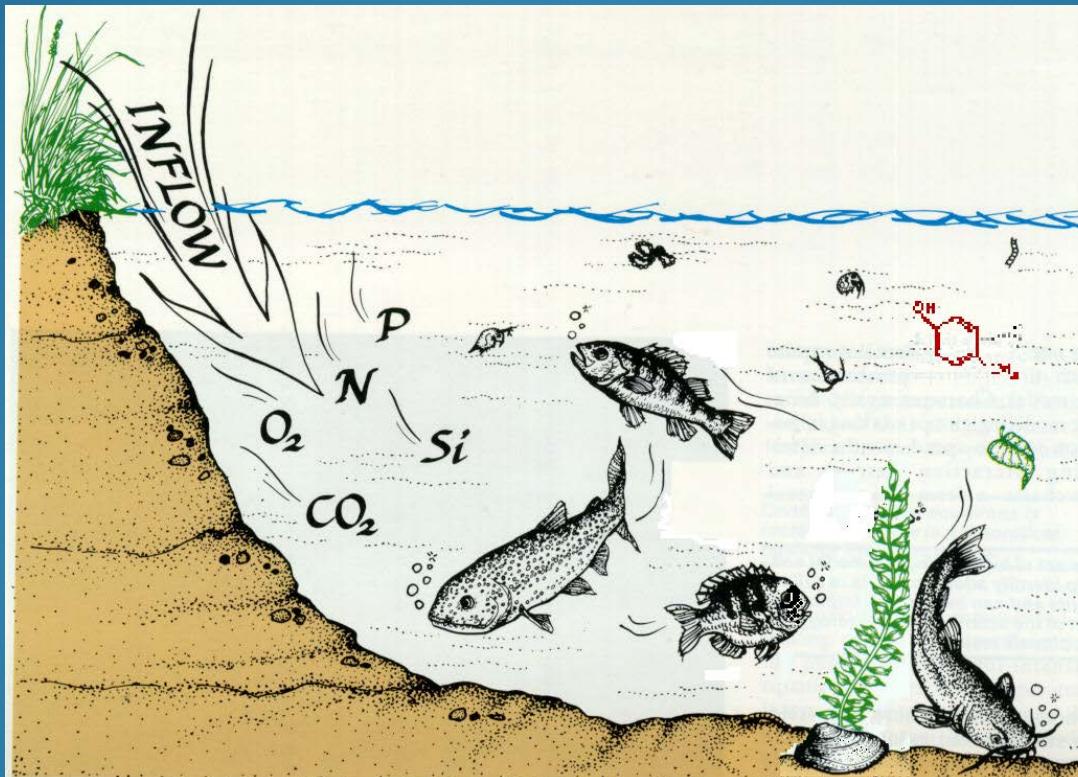


# AQUATOX: Linking Water Quality with Aquatic Life

February 11, 2014

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# Outline

- Model capabilities
  - Introduction
  - Physics and Chemistry
  - Biology
  - Fate and Effects of Chemicals
  - Interface and Output
- Example Applications
  - Tenkiller Reservoir, OK
  - Lake Hartwell, GA/SC
- Wrap-up and model future

# Acknowledgements

- Dr. Richard Park, Eco Modeling: model creator and developer
- Jonathan Clough, Warren Pinnacle Consulting: chief programmer

# Introduction to AQUATOX

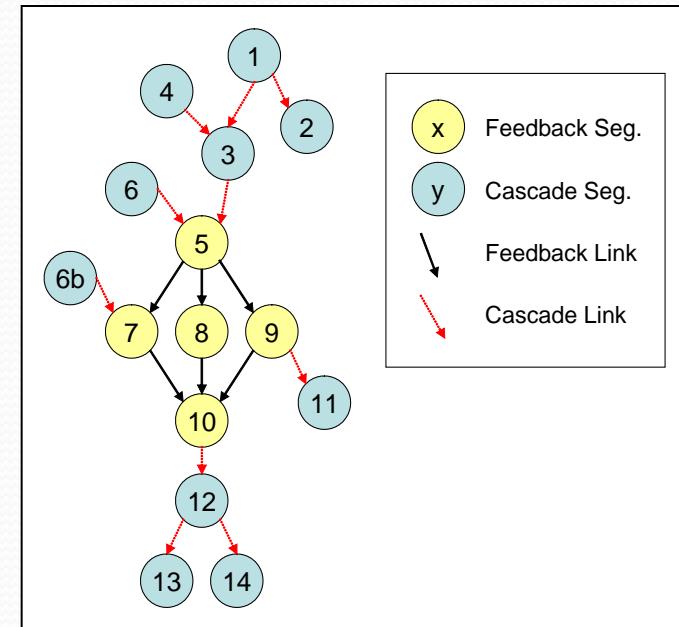
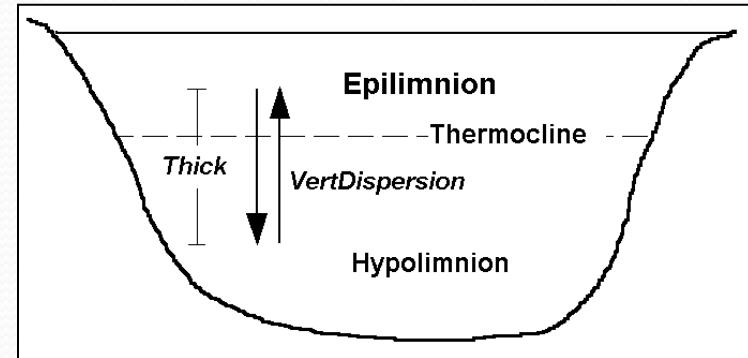
# What is AQUATOX?

- Mechanistic simulation model for aquatic ecosystems
  - Streams, rivers, lakes, reservoirs, estuaries
- Fate and effects of multiple stressors
  - Nutrients
  - Organic toxicants
  - Suspended and bedded sediments
  - Flow
  - Temperature

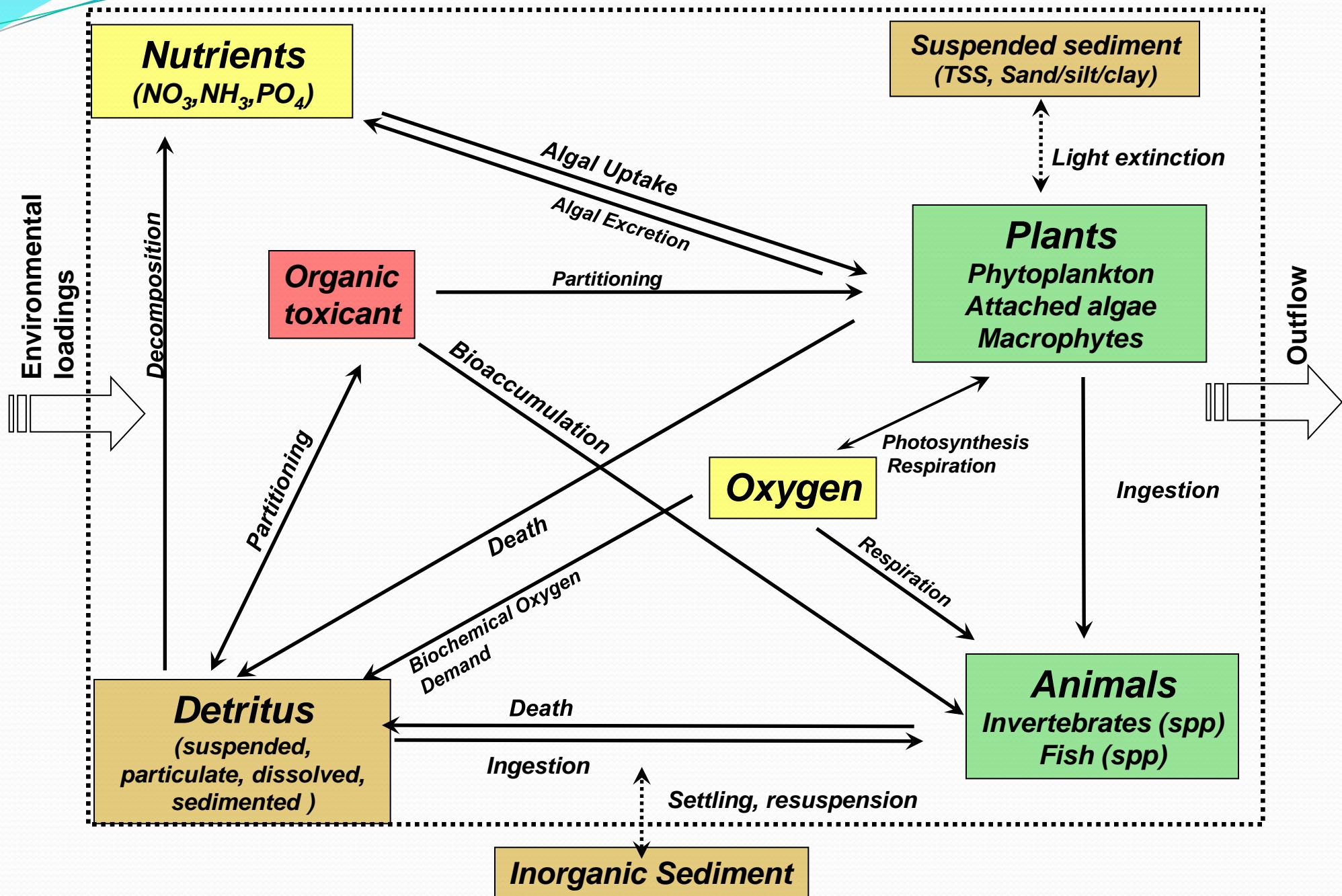


# AQUATOX Structure

- Time-variable
  - usually daily reporting time step
  - can run from few days to decades
- Spatially simple, but:
  - thermal stratification
  - salinity stratification
  - can link multiple segments together
- Modular and flexible
  - model only what is necessary
  - simple to complex food web
- Control vs. perturbed simulations



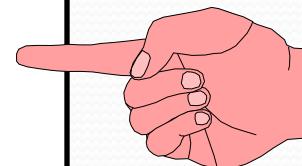
# AQUATOX Simulates Ecological Processes & Effects within a Volume of Water Over Time



- Site characteristics
- Biological characteristics
- Chemical characteristics
- Environmental loadings
  - Multiple sources
  - Variable or constant
- Watershed loads from BASINS (*opt.*)
- Library or user-supplied

default or  
user-supplied

## AQUATOX Inputs



## AQUATOX Outputs



- Biomass
- Pollutant concentrations
- Tissue concentrations & BAFs
- Process rates
- Direct & indirect effects
- Time variable

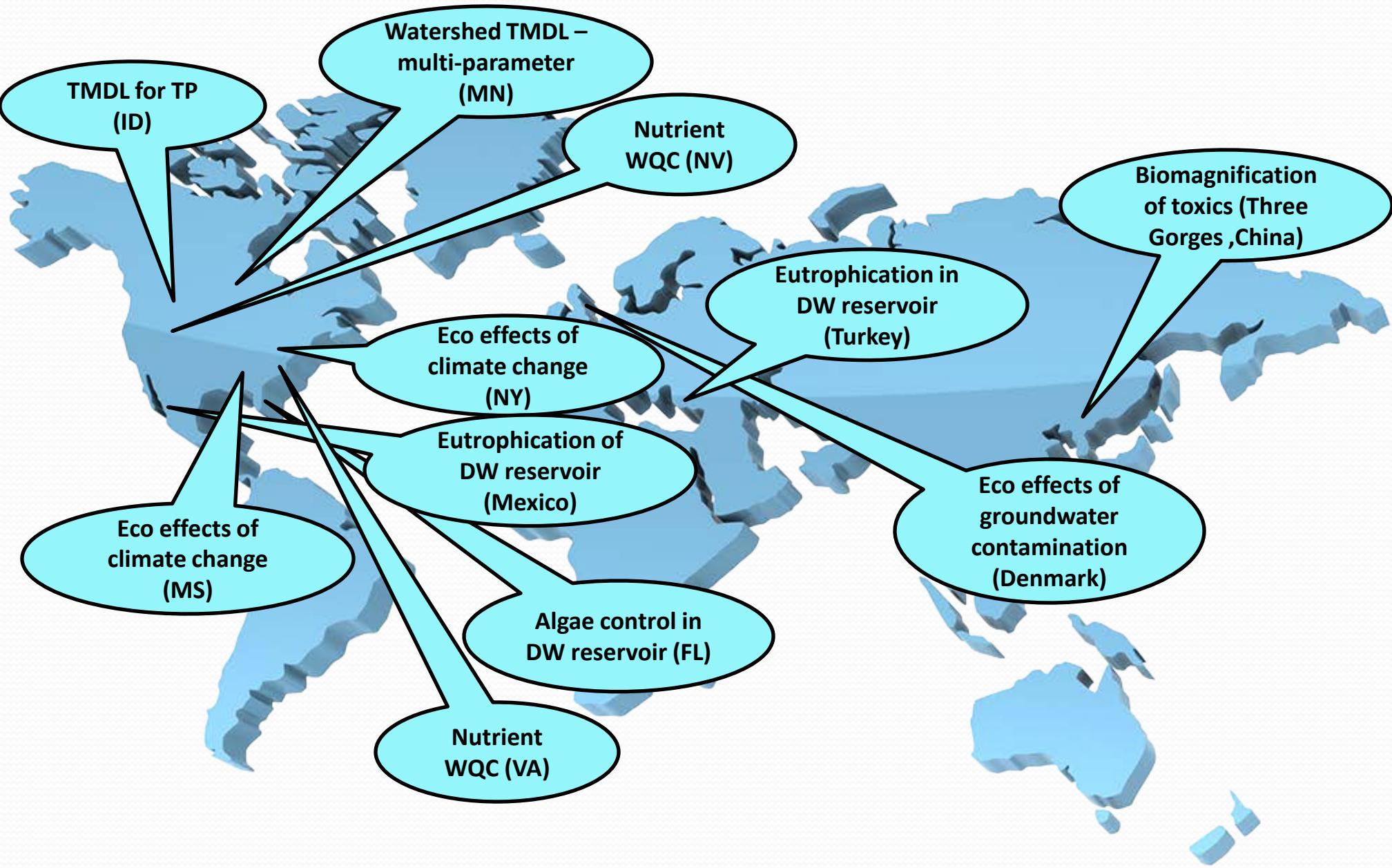
# Why AQUATOX?

- A truly integrated eutrophication, contaminant fate and effect model
  - “is the most complete and versatile model described in the literature” (Koelmans et al. 2001)
- Comparison with other models
  - Includes more biological components than water quality models such as WASP7 or QUAL2K
  - CASM models toxic effects but not fate
- Comprehensive bioaccumulation model

# One model, many questions

- Many waters are impaired, with multiple stressors
- To restore them we need to know:
  - Relative importance of stressors?
  - Combined effects?
  - Predicted effects of management actions?
    - Better water quality
      - Fewer and/or smaller algae blooms
      - More oxygen
    - Restore fisheries
    - Will the fish be safe to eat?
  - What is the best management scenario?
    - Which combinations of measures will work best?
    - Any unintended consequences?
  - How long will recovery take?

