

# AQUATOX Short Course

SETAC Meeting, Tampa Florida

November 16, 2008



*Richard A. Park, Eco Modeling, Diamondhead MS*

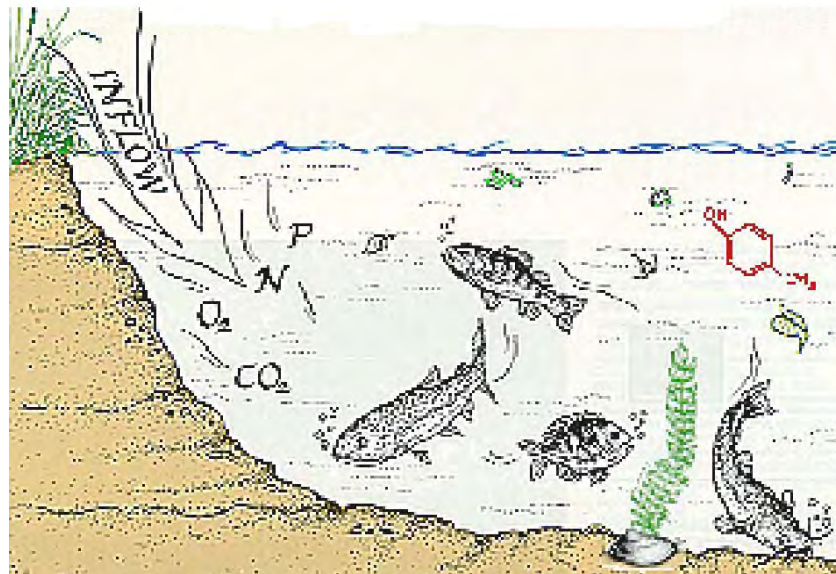
*dickpark@CableOne.net*

*Jonathan S. Clough, Warren Pinnacle Consulting, Warren VT*

*jclough@warrenpinnacle.com*

*Marjorie Coombs Wellman, Office of Water, US EPA, Washington DC*

*wellman.marjorie@epamail.epa.gov*



# Introduction 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

# 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)
  - CATS-5 (Traas et al. 2001) is similar; models microcosms
  - CASM (Bartell et al. 1999) models toxic effects but not fate
- Can simulate many more types of organisms with more realism than most other water quality models
  - WASP6 models total phytoplankton and “benthic algae” (Wool et al. 2004); zooplankton are just a grazing term
  - QUAL2K models phytoplankton and “bottom algae” (Chapra and Pelletier 2003); no animals
- Very comprehensive bioaccumulation model

# 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

# Potential Applications for AQUATOX

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

# Regulatory Endpoints Modeled

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

# 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
- Using the linkage to BASINS, evaluate effects of agricultural practices
  - Will target chlorophyll *a* concentrations be attained after BMPS are implemented?
  - Will land use changes from agriculture to residential use increase or decrease eutrophication effects?



# Potential Applications of AQUATOX *toxic substances*

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

# Potential Applications

## *aquatic life support*

- Estimate recovery time for fish or invertebrates after reducing pollutant loads
- Evaluate potential ecosystem responses to invasive species and mitigation measures
  - Will native species disappear?
  - Will there be changes in ecosystem “services”?
  - What are the potential effects and half-life of a biocide?
- *Coordinate with biological criteria program*
  - *Estimate biological metrics*
  - *Simulate reference conditions where none exist*
  - *Evaluate biological potential*

# Comparison of Dynamic Risk Assessment Models

State Variables & Processes	AQUATO X	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

# Comparison of Bioaccumulation Models: Biotic State Variables

Table 3.2. Comparison of Bioaccumulation State Variables								
	AQUATOX Release 2	BASS v 2.1	Biotic Ligand 1.0.0	Ecofate 1.0b1, Gobas	EMCM 1.0	RAMAS Ecosystem	QEAFFDCHN 1.0	TRIM.FaTE v 3.3
<b>BIOTIC STATE VARIABLES</b>								
<b>Plants</b>								
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	★				★			★
<b>Animals</b>								
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								★

## What AQUATOX does *not* do

- It does not model metals
  - **Hg was attempted, but unsuccessful**
- It does not model bacteria or pathogens
  - **microbial processes are implicit in decomposition**

# AQUATOX Structure

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

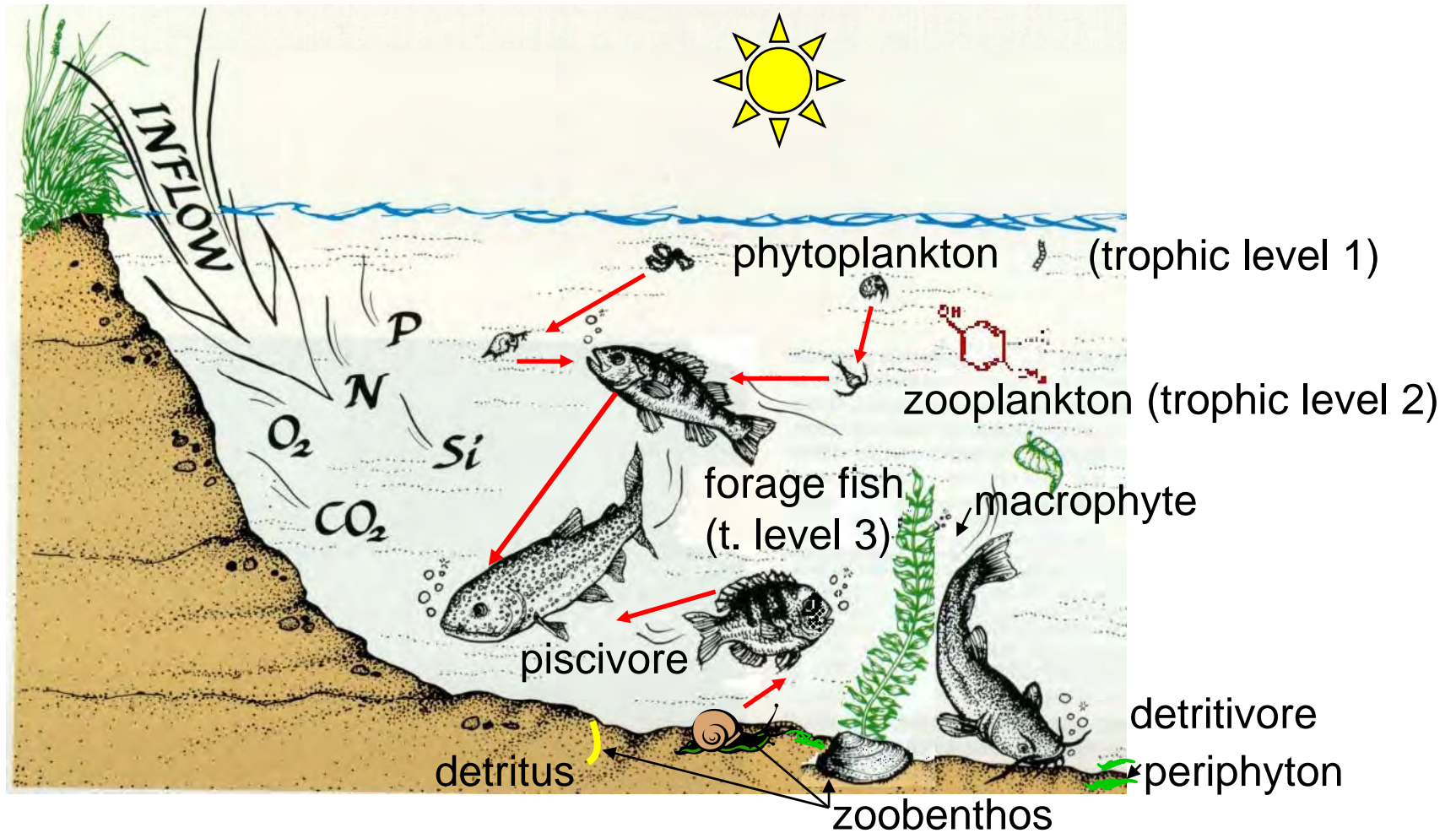


# Processes Simulated

- **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



# Ecosystem components



# State Variables in Coralville, Iowa, Study

Phosphate	Ammonia	Nitrate & Nitrite	Carbon Dioxide	Oxygen
Phytoplankton Blue-green Toxicant	Phytoplankton Diatom Toxicant	Periphyton Diatom-Green Toxicant	Macrophyte water milfoil, Toxicant	
Zoobenthos midges, oligochaetes Toxicant	Zoobenthos Grazer: snails Toxicant	Herbivorous Zooplankton cladocerans Toxicant	Predatory Invertebrate zooplankton Toxicant	
Bottom Fish catfish, buffalofish Toxicant	Forage Fish shad, bluegill Toxicant	Piscivore walleye Toxicant	Multi-aged Piscivore bass Toxicant	
Refractory Diss. Detritus Toxicant	Labile Diss. Detritus Toxicant	Dissolved Org. Toxicants (up to 20)	Refractory Susp. Detritus Toxicant	Labile Susp. Detritus Toxicant
Refractory Sed. Detritus Toxicant	Labile Sed. Detritus Toxicant	Buried Refrac. Sed. Detritus Toxicant		Total Susp. Solids (minus algae)

# State Variables in Experimental Tank

Phosphate

Ammonia

Nitrate & Nitrite

Carbon Dioxide

Oxygen

Macrophyte  
water milfoil  
Toxicant

Refractory  
Diss. Detritus  
Toxicant

Labile  
Diss. Detritus  
Toxicant

Dissolved  
HCB

Refractory  
Susp. Detritus  
Toxicant

Labile  
Susp. Detritus  
Toxicant

Refractory  
Sed. Detritus  
Toxicant

Labile  
Sed. Detritus  
Toxicant

# 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

# Demonstration 1

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

- Installation Considerations
- The “APS” file unit
- Looking at a few Parameters
- Libraries of Parameters
- Looking at Model Output vs. Observed
- Setup Screen
- Integrated Help-File and Users Manual

# What are the Analytical Capabilities?

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

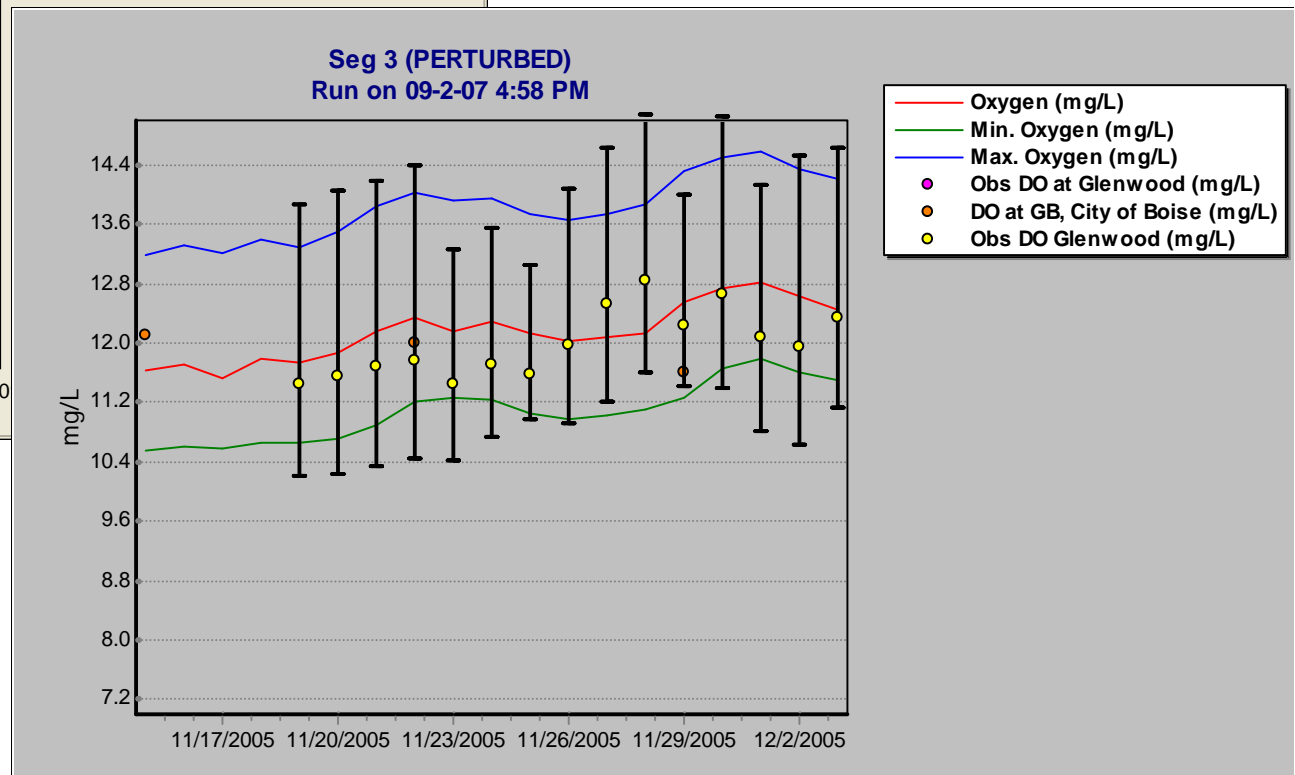
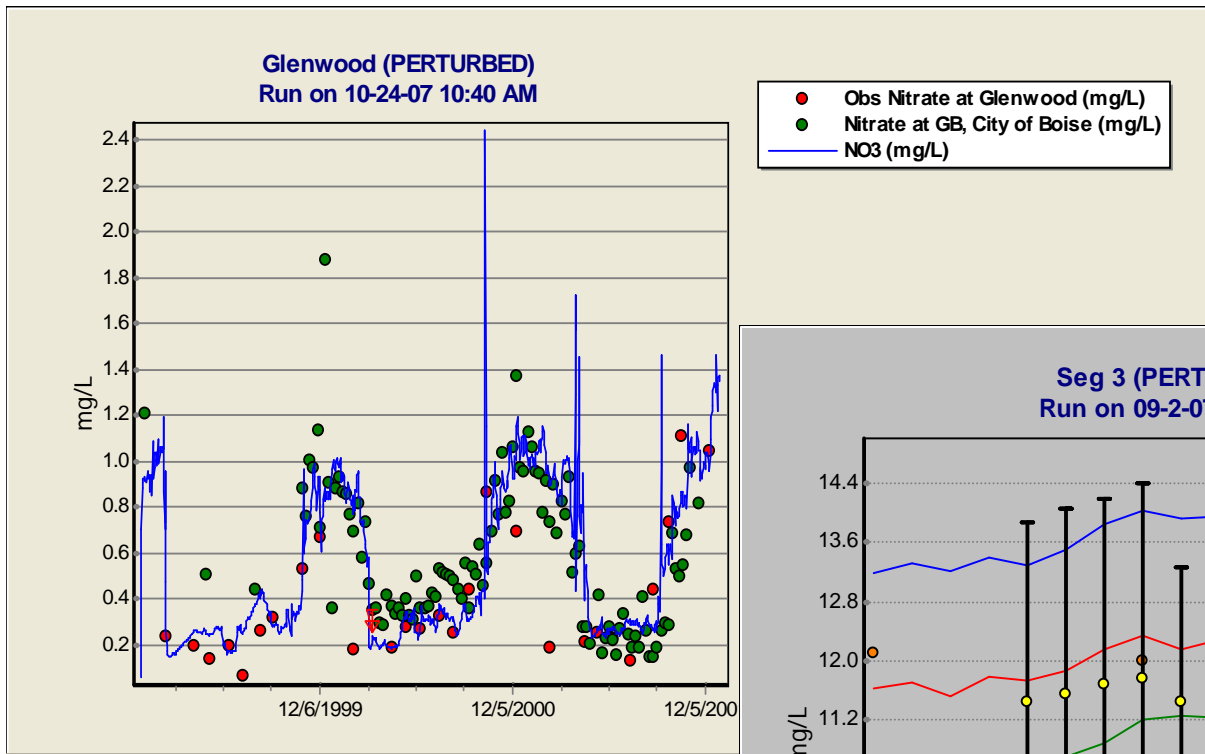
# The Many Types of AQUATOX Output

(in order of output list)

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

# Graphical Analysis

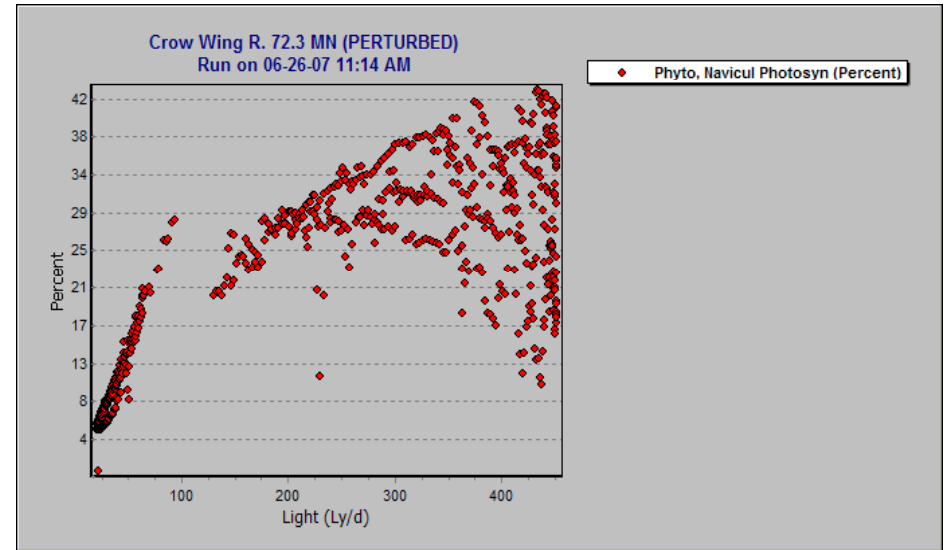
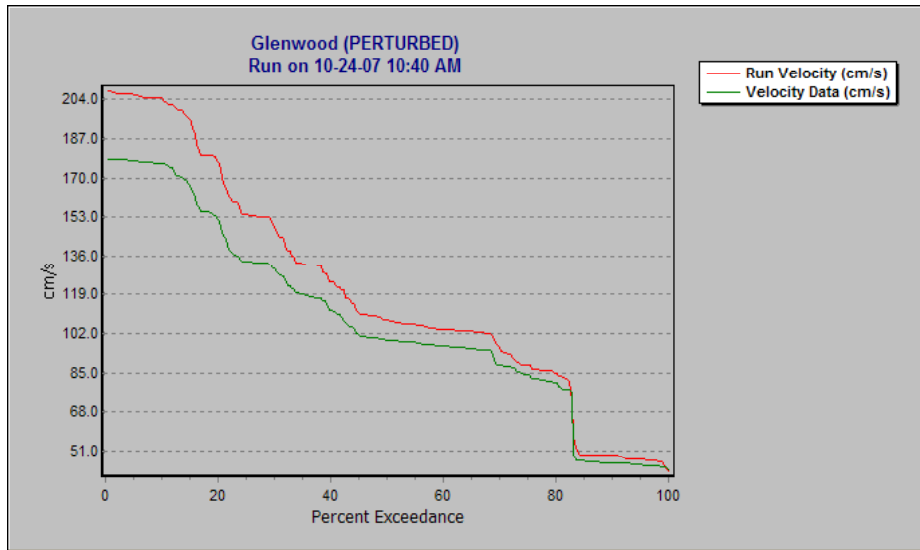
Compare observed data to model output





