull distribution and also the magnitude of the LC50 in question. For this reason, rather than have a user enter "the slope at LC50" into the chemical record, AQUATOX asks that the user enter a "slope factor" defined as "the slope at LC50 multiplied by LC50." In the above example, the user would enter a slope factor of 1.0 and then, given an LC50 of 1 or an LC50 of 100, the above curve would be generated.

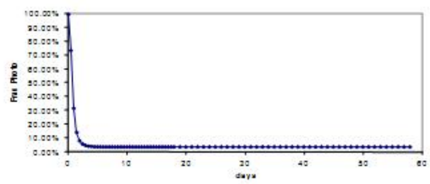
When modeling toxicity based on external concentrations, organisms are assumed to come to equilibrium with external concentrations (or the toxicity is assumed to be based on external effects to the organism).

Spreadsheet Demo

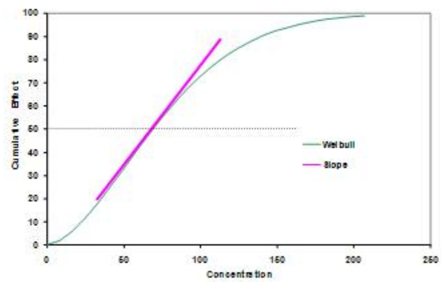
AQUATOX is distributed with two spreadsheets useful in understanding the model's toxicity components

AQUATOX_Internal_Toxicity_Model.xls





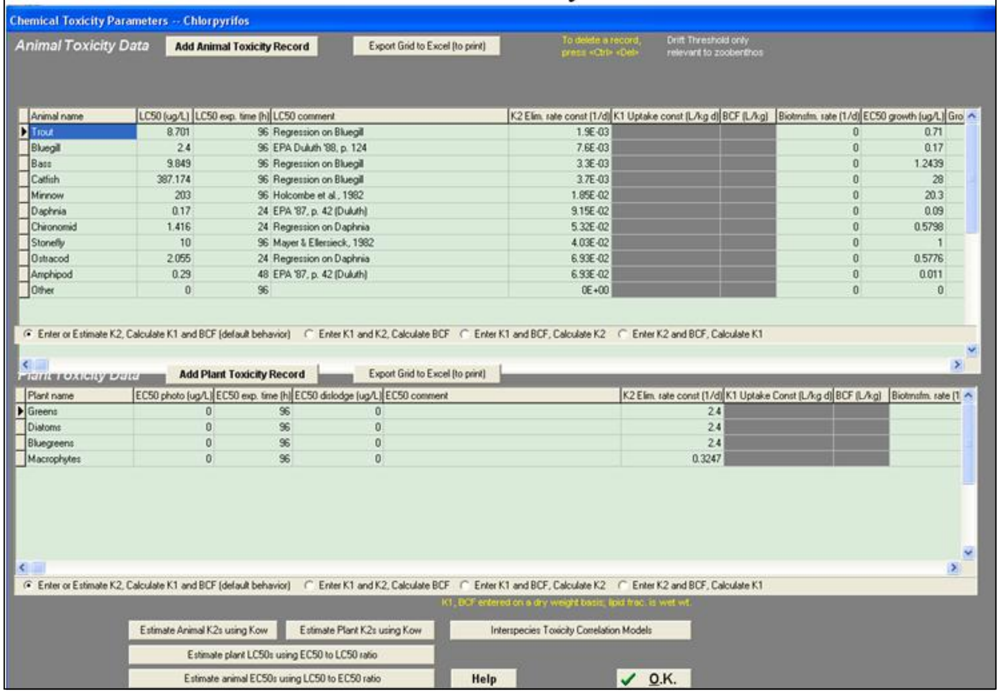
AQUATOX_External_Toxicity_Model.xls



These spreadsheets are simplifications of AQUATOX, in that they represent a constant toxicant water concentration, rather than being subject to the various fate processes normally simulated.

These Excel spreadsheets are located in the STUDIES directory of your AQUATOX installation location.

Chemical Toxicity Screen



This screen is where all of the important chemical toxicity parameters are located. To get to this screen go to Chemical Underlying Data and select the "Toxicity Data" button.

There are multiple options for entering uptake rate constant (k1), the elimination rate constant (k2) and the bioconcentration factor (BCF) or allowing the model to calculate these parameters (BCF=k1/k2).

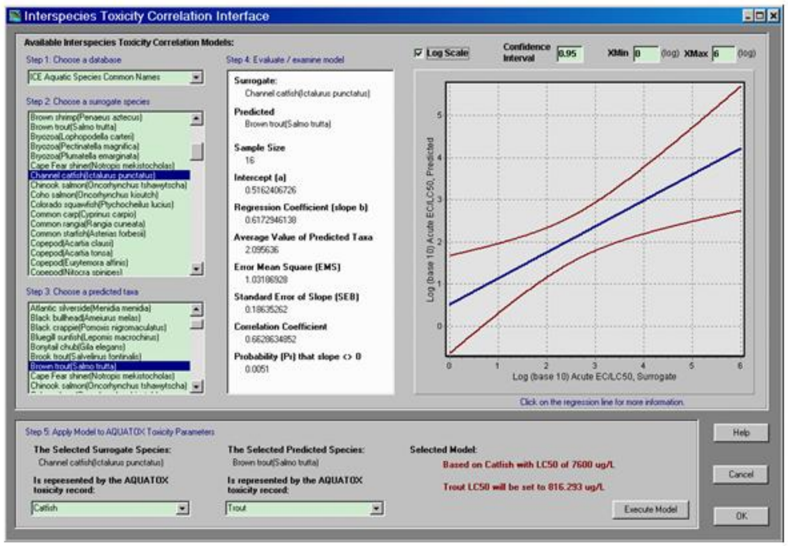
Additionally, elimination rates may be estimated using the octanol water partition coefficient (Kow).

Fish and invertebrate regressions (i.e. estimating toxicity from one species to another) are available for many organisms using the ICE database (see next slide).

As explained previously, by entering both LC_{50} and EC_{50} values for a species the application factor can be computed. The user has the option of applying that same ratio to the rest of the species in the animal or plant toxicity screen using the buttons **Estimate animal LC50s**... and **Estimate plant EC50s...**.

Release 3: Additional Toxicity Features

- **Integration with ICE: a large EPA database of toxicity regressions**



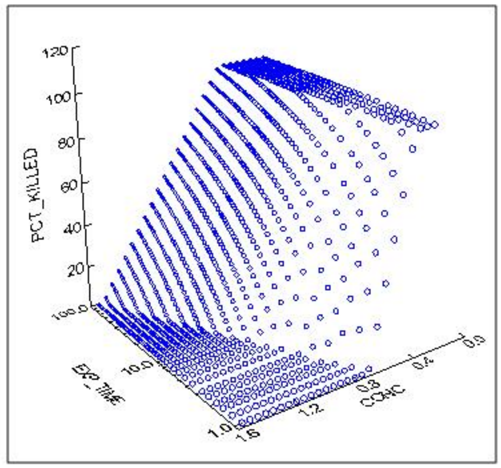
http://www.epa.gov/ceampubl/fchain/webice/index.htm

Release 3: Additional Toxicity Features

- Integration with ICE: a large EPA database of toxicity regressions
- **Dissolved Oxygen effects**

A 3D model of effects that is a function of exposure time and oxygen concentration.

Includes non-lethal effects on consumption and reproduction



U.S. Environmental Protection Agency. 1986. Ambient Water Quality Criteria for Dissolved Oxygen. Pages 62. Office of Water, Washington D.C.

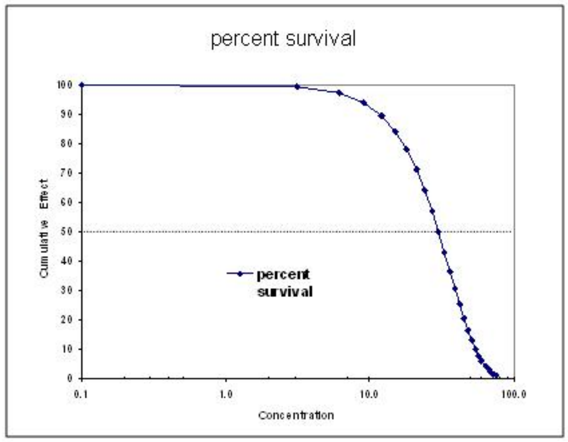
U.S. Environmental Protection Agency. 2000. Ambient Aquatic Life Water Quality Criteria for Dissolved Oxygen (Saltwater): Cape Cod to Cape Hatteras. Pages 55. Office of Water, Washington DC.

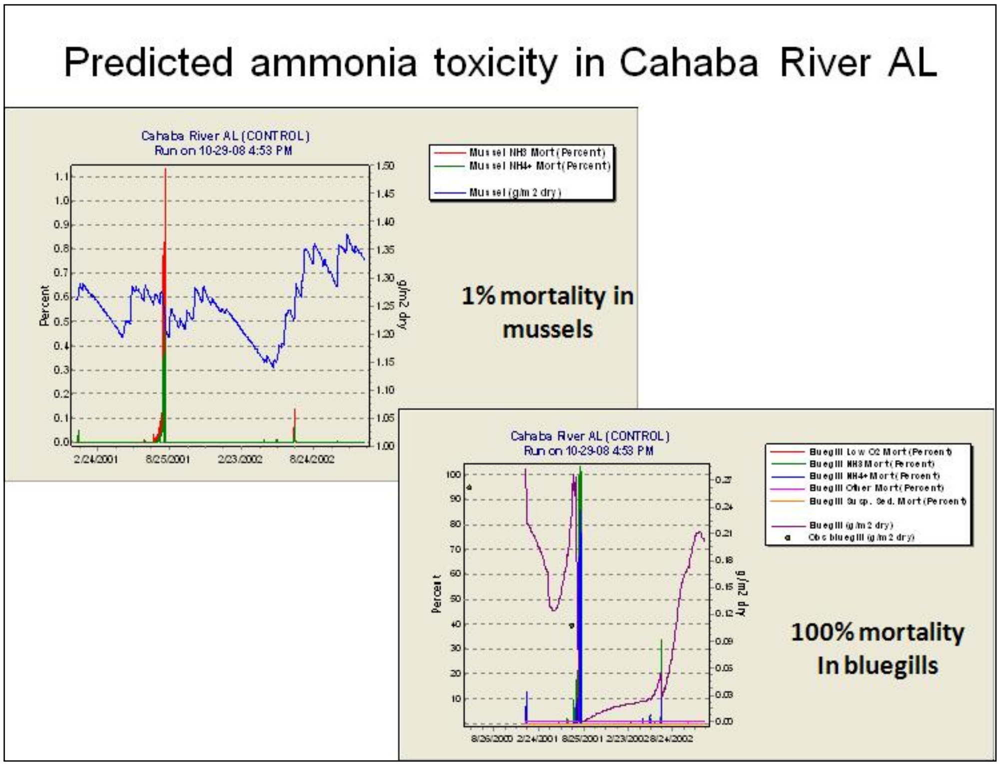
Release 3: Additional Toxicity Features

- Integration with ICE: a large EPA database of toxicity regressions
- Dissolved Oxygen effects
- Ammonia effects