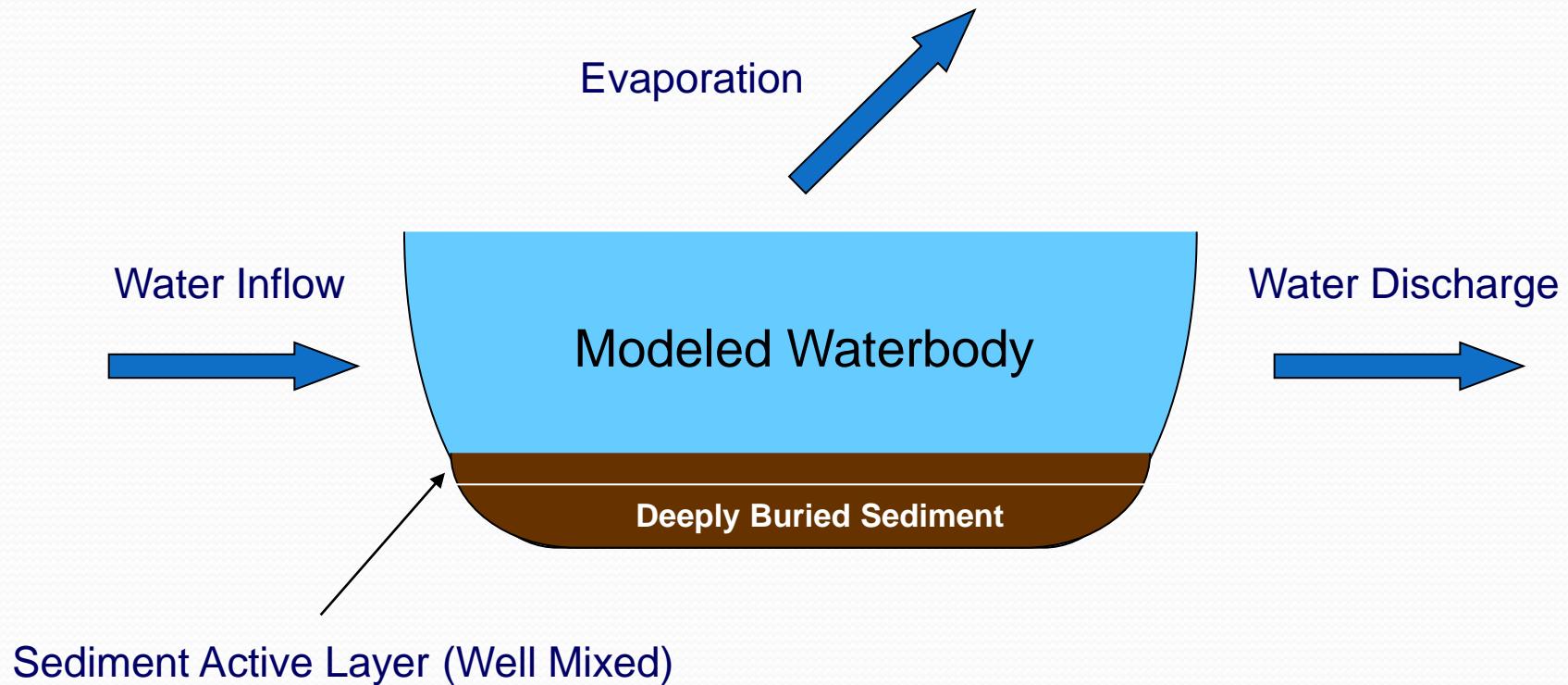
# Worldwide applications



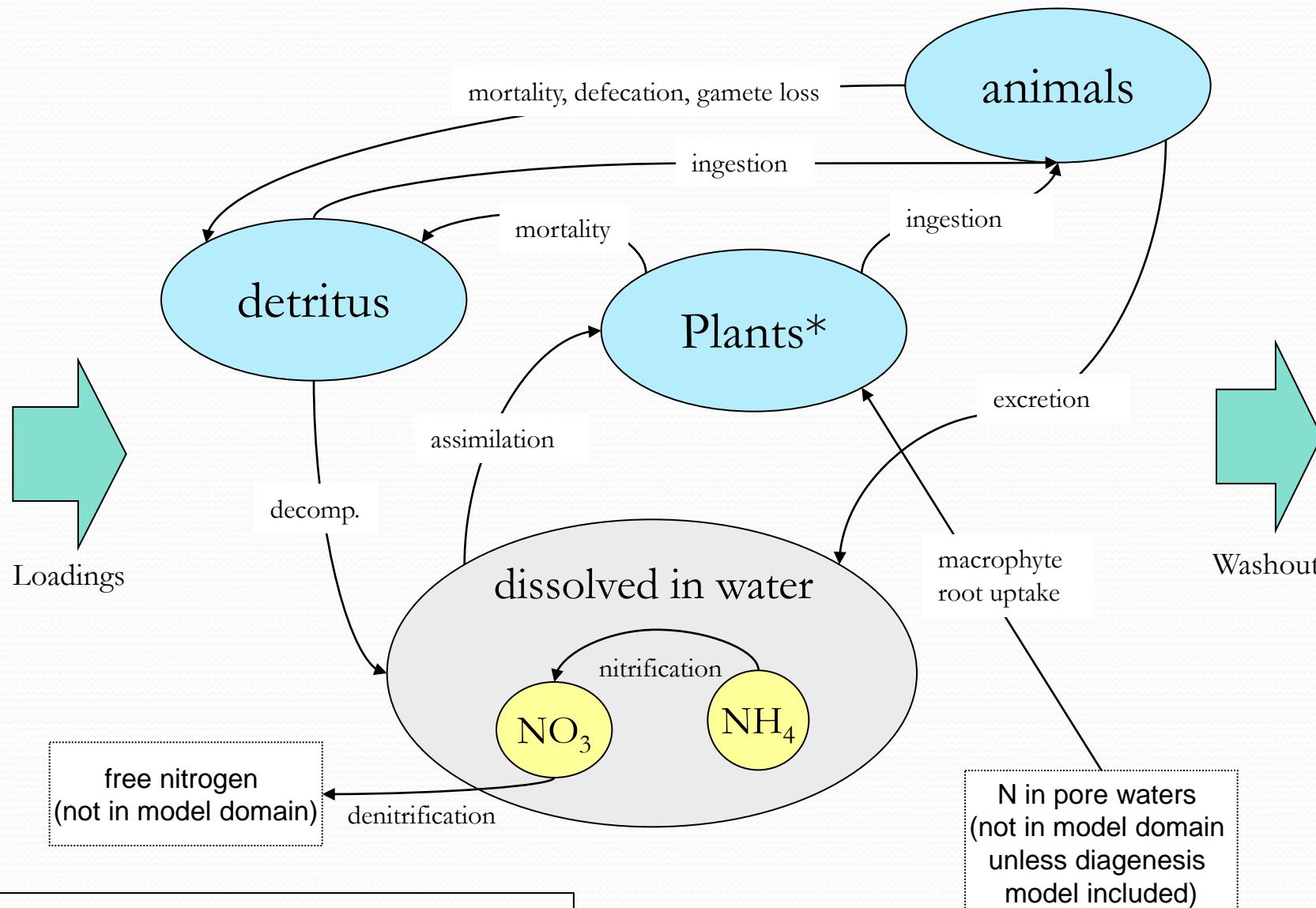
# Physics and Chemistry in AQUATOX

# Physical Characteristics of a Site

## Water Balance and Sediment Structure



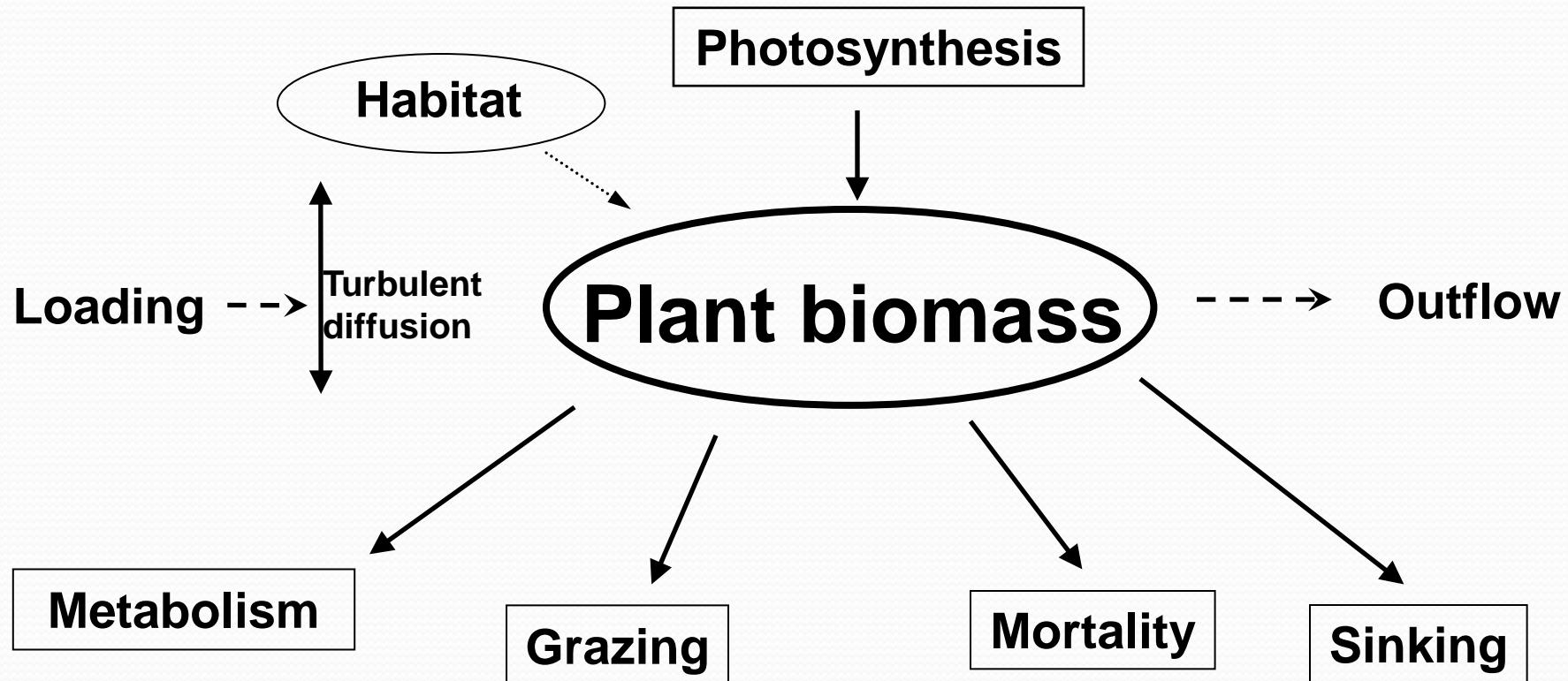
# Nitrogen Cycle in AQUATOX



\* : includes nitrogen fixation by cyanobacteria

# Biology in AQUATOX

# How AQUATOX Models Plants

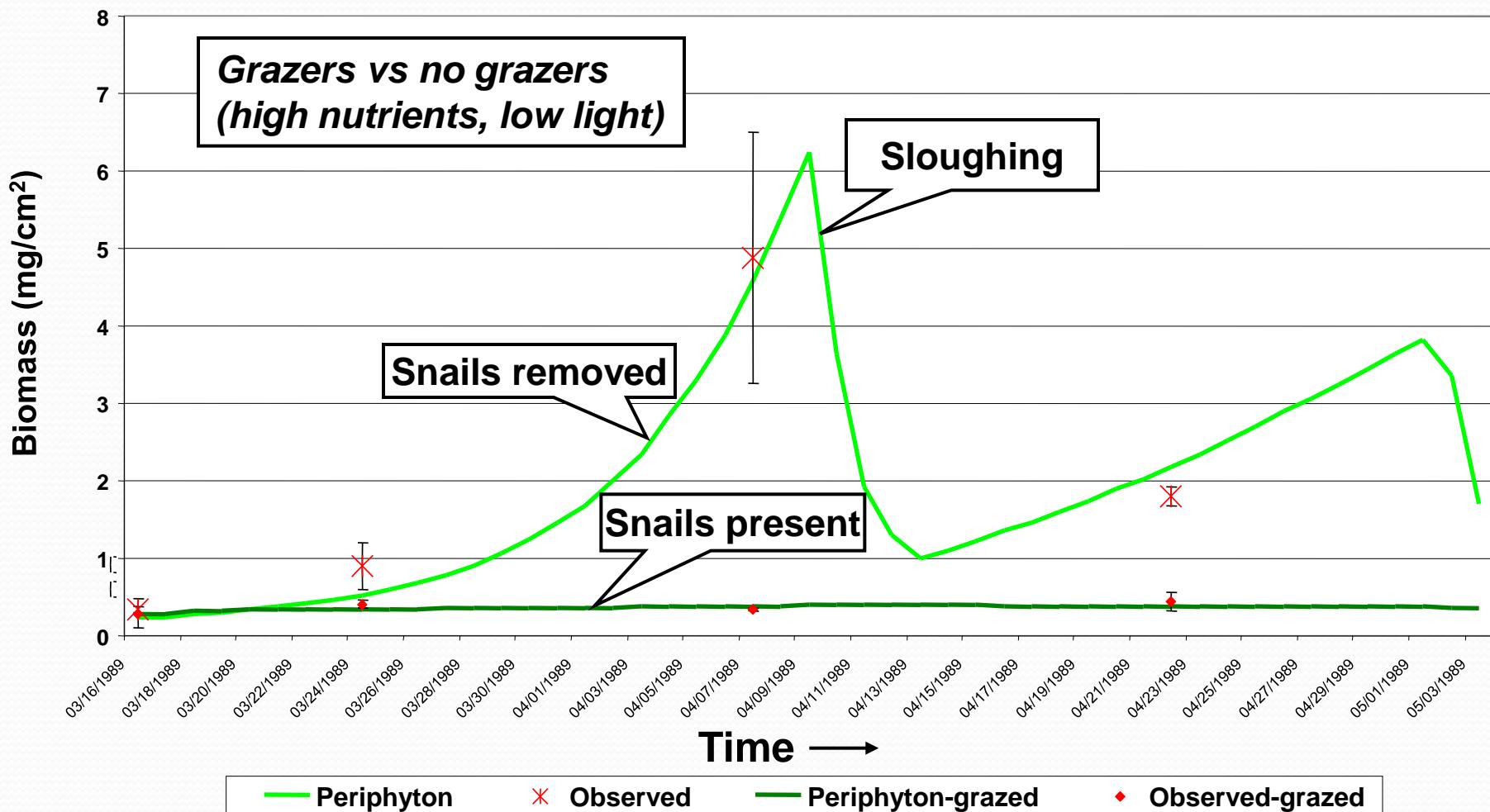


# Multiple plant groups

- Phytoplankton
  - greens, cyanobacteria, diatoms or “other”
- Periphyton
  - greens, diatoms, cyanobacteria, or “other”
  - include live material and detritus
  - snails & other animals graze it heavily
  - subject to sloughing, *even at relatively low velocity*
- Macrophytes
  - benthic, rooted-floating, or free-floating
  - heavy growths have significant effect on light climate
  - may act as refuge from predation for animals
  - leaves can provide significant surface area for periphyton growth