# Graphical Analysis

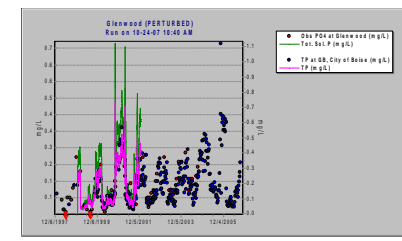
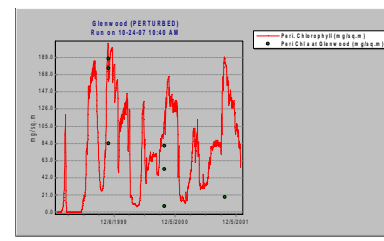
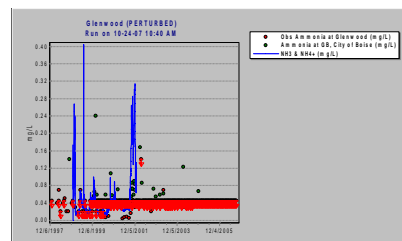
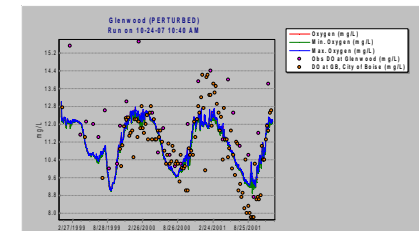
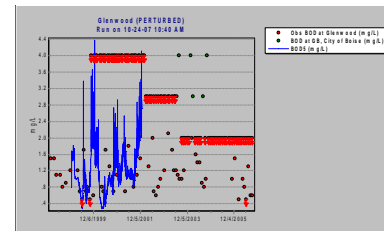
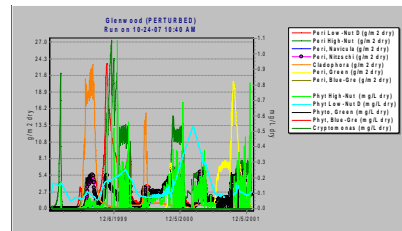
Percent exceedance, duration, scatter plots, log-scale graphs



Graph Library saved within simulation

**New Graph**

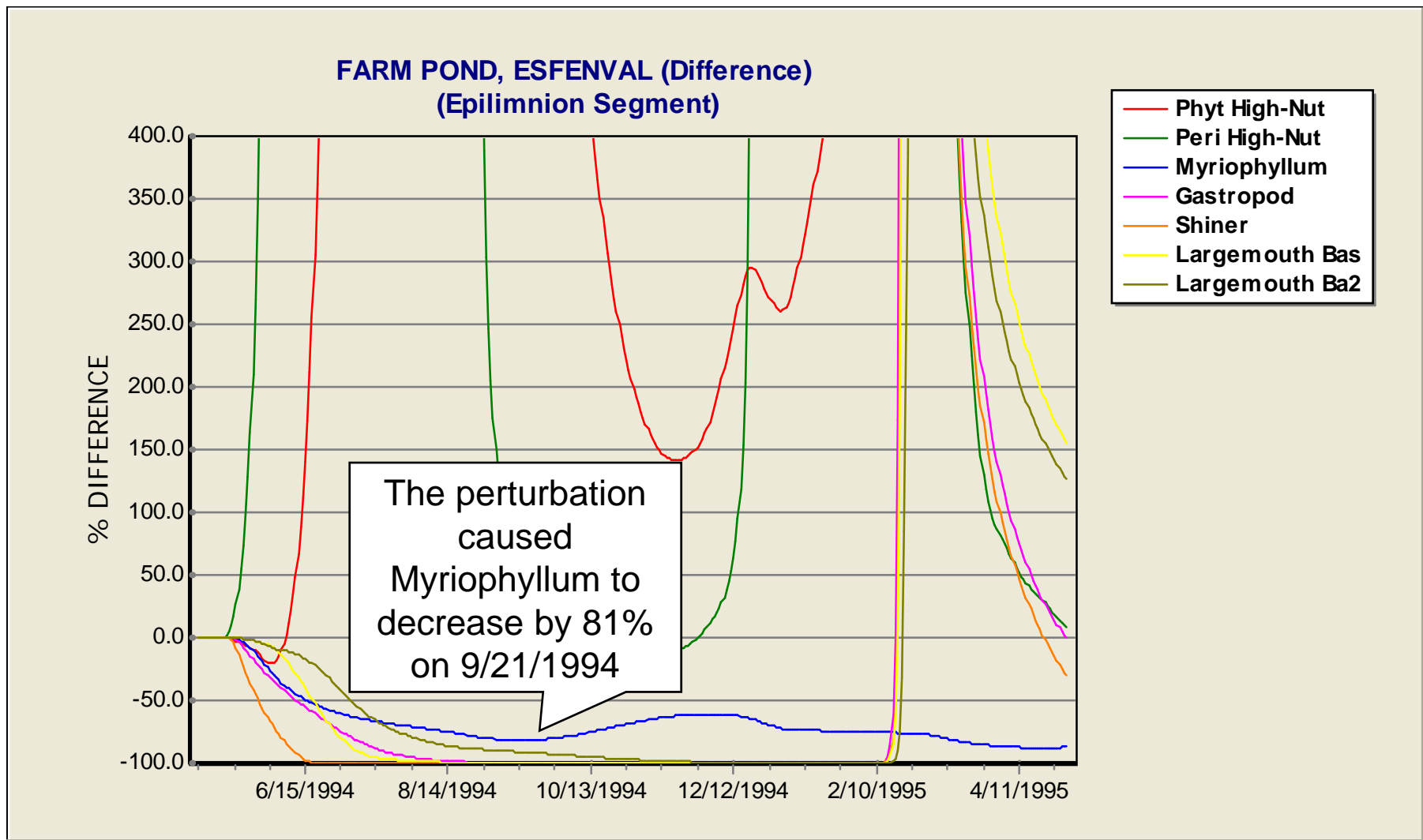
- All Plants
- Ammonia Summary
- BOD Summary
- peri chla2
- oxygen
- TP & PO4
- nitrate
- Chlorophyll a
- Velocity
- NZMS
- Dissolved Oxygen
- New Graph



# Comparing Scenarios: the “Difference” Graph

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

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



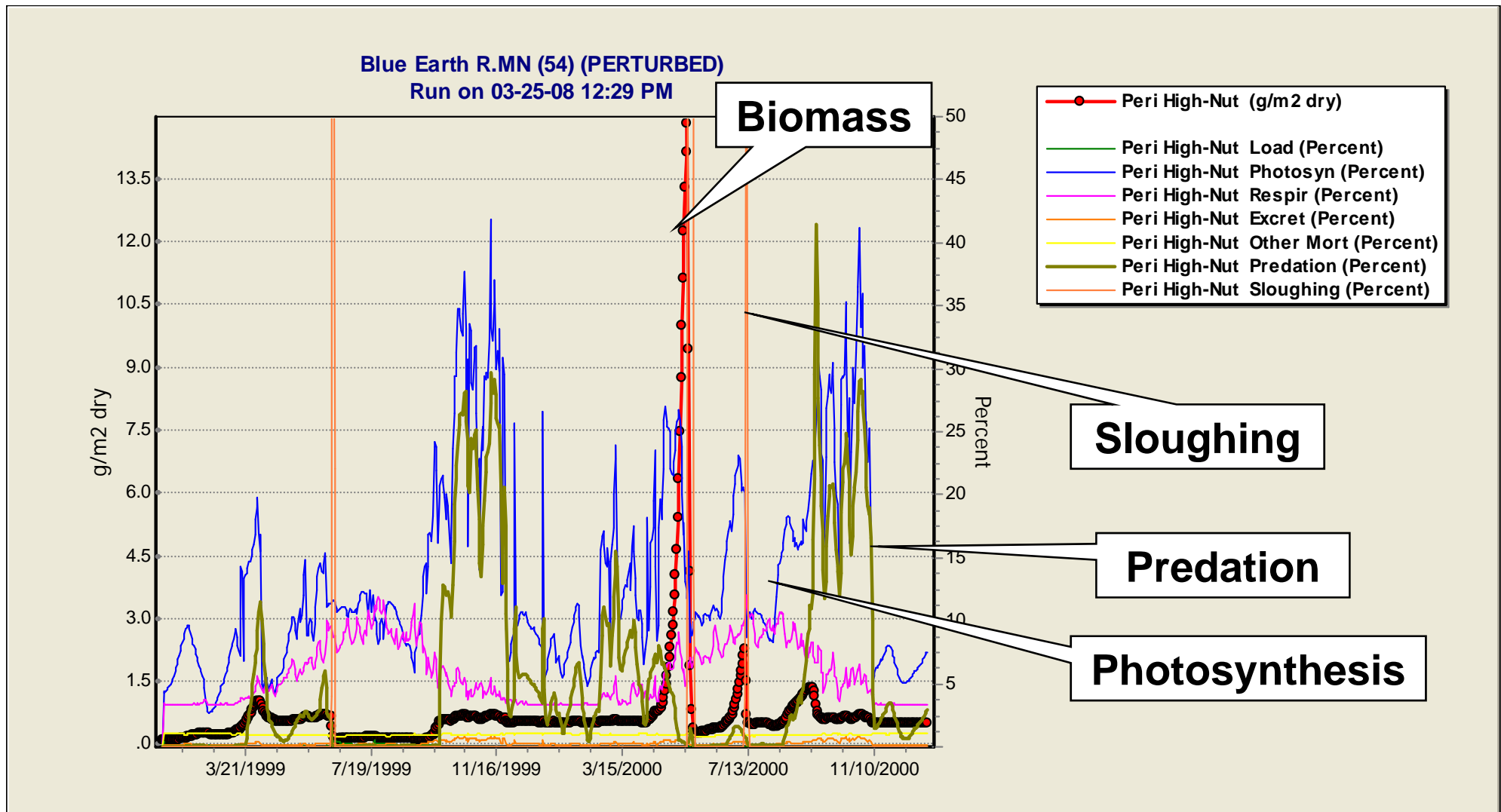
# Process Rates

- concentrations of state variables are solved using partial differential equations (Tech. Doc.)
- e.g. the equation for periphyton concentrations is

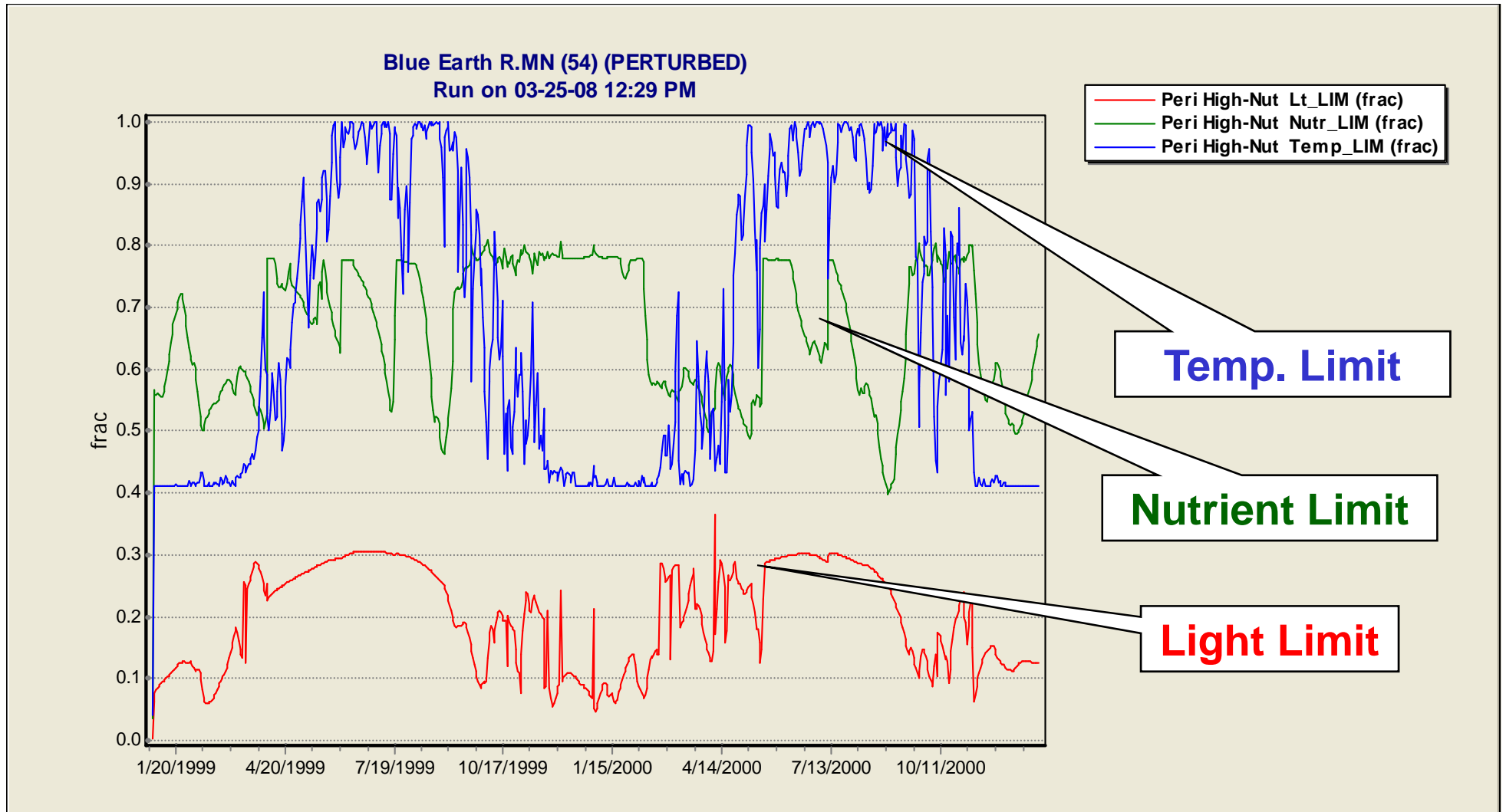
$$\frac{dBiomass_{Peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion - Mortality - Predation + Sed_{Peri}$$

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

# Rates Plot Example: Periphyton

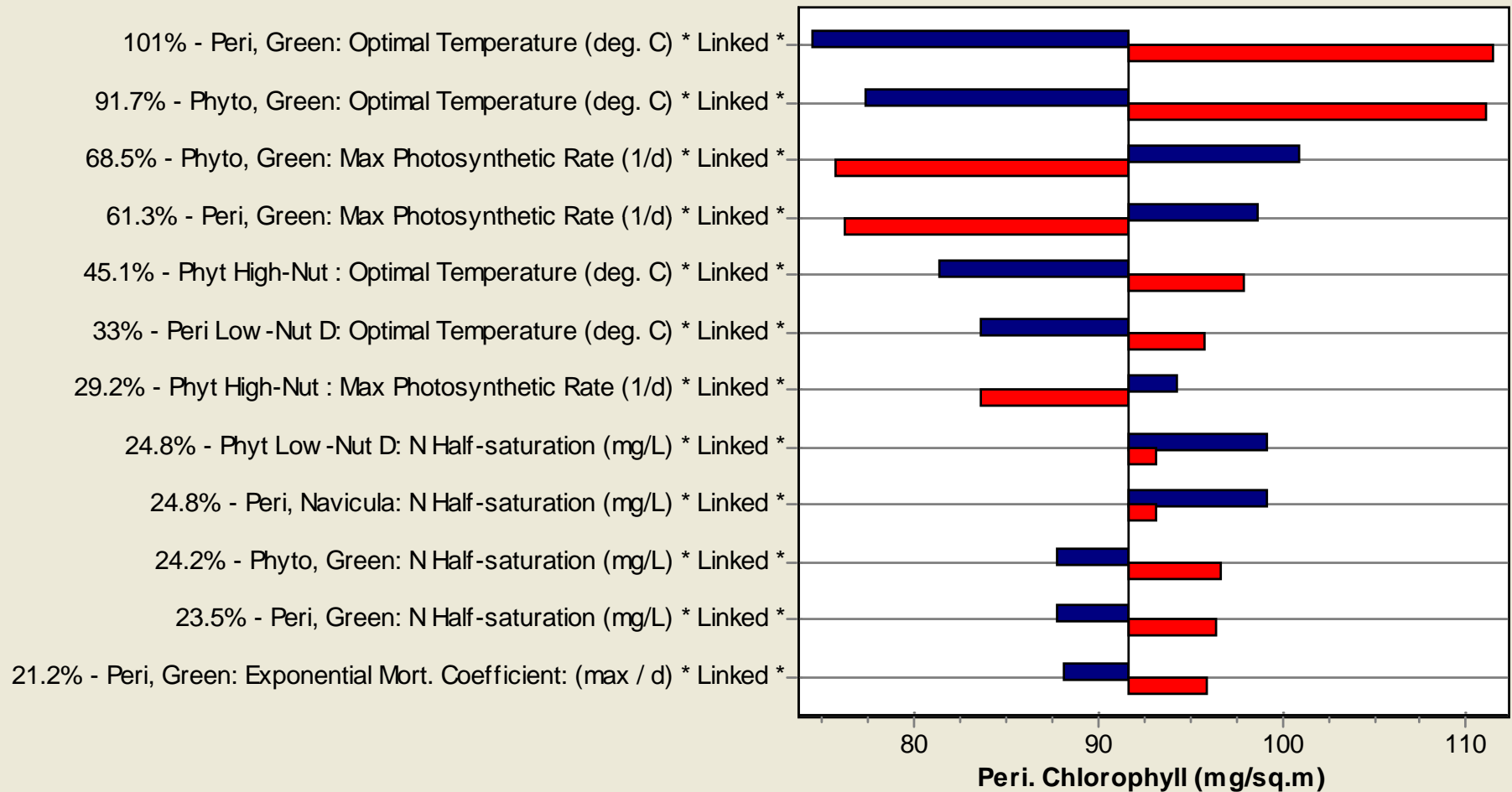


# Limitations to Photosynthesis May also be Graphed



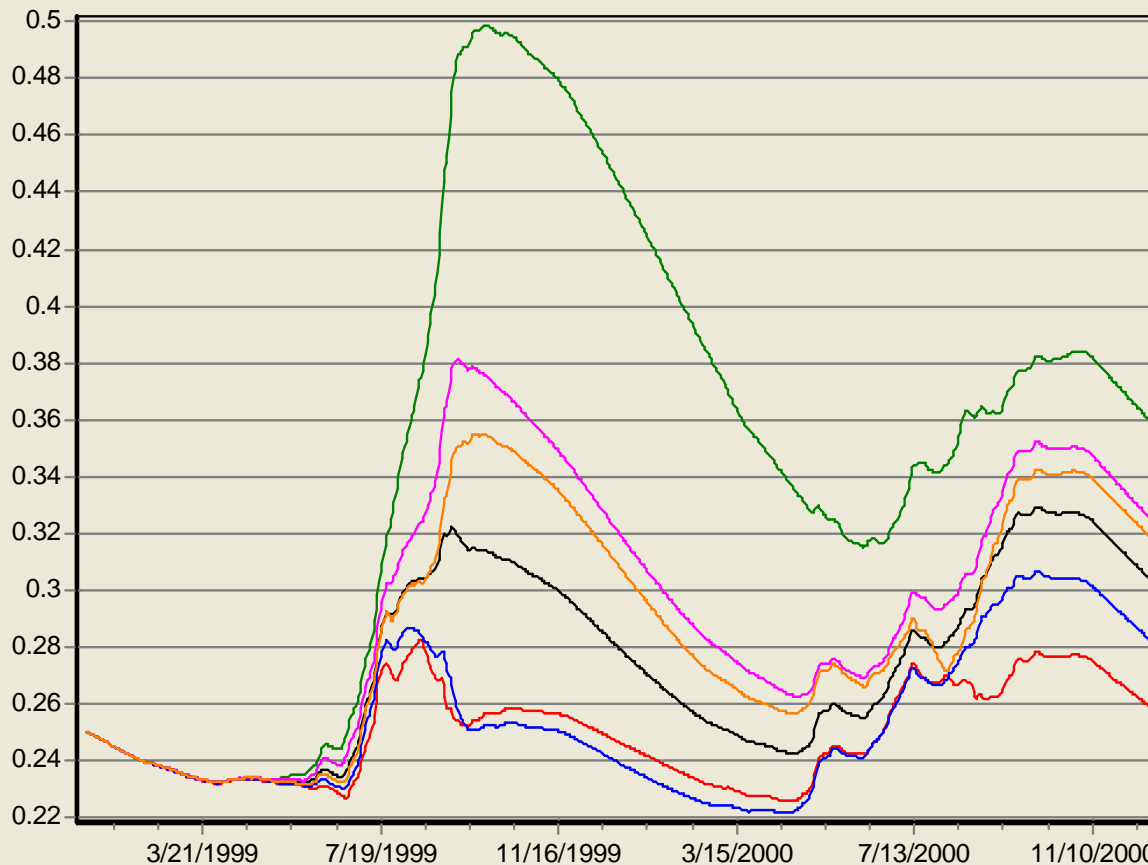
# Integrated Nominal Range Sensitivity Analysis with Graphics