External Toxicity Model Utilized

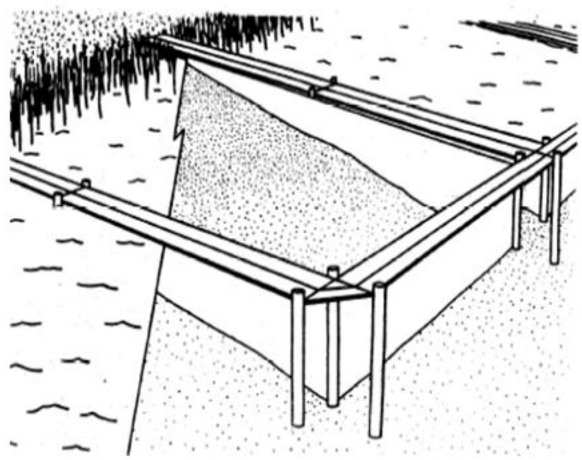
Effects from un-ionized and
ionized ammonia are additive



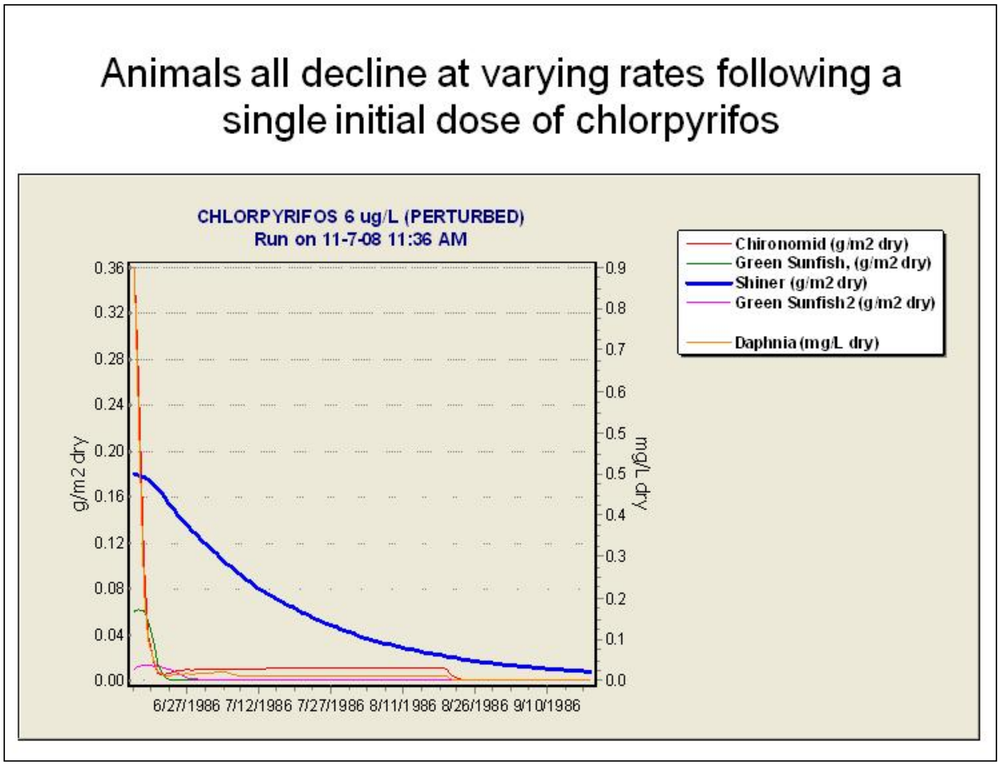


Young mussels are very sensitive to ammonia (LC50 = 0.165), but adults appear to be tolerant (LC50 = 17 mg/L), so the default of 10 mg/L was used for mussels. Bluegill LC50 = 0.62 mg/L.

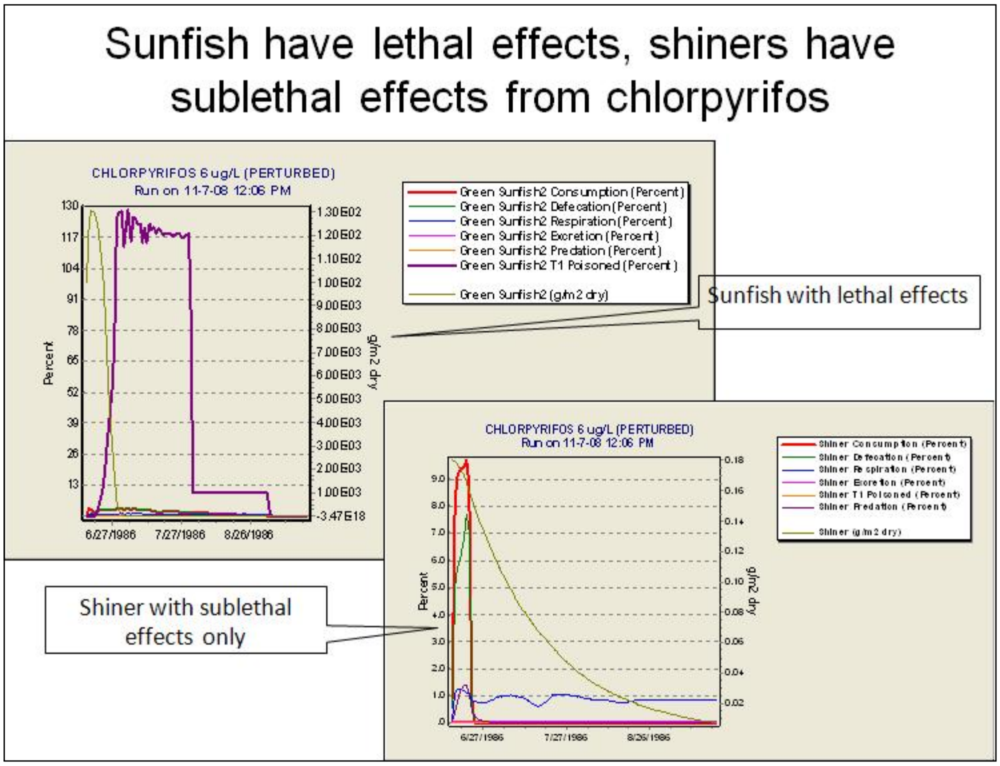
Returning to the Enclosure in Duluth MN . . .



We have seen the simulated chemical fate and bioaccumulation of chlorpyrifos in the mesocosm, now we'll look at the simulated toxic effects.

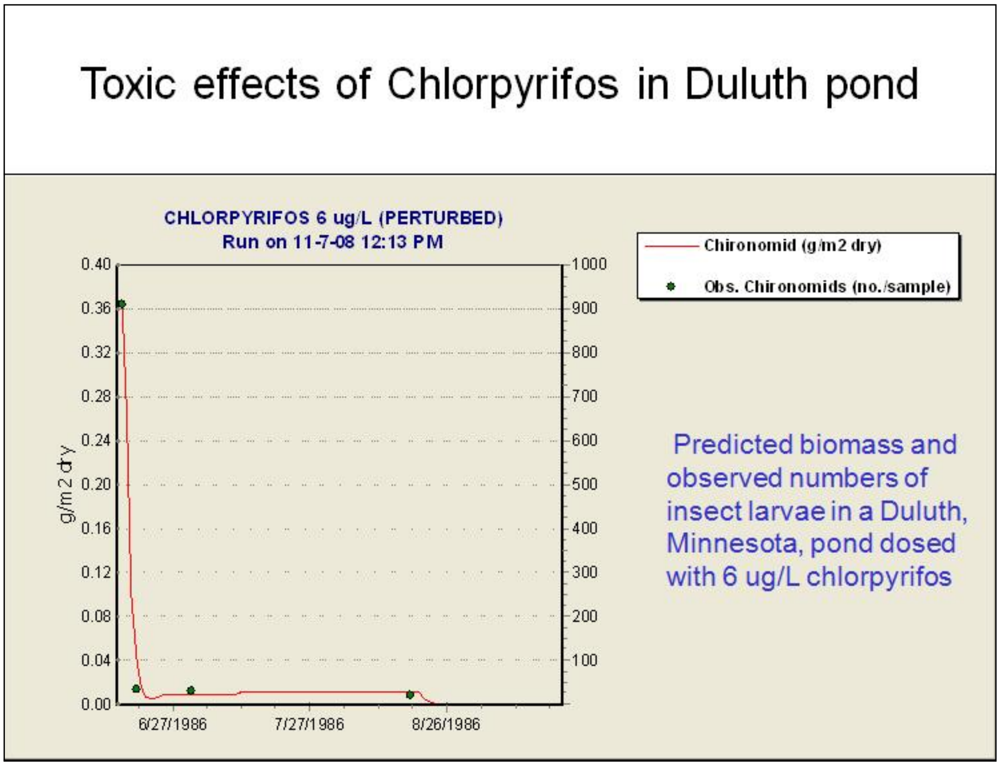


Shiners are most tolerant to chlorpyrifos according to toxicity data. Chironomids and *Daphnia* are most sensitive.

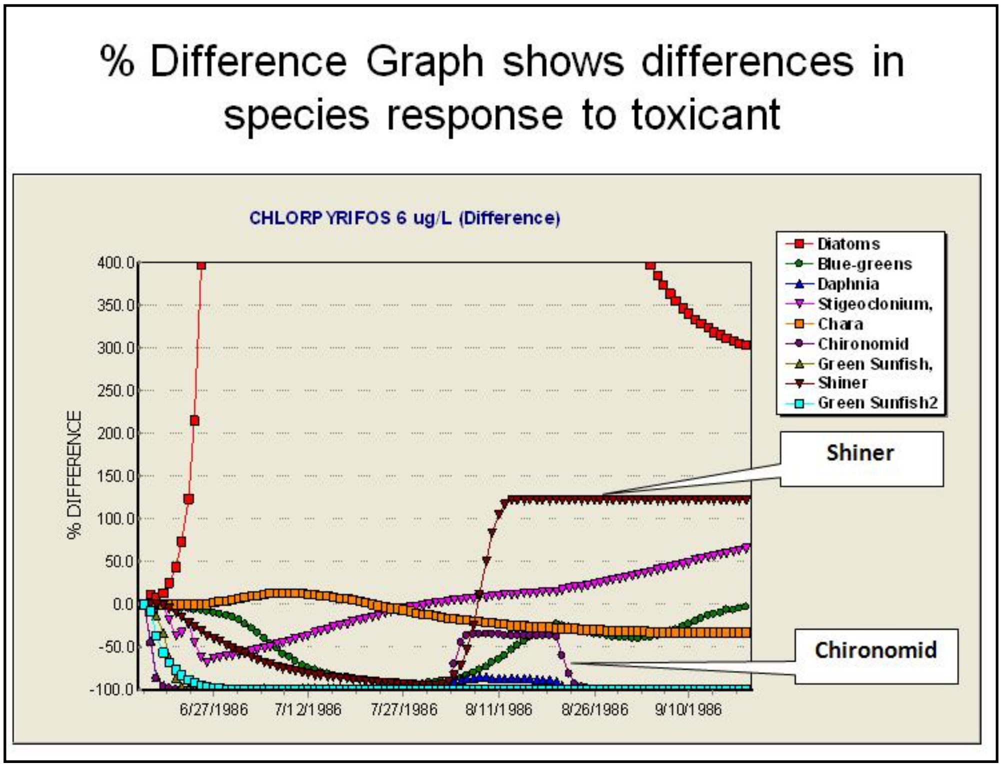


Sunfish have a low tolerance to chlorpyrifos (LC50 = 2.4 ug/L), so bioaccumulation is followed by significant mortality with gradual recovery.