# Periphyton Controlled by Multiple Independent Factors

One important factor is grazing by snails  
another is sloughing



# Modeling Animals in AQUATOX

## Consumption

- maximum feeding rates
- availability & preferences
- reductions due to stress

## Vertical migration

## Loadings →

## → Washout

## Metabolism

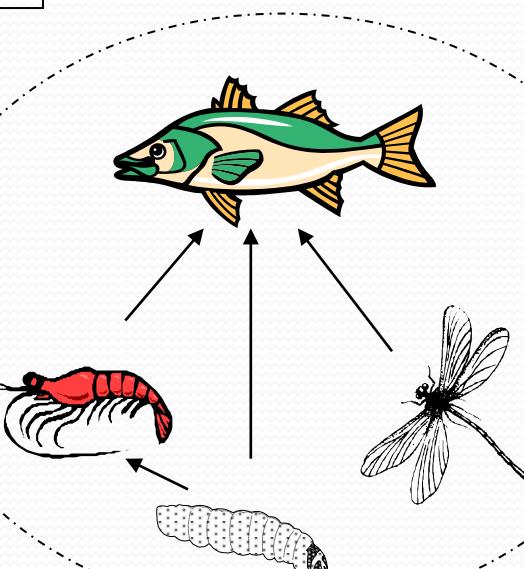
- defecation
- excretion
- respiration

## Reproduction

- gamete loss
- promotion
- emergence

## Mortality

- predation
- natural mortality
- toxicity



# Multiple Animal Groups

- Zooplankton
- Benthic invertebrates
- Benthic insects
- Fish, with multiple year classes

# Foodweb Model specified as Trophic Matrix

AQUATOX-- Trophic Interaction Matrix

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

Show Preferences

Show Egestion Coefficients

Show Comments

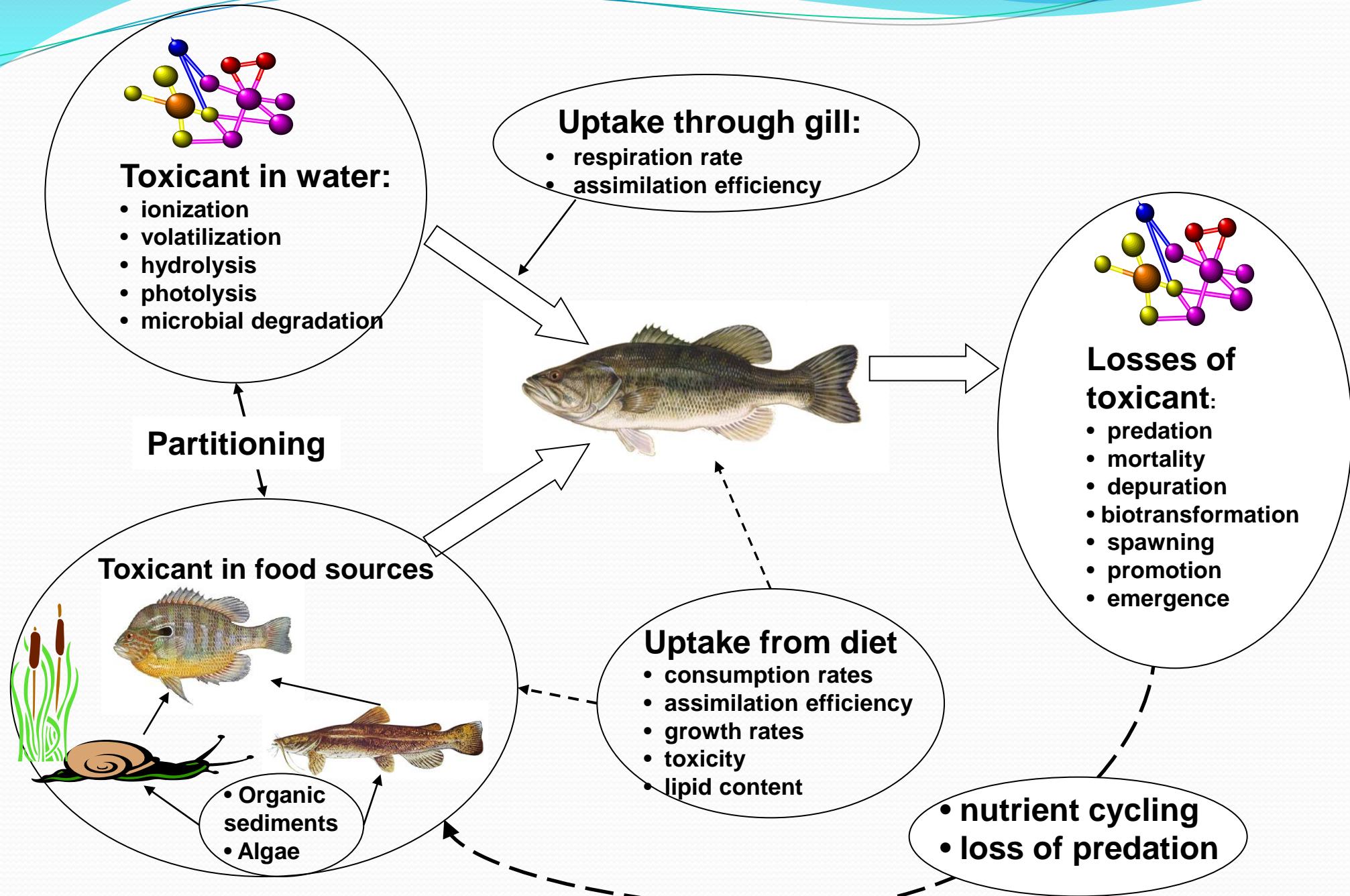
	Tubifex tubifex	Daphnia	Rotifer, Brach	Predatory Z	Shad	Bluegill	White Perch	Catfish	Largemouth Bas	Largemouth Ba2	Walleye
R detritus sed	50.0							1.2			
L detritus sed	50.0							4.7			
R detritus part					12.5				2.1		
L detritus part		30.0	40.0		12.5	3.9	0.5		2.1		
Cyclotella nan		35.0	5.0		12.5						
Greens		30.0	5.0		12.5						
Phyt, Blue-Gre					12.5						
Cryptomonad		5.0	50.0								
Tubifex tubifex						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 Zoopl					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		

# Fate and Effects of Chemicals in AQUATOX

# Modeling Toxicity

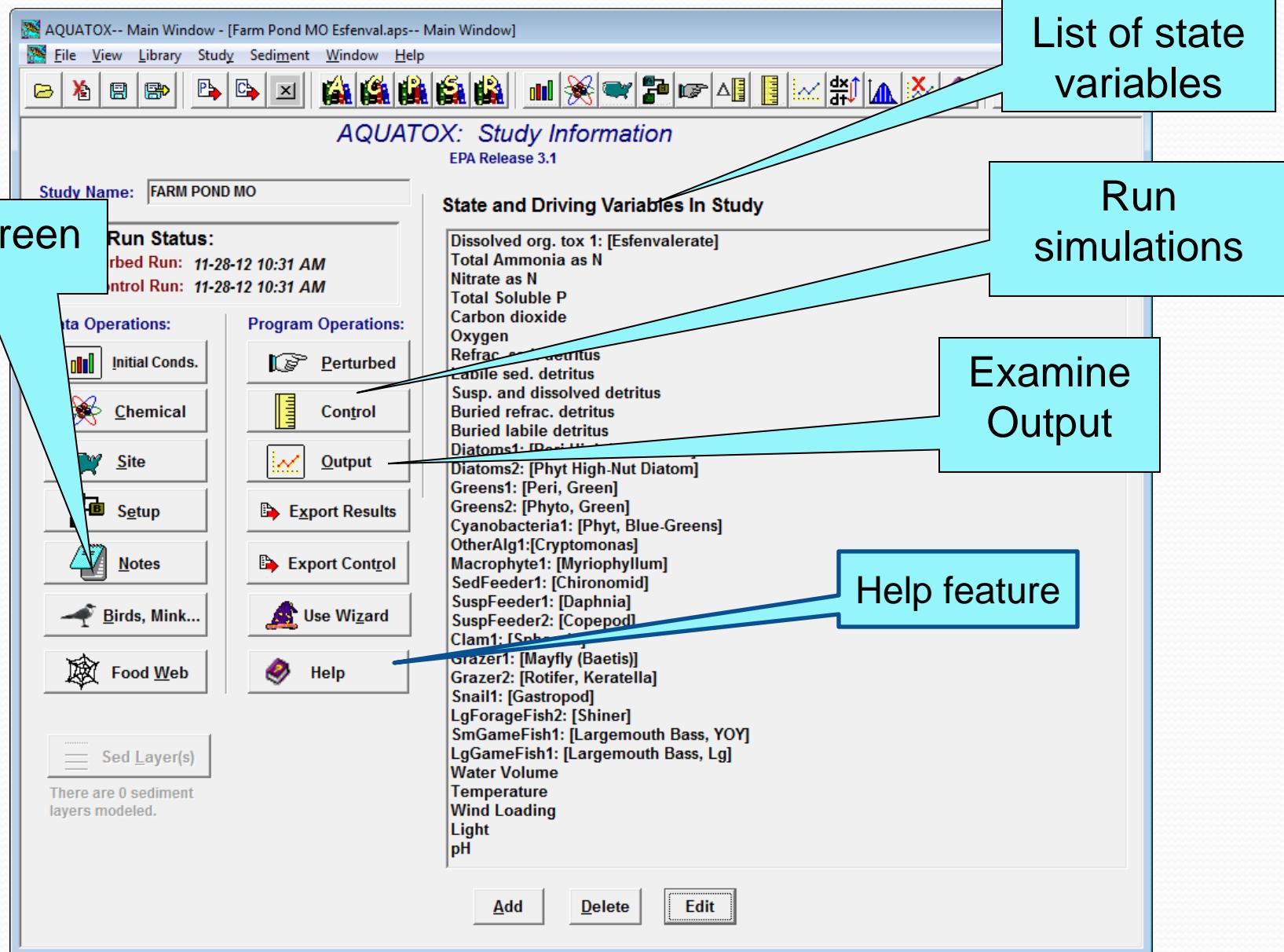
- Organic toxicants
- ≤ 20 chemicals simultaneously
- Lethal and sublethal effects
- Acute and chronic toxicity
- Effects based on total internal concentrations
- Option to model external toxicity
  - Useful if uptake and depuration are very fast (as with herbicides)
- Ecological effects – direct and indirect
  - Non-target organisms
  - Food web disturbances
  - Unintended consequences?

# Fate and Bioaccumulation in AQUATOX



# AQUATOX Interface and Output

# AQUATOX Interface: Main Screen



The screenshot shows the AQUATOX software interface. At the top is a menu bar with File, View, Library, Study, Sediment, Window, and Help. Below the menu is a toolbar with various icons. The main window title is "AQUATOX-- Main Window - [Farm Pond MO Esferval.aps-- Main Window]". The title bar also displays "AQUATOX: Study Information" and "EPA Release 3.1". A study name field shows "Study Name: FARM POND MO". Below this is a "Run Status:" section indicating a "Perturbed Run: 11-28-12 10:31 AM" and a "Control Run: 11-28-12 10:31 AM". On the left, there's a sidebar with "Data Operations" (Initial Conds., Chemical, Site, Setup, Notes) and "Program Operations" (Perturbed, Control, Output, Export Results, Export Control, Use Wizard, Help). A message at the bottom of the sidebar says "There are 0 sediment layers modeled." To the right, a large list titled "State and Driving Variables In Study" includes: Dissolved org. tox 1: [Esfenvalerate], Total Ammonia as N, Nitrate as N, Total Soluble P, Carbon dioxide, Oxygen, Refrac. detritus, Labile sed. detritus, Susp. and dissolved detritus, Buried refrac. detritus, Buried labile detritus, Diatoms1: [Diatom], Diatoms2: [Phyt High-Nut Diatom], Greens1: [Peri, Green], Greens2: [Phyto, Green], Cyanobacteria1: [Phyt, Blue-Greens], OtherAlg1:[Cryptomonas], Macrophyte1: [Myriophyllum], SedFeeder1: [Chironomid], SuspFeeder1: [Daphnia], SuspFeeder2: [Copepod], Clam1: [Sphaerium], Grazer1: [Mayfly (Baetis)], Grazer2: [Rotifer, Keratella], Snail1: [Gastropod], LgForageFish2: [Shiner], SmGameFish1: [Largemouth Bass, YOY], LgGameFish1: [Largemouth Bass, Lg], Water Volume, Temperature, Wind Loading, Light, pH. Buttons for Add, Delete, and Edit are at the bottom of this list. Callout boxes with arrows point from the text to specific features: "Setup screen" points to the sidebar; "List of state variables" points to the variable list; "Run simulations" points to the "Control" button; "Examine Output" points to the "Output" button; and "Help feature" points to the "Help" button.