**Sensitivity of Peri. Chlorophyll (mg/sq.m) to 20% change in tested parameters**  
**3/21/2008 9:56:56 AM**



# Integrated Latin Hypercube Uncertainty Analysis with Graphics

Smallmouth Bas (g/m<sup>2</sup>)  
3/21/2008 10:15:57 AM



- Mean
- Minimum
- Maximum
- Mean - StDev
- Mean + StDev
- Deterministic

can represent all  
“point  
estimate”  
parameters as  
distributions

**Distribution Information**  
*Phyt, Blue-Gre: Max Ph... synthetic Rate (1/d)*

Probability  Cumulative Distribution

**Distribution Type:**

- Triangular
- Uniform
- Normal
- Lognormal

**Distribution Parameters:**

Mean

Std. Deviation

For this parameter, in an Uncertainty Run:

- Use a Distribution
- Use a Point Estimate

Help

# Applications in Nutrient Analysis

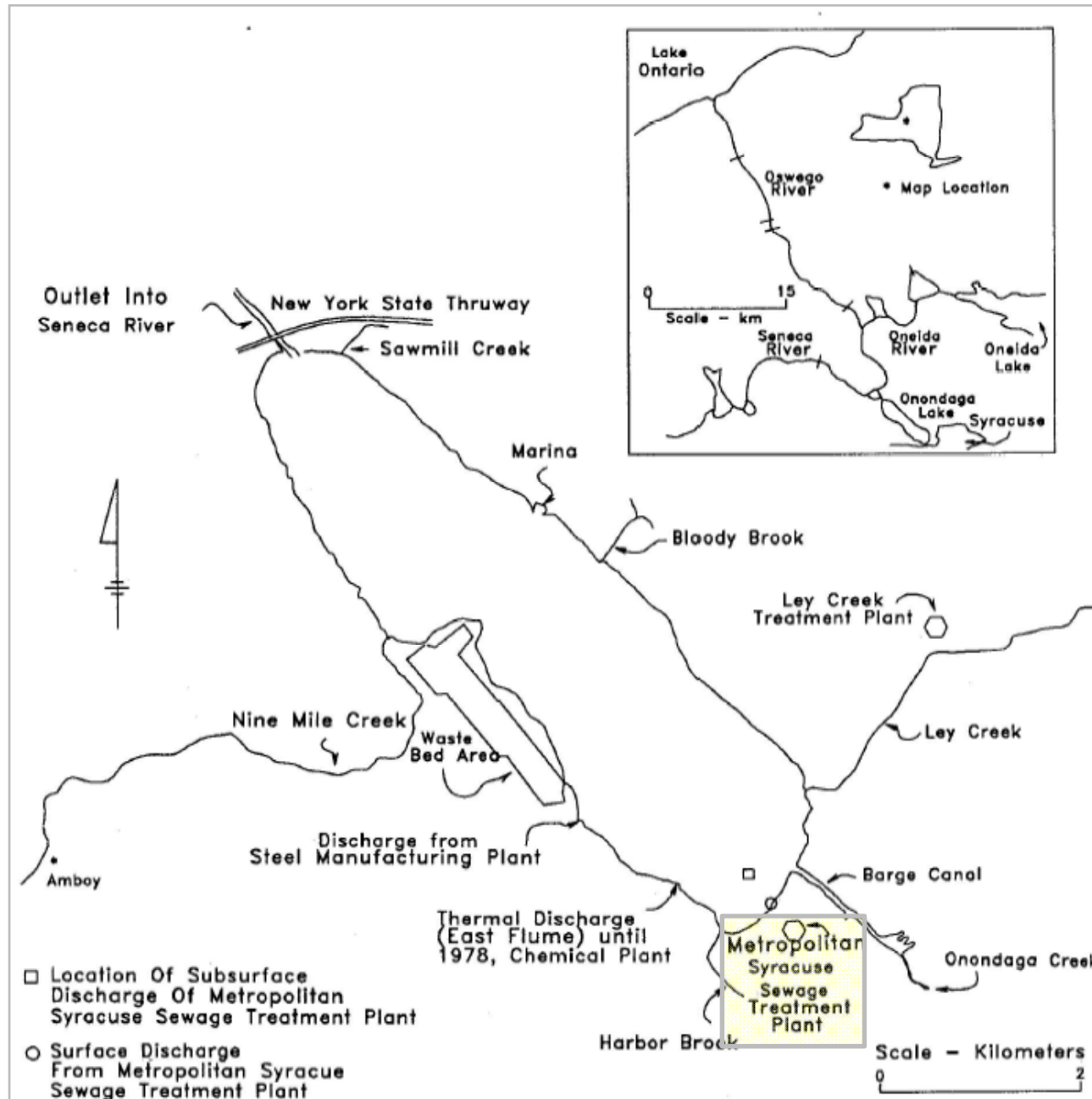
- Lake Onondaga, NY
- Rum, Blue Earth, Crow Wing Rivers, MN
- Cahaba River, AL
- Lower Boise River, ID
- Lake Tenkiller, OK



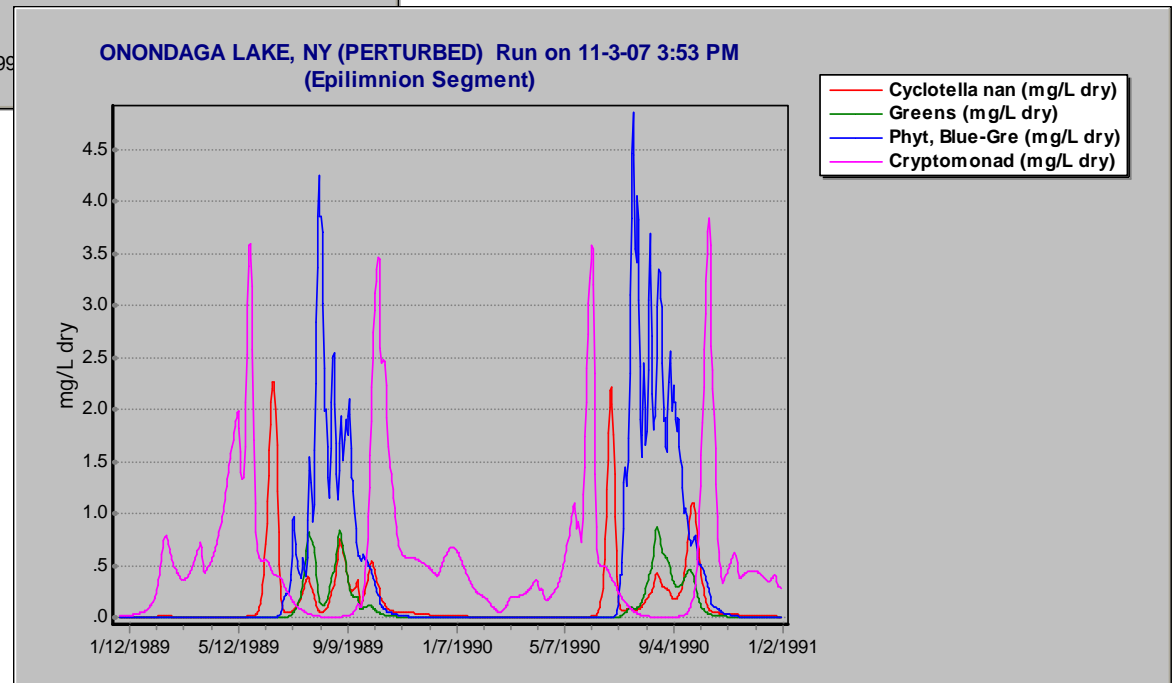
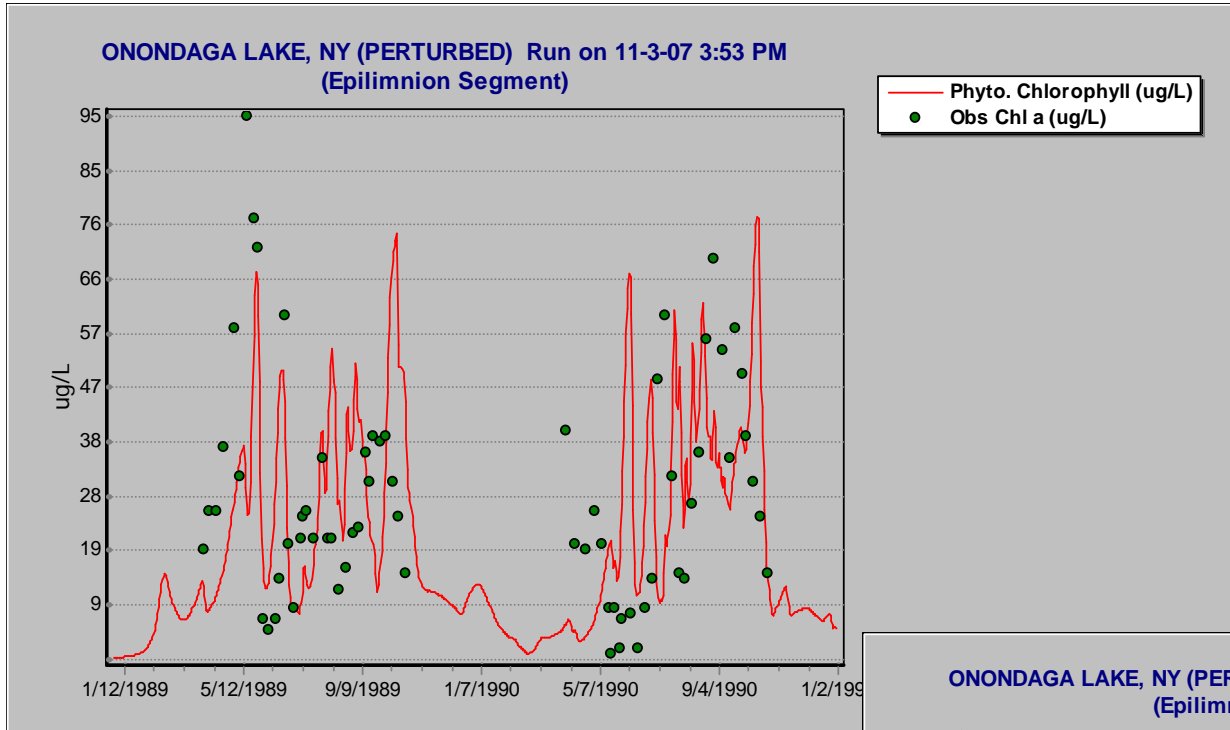
# Lake Onondaga, NY

- AQUATOX Validation Site
- “Most polluted lake in U.S.”
  - nutrient inputs from wastewater treatment plant (“Metro”) & combined sewers
  - successive algal blooms
  - hypoxia in hypolimnion
  - build-up of organic sediments in bottom
  - high mercury levels (not modeled at present)
  - high salinity