Shiners are tolerant of chlorpyrifos (LC50 =203 ug/L) and exhibit no mortality with an initial dose of 6 ug/L chlorpyrifos; they do exhibit sublethal toxicity in the form of decreased consumption and assimilation; loss of forage is a predicted indirect effect. Predicted recovery of sunfish eventually leads to high predation on shiners.

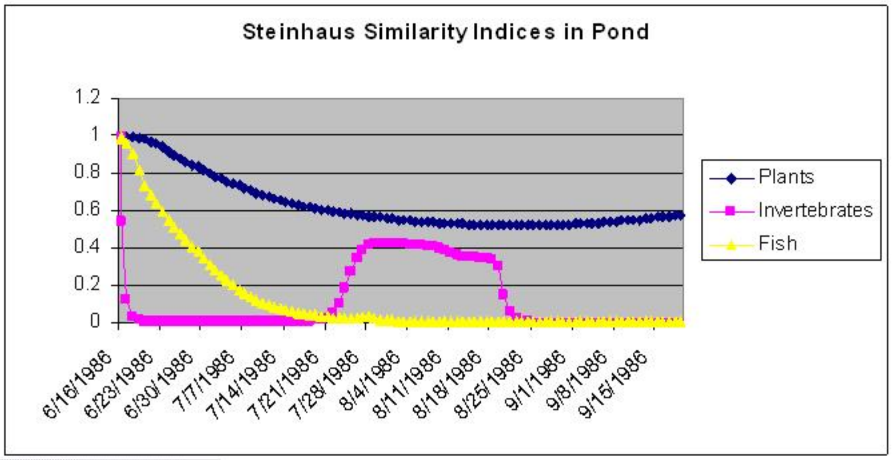


In a validation study 6 ug/L initial dose of chlorpyrifos in a pond resulted in a decline in predicted insect biomass, which compared favorably to decline in observed numbers of insects.



An initial 6 ug/L chlorpyrifos in the pond has an immediate impact on the invertebrates and sunfish. Removal of predation causes an explosive increase in diatoms; shiners recover, partly in response to chironomid recovery half way through the simulation period.

Steinhaus Indices show ecosystem impacts predicted by the model



$$S = \frac{2 * \sum_{k=1}^{n} Min(a_{1,k}, a_{2,k})}{\sum_{k=1}^{n} a_{1,k} + \sum_{k=1}^{n} a_{2,k}}$$

Coefficients of similarity are used to determine whether the composition of two communities is similar. The Steinhaus coefficient or similarity index (S) is based on the species abundances (in this case indicated by the species specific daily biomass) common to two communities, where $a_{i,k}$ is abundance of species k in sample I.

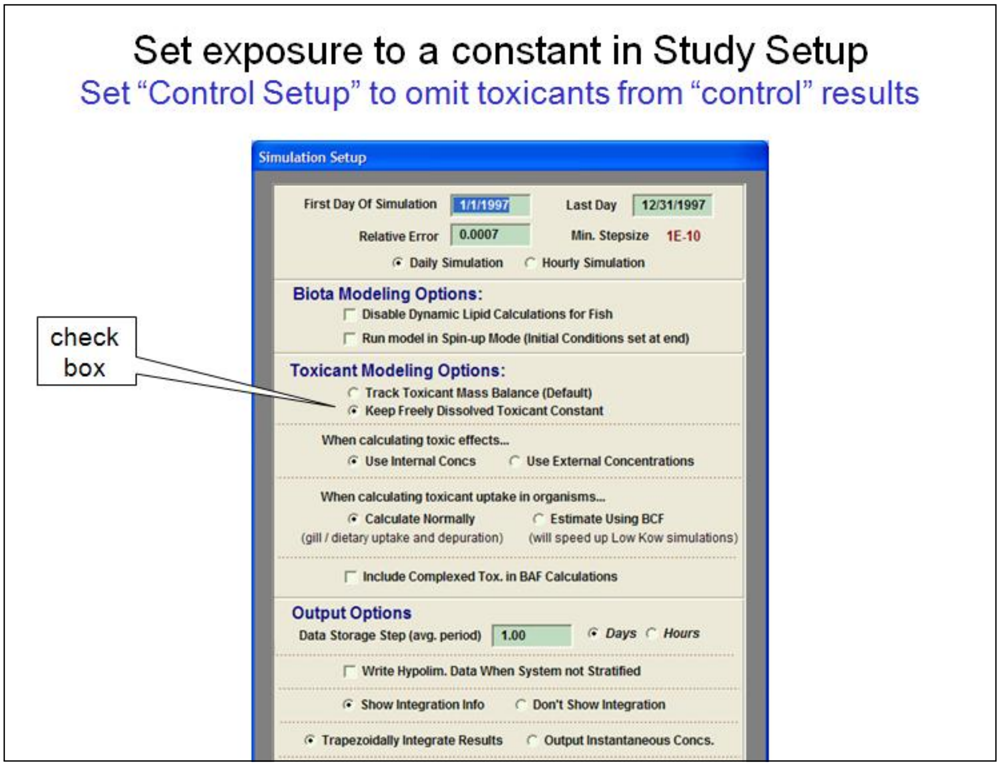
The Steinhaus coefficient may be calculated from the Graph Menu; the values will export to EXCEL. You can then graph the Steinhaus values over time.

Chlorpyrifos in Stream

Objective: analyze direct and indirect ecotoxicological effects with model

- Assessment of chlorpyrifos in a generic stream
  – small stream in corn belt
  – exposure to constant level of Chlorpyrifos assessed (0.4 ug/L)
  – optionally simulate with the initial condition of 0.4 ug/L as a one-time dose

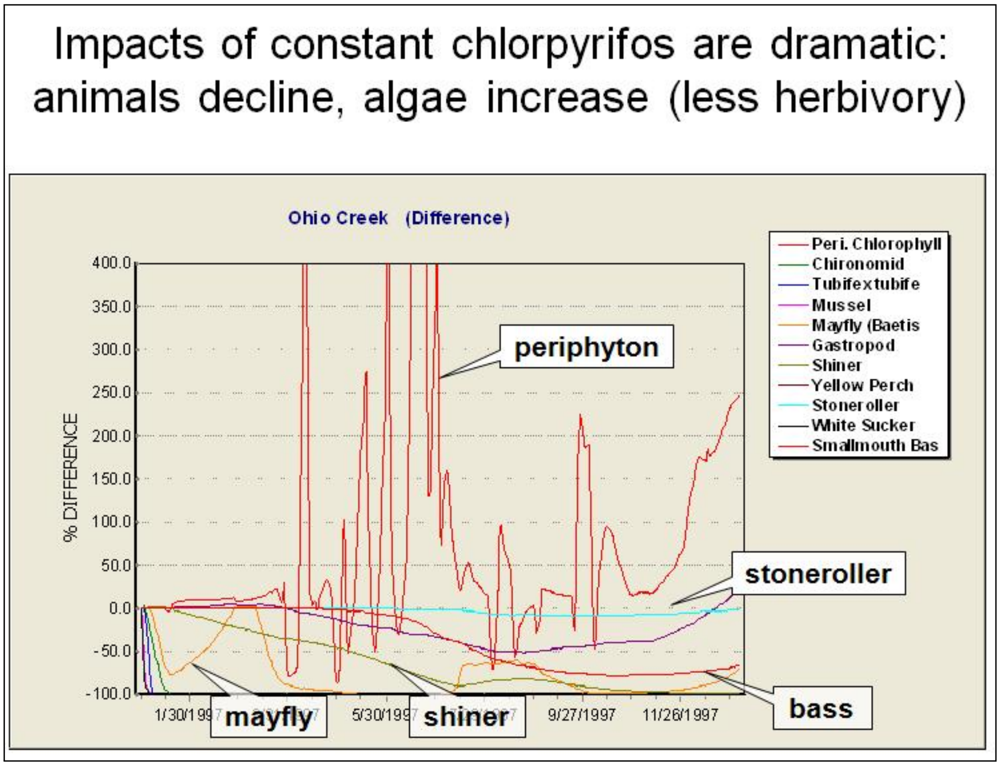
Having examined the predicted responses of a pond ecosystem to a large dose (6 ug/L) of chlorpyrifos, let's now examine the simulated response in a "generic" stream to a constant level at a low dose (0.4 ug/L) and, optionally, to an initial low dose of 0.4 ug/L.



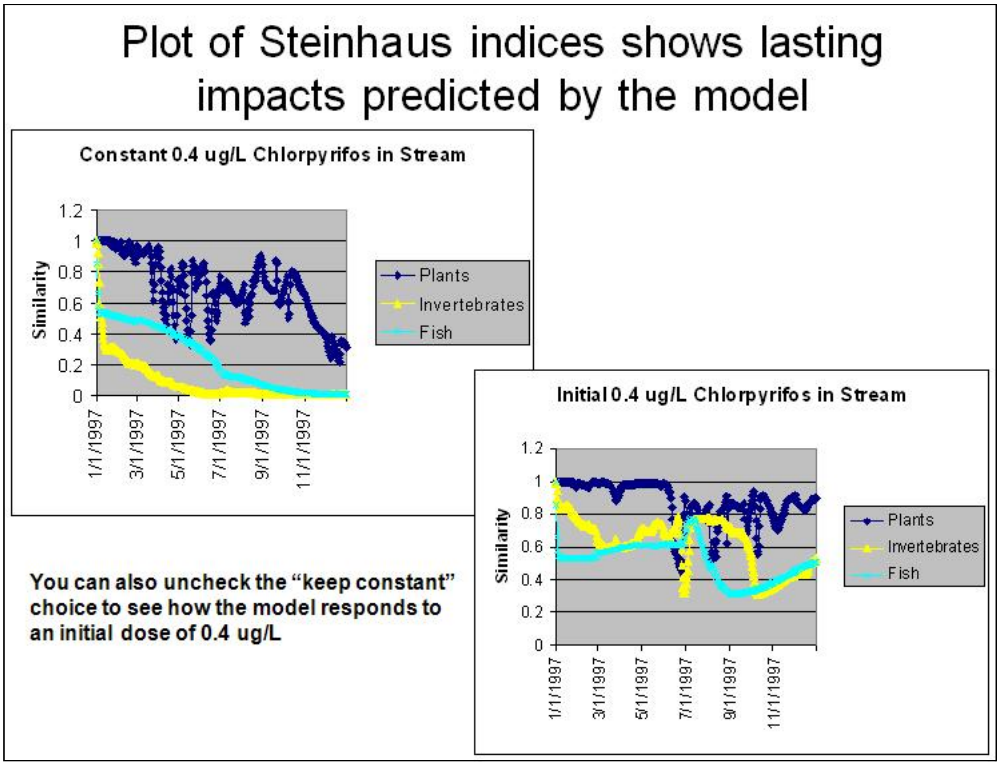
If you wish to try this yourself, open a study with a chemical attached, such as ***Ohio stream Chlorpyrifos.aps*** Then, in Main Screen click on **Study Setup**

Check button **Keep Freely Dissolved Contaminant Constant**. Alternatively, by not choosing the button, and in the absence of loadings, the model will take the initial condition as a one-time dose.