Setup screen

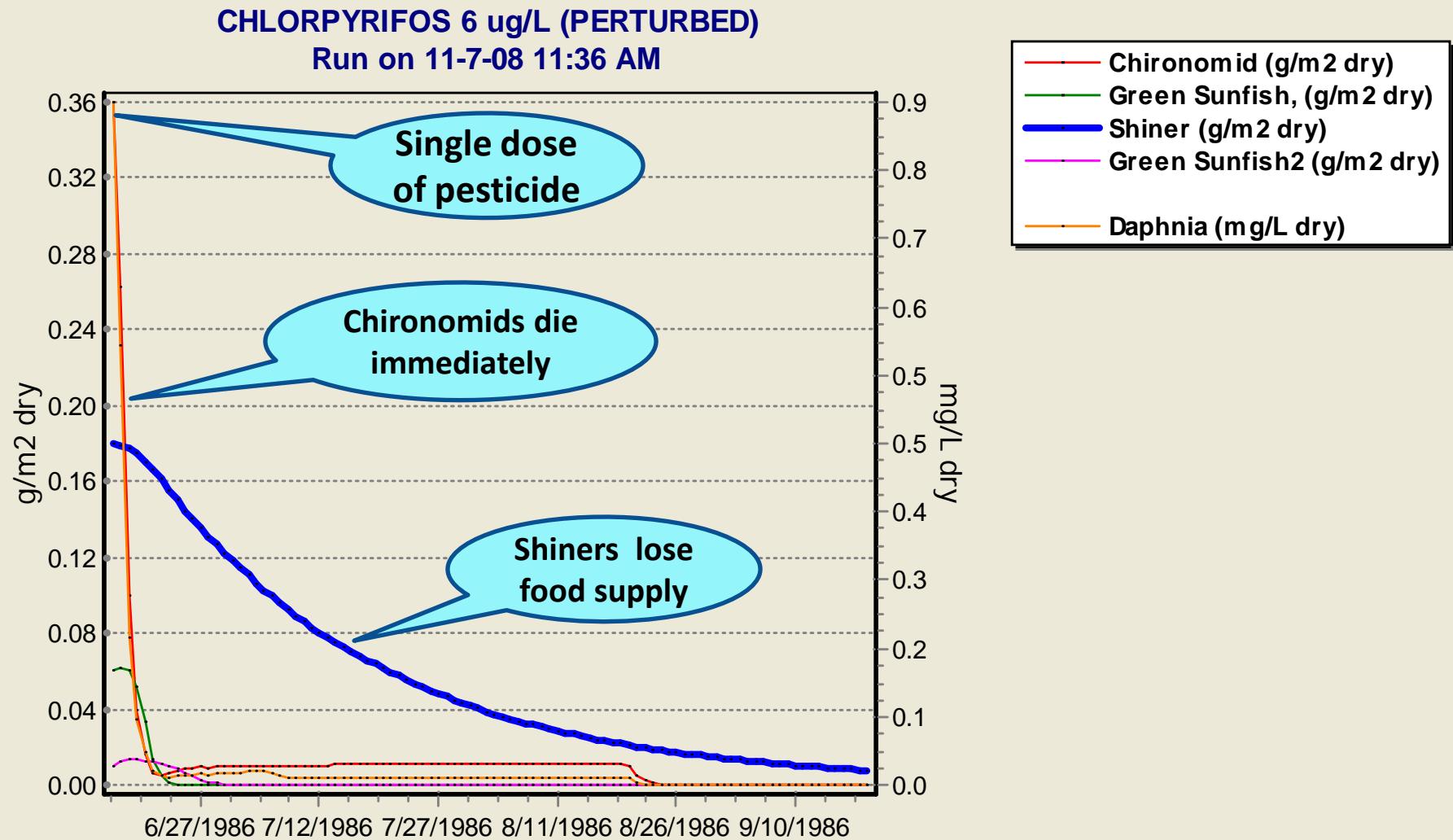
List of state variables

Run simulations

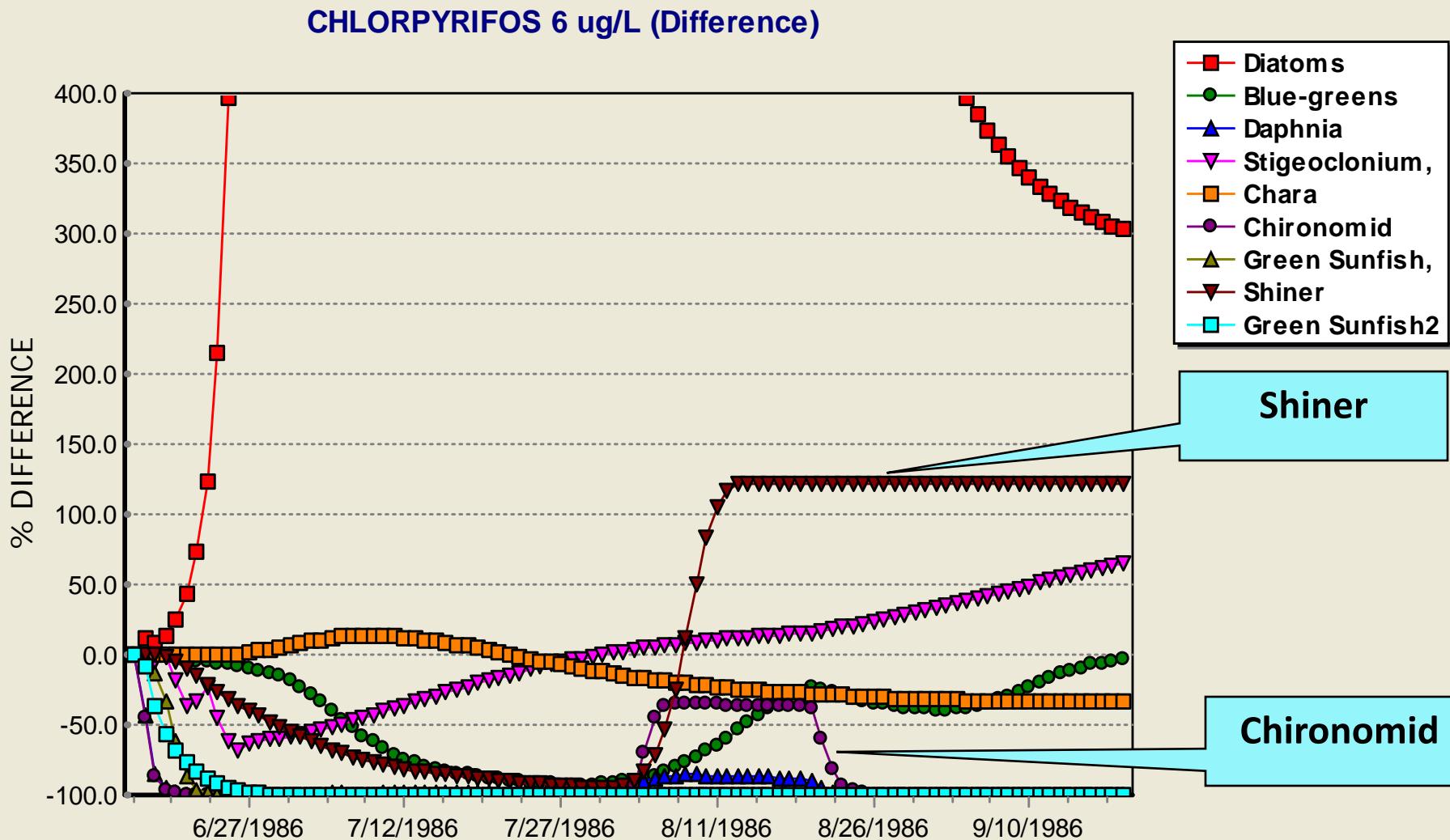
Examine Output

Help feature

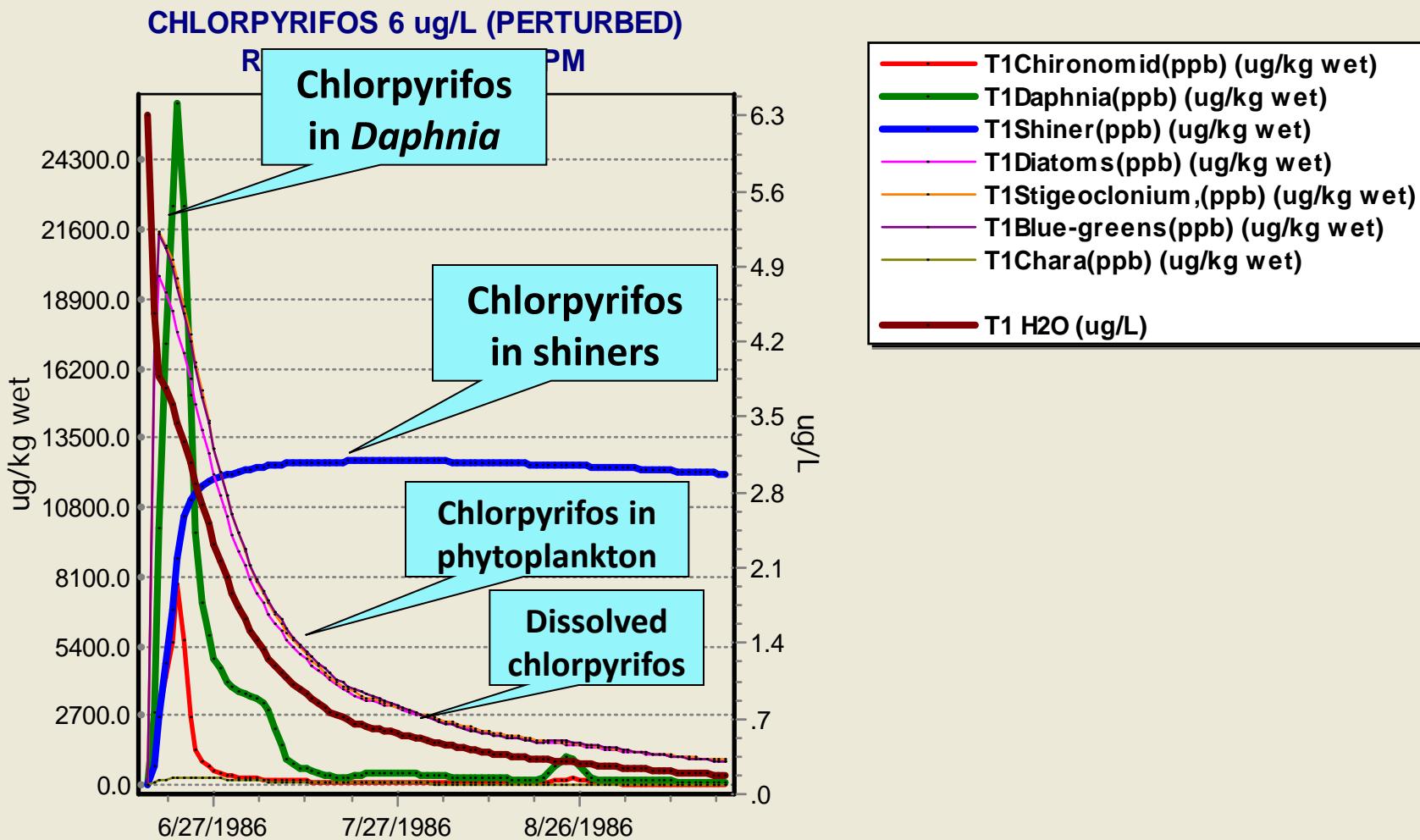
# Output: Animals decline at different rates following single dose of chlorpyrifos



# % Difference Graph shows relative differences



# Track concentrations in tissues and water



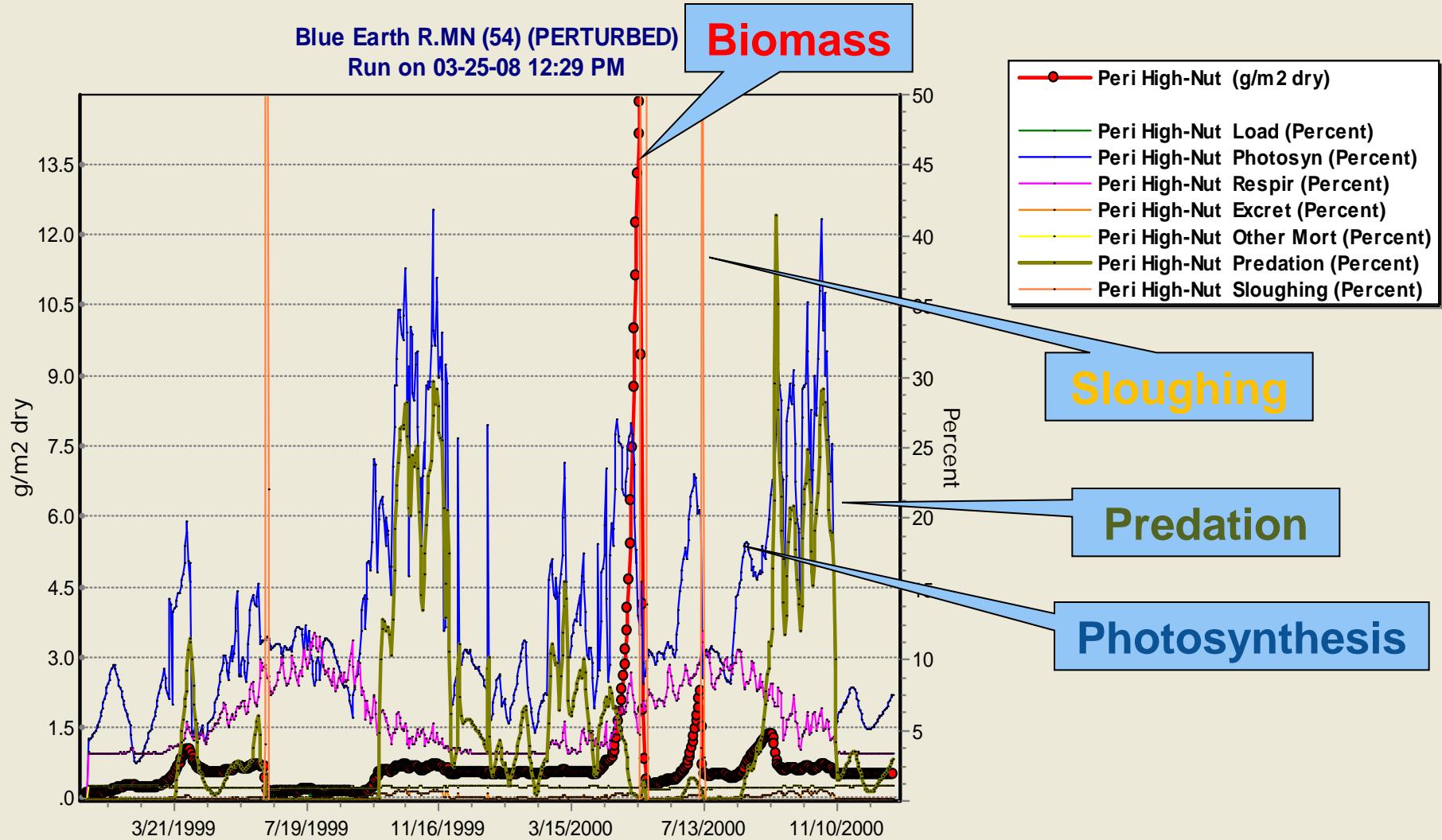
# Process Rates

- Concentrations of state variables are solved using differential equations
  - Equation for periphyton concentrations is:

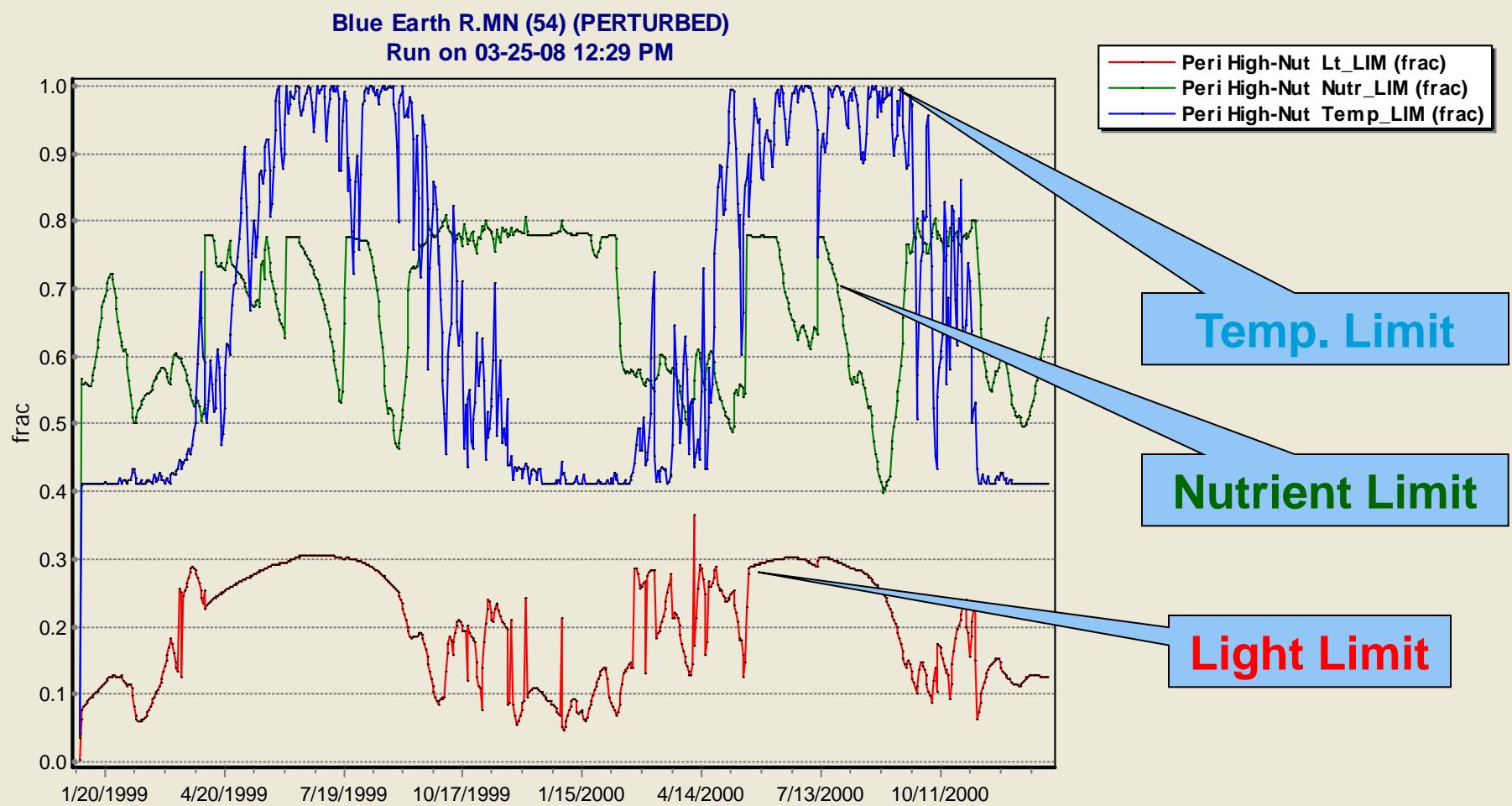
$$\frac{d\text{Biomass}_{\text{Peri}}}{dt} = \text{Loading} + \text{Photosynthesis} - \text{Respiration} - \text{Excretion} \\ - \text{Mortality} - \text{Predation} + \text{Sed}_{\text{Peri}} - \text{Slough}$$

- Individual terms of these equations can be saved and graphed

# Periphyton Rates show importance of grazing and sloughing



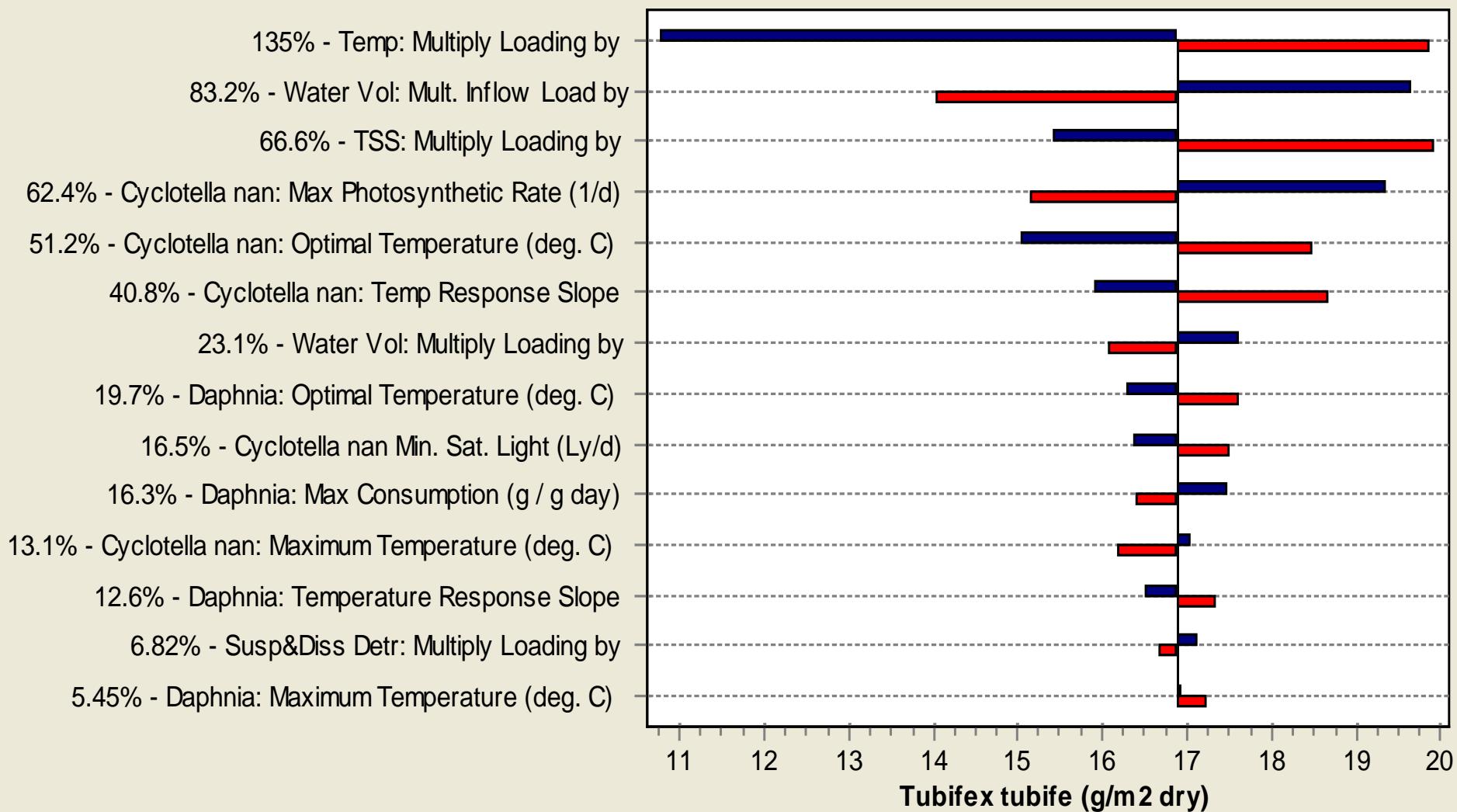
# Limitations to Photosynthesis can also be Graphed



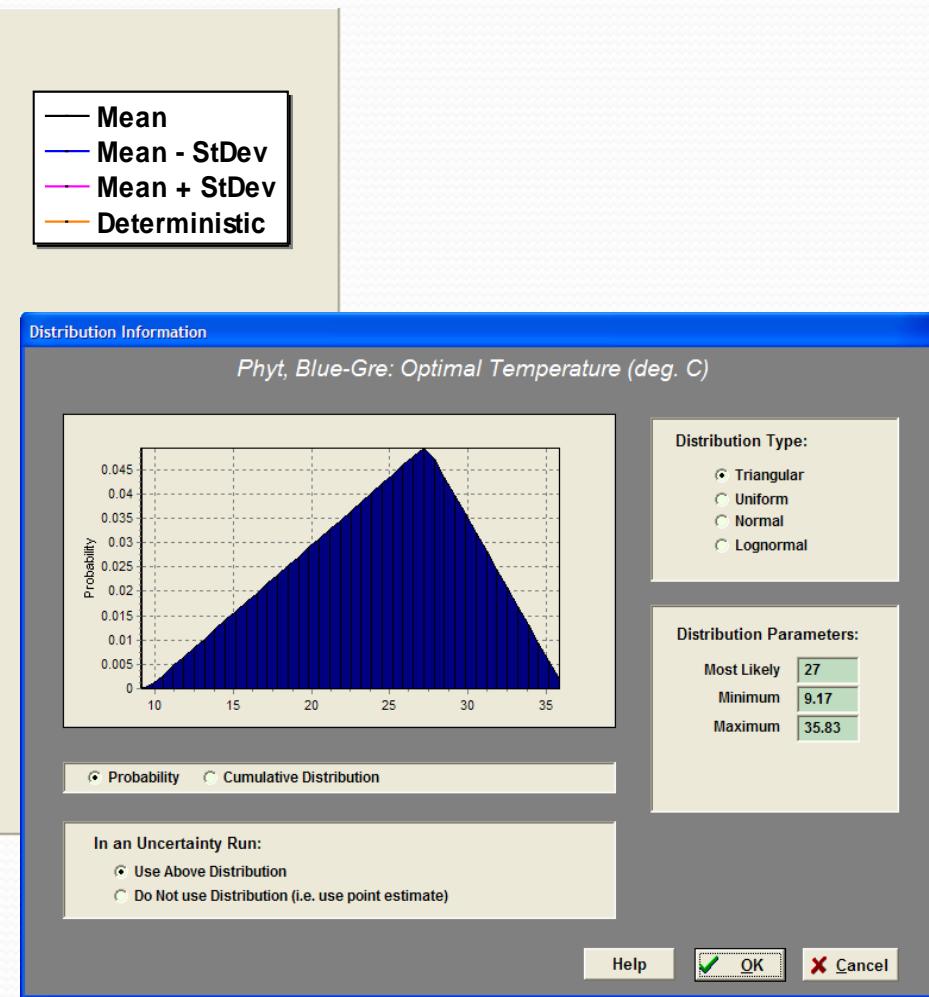
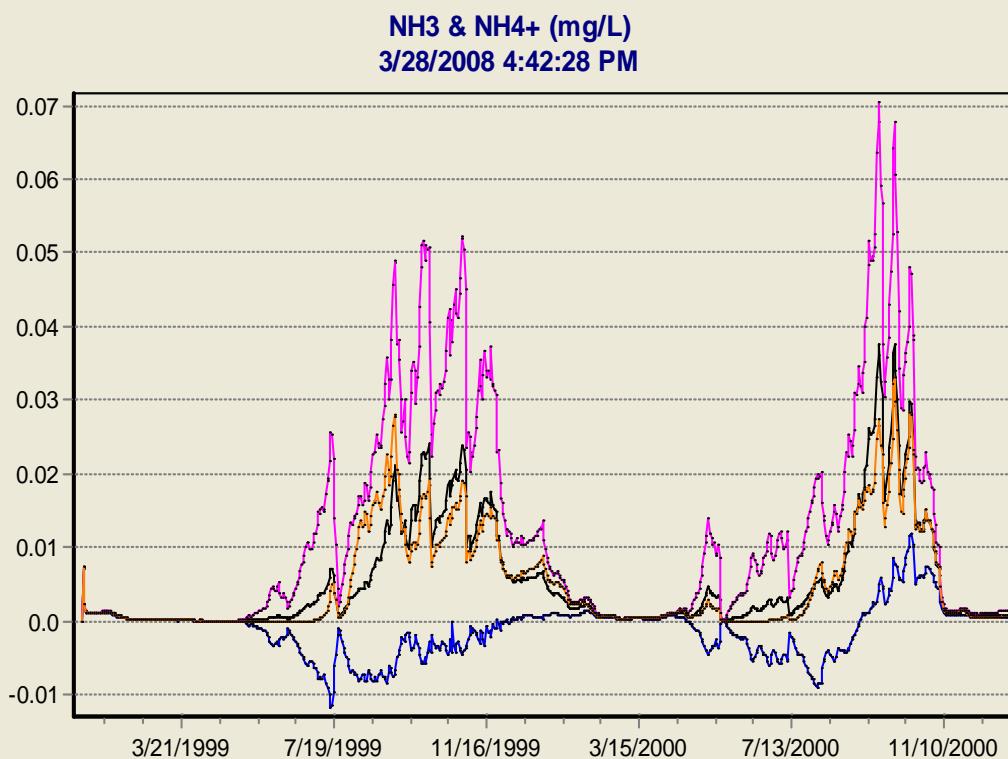
# Automated Sensitivity Analysis

Sensitivity of *Tubifex tubife* (g/m<sup>2</sup> dry) to 20% change in tested parameters

3/28/2008 3:31:16 PM



# Integrated Uncertainty Analysis Capability



# Example Applications of AQUATOX

- Eutrophication in TenKiller Lake Reservoir, OK
- PCB bioaccumulation in Lake Hartwell, SC/GA

# Application of AQUATOX to Eutrophic Reservoir

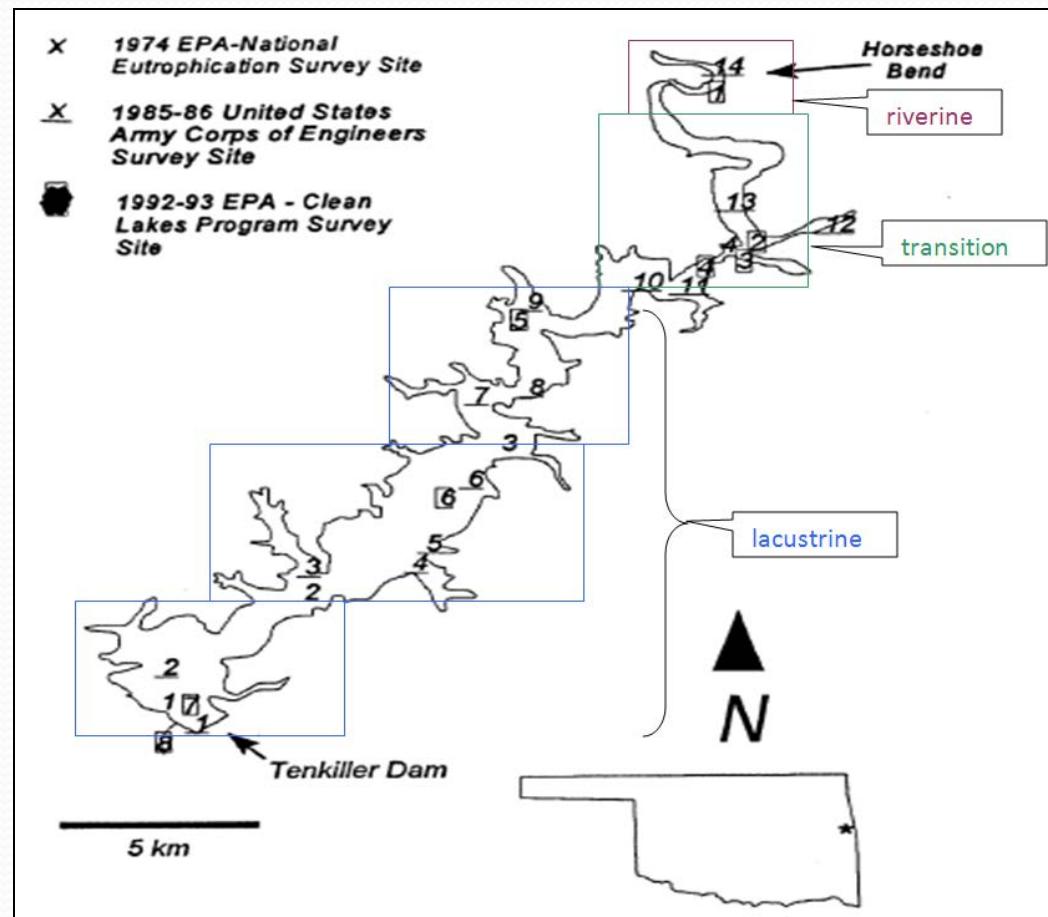
- Tenkiller Lake in eastern Oklahoma formed by the damming of the Illinois River
- On Oklahoma's 303d list as impaired for phosphorus
- Nutrient concentrations and water clarity indicate eutrophic conditions
- Example of:
  - Multiple linked segments (complex system)
  - Linkage to watershed and hydrodynamic model
  - Scenario testing