# Lake Onondaga NY, heavily polluted

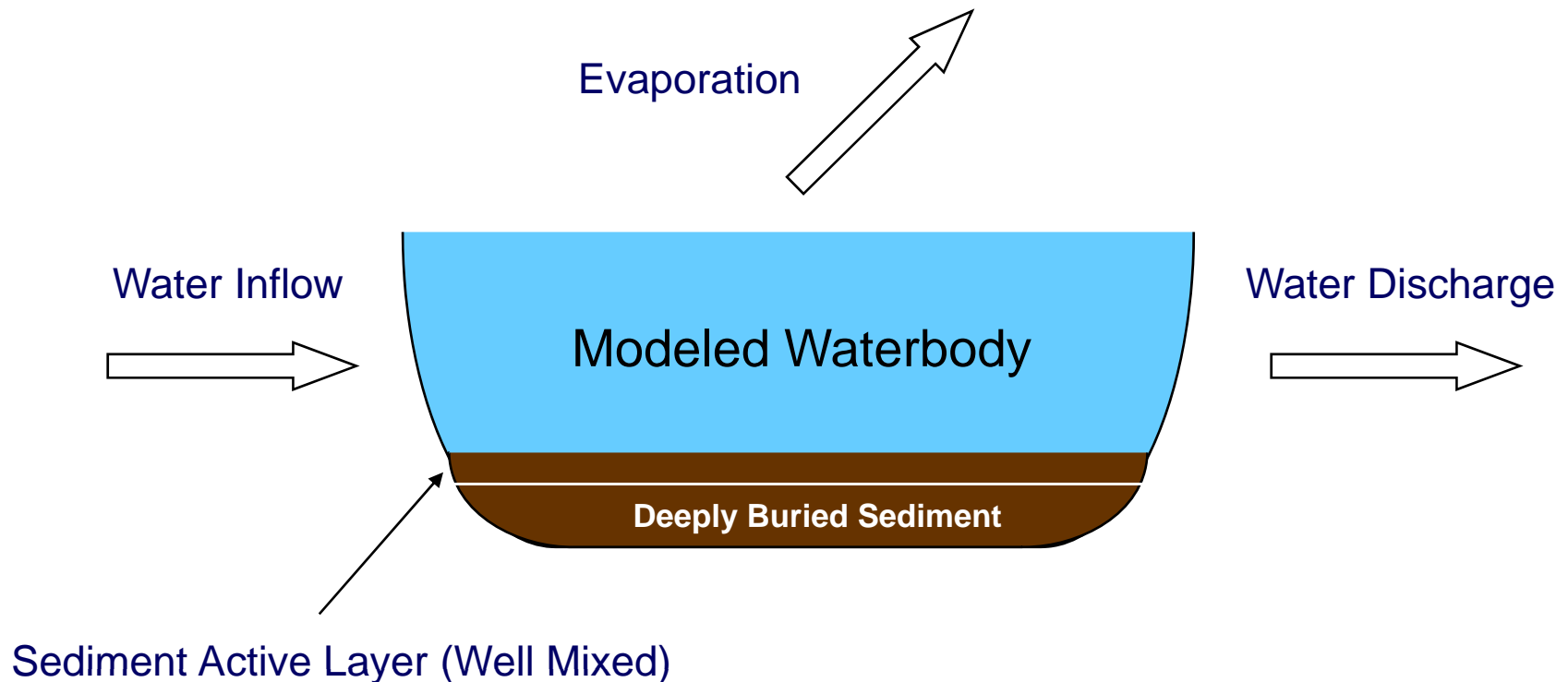


# Lake Onondaga is very productive with succession of algal groups

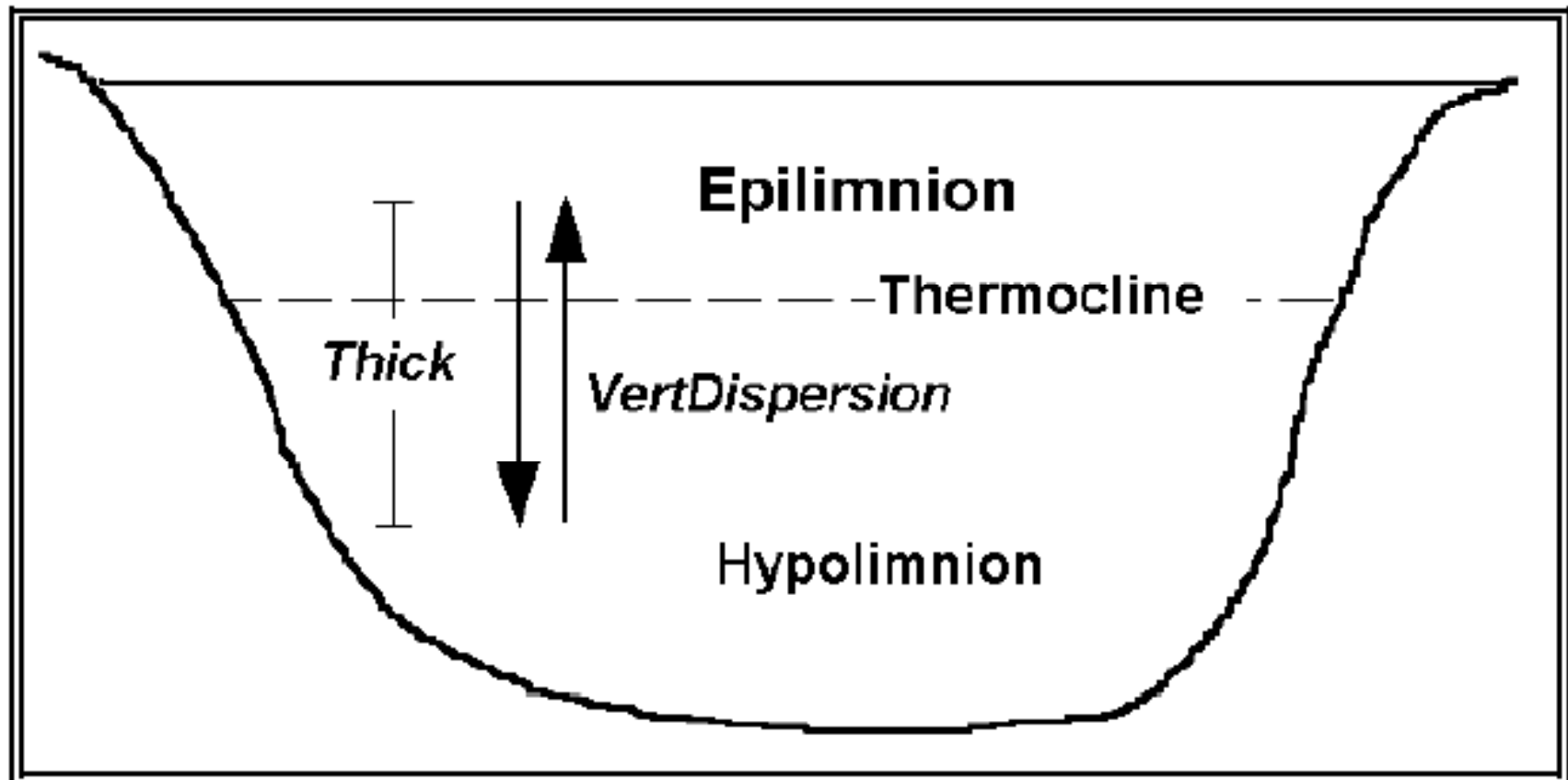


# Physical Characteristics of a Site

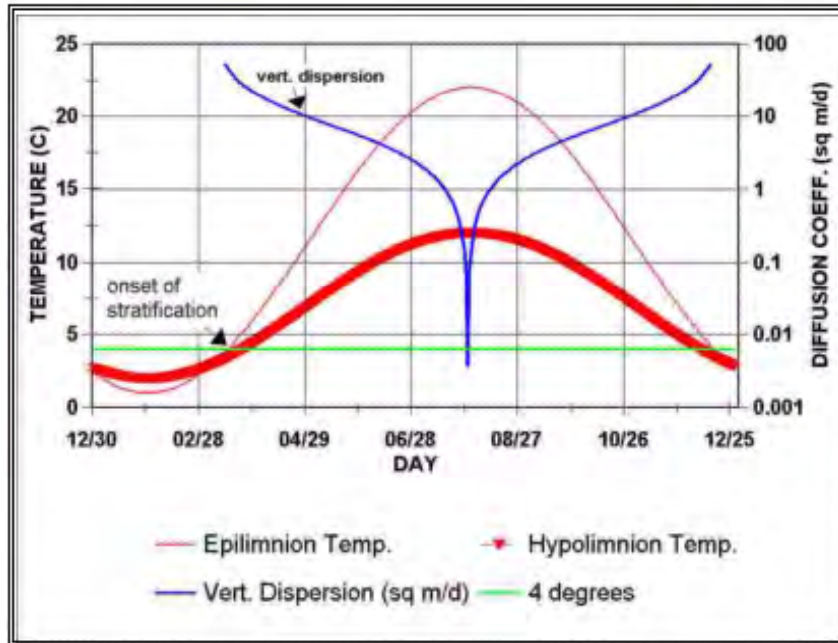
## Water Balance and Sediment Structure



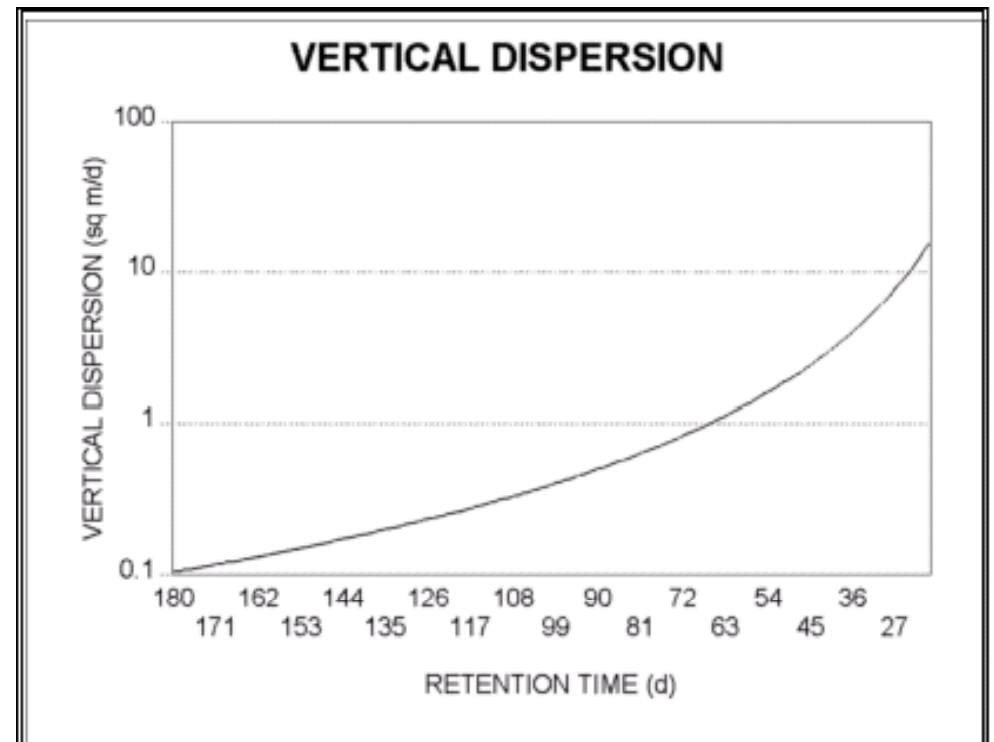
# Thermal Stratification in a Lake



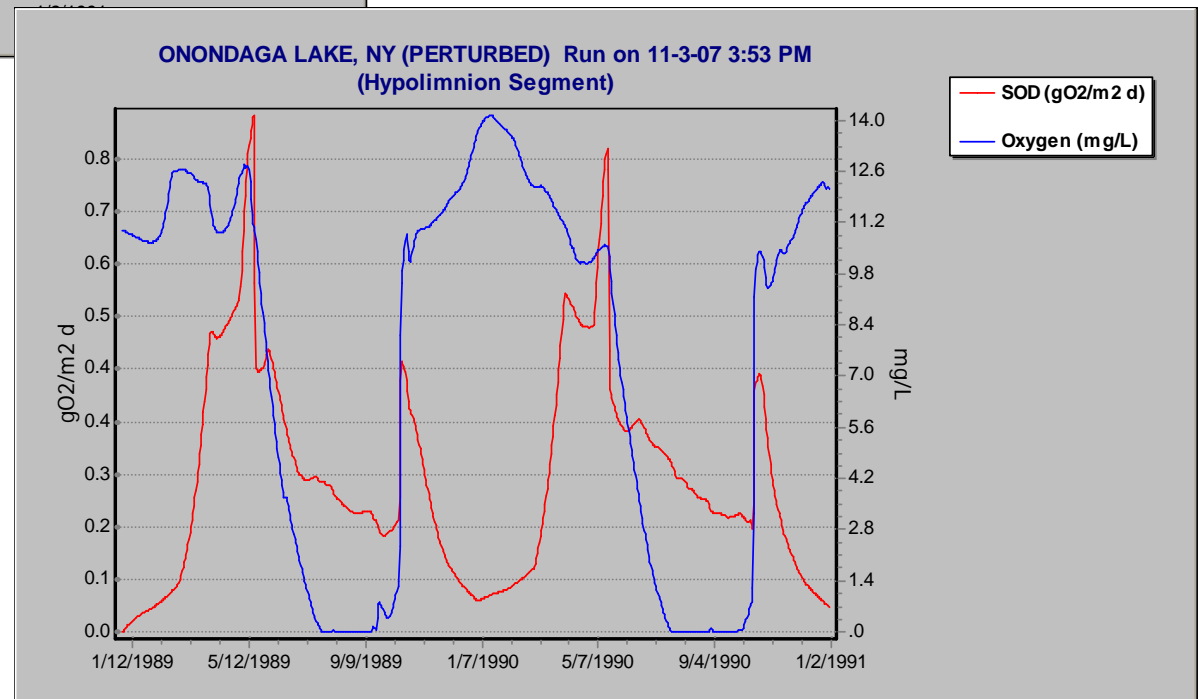
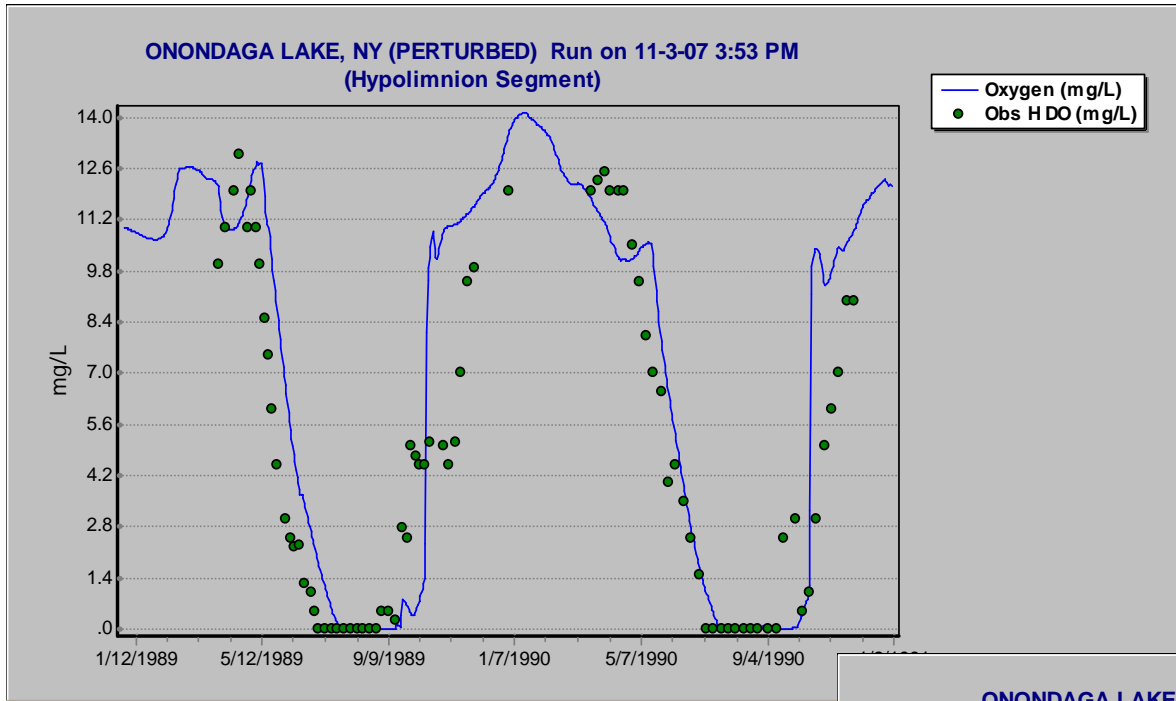
# Stratification is a Function of Temperature Differences



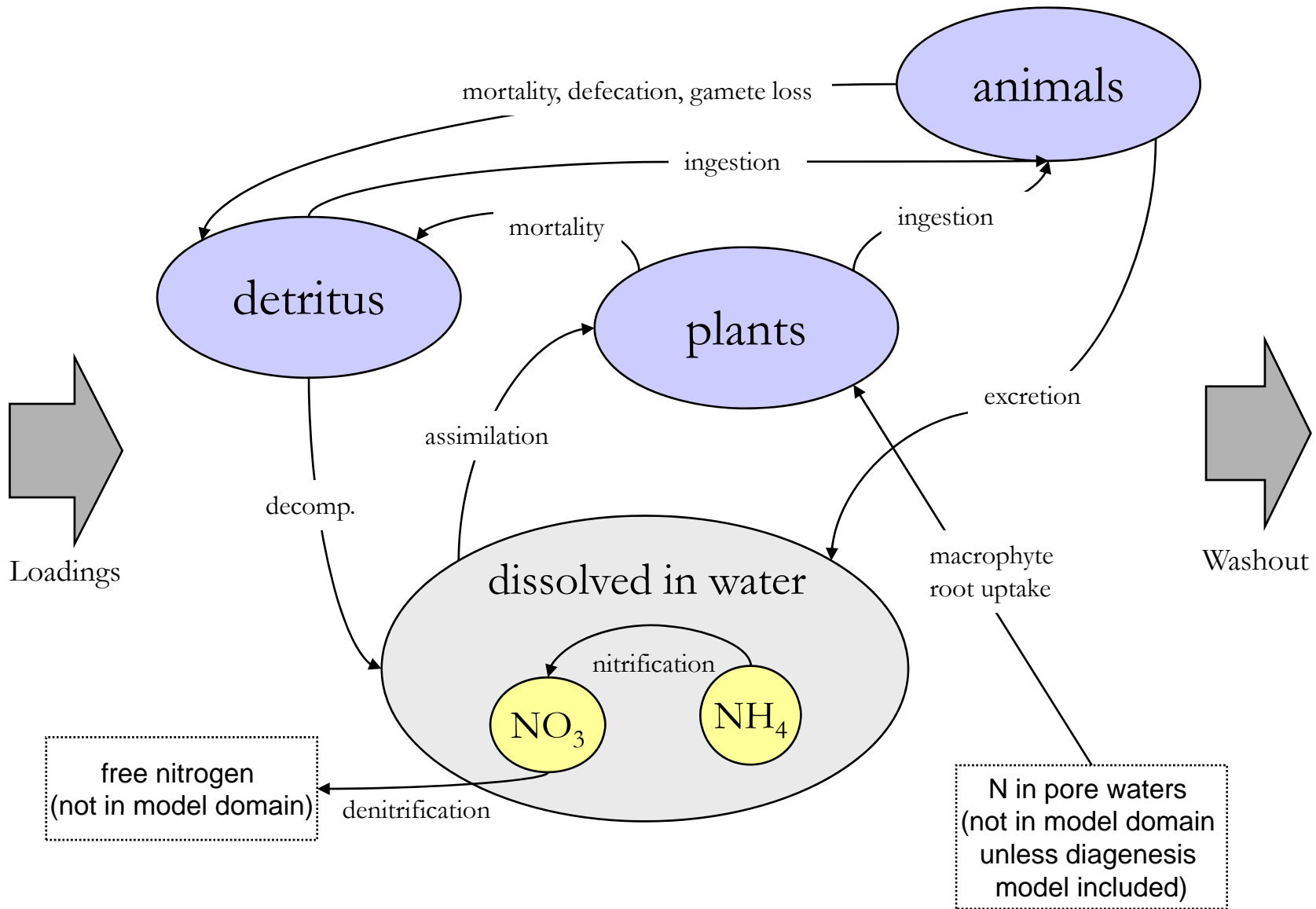
# Stratification is also a Function of Discharge



# Hypolimnion goes anoxic with high SOD



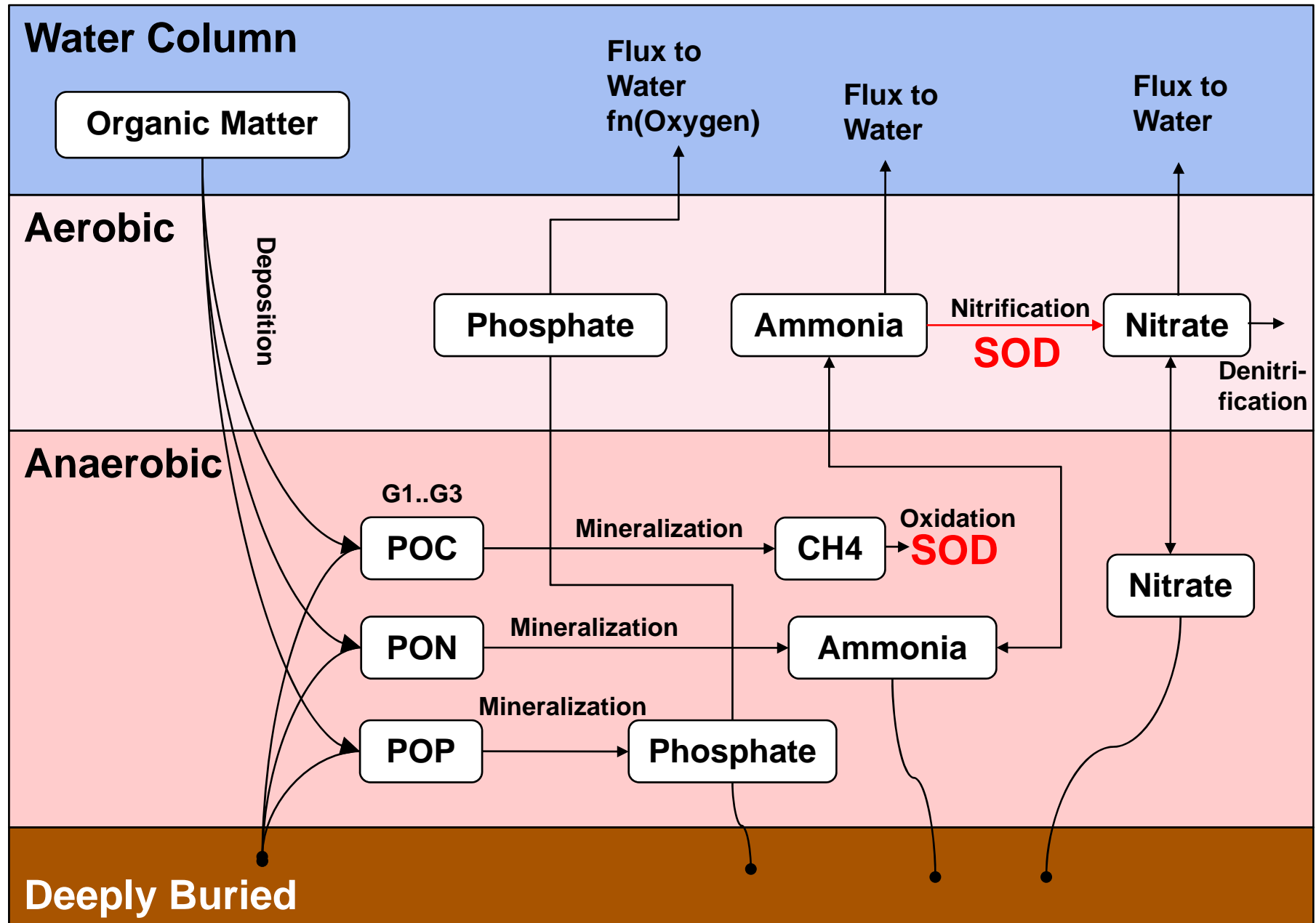
# Nutrient Cycle in AQUATOX (Nitrogen)





# Release 3: Optional Sediment Diagenesis Model

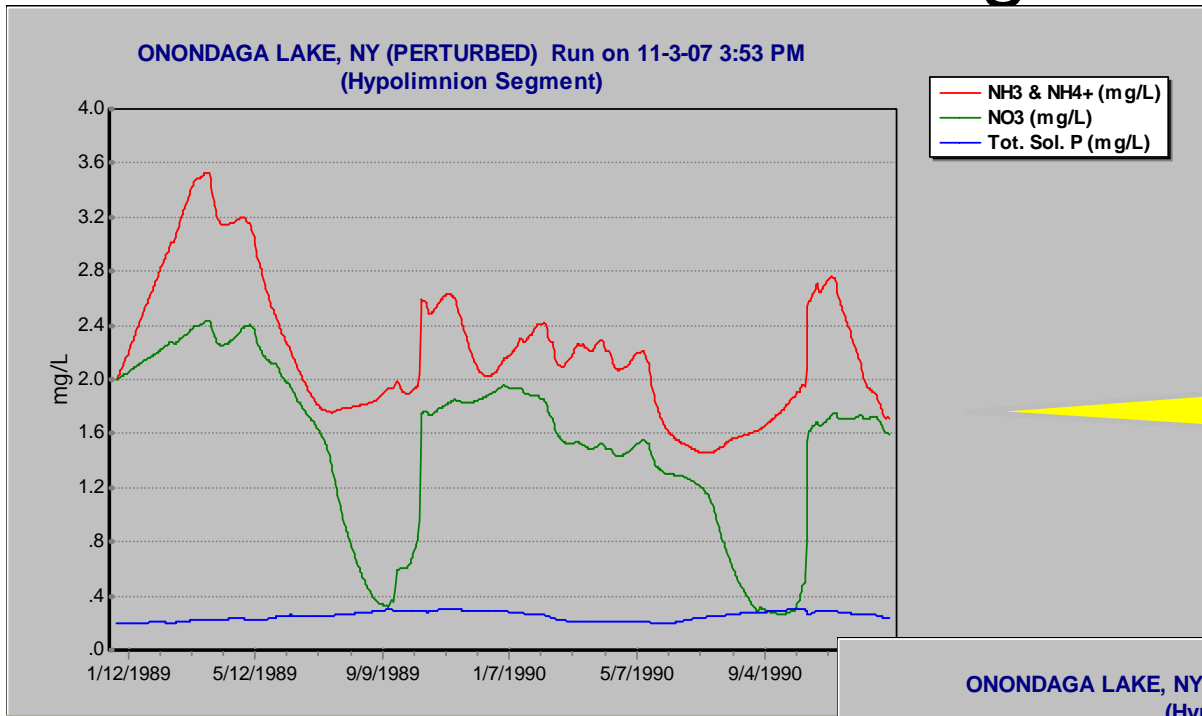
A complex model of nutrient regeneration in the sediment bed based on decay of POM and nutrient reactions in the pore waters (DiToro, 2001)