To compare control (with no toxicant) to perturbed with constant or initial dose, in **Control Setup** check **All Organic Toxicants** boxes (so Control will not have chlorpyrifos)



The best indication of the impacts are to be seen in a **Difference** graph that compares the perturbed with the control. To get this you have to run the simulations for the same period. Note that most of the invertebrates disappear quickly, followed by the fish. Shiners and stonerollers share the same toxicity record ("Minnow"), so the relative decline of shiners is due to loss of invertebrate food base and not direct toxicity whereas stonerollers, which graze periphyton, are unaffected.

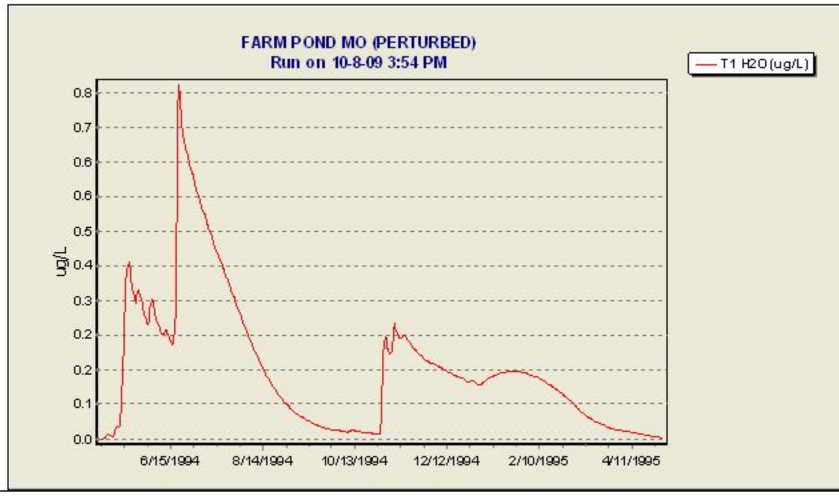


Coefficients of similarity are used to determine how similar the composition of control and perturbed communities is. The Steinhaus coefficient or similarity index (S) is based on the species abundances (in this case indicated by the species specific daily biomass) common to two communities.

The chronic exposure to 0.4 ug/L chlorpyrifos is predicted to lead to the eventual disappearance of invertebrates followed by fish. An acute exposure of 0.4 ug/L is predicted to result in a significant change in the animals (about 50% similarity compared to the control) that lasts at least a year.

Farm Pond MO, Esfenvalerate

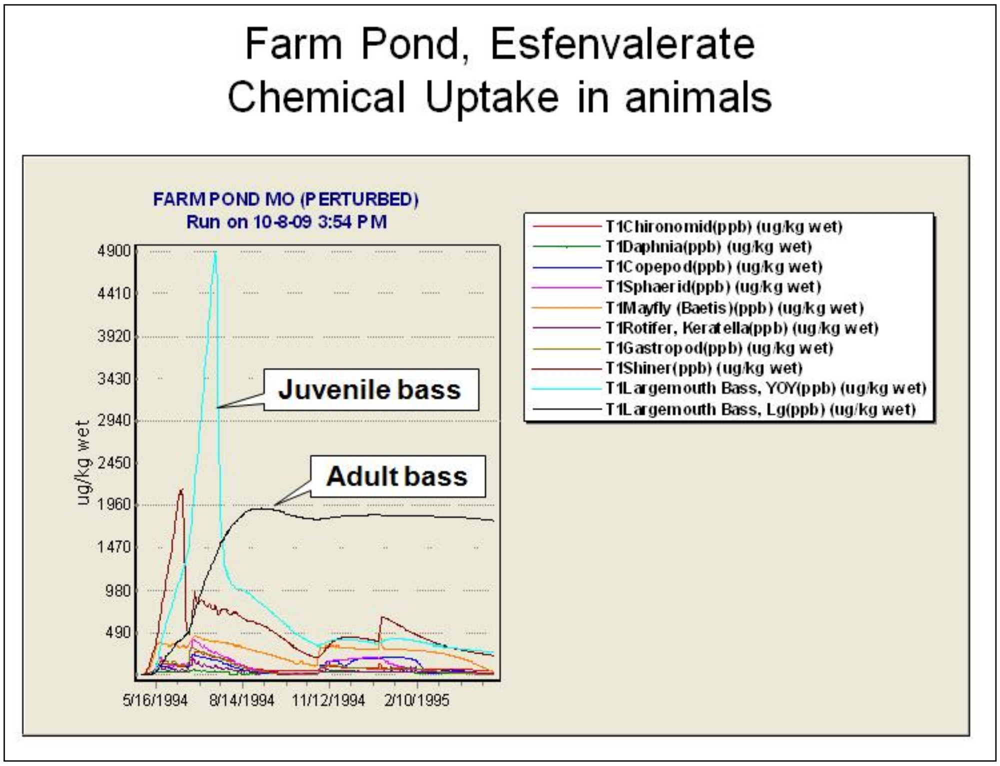
- Loadings from PRZM for adjacent cornfield
- Worst case scenario for runoff of pesticide predicted by PRZM



The assumptions in setting up this hypothetical case is that it is a typical farm pond located adjacent to and receiving runoff from a corn field in Missouri. The Pesticide Root Zone Model (PRZM) was run to obtain loadings for AQUATOX using the worst-case scenario out of 20 years (rain with runoff immediately after pesticide applications).

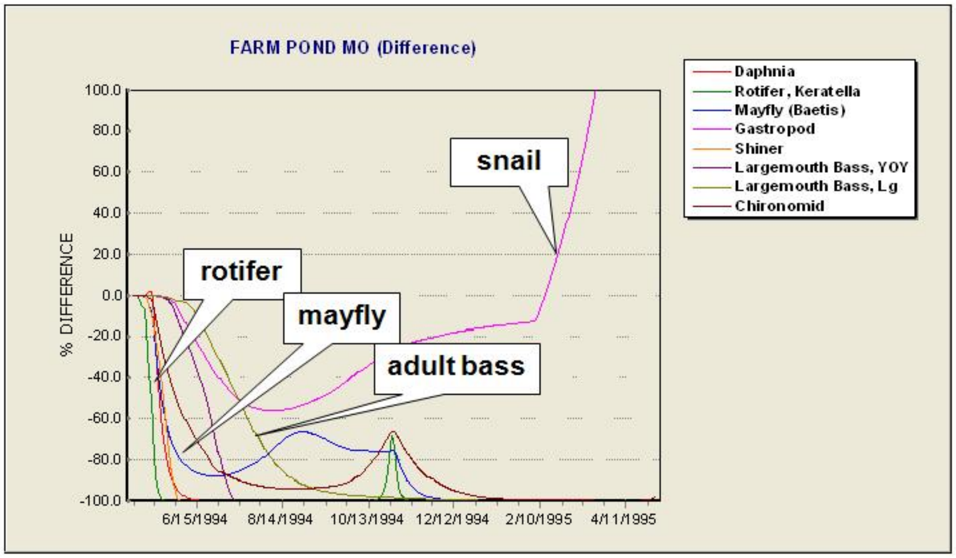
From http://extoxnet.orst.edu/pips/esfenval.htm: " Esfenvalerate is a synthetic pyrethroid insecticide which is used on a wide range of pests such as moths, flies, beetles, and other insects. It is used on vegetable crops, tree fruit, and nut crops."

Esfenvalerate is listed as very highly toxic to aquatic animals., and this was reflected in the toxicity data used in the model.

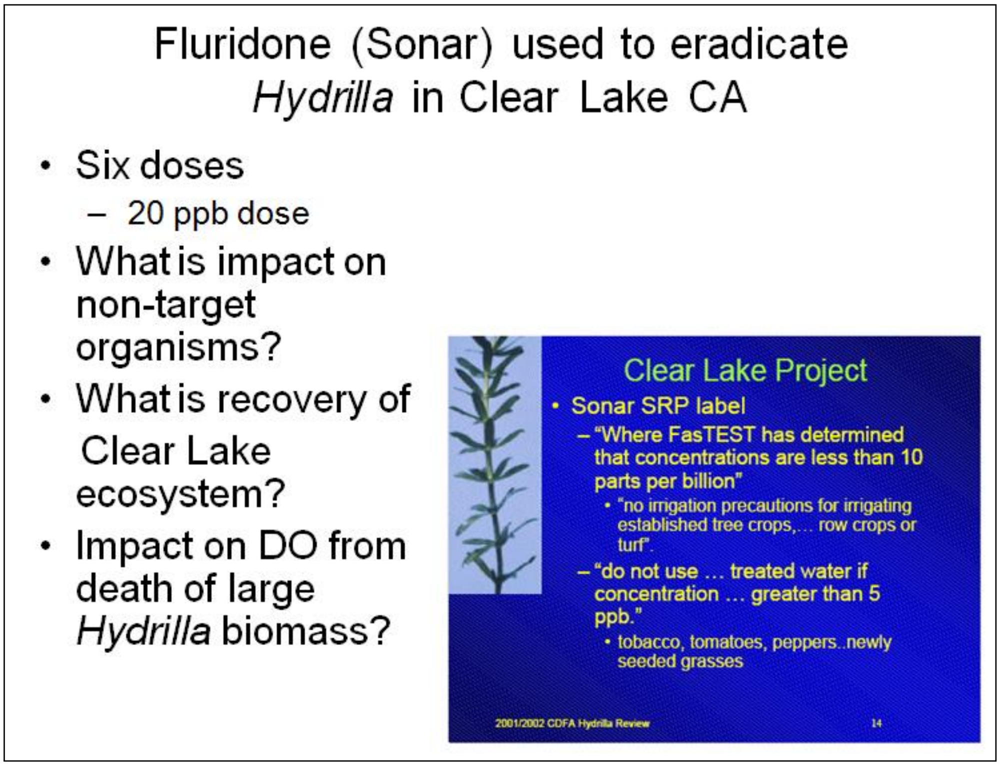


Juvenile bass are predicted to bioaccumulate esfenvalerate quickly because of bioenergetics (i.e they respire and consume more food per body weight); adult bass are predicted to bioaccumulate more slowly but to retain the pesticide due to lower clearance rate.