# Incoming waters very rich in algae

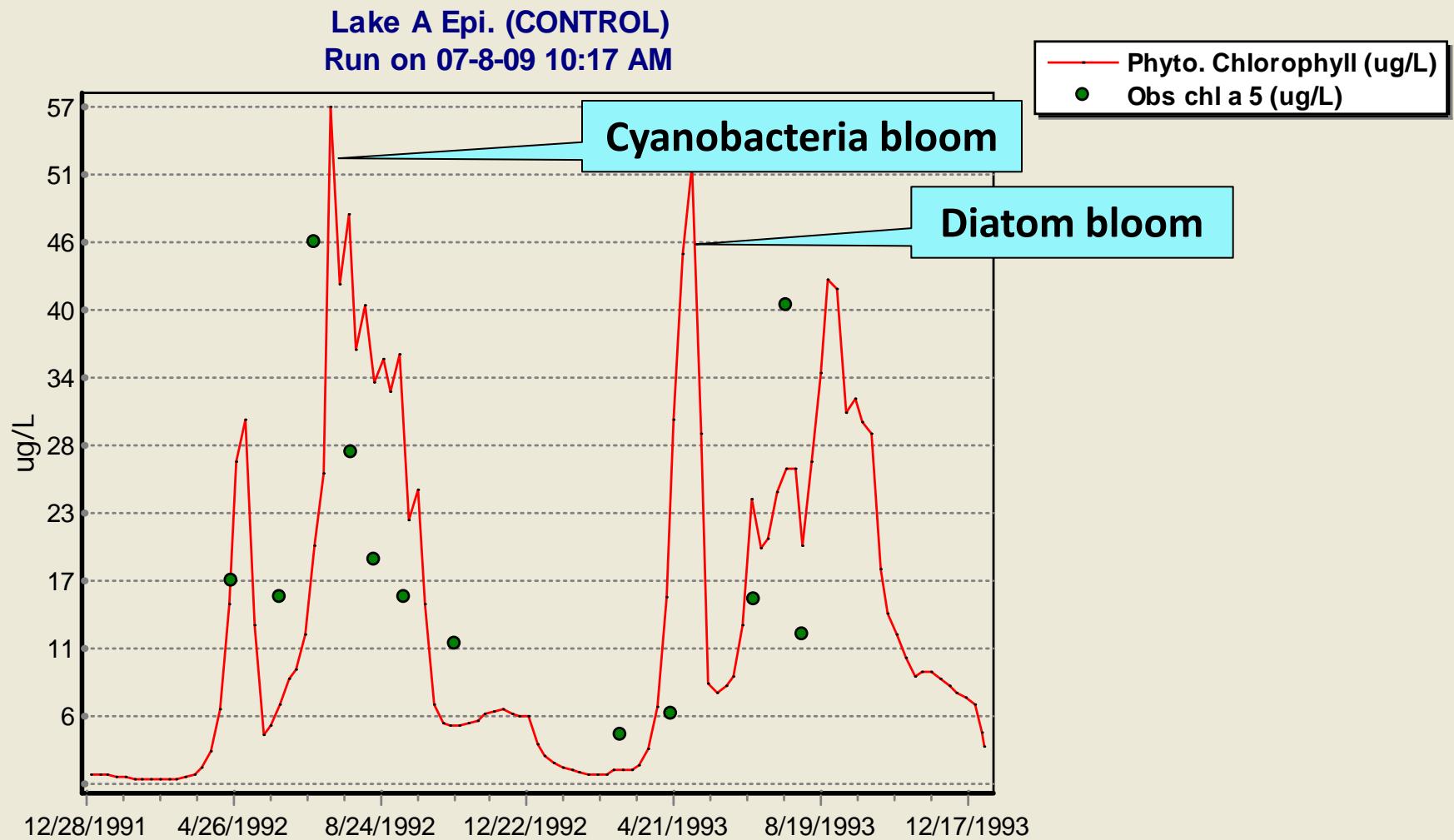


# Tenkille Lake Application

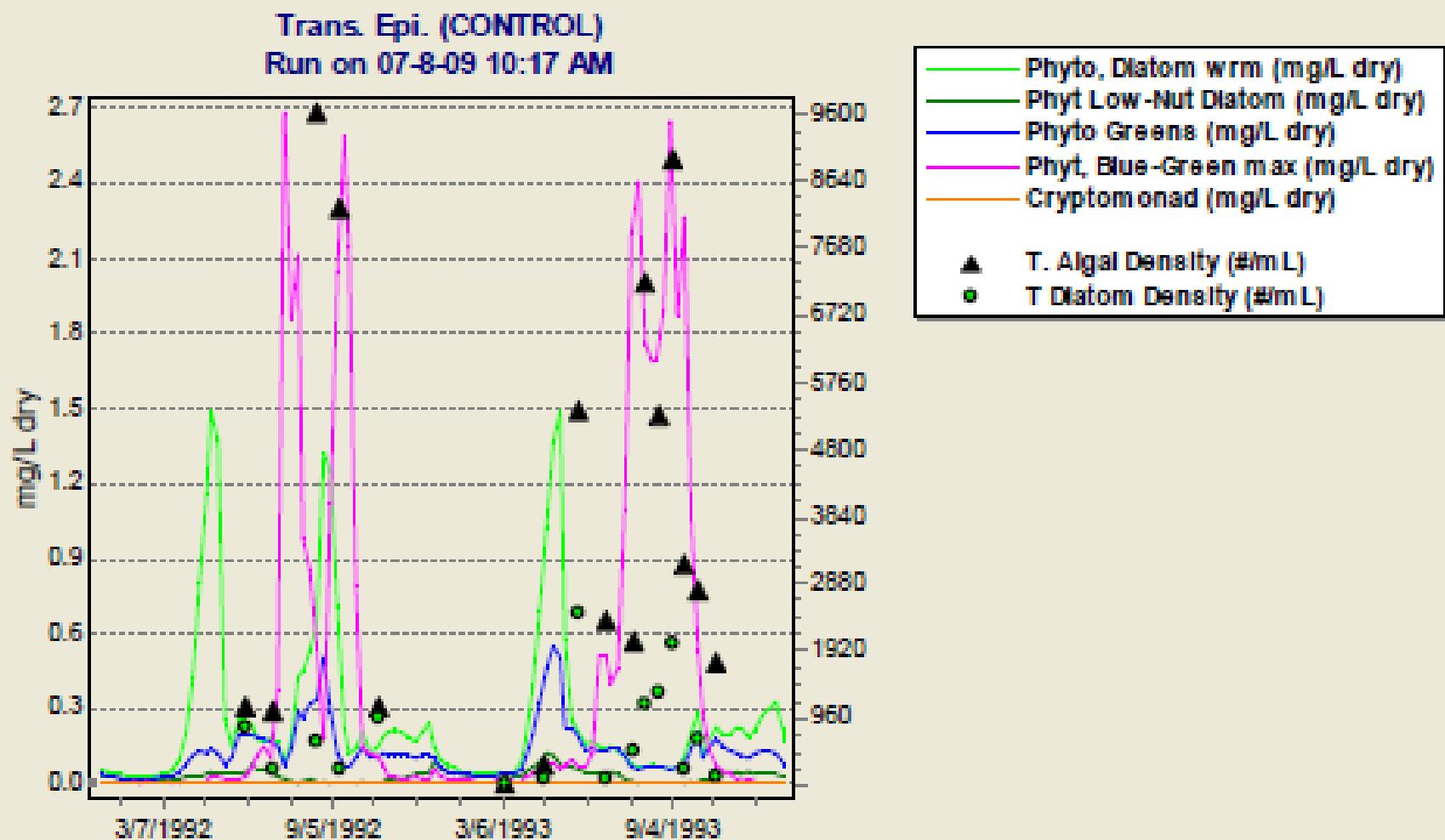
- River-reservoir system divided into nine segments
  - Riverine
  - Vertically stratified transition zone
  - Three vertically stratified lacustrine segments
- AQUATOX linked to HSPF (watershed) and EFDC (in-lake hydrology) models
- Tested scenarios to predict chlorophyll *a* levels based on different nutrient, BOD and sediment loadings (BMPs)