# Key Points: Diagenesis Model

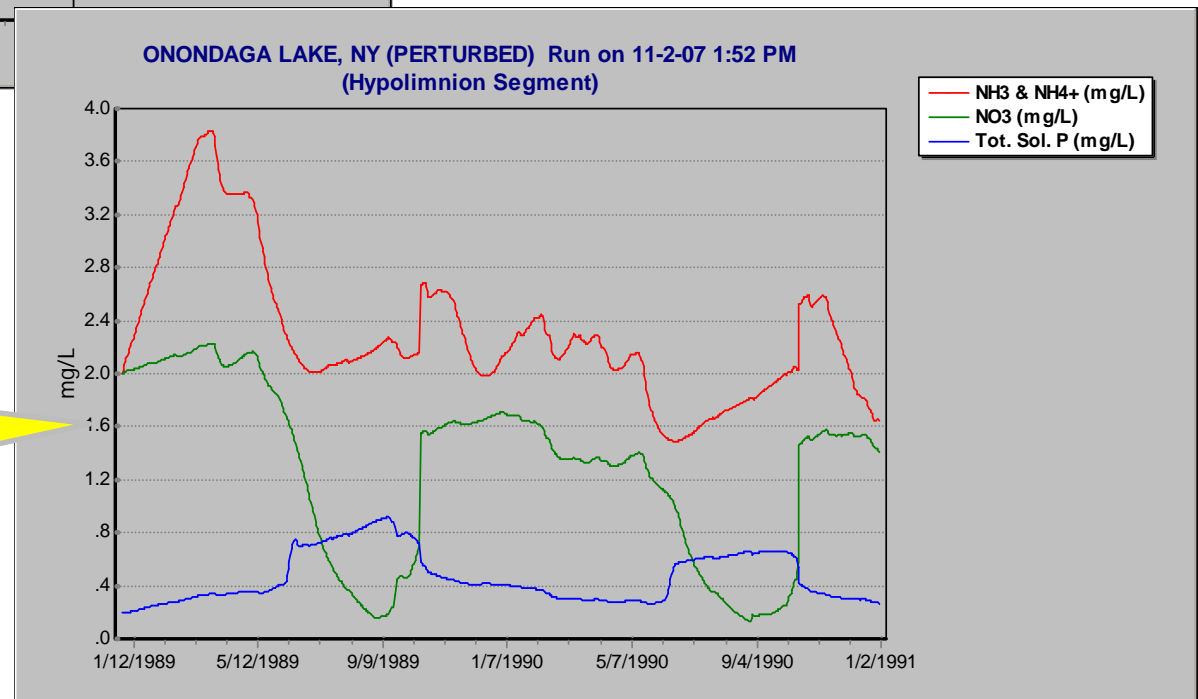
- Two sediment layers: thin aerobic and thicker anaerobic
- When oxygen is present, the diffusion of phosphorus from sediment pore waters is limited
  - Strong P sorption to oxidated ferrous iron in the aerobic layer (iron oxyhydroxide precipitate)
  - Under conditions of anoxia, phosphorus flux from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

# Hypolimnion $\text{PO}_4$ is better modeled by sediment diagenesis model



“Classic” AQUATOX model

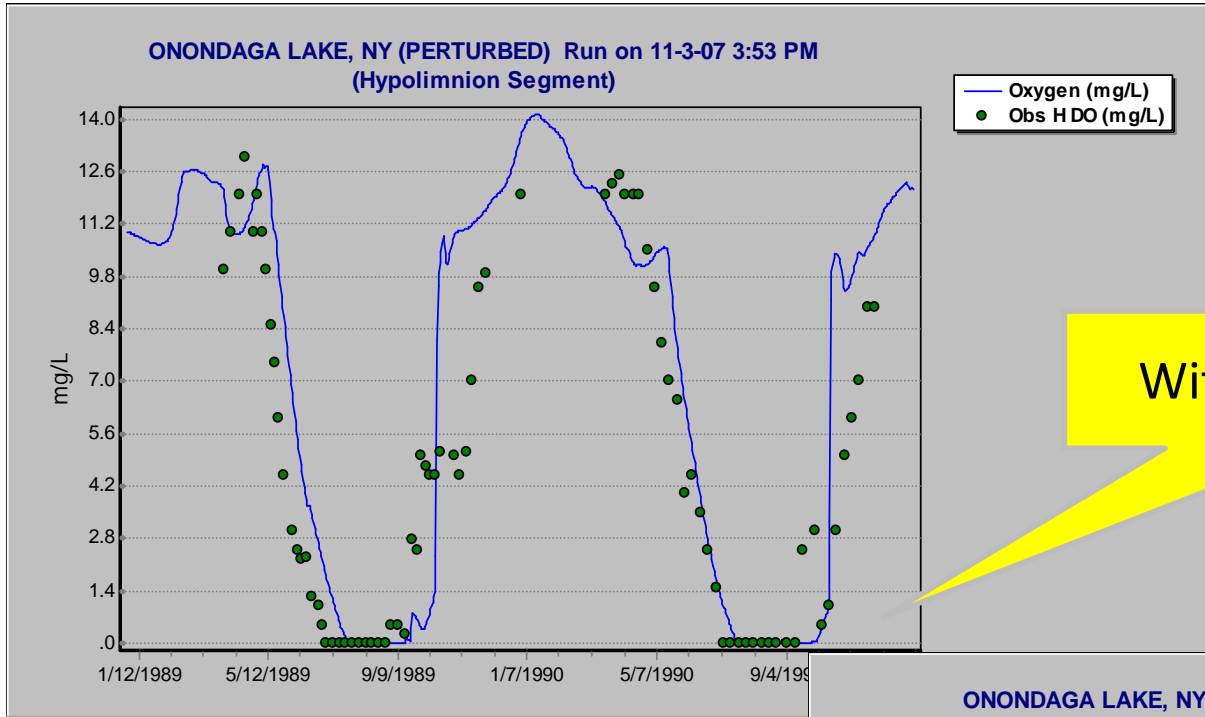
Sediment diagenesis model



# Nutrient Effects on Simulations

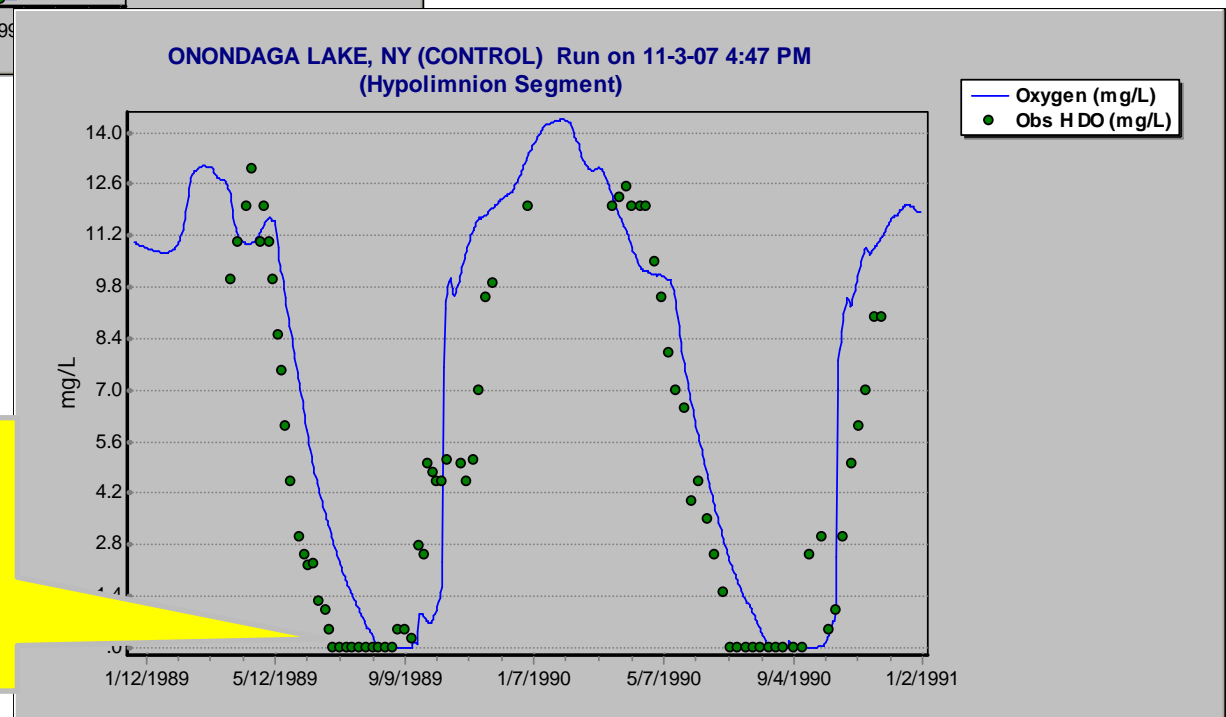
- Direct effects on algal growth rates
  - Maximum growth rates often limited by nutrients
  - Degree of limitation may be tracked and plotted
- Indirect repercussions throughout the foodweb due to bottom-up effects
- Light climate changes due to algal blooms
- Algal composition will be affected
- Decomposition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

# What if Metro WWTP effluent were diverted?

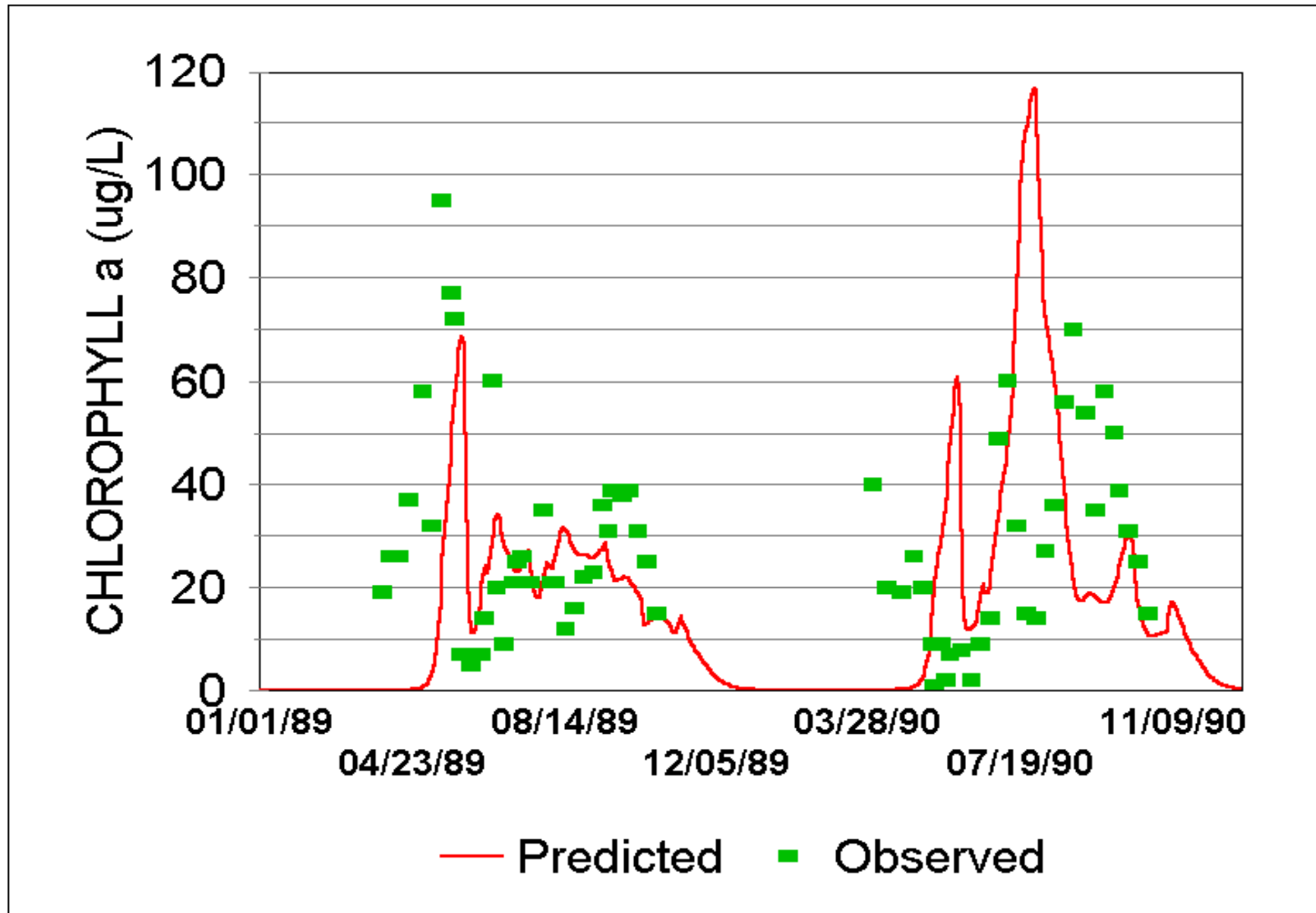


With Metro effluent

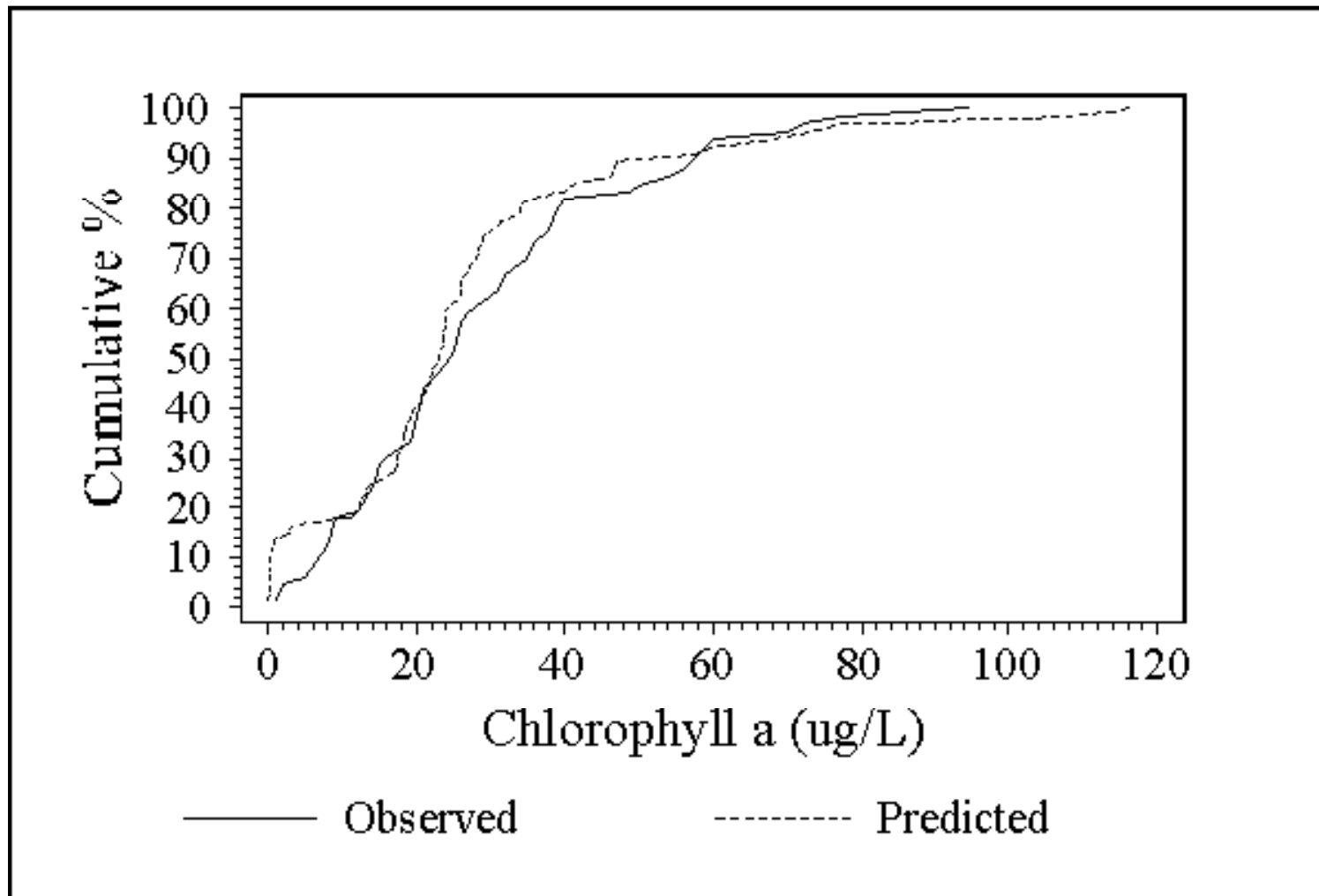
With Metro diversion,  
in first 2 years anoxia is  
delayed 1 month



# Validation of AQUATOX with Lake Onondaga Data—visual test



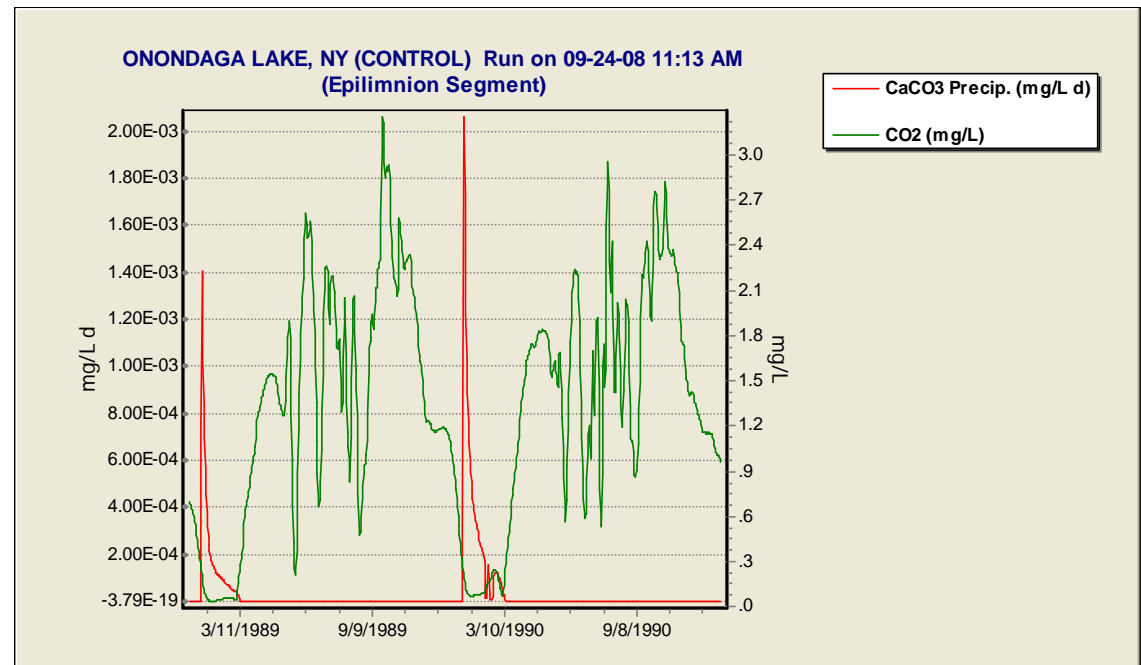
# Validation with chlorophyll a in Lake Onondaga, NY