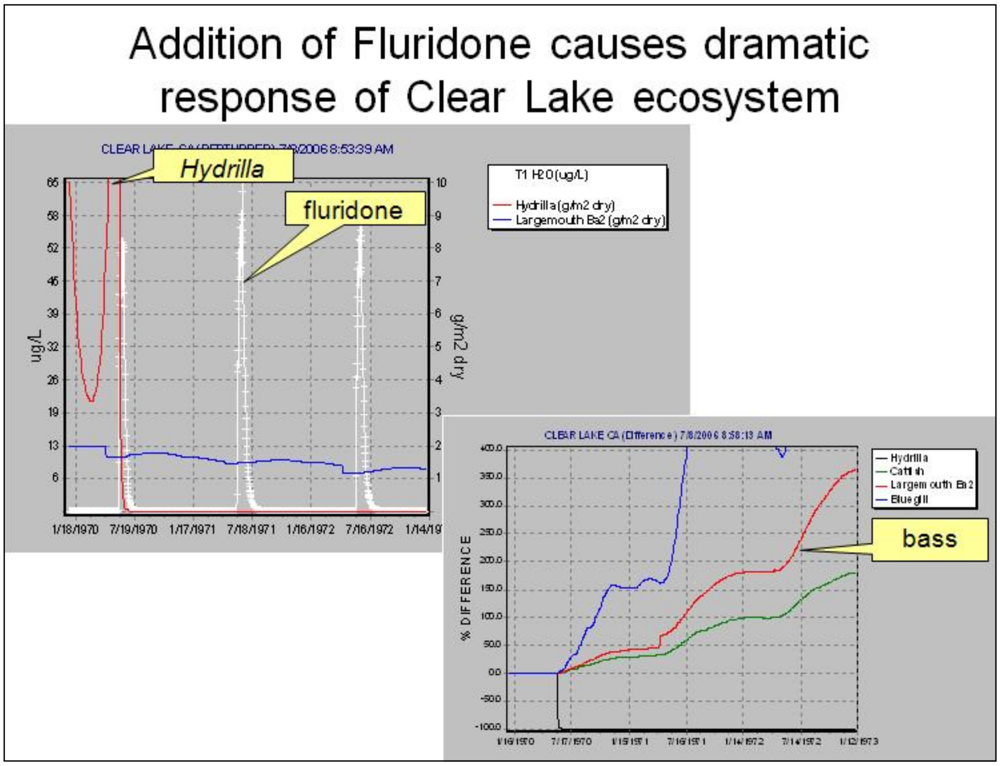
Farm Pond, Esfenvalerate Difference Graph



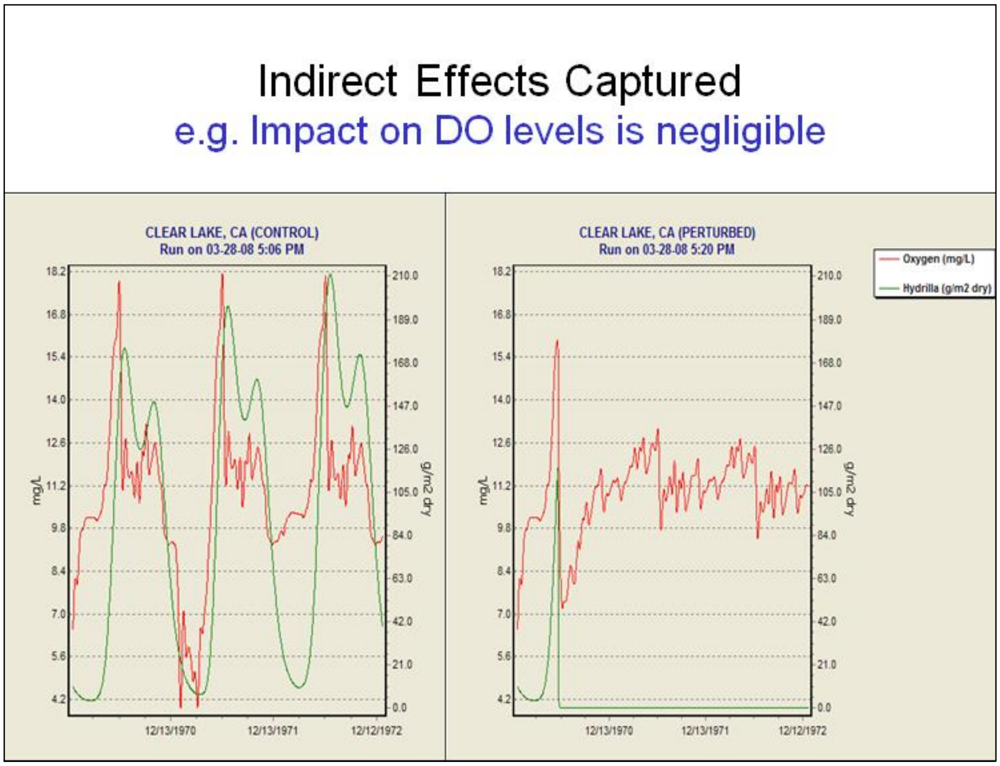
A difference graph shows the rapid decline and almost total extinction of all smaller animals except snails, which are tolerant and benefit from reduced competition for periphyton. Adult bass decline slowly because of slower bioaccumulation.



Sonar (fluridone) has been used successfully in Clear Lake to eradicate *Hydrilla*. Although *Hydrilla* did not appear until 1994, we will use the study set up with 1970-1971 data. Note that the fluridone loadings are for 1971 but without bracketing the simulation period with 0 loadings, the loadings are repeated in each of the three years. You can easily change this in the supplied study if you wish. Also note that we are modeling the entire lake for convenience; in reality, *Hydrilla* spread slowly, so only selected areas needed to be treated; our simulation is, therefore, a worst-case scenario.



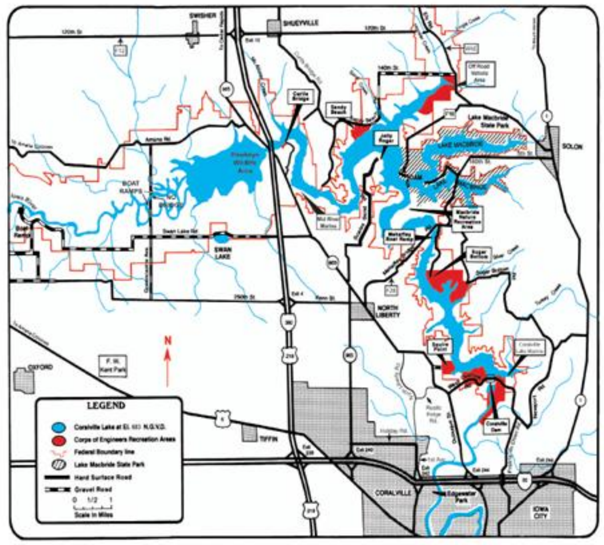
Fluridone kills off *Hydrilla*, leading to predicted much slower decline if not recovery of fisheries.



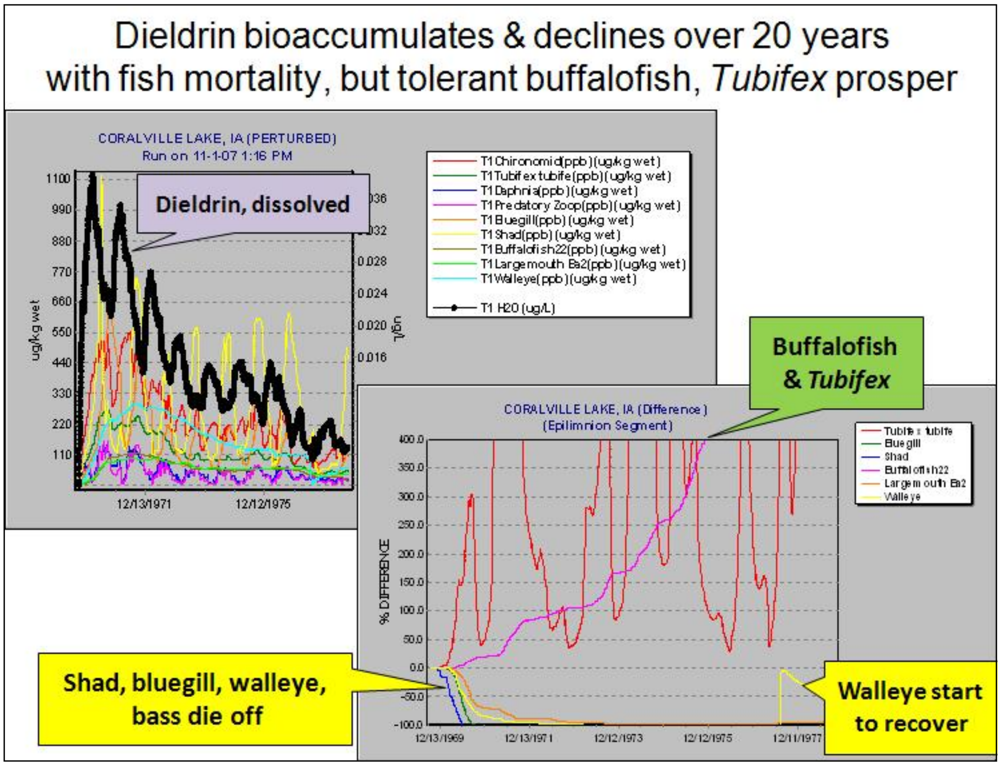
Death of *Hydrilla* due to the fluridone is not predicted to have serious impact on dissolved oxygen. Production of detritus by *Hydrilla* is predicted to impact DO more with seasonal dieoff.

Coralville Reservoir Iowa
long-term contamination with dieldrin

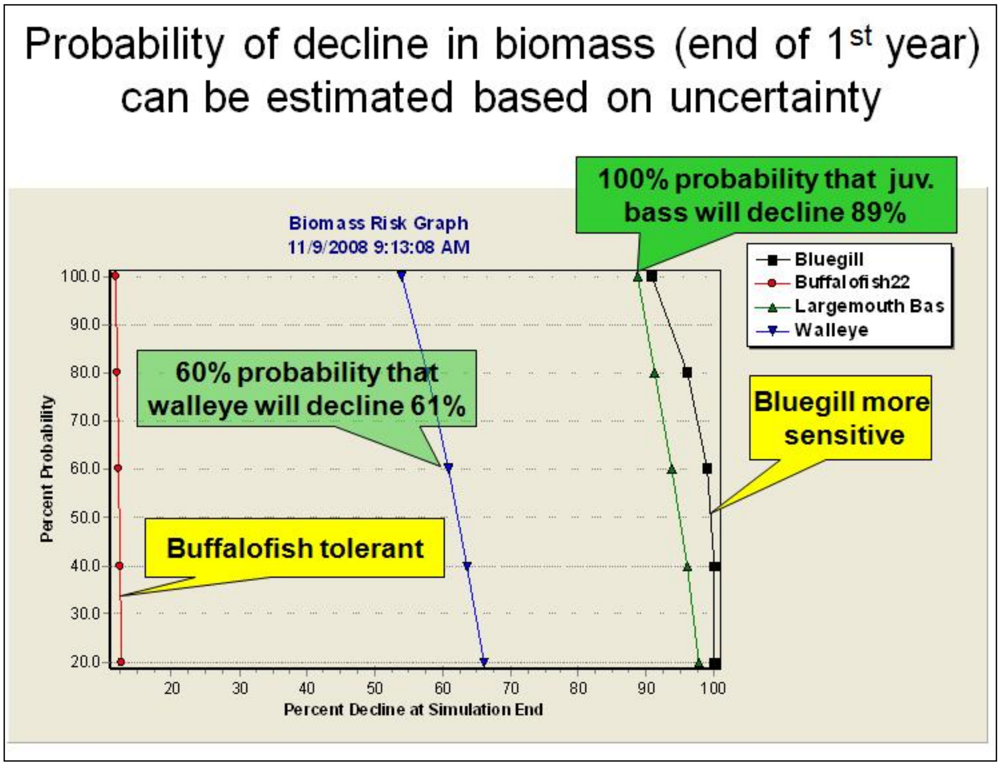
- Run-of-river
- Flood control
- 90% of basin in agriculture
  - Nutrients
  - Pesticides
  - Sediment



Coralville is a shallow, run-of-the river reservoir built in 1958 for flood control. It captures large quantities of agricultural runoff. Most dangerous is dieldrin, a chlorinated hydrocarbon insecticide, which is also a degradation product of the pesticide aldrin. It was widely used from 1950 to 1974 and was banned for most uses in 1985.