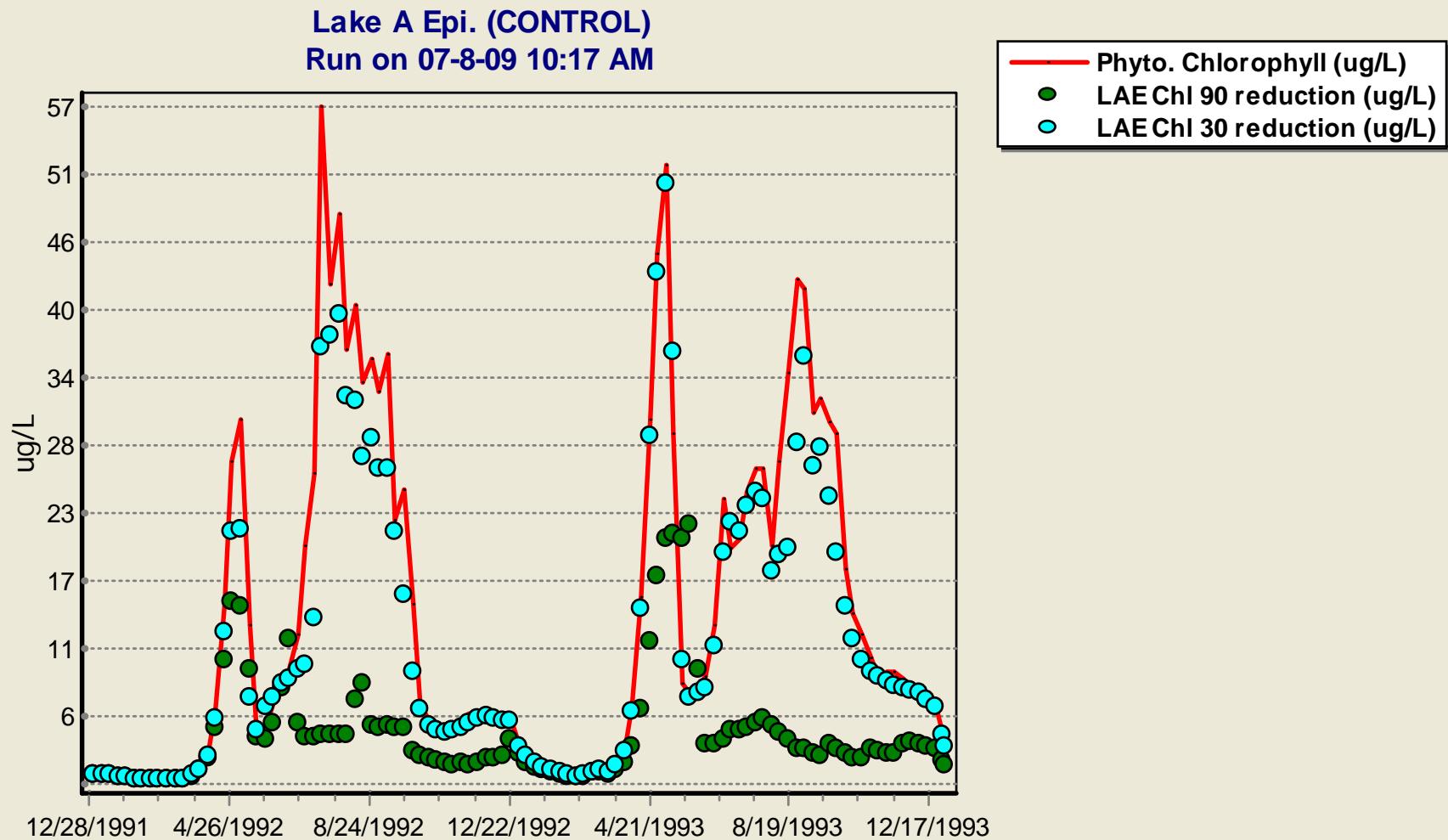
# Simulated & observed chlorophyll a



# Simulated & observed algal composition

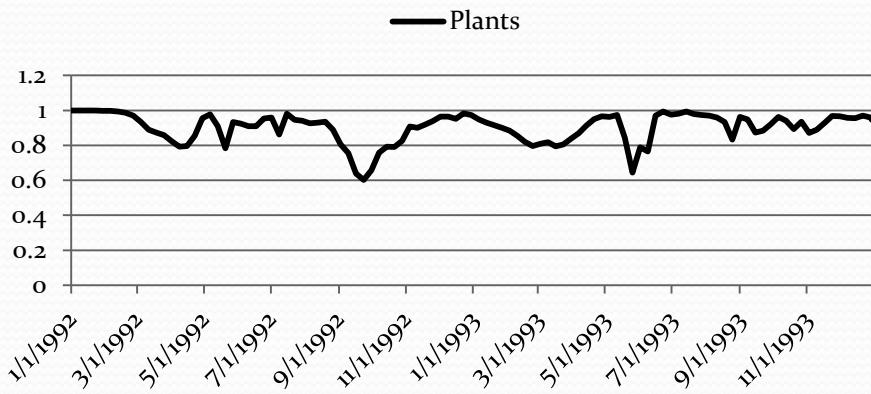


# Predicted chl *a* levels under increasing load reductions of TP

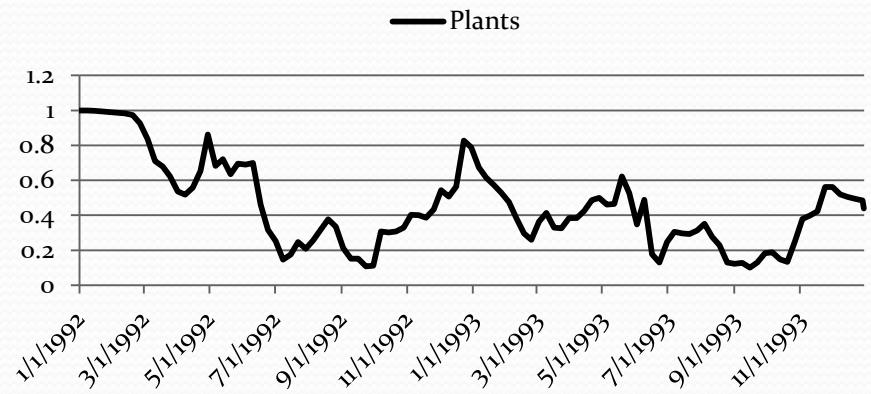


# Steinhaus Similarity Index illustrates increasingly dramatic changes in algal community

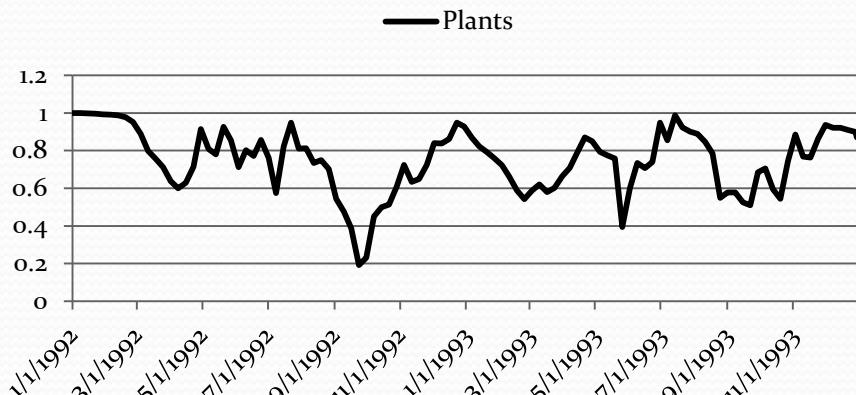
Baseline vs 30% TP reduction



Baseline vs 90% TP Reductions

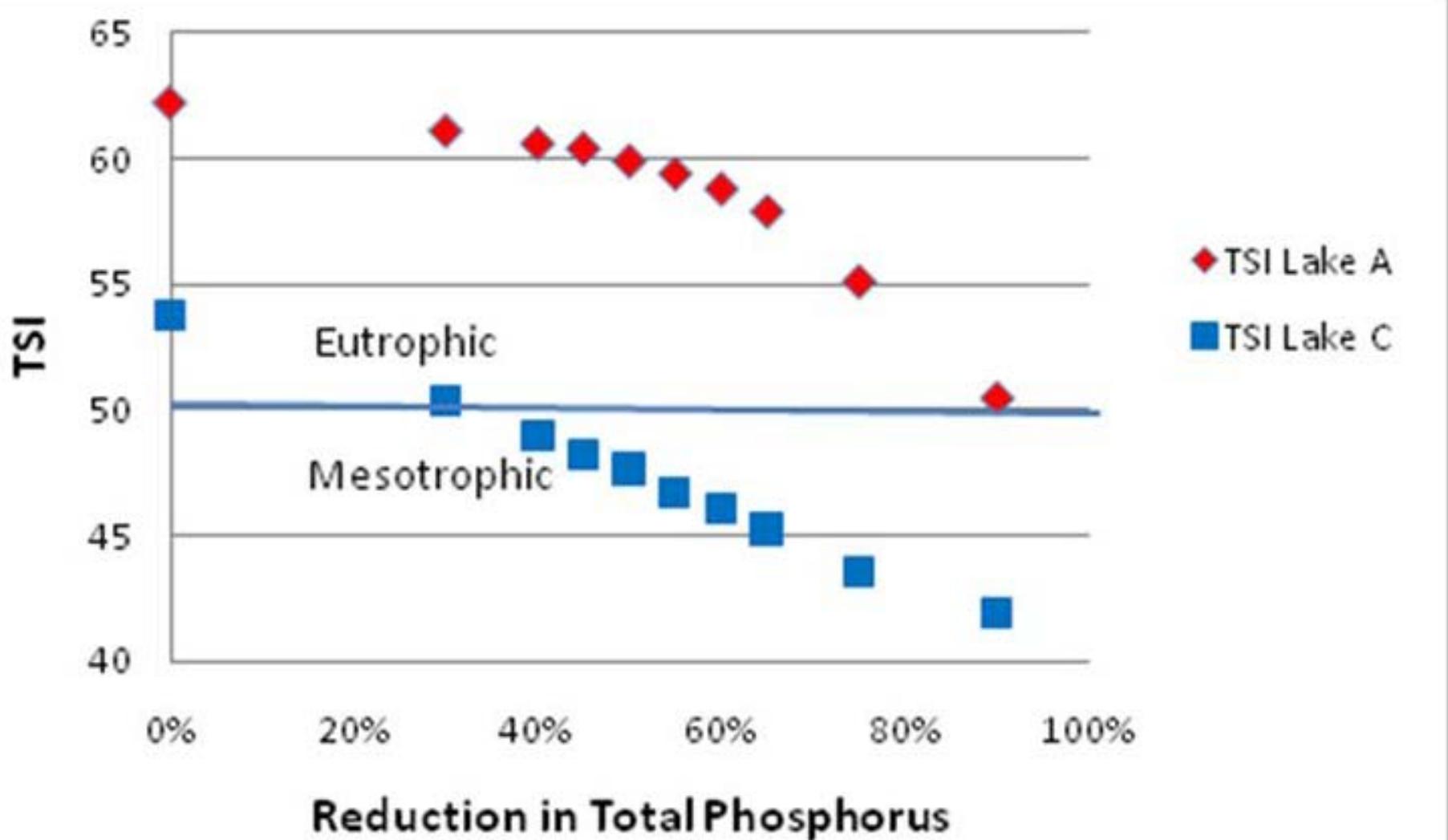


Baseline vs 60% TP Reduction



30% reduction in TP has relatively minor effect on the composition of the algal community

# Trophic State Indices show differences between lake segments

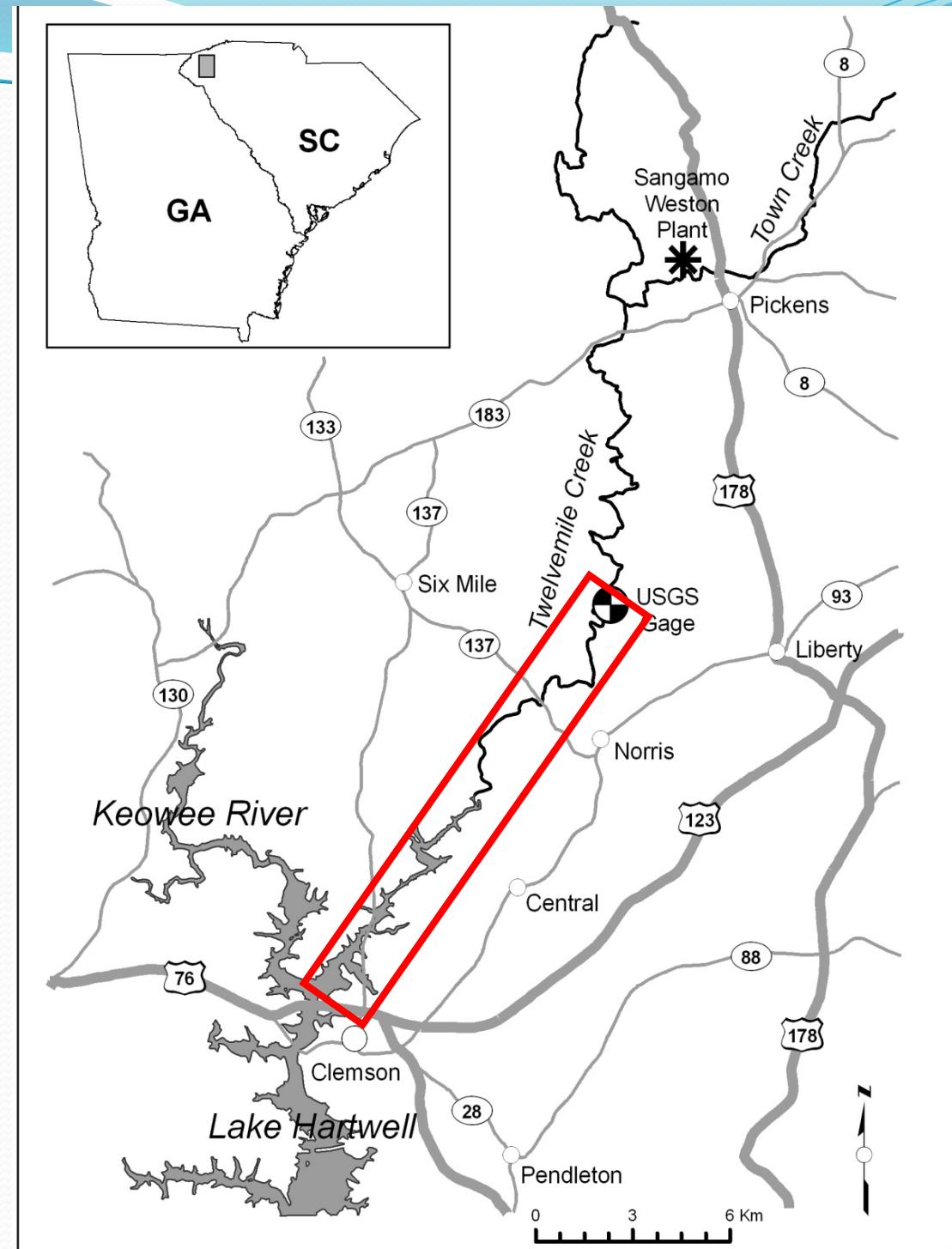


# Ecosystem Modeling for PCBs in Lake Hartwell



# Study Site

- Sangamo-Weston Superfund Site discharged 400,000 lbs of PCBs in creek from 1955-1990s
- Creek/lake treated via Monitored Natural Recovery
- PCBs have declined since 1995 in lake sediment but not in all fishes (5-10ppm)



(modified)

# AQUATOX: Study Information

EPA Release 3.1

Study Name: Lake Hartwell TCA

## Model Run Status:

Perturbed Run: 03-18-13 1:04 PM

Control Run: 03-18-13 10:55 AM

## Data Operations:



Initial Conds.



Chemical



Site



Notes

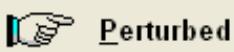


Birds, Mink...



Food Web

## Program Operations:



Perturbed



Control



Output



Export Results



Export Control



Use Wizard



Help

Model is set up to run in sensitivity mode.

## State and Driving Variables In Study

Dissolved org. tox 1: [PCB Hartwell]

Total Ammonia as N

Nitrate as N

Total Soluble P

Carbon dioxide

Oxygen

Tot. Susp. Solids

Refrac. sed. detritus

Labile sed. detritus

Susp. and dissolved detritus

Buried refrac. detritus

Buried labile detritus

Diatoms1: [Diatoms]

Greens1: [Greens]

SedFeeder1: [Chironomid]

SuspFeeder1: [Daphnia]

Grazer1: [Isonychia]

PredInv1: [Chaoborus]

LgForageFish1: [Shad\_BR]

LgGameFish1: [Largemouth Bass, Lg]

LgGameFish2: [Bluegill\_BRI]

Water Volume

Temperature

Wind Loading

Light

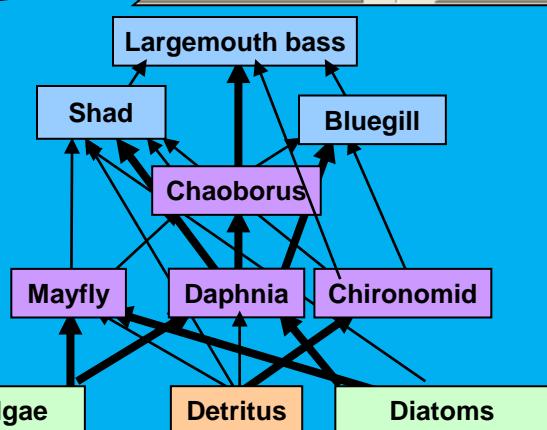
pH

Based on data

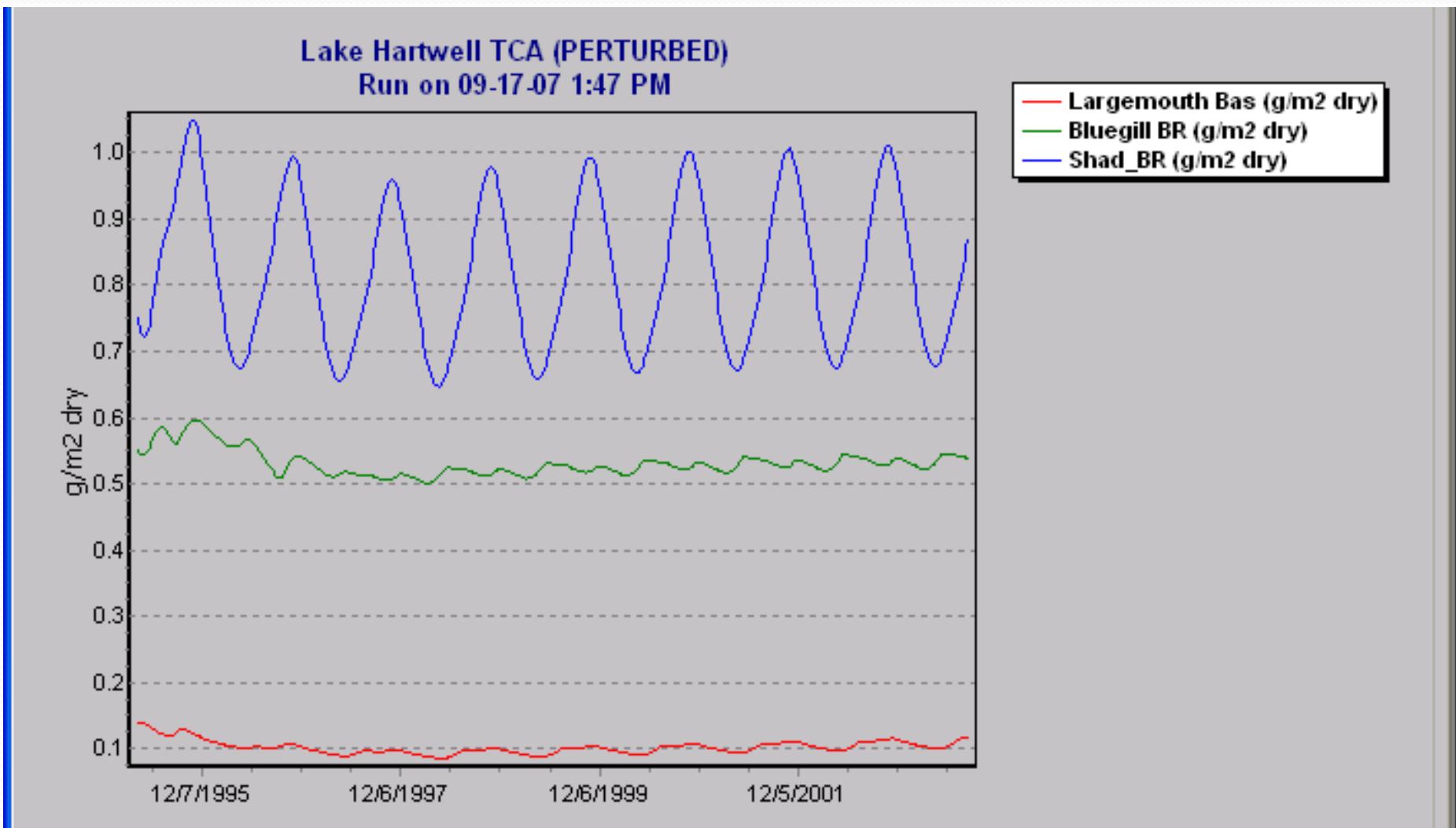
N, P, oxygen, TSS  
(EPA STORET)