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

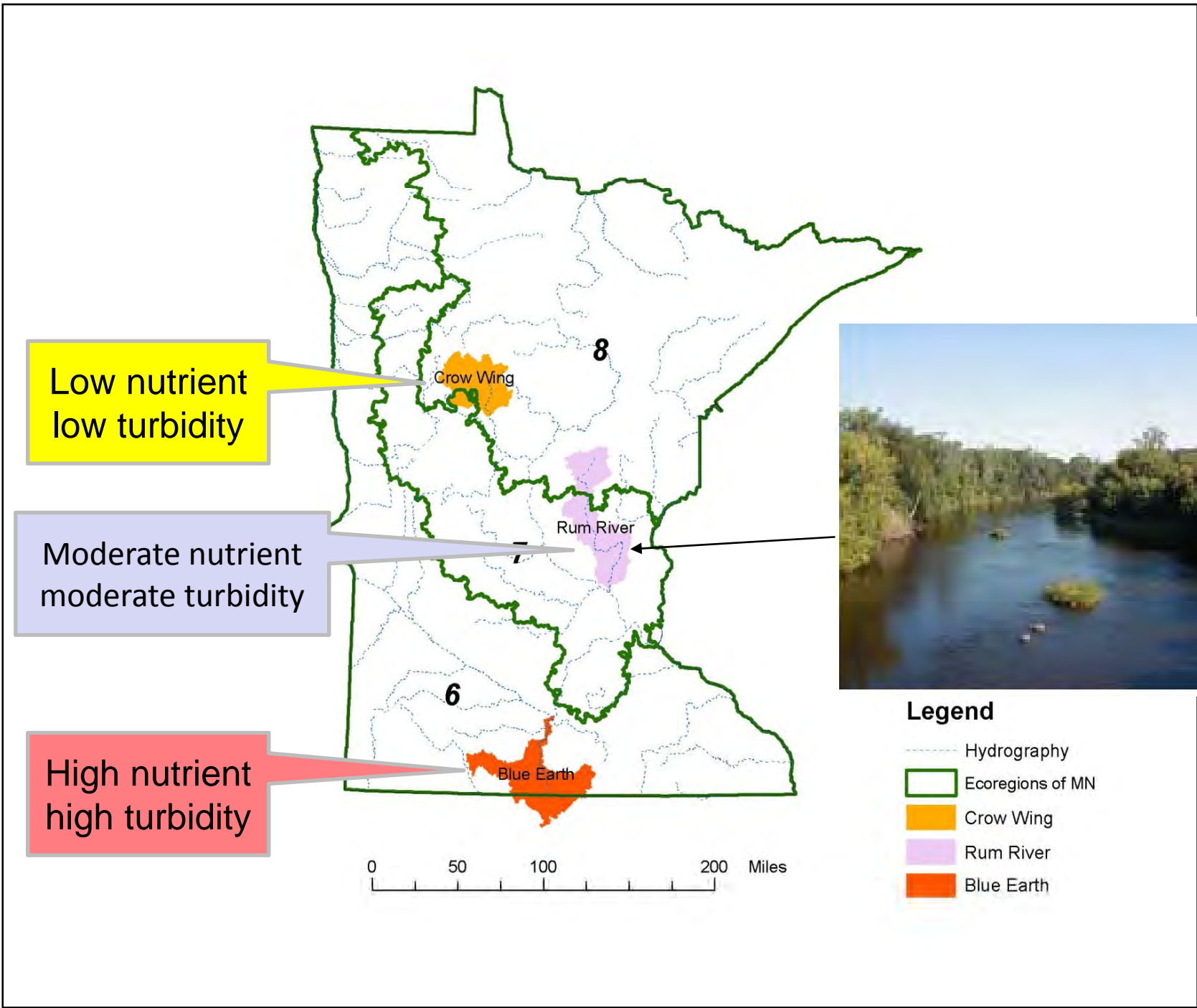
# Release 3 Addition: Calcium Carbonate Precipitation

- Predicted as a function of pH and algae type
  - When pH exceeds 8.25, precipitation is predicted
  - Precipitation rate is dependent on photosynthesis rate in precipitating algae
- $\text{CaCO}_3$  sorbs phosphate from the water column





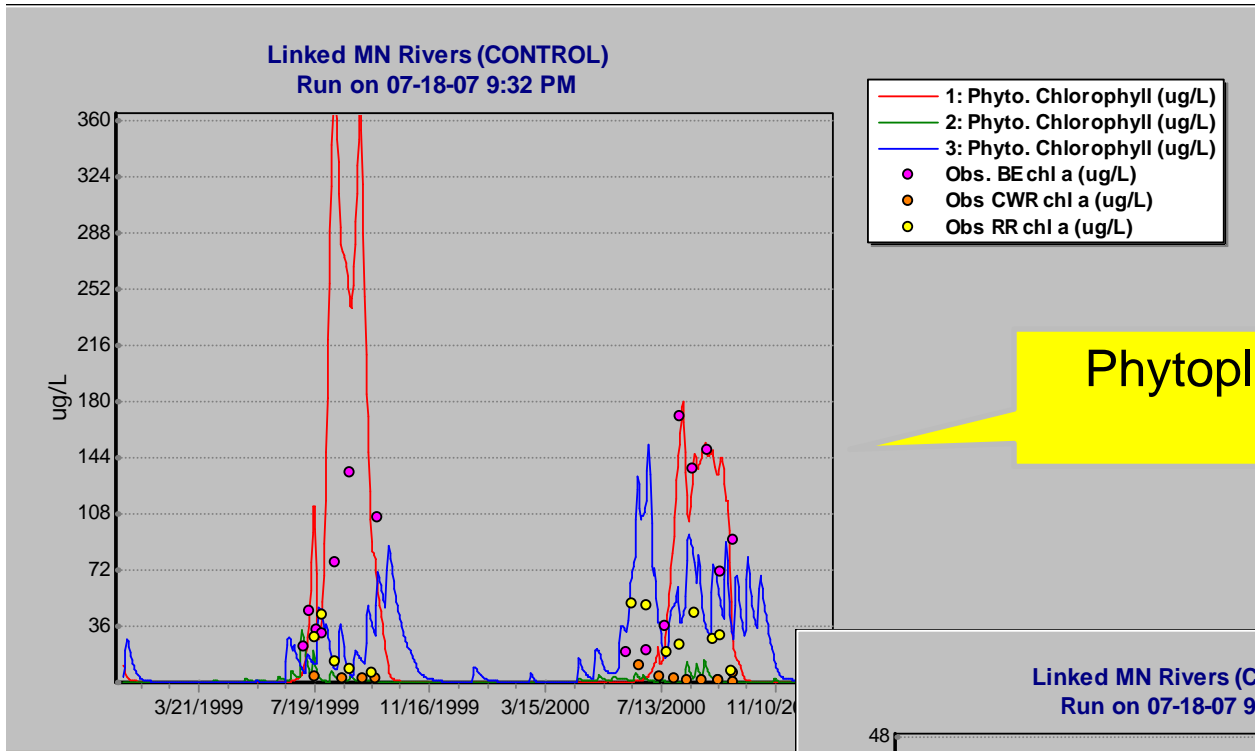
# Minnesota Nutrient Sites



# Calibration Strategy for Minnesota Rivers

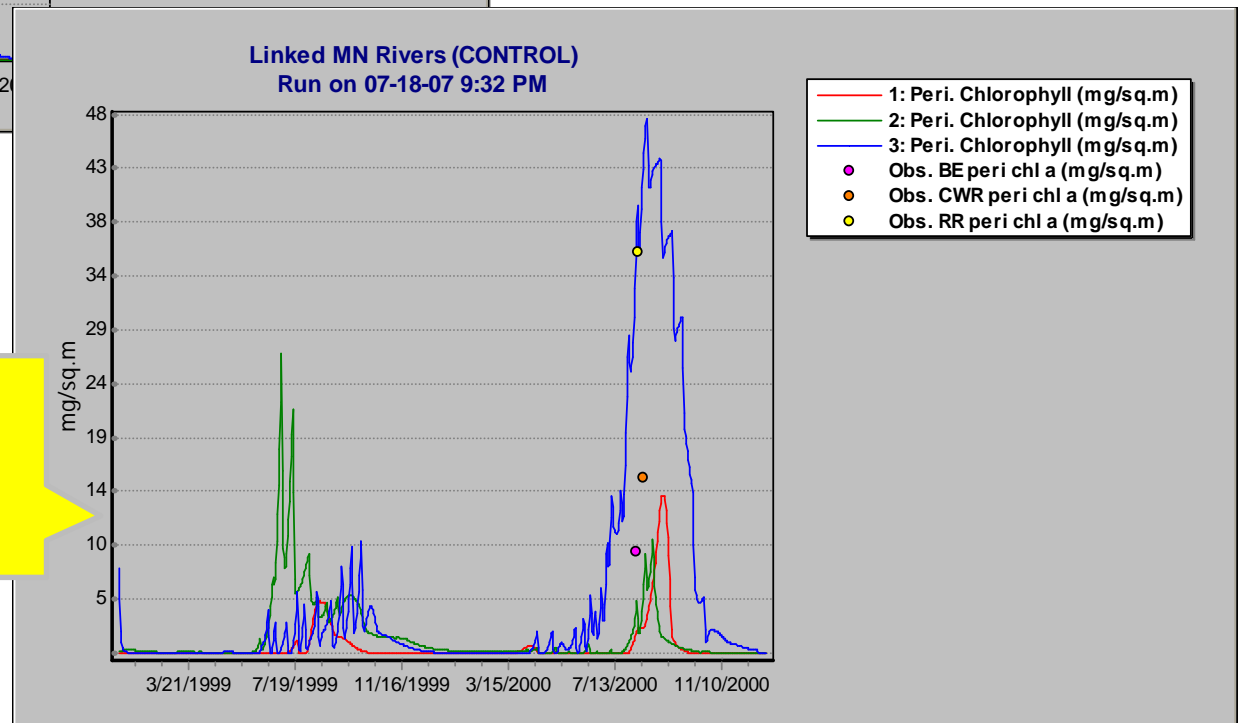
- Must be able to simulate *changing* conditions!
- Add plants and animals representative of both low- (Crow Wing) and high-nutrient (Blue Earth) rivers
- Iteratively calibrate key parameters for each site and cross-check to make sure they still hold for other site
- When goodness-of-fit is acceptable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

# Chlorophyll a Trends in MN Rivers



Phytoplankton follow nutrient trend

Periphyton reach maximum in Rum River with moderate nutrients and turbidity



# Modeling Phytoplankton

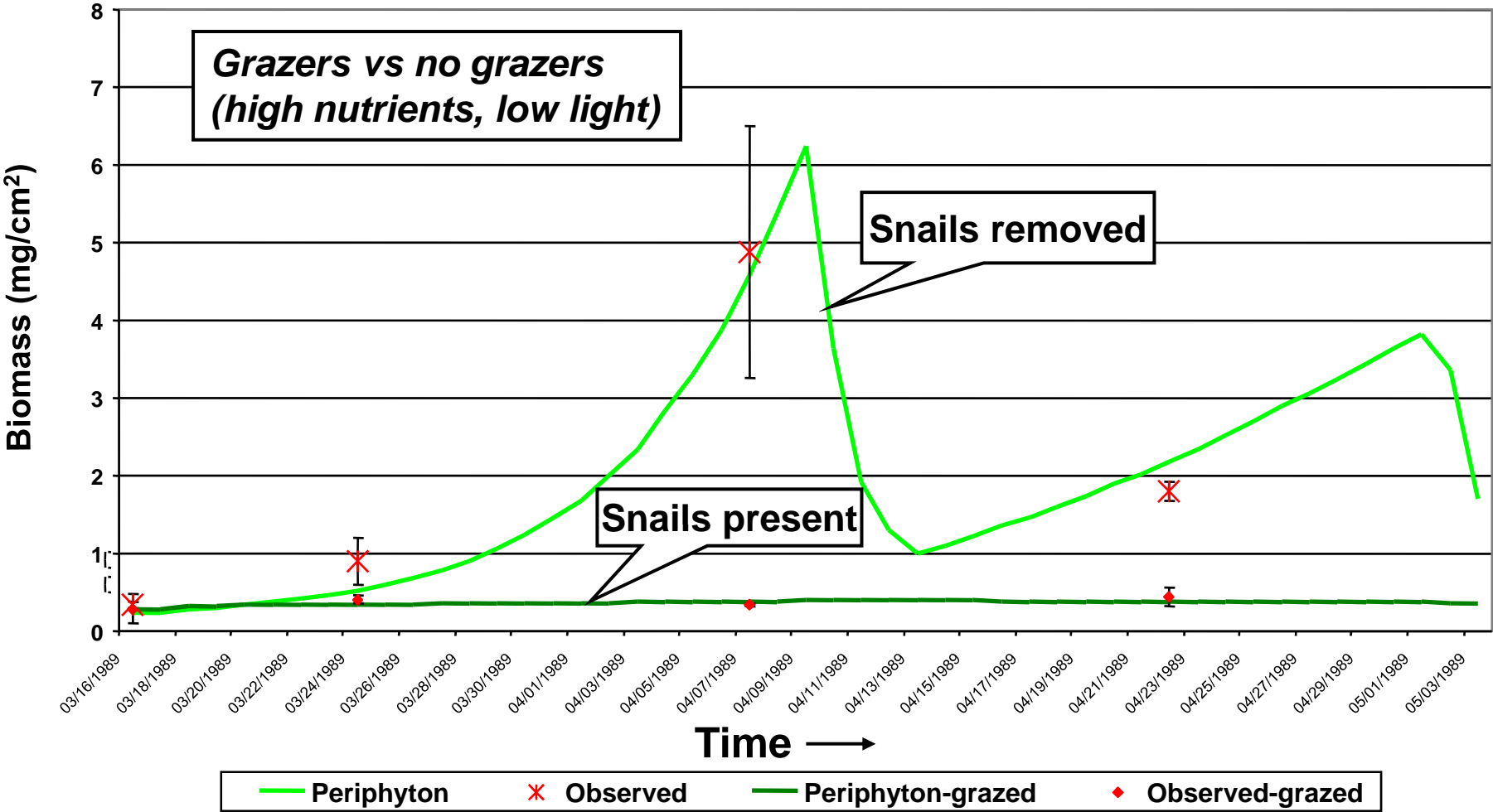
- Phytoplankton may be greens, blue-greens, diatoms or “other algae”
- Subject to sedimentation, washout, and turbulent diffusion
- In stream simulations, assumptions about flow and upstream production are important

# 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

# Several Independent Factors Affect Periphyton

One important factor is Grazing by Snails



# Modeling Macrophytes

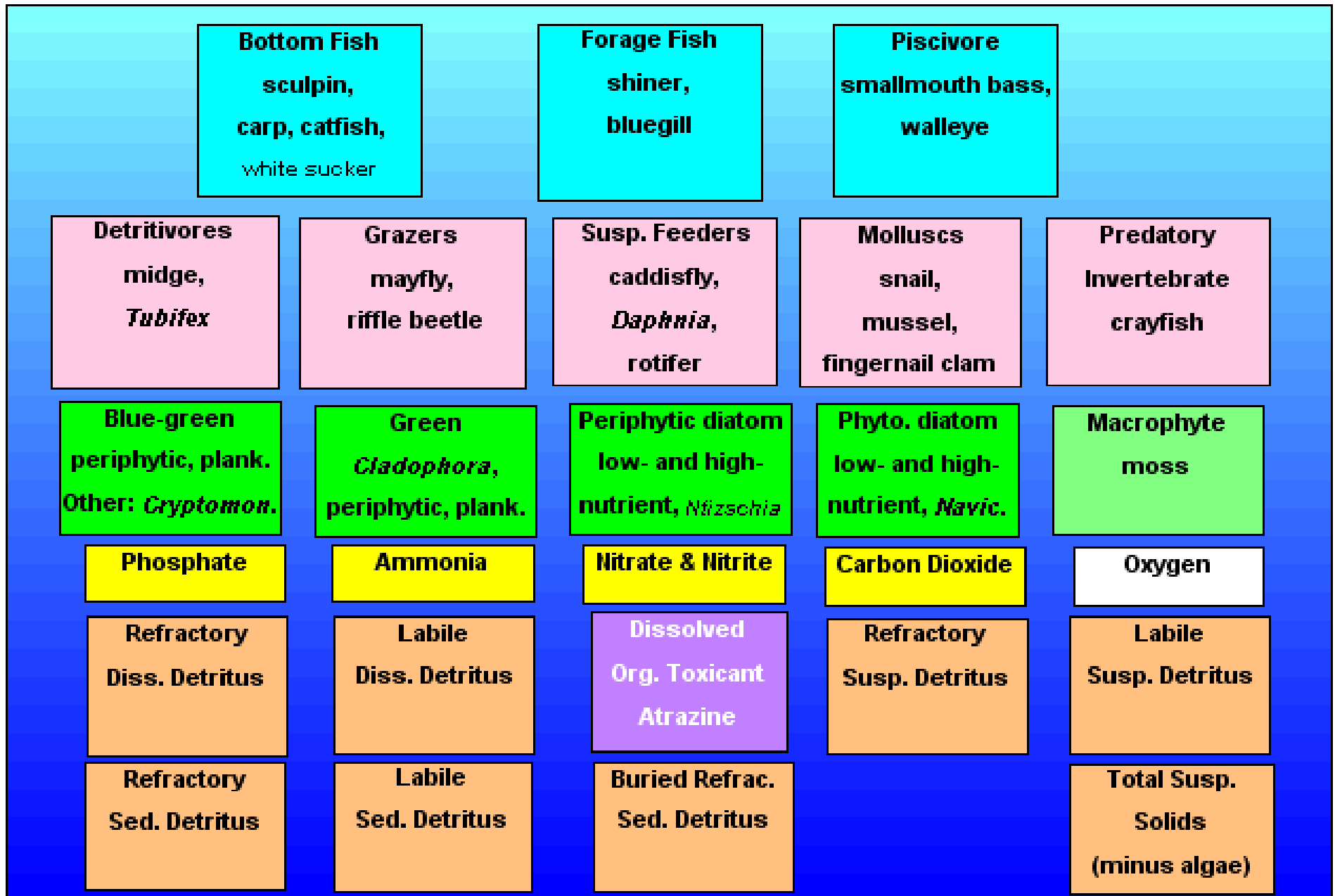
- Macrophytes may be specified as benthic, rooted-floating, or free-floating
- Macrophytes can have significant effect on light climate and other algae communities
- Root uptake of nutrients is assumed and mass balance tracked
- May act as refuge from predation for animals
- Moss are a special category