Buffalofish are tolerant of dieldrin and prospered—so much so that there was a commercial fishery on Coralville until it was realized that the levels of dieldrin in the tissue was quite high! The model predicted the eventual recovery of bass; and, in fact, Coralville is known for the best bass fishing in Iowa!



AQUATOX can estimate probability of decline, which is a very powerful tool for risk assessment. In this example, using a distribution of loadings of dieldrin, we see that bluegill are the most sensitive to dieldrin and buffalofish are the least sensitive. Walleye are of intermediate sensitivity, as suggested by their recovery shown in the previous slide.

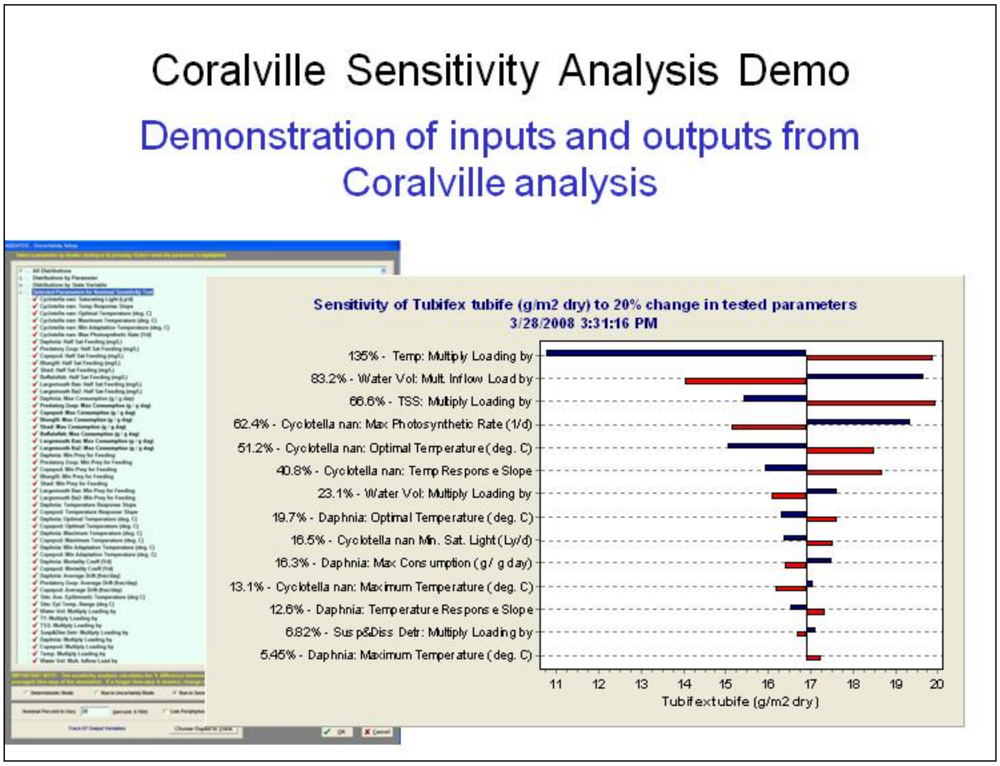
Uncertainty and Sensitivity Analysis

- "Sensitivity" refers to the variation in output of a mathematical model with respect to changes in the values of the model inputs (Saltelli, 2001).
- Sensitivity analysis provides a ranking of the model input assumptions with respect to their relative contribution to model output variability or uncertainty (EPA, 1997).
- A comprehensive sensitivity analysis of AQUATOX has been performed for diverse sites.

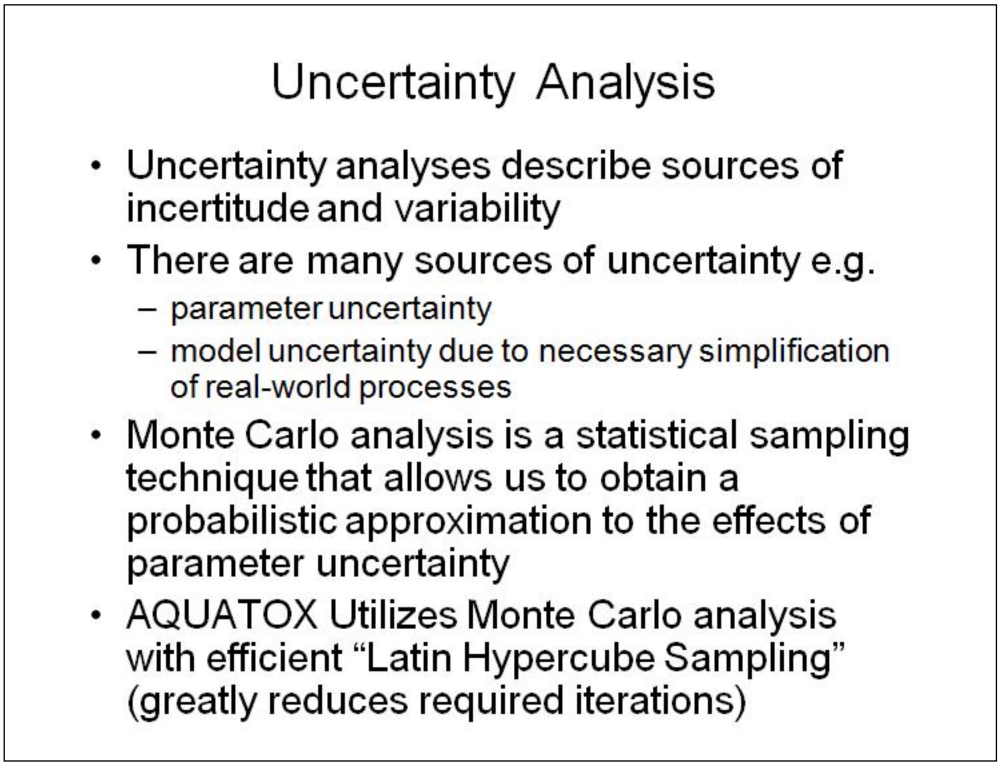
See slides 32 and 96 for examples of nominal range sensitivity analysis.

EPA (U.S. Environmental Protection Agency). 1997. *Guiding Principles for Monte Carlo Analysis*. Risk Assessment Forum, U.S. Environmental Protection Agency. EPA/630/R-97/001. March 1997.

Saltelli, A. 2001. Unpublished manuscript. Sensitivity Analysis for Importance Assessment. Proceedings of a workshop held June 11-12, 2001, at North Carolina State on "Sensitivity Analysis Methods." Joint Research Centre of the European Communities in Ispra. 36
http://www.ce.ncsu.edu/risk/pdf/saltelli.pdf

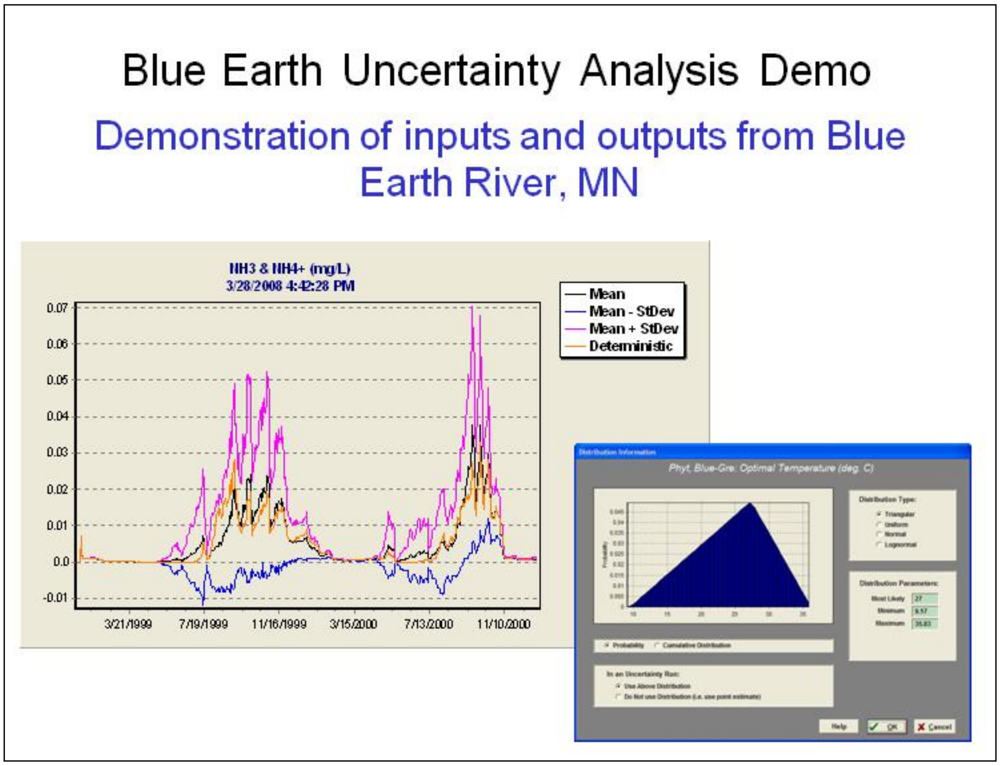


Using the Coralville study, we will have a quick demonstration of setting up a sensitivity analysis.



EPA (U.S. Environmental Protection Agency). 1997. *Guiding Principles for Monte Carlo Analysis*. Risk Assessment Forum, U.S. Environmental Protection Agency. EPA/630/R-97/001. March 1997.

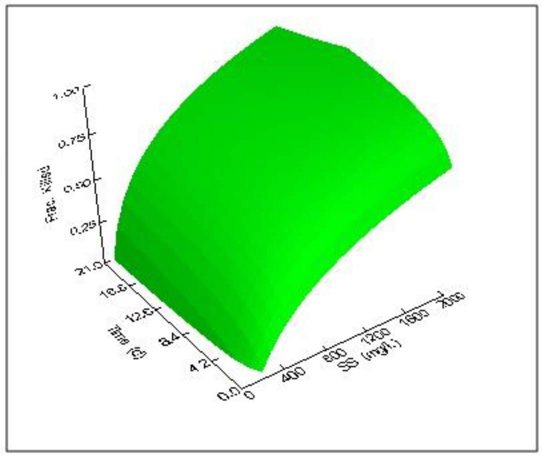
A formal uncertainty analysis often follows a sensitivity analysis as the modelers may limit the parameters they are varying to those that have proven to be sensitive over the range of uncertainty.