Algae  
Invertebrates  
Fish

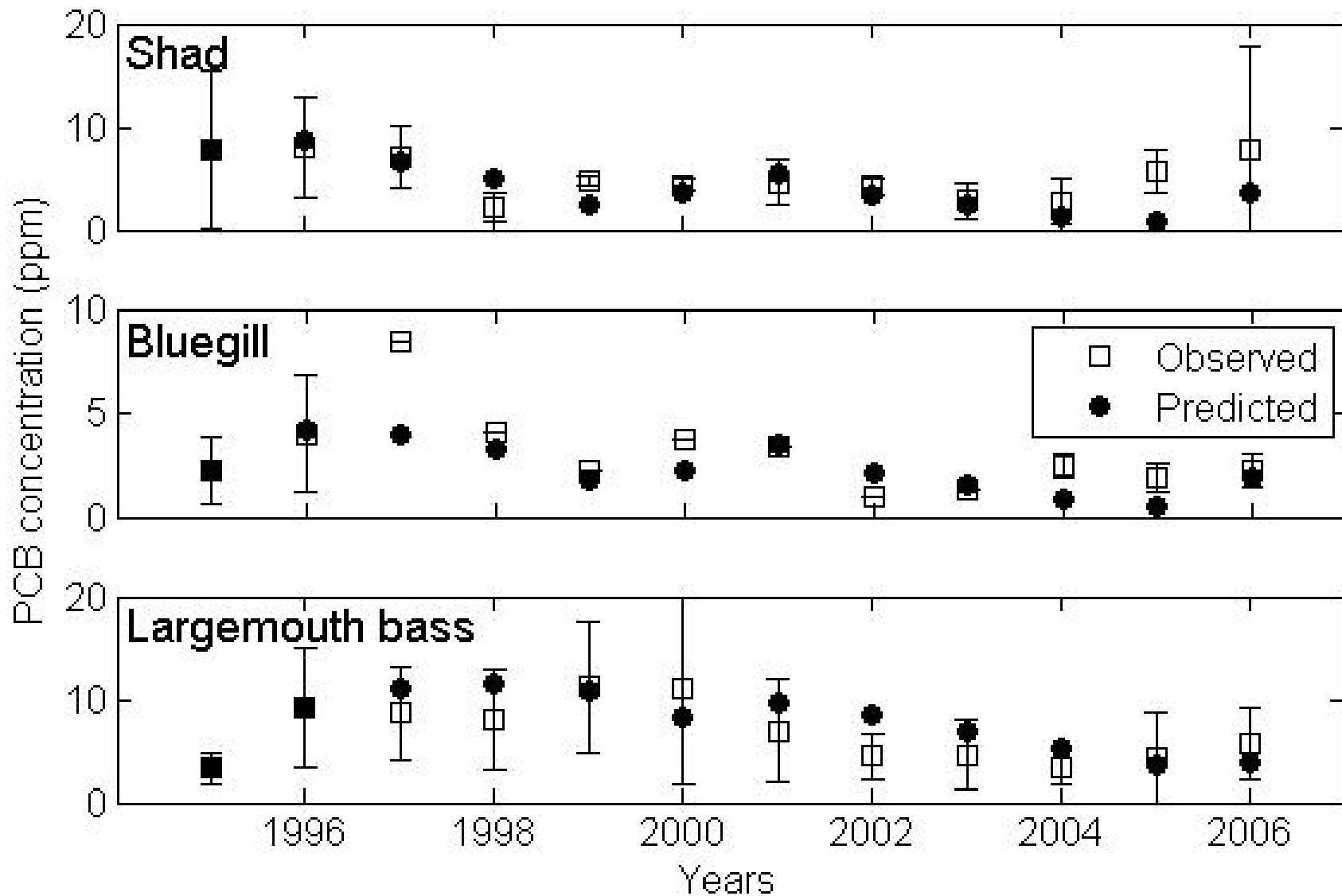
Flow (USGS gage)  
Climate (NOAA)



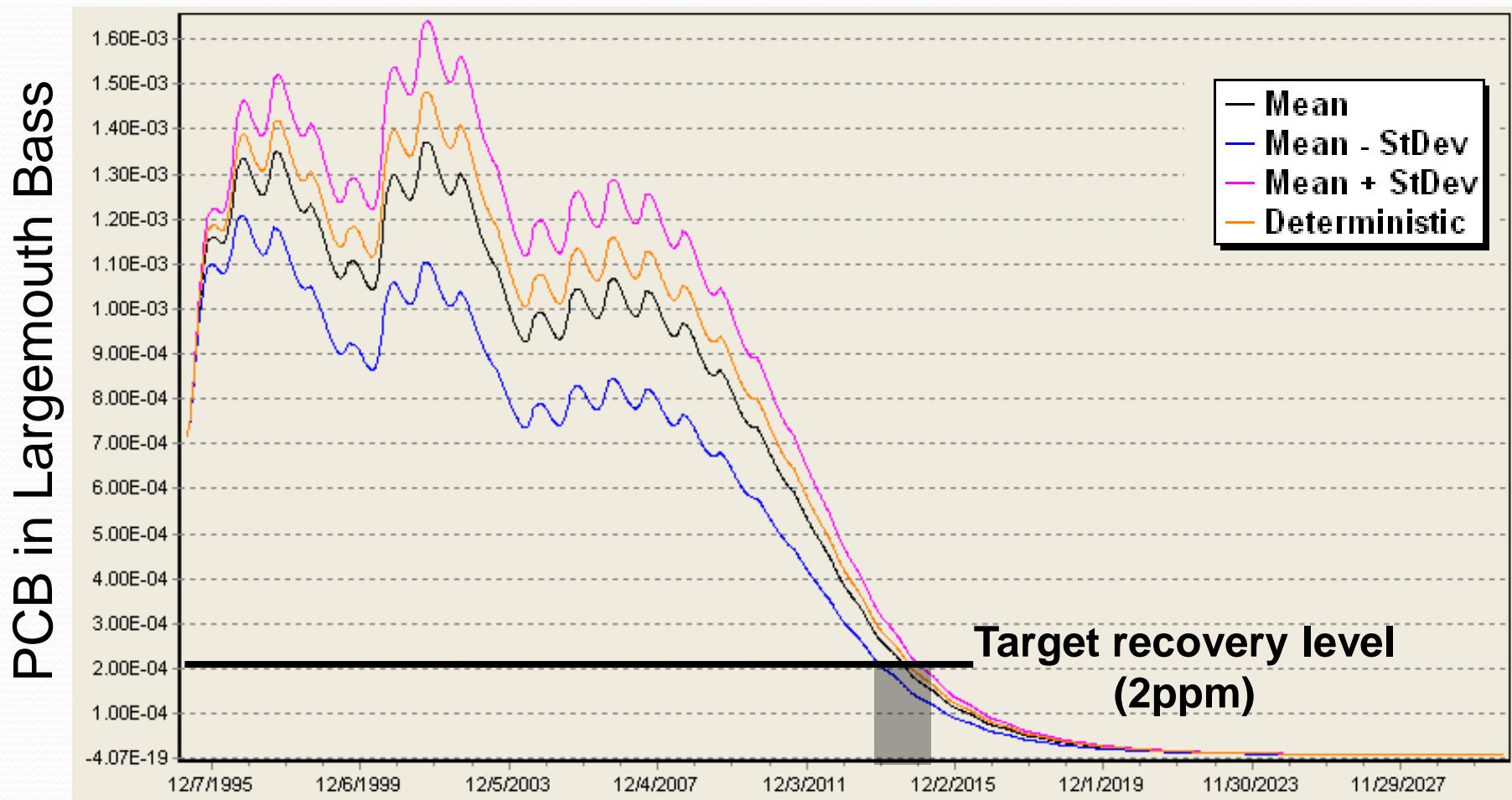
# Predicted fish biomass is calibrated to observed values



# Predicted PCB in fish is similar to observed

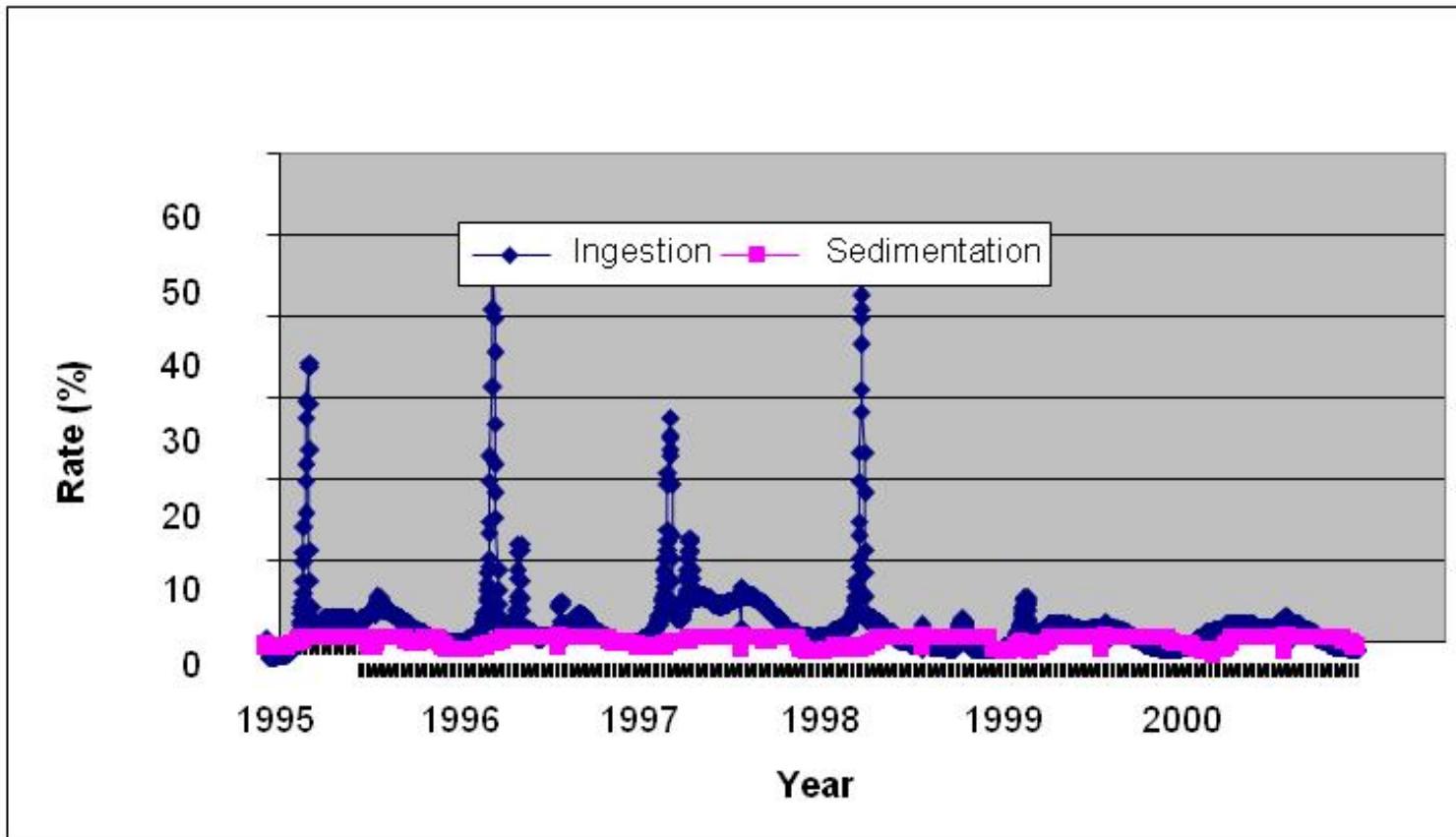


# Future Prediction with Uncertainty



# Fate of Input Detritus

- Ingested (14%) > Sedimented (4%)



# Results

When will fish recover?

- ✓ Summer/Fall 2013

Why are fish still contaminated while sediment is recovering?

- ✓ Due to contaminated input detritus



# Sensitivity of PCB Concentration in Fish to 10% ↑Temperature



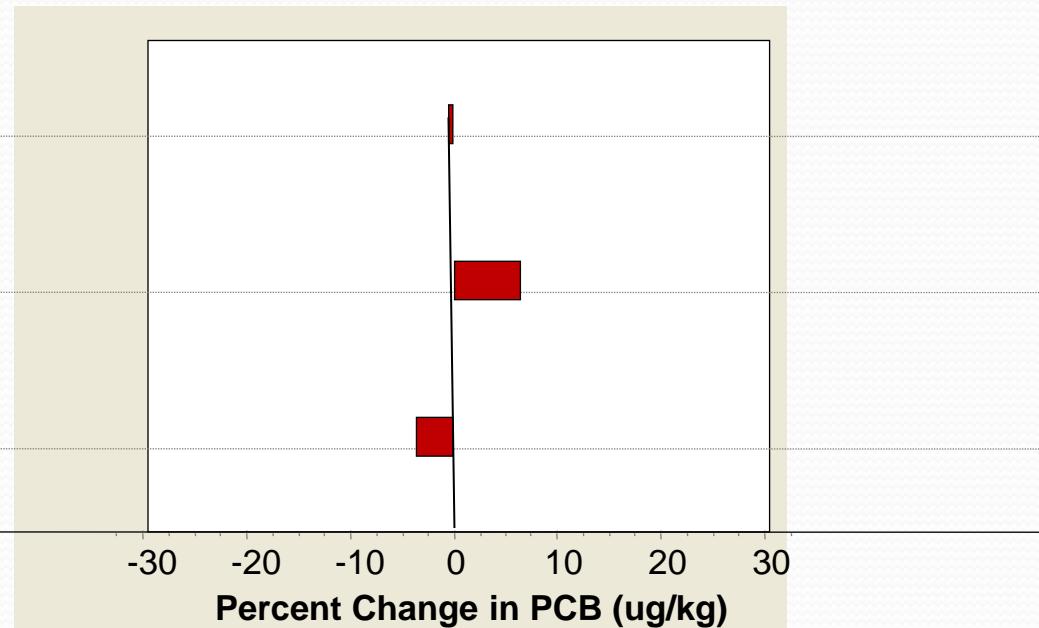
Largemouth Bass



Shad



Bluegill



# Wrap-up and Model Future

# User Support

- Technical support materials on web site  
<http://water.epa.gov/scitech/datait/models/aquatox/index.cfm>
  - Technical notes
  - Data sources
  - Workshop materials
  - Annotated bibliography (*newly updated*)
  - Sensitivity analysis report (*new*)
  - Set up guide (*in draft*)
- AQUATOX listserver (>350 subscribers)
- One-on-one technical support available (subject to future funding)

# Applicability to Sustainable and Healthy Communities Research Program

- *Contaminated sites*
- *Nitrogen plus climate change*
- *Ecosystem Services*
  - *Food and Recreation*
  - *Biodiversity and Wildlife habitat*
  - *Aesthetic*



# Thanks For Your Attention

- Marjorie Coombs Wellman, Office of Water, US EPA,  
[wellman.marjorie@epa.gov](mailto:wellman.marjorie@epa.gov)
- Brenda Rashleigh, Office of Research and Development,  
US EPA, [rashleigh.brenda@epa.gov](mailto:rashleigh.brenda@epa.gov)
- <http://water.epa.gov/scitech/datait/models/aquatox/index.cfm>