# Calibration of Plants

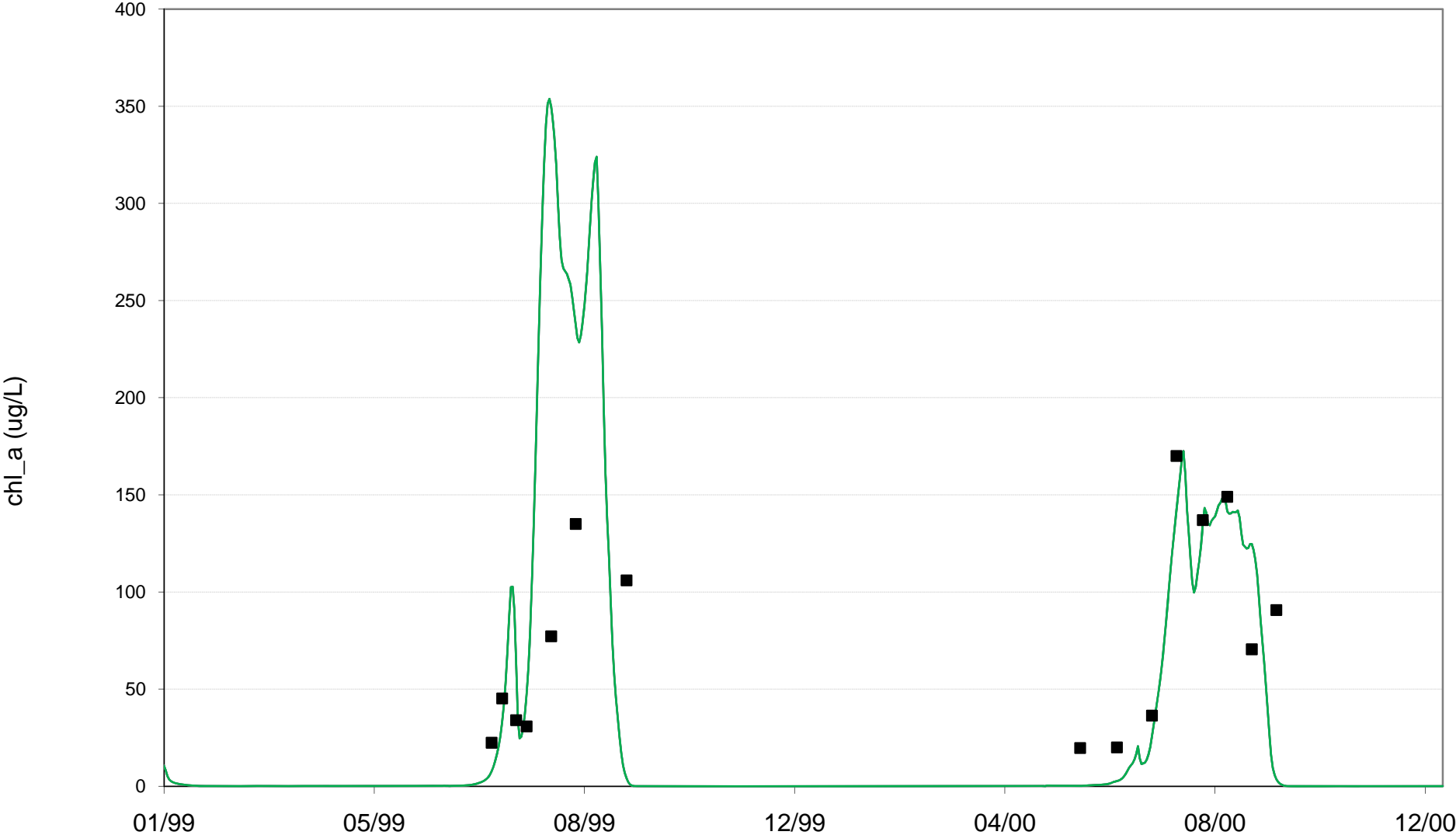
- algae are differentiated on basis of:
  - nutrient half-saturation values
  - light saturation values
  - maximum photosynthesis
- MN project has developed new parameter sets that span nutrient, light, and PMax
- phytoplankton sedimentation rates differ between running and standing water
- critical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



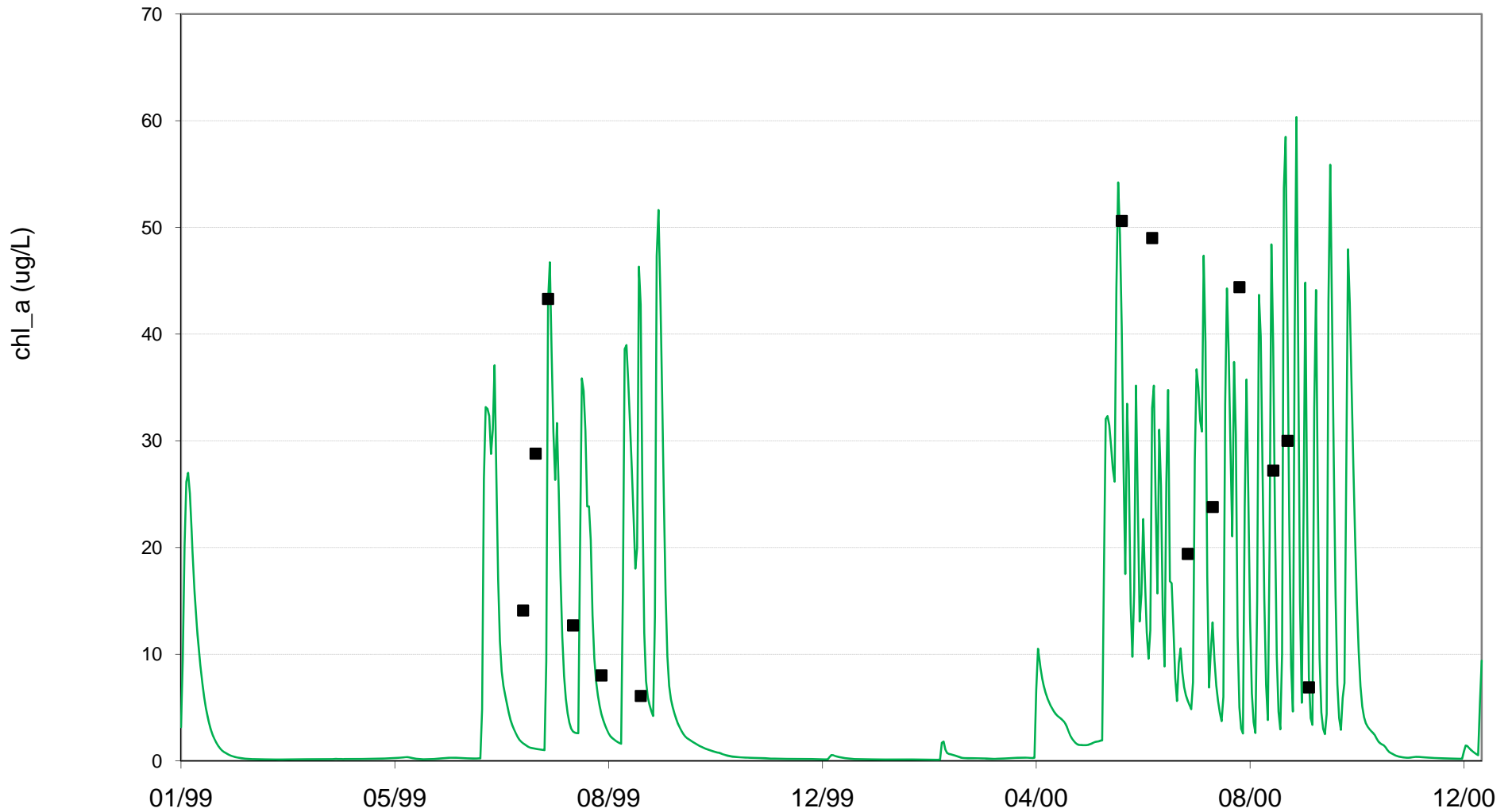
# State variables in MN rivers simulations



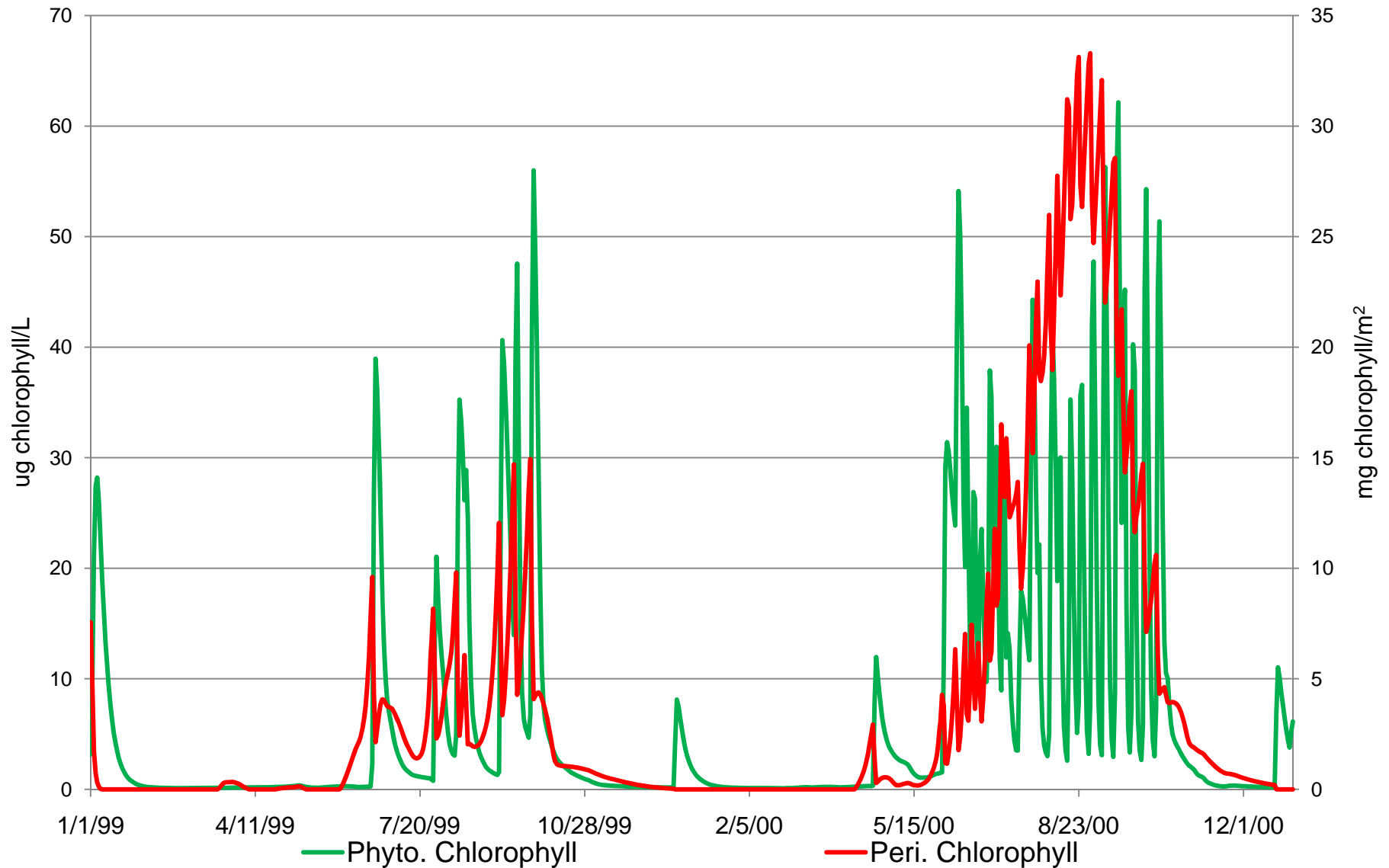
# Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Blue Earth River at mile 54



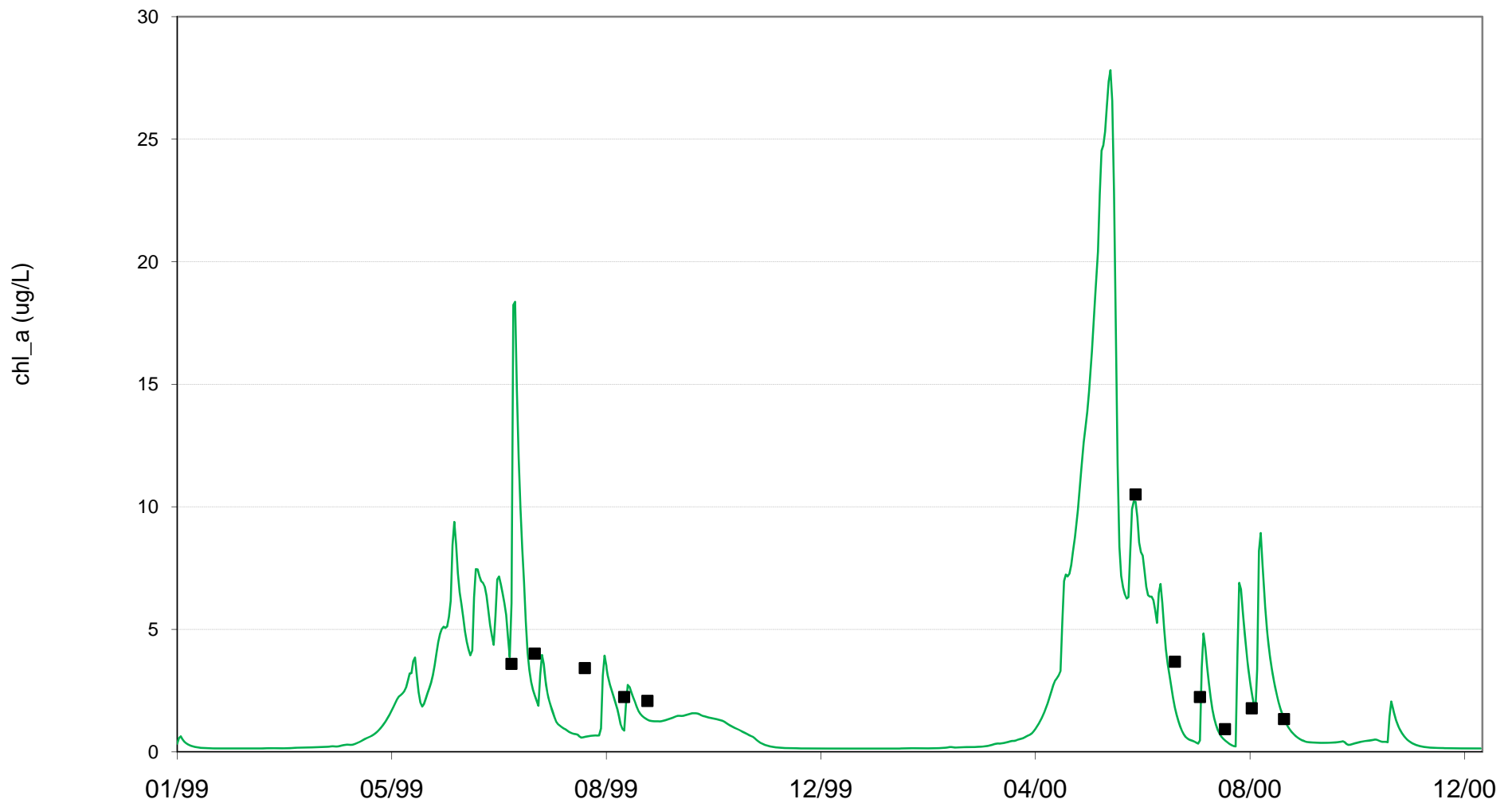
# Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Rum River at mile



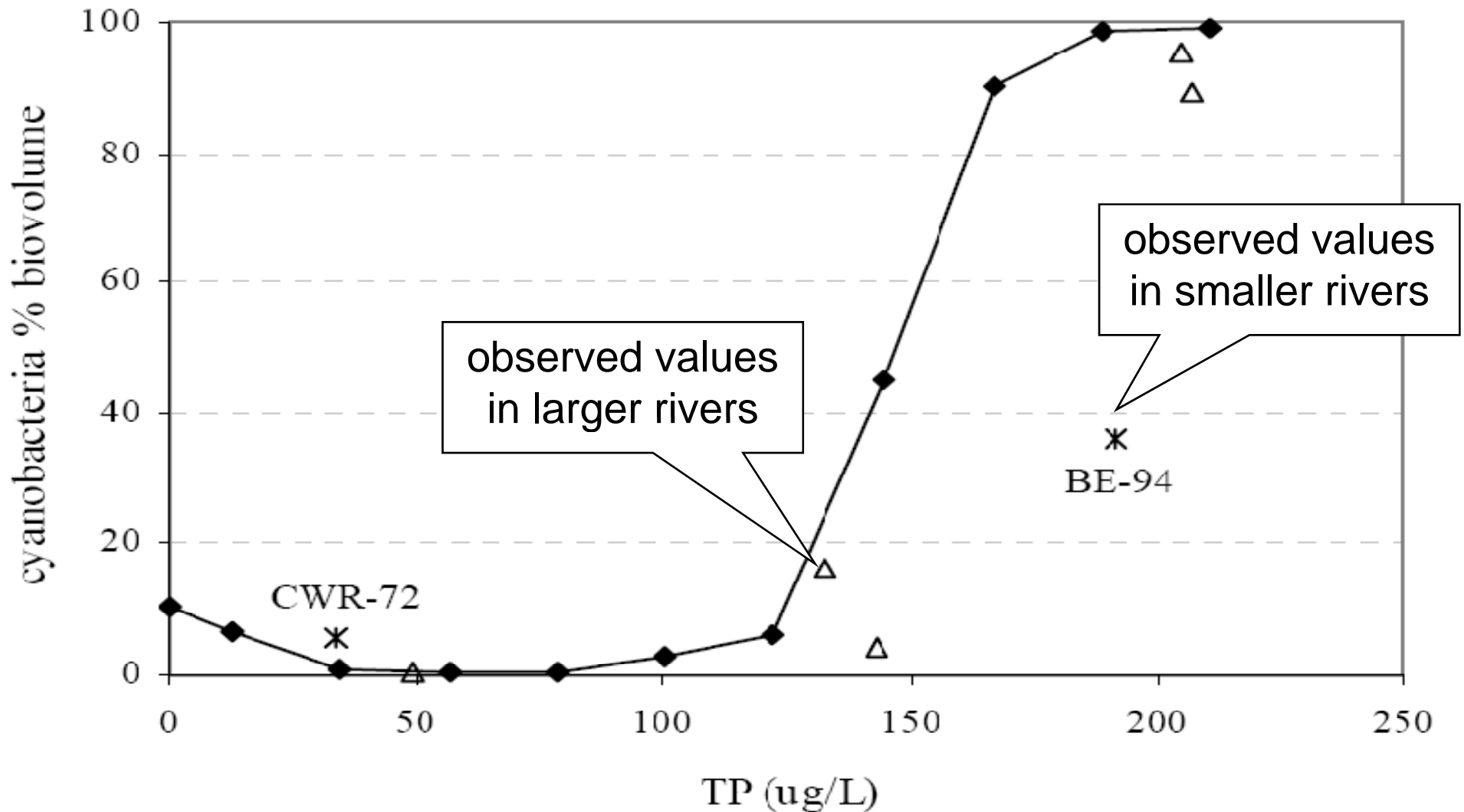
# Sestonic algae are largely a result of sloughed periphyton in this shallow river