Input utilizes a graphical interface with several possible distributions for each of the loadings or parameters being tested. Output includes graphs of the deterministic, mean, +- 1 standard deviation, maximum, and minimum values. Output can also be shown as a biomass risk graph (see slide 171). Furthermore, output for each iteration of the analysis can be saved as csv files (in Release 3.1).

Sediment Effects Overview

- Suspended and bedded sediment effects
  - **Mortality**
    - Highly Sensitive
    - Sensitive
    - Intolerant
    - Tolerant

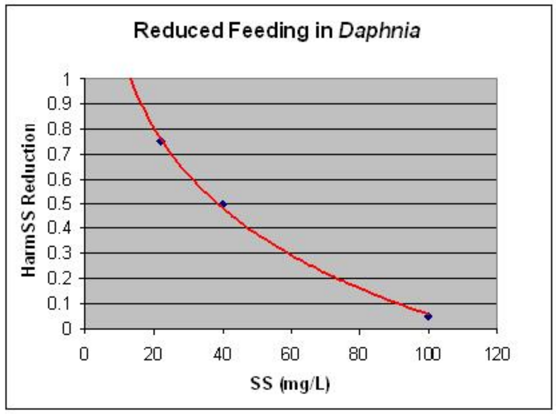


AQUATOX can simulate the effects of sediments, either suspended in the water column or deposited on the bottom; it is especially appropriate for streams, although some of the functions are generally applicable.

Sediment Effects Overview

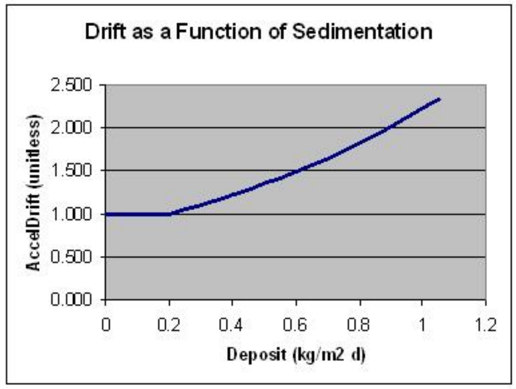
- Suspended and bedded sediment effects
  - Mortality
  - **Reduced Feeding**

- Dilution effect
- Direct effects due to clogging of filter feeding apparatus



Sediment Effects Overview

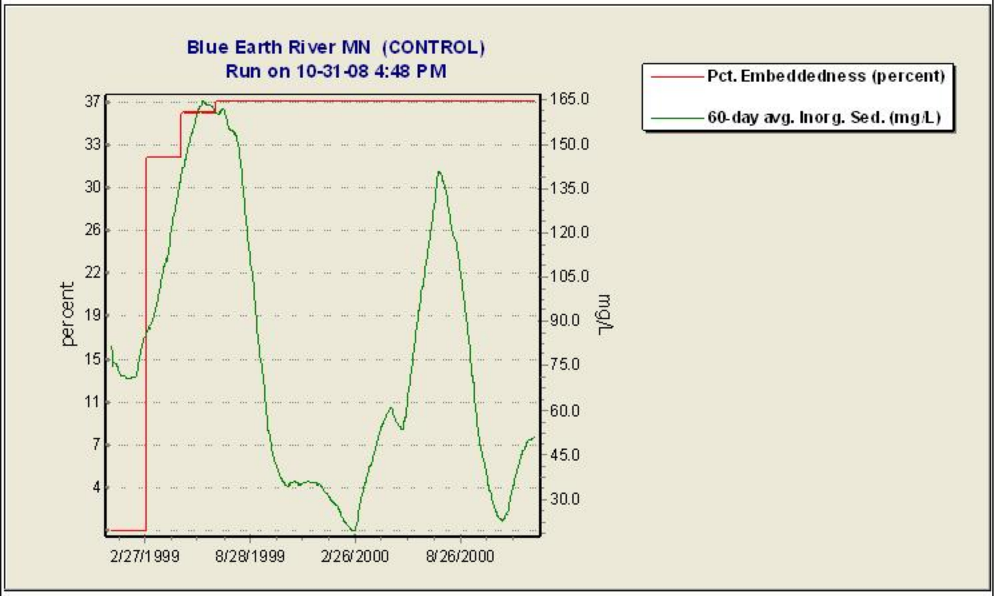
- Suspended and bedded sediment effects
  - Mortality
  - Reduced Feeding
  - **Increased drift of benthos due to sedimentation**



Sediment Effects Overview

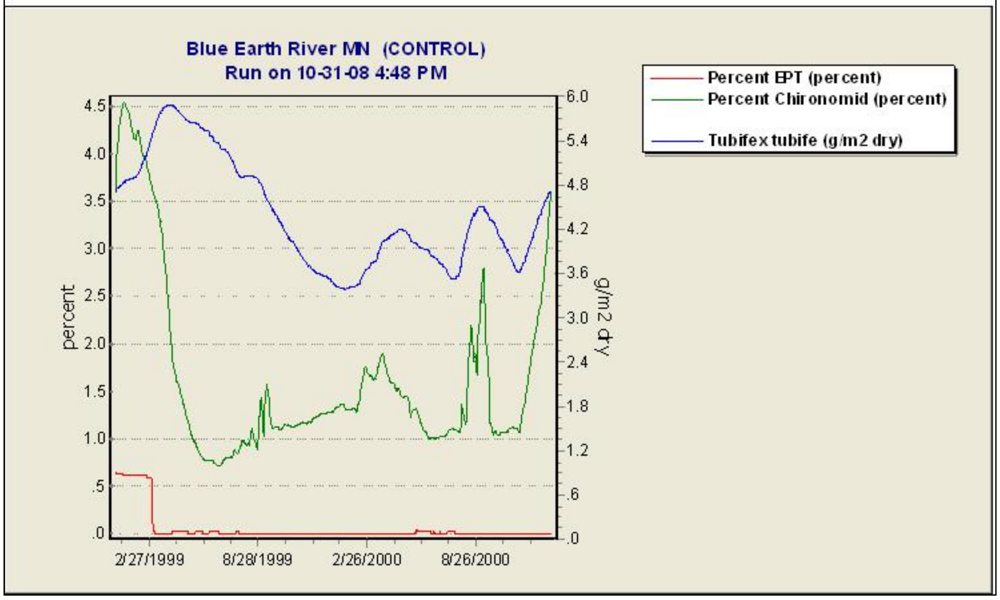
- Suspended and bedded sediment effects
  - Mortality
  - Reduced Feeding
  - Increased drifting of grazers due to sedimentation
  - **Deposition of fines and their effect on invertebrates and salmonid reproduction**
    - Percent Embeddedness calculated as a function of 60-day average TSS

Percent embeddedness is computed from 60-day deposition rate (a function of TSS)

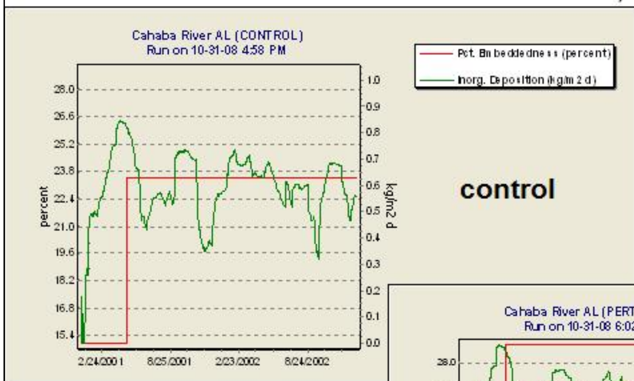


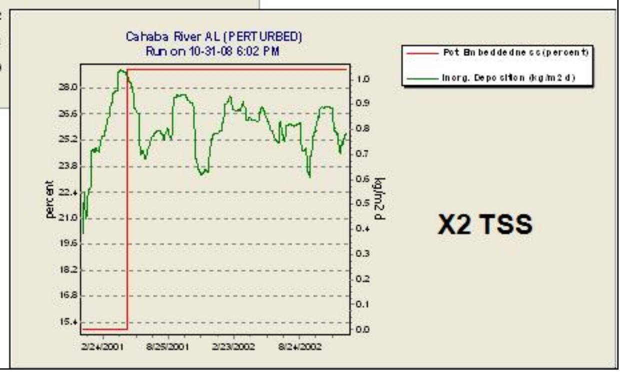
Percent Embeddedness = % sediment surrounding pebbles

Mayflies, stoneflies, & caddisflies (EPT) are sensitive to embeddedness; chironomids & oligochaetes are not