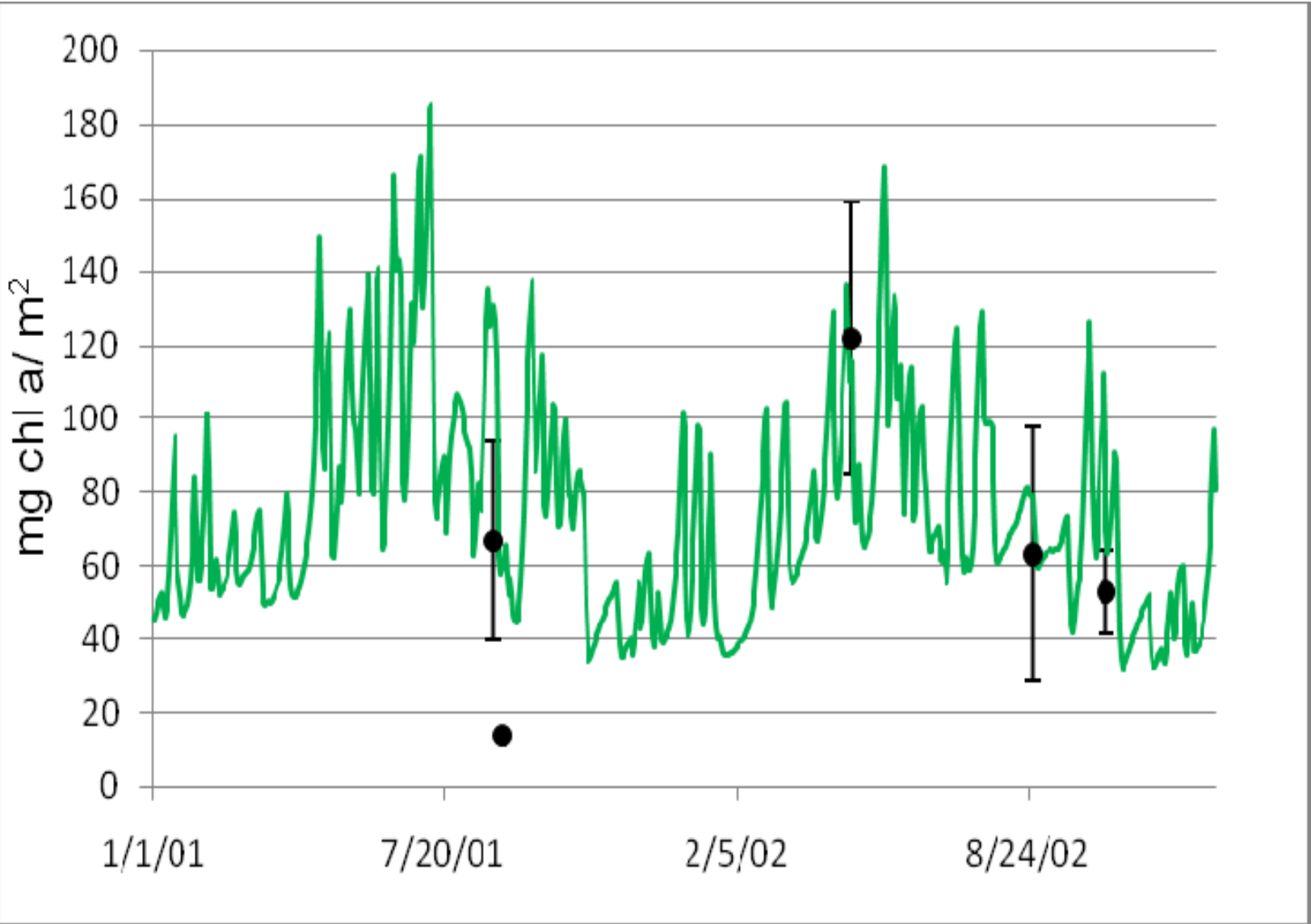
# Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Crow Wing at mile 72



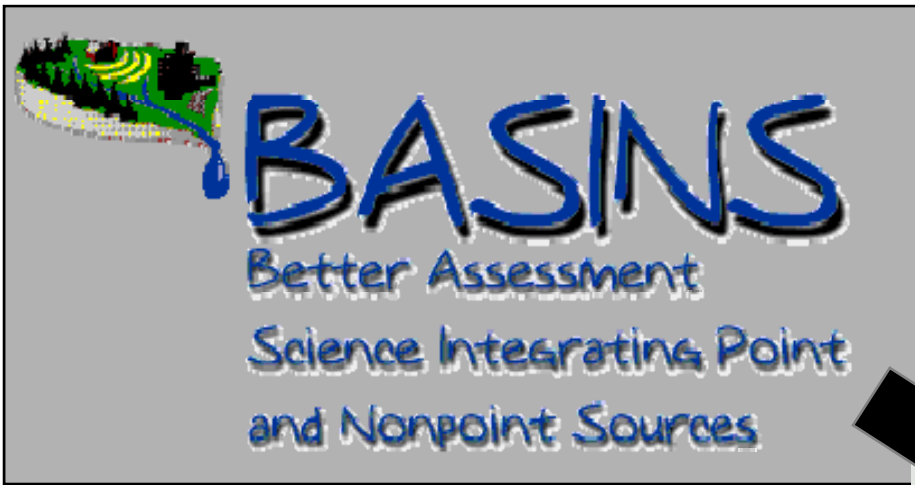
# Summer mean percent Phytoplankton composed of cyanobacteria-- BE-54 simulations with fractional multipliers on TP, TN, and TSS



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



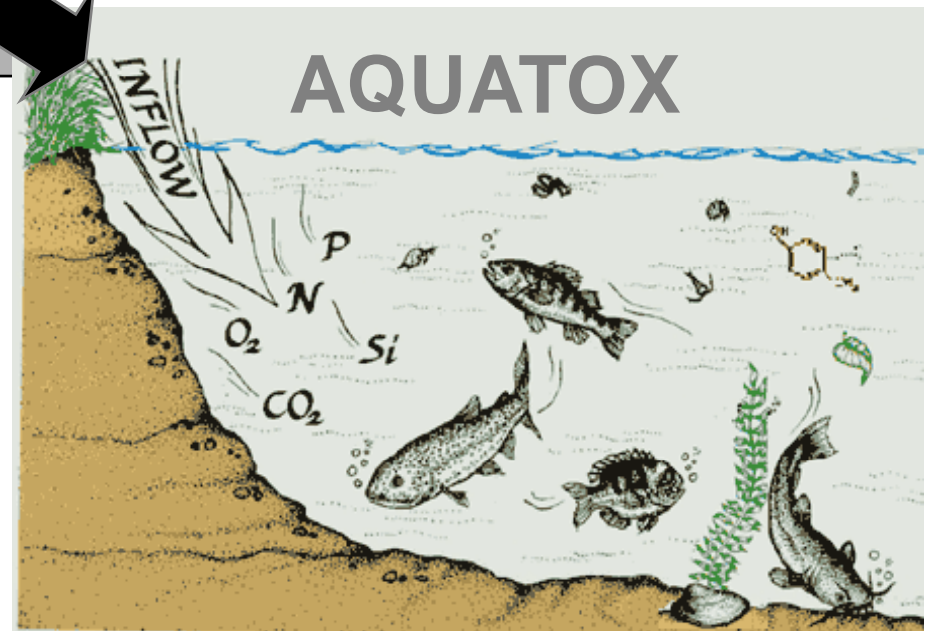
# AQUATOX BASINS Linkage



Integrates point/nonpoint source analysis with effects on receiving water and biota

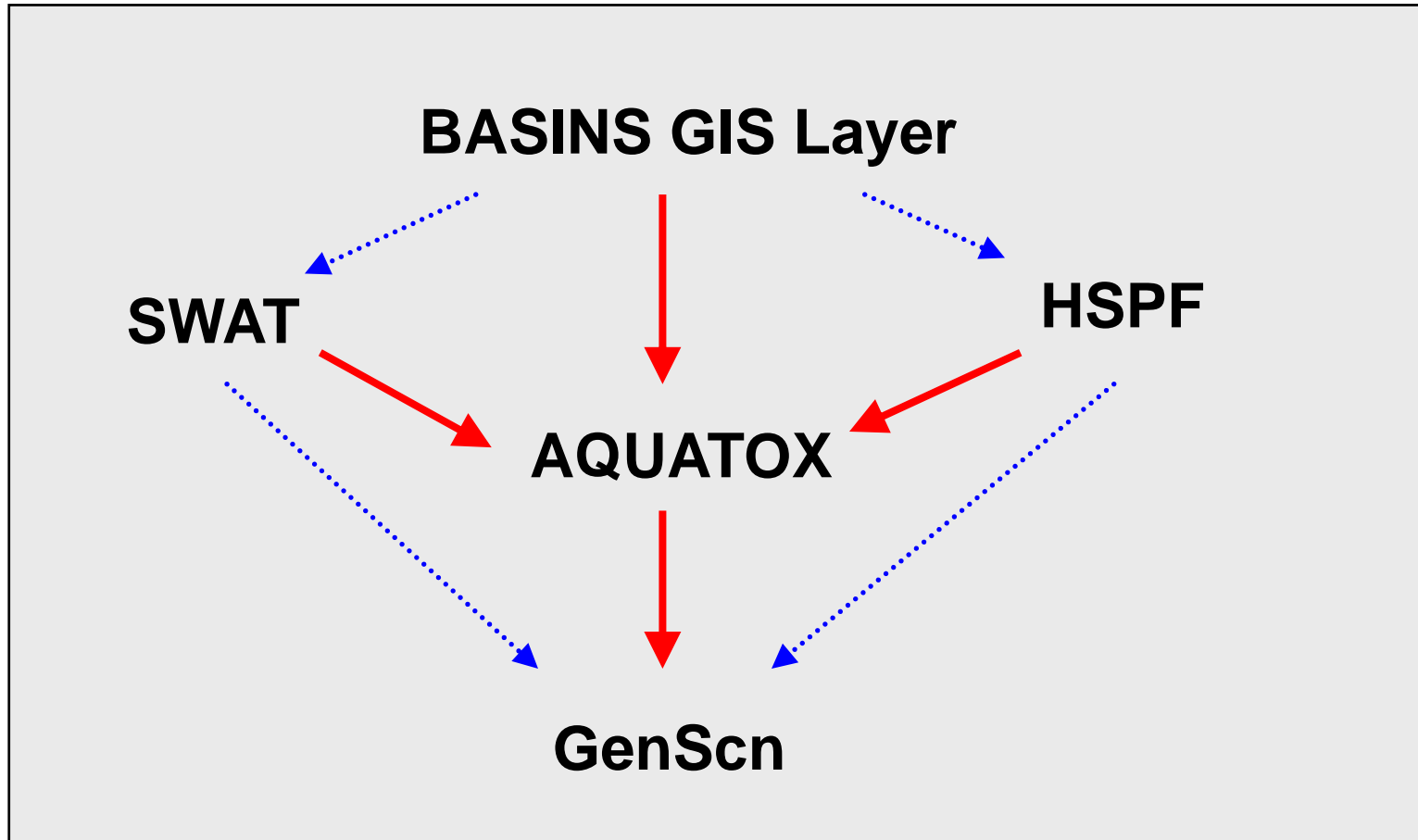
Provides time series loading data and GIS information to AQUATOX

Creates AQUATOX simulations using physical characteristics of BASINS watershed





# Linkages Between Models



.....>  
**Linkage within BASINS**

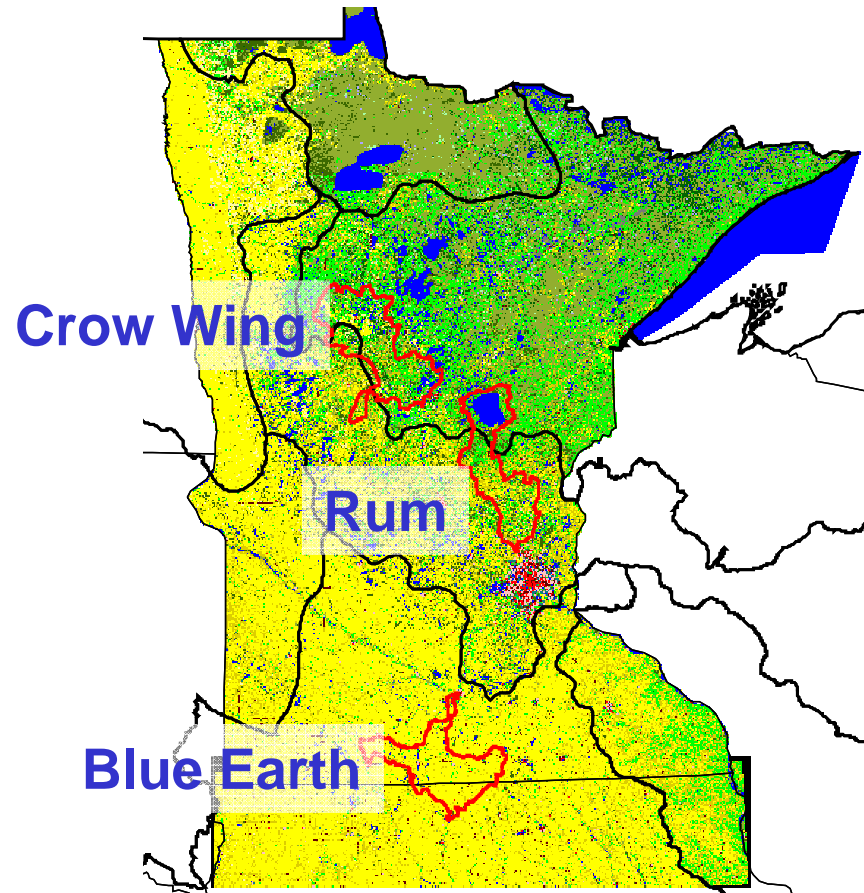
————>  
**Linkage to AQUATOX**

# Use of AQUATOX in development of water quality criteria

- 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 algae blooms)

# Modeling Case Study: Minnesota

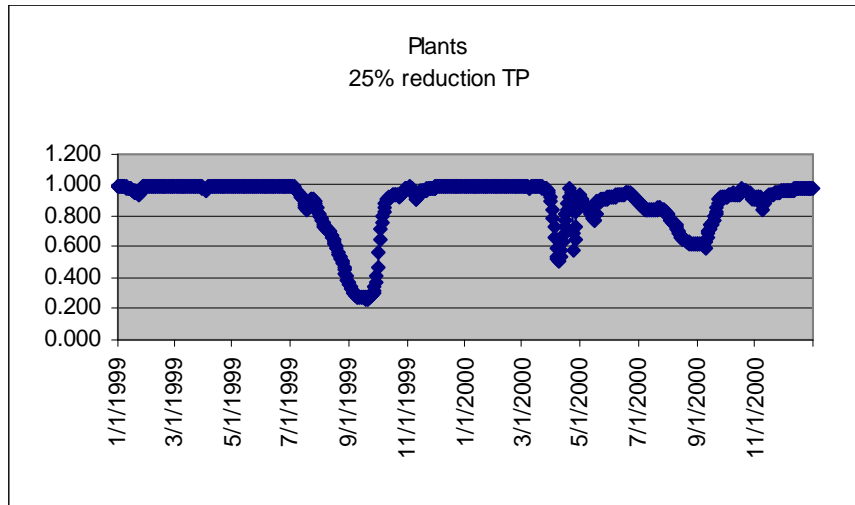
- **MPCA collected monitoring data from rivers in different ecoregions:**
  - nutrients, BOD, water clarity, chlorophyll a
  - phytoplankton, periphyton, fish & invertebrate IBI scores.



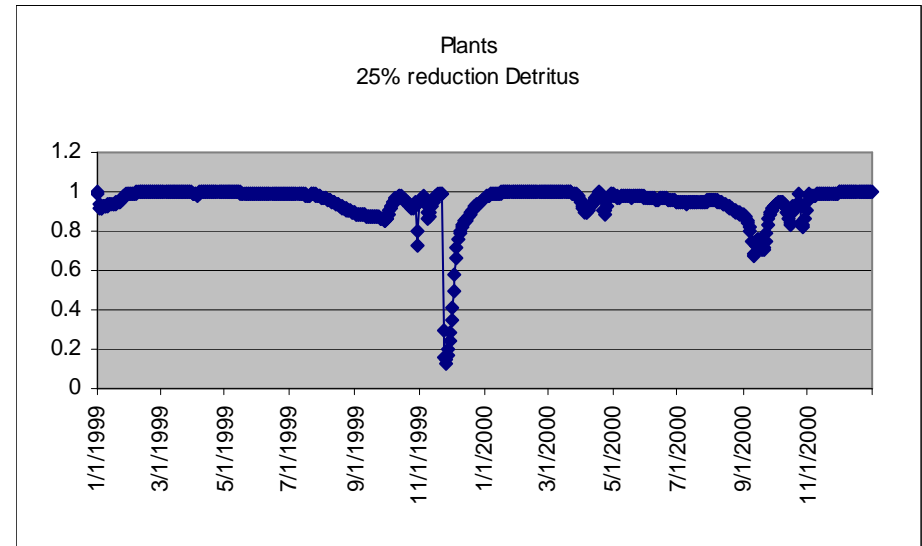
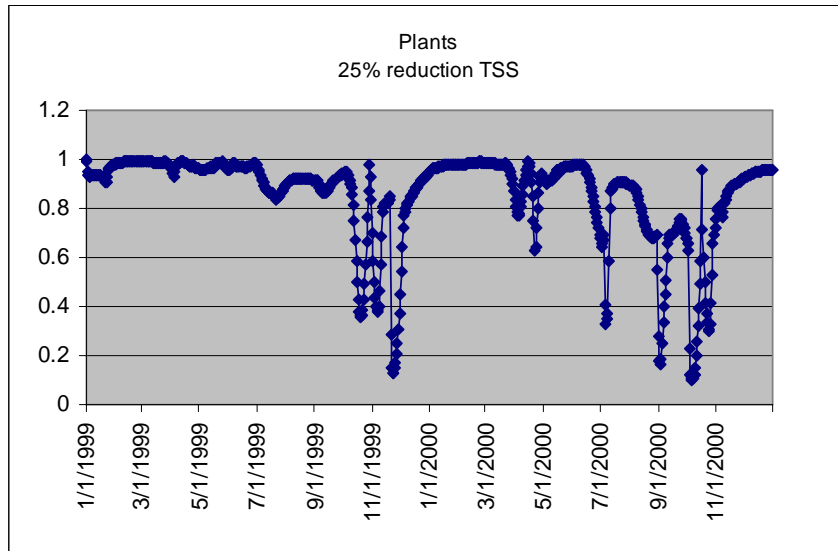
# Example Nutrient Analyses from MN

- Calibrated AQUATOX across nutrient gradient
- Set up HSPF, linked loadings to AQUATOX
- Ran iterative simulations with various nutrient reductions
- Applied 2 ways of developing nutrient target
  - Accept the ecoregion chl *a* target, use AQUATOX to get corresponding TP level
  - Use AQUATOX to develop chl *a* and TP target based on algal species composition
- Ran HSPF with various likely pollutant reductions from BMPs
  - Will chl *a* and/or TP target be achieved under any of these scenarios?

# Steinhaus Similarity Indices show changes in algal community



**Differences in TSS and TP loadings have significant effects on algal community; BOD appears to have some effect, though of much shorter duration**



# What reductions in TP will result in attainment of long term chl. a target?

*Start with reference condition chl. a value (7.85 ug/L)*

Parameter	Reported min	Reported max	25 <sup>th</sup> Percentile (all seasons)	AQUATOX 6-yr average
<b>TP (ug/L)</b>	11.25	1720	<b>118.13</b>	<b>268</b>
<b>Chl a (ug/L)</b>	3.76	90.6	<b>7.85</b>	<b>18.3</b>

# Effect of Load Reductions on Blue Earth Mean Chlorophyll *a*

TP/TSS multiplier	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

} **7.85 ug/L**

# Target Development

## Method #1

- Model results suggest that **> 80%** reduction of TP (coupled with TSS reductions) required to attain 7.85 ug/L
- 304(a) recommendations suggest a **56%** reduction of TP would be necessary