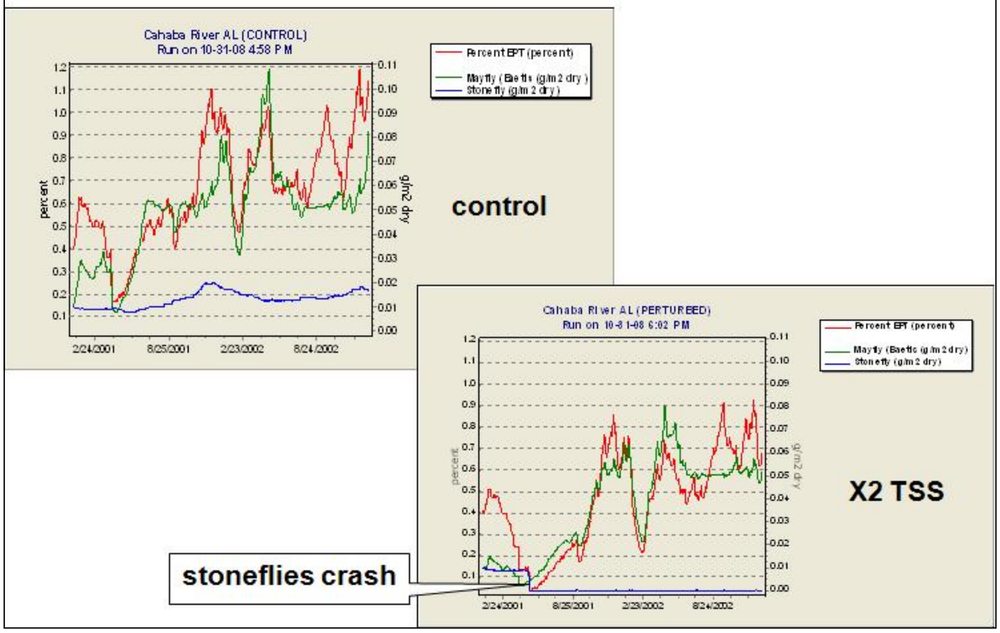


Doubling TSS increases embeddedness in Cahaba River, AL





Doubling TSS loadings adversely impacts insect community in Cahaba River, AL



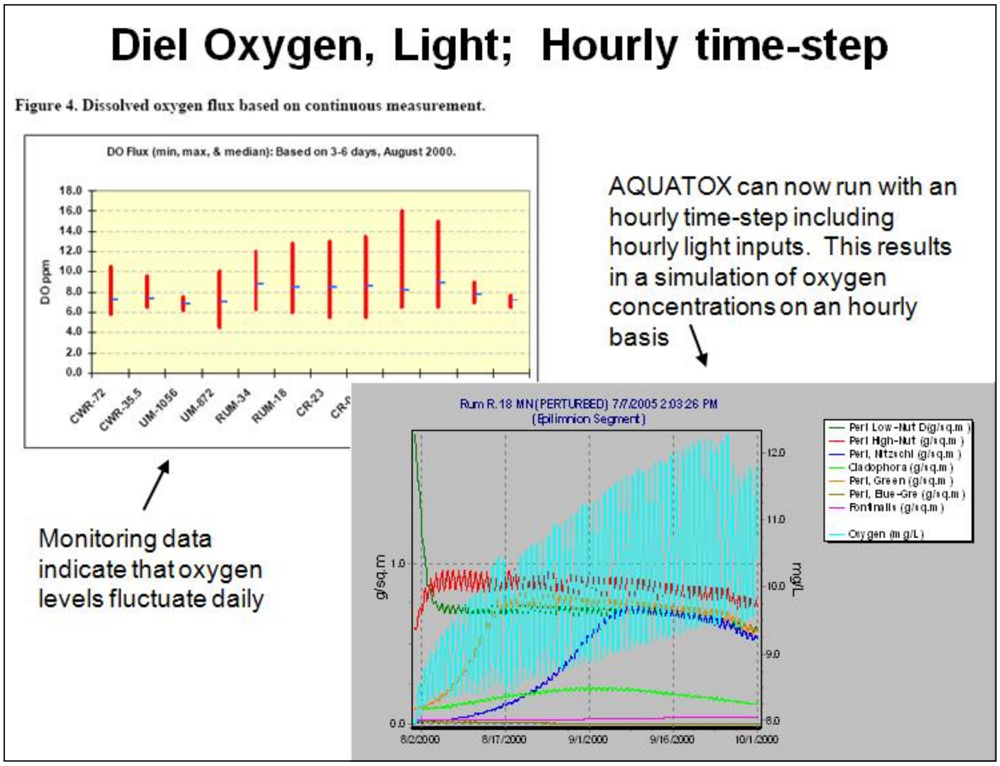
Closure

- Topics not yet covered (time-permitting)
  - Diel Oxygen
  - Sand-Silt-Clay model
  - Multi-layer sediment model
- Final Q&A

Please Keep in Touch!

- Applications help drive enhancements, example studies and data libraries
- Growing user community builds robustness and confidence
- Continued model and user support
  - One-on-one technical support is available
  - AQUATOX listserver
- Visit the AQUATOX web site
  - http://water.epa.gov/scitech/datait/models/aquatox/index.cfm
  - Citations of articles using or reviewing AQUATOX
  - Data sources

Listserver URL:
http://water.epa.gov/scitech/datait/models/aquatox/listserv.cfm

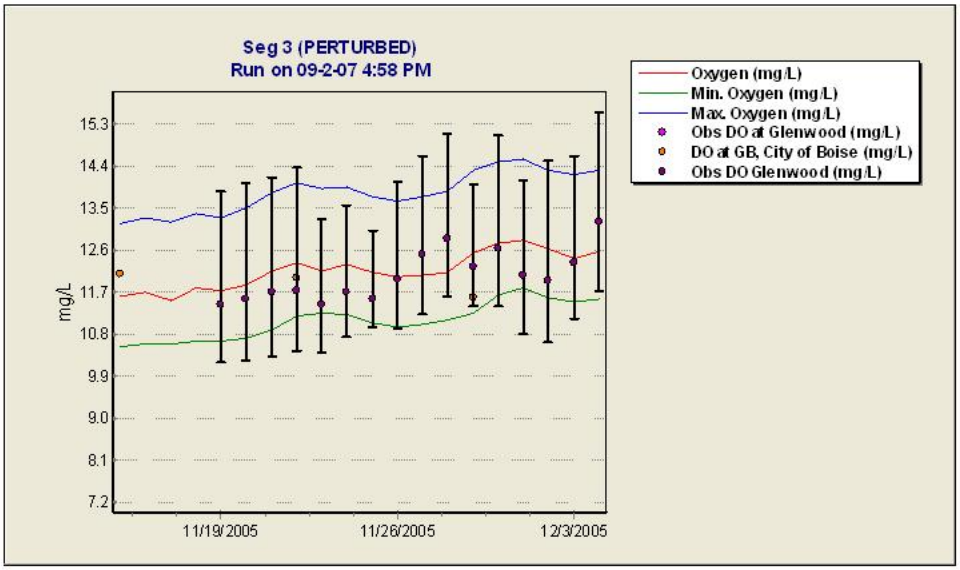


Photosynthesis can be calculated on an hourly basis.

The Light Limitation calculation is modified for hourly simulations to remove the now irrelevant photoperiod.

Stress due to low light-conditions continues to be calculated with an average daily light value.

Diel Oxygen, Hourly Time-step



Predicted and observed diel dissolved oxygen at Glenwood Bridge, Lower Boise River, Idaho. This is applicable during low-flow when photosynthesis is dominant within the reach. However, during high flow the DO is completely dominated by loadings from upstream. You should always check the retention times for a particular reach.

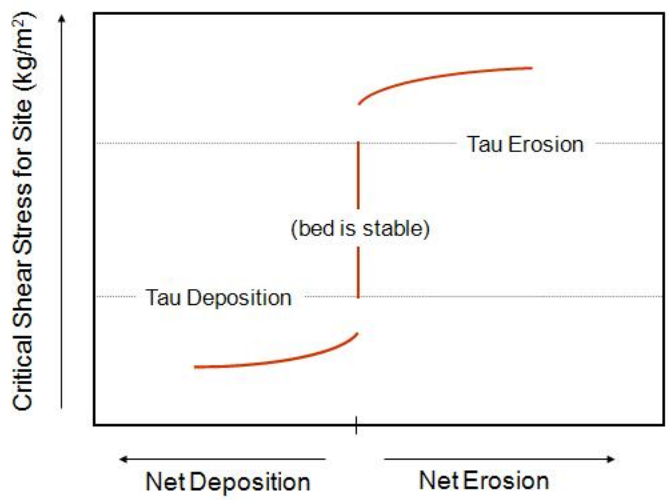
Modeling Inorganic Sediments (sand, silt, and clay)

- Stream simulations only
- Scour, deposition and transport of sediments
- River reach assumed short and well mixed
- Daily average flow regime determines shear stresses
- Feedback to biota through light limitation, sequestration of chemicals, and now direct sediment effects

The sediment transport component of AQUATOX simulates scour, deposition and transport of sediments and calculates the concentration of sediments in the water column and sediment bed within a river reach. For running waters, the sediment is divided into three categories according to the particle size: 1) sand, with particle sizes between 0.062 to 2.0 millimeters (mm), 2) silt (0.004 to 0.062 mm), and 3) clay (0.00024 to 0.004 mm). Wash load (primarily clay and silt) is deposited or eroded within the channel reach depending on the daily flow regime. Sand transport is also computed within the channel reach. At present, inorganic sediments in standing water are computed based on total suspended solids loadings.

Output variables resulting from the inclusion of sand/silt/clay include suspended sand, silt and clay, bed sheer, and bed depth.

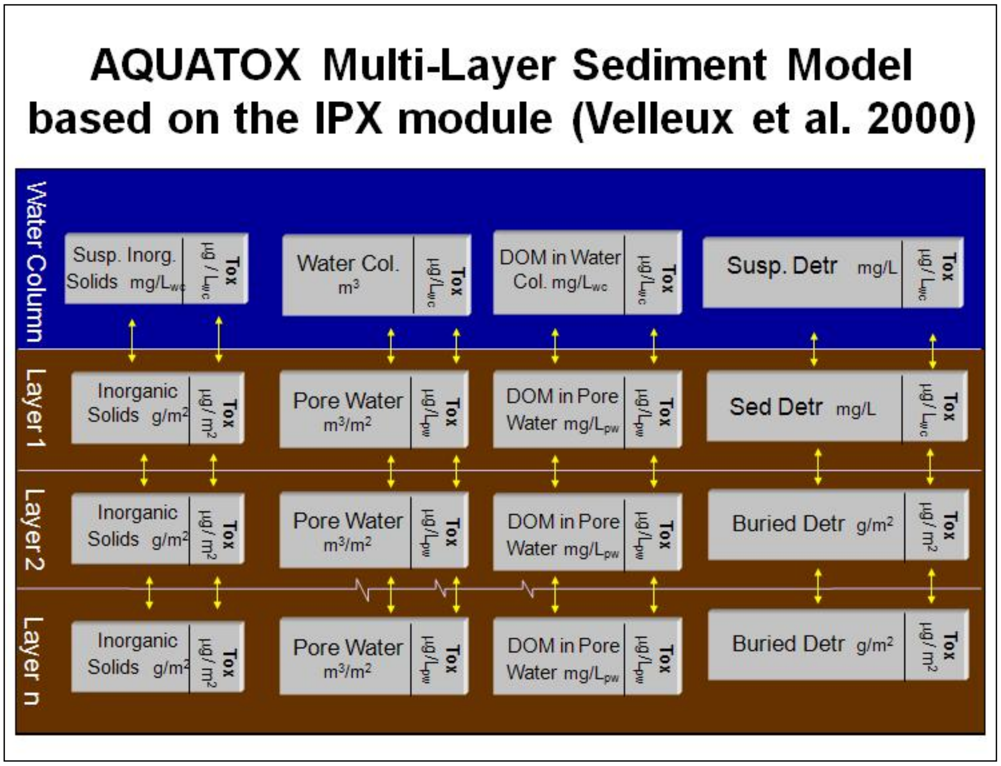
Critical Shear Stress for Erosion and Deposition Key Parameters



These two parameters are specified for silt and clay and can be found in the Stream section of the Site underlying data. This section of model is identical to HSPF. These parameters can be highly site-specific and are usually used as calibration parameters when calibrating the HSPF inorganic sediment model.

The river reach is assumed to be short and well mixed so that concentration does not vary longitudinally. Flow routing is not performed within the river reach. The daily average flow regime determines the amount of scour, deposition and transport of sediment. Scour, deposition and transport quantities are also limited by the amount of solids available in the bed sediments and the water column.

When the inorganic sediments model is included in a stream simulation, particulate detritus moves to and from the bed to and from the water column along with the deposition and resuspension of the Cohesives compartment.



- From left to right each sediment layer is composed of inorganic solids, water, dissolved organic matter, and organic solids. Each category can have toxicant sorbed to it, or in the case of water, dissolved within it.
- In this case the top layer (Layer 1) is the active layer and interacts with the water column through scour, deposition and diffusion. This layer changes height and if it gets too big it is split into two layers; if it gets too small it is joined with the layer below it.
- Lower layers only interact through pore-water diffusion.

Velleux, M., S. Westenbroek, J. Ruppel, M. Settles, and D. Endicott. 2000. A User's Guide to IPX, The In-Place Pollutant Export Water Quality Modeling Framework, Version 2.7.4. US Environmental Protection Agency, Grosse Ile, MI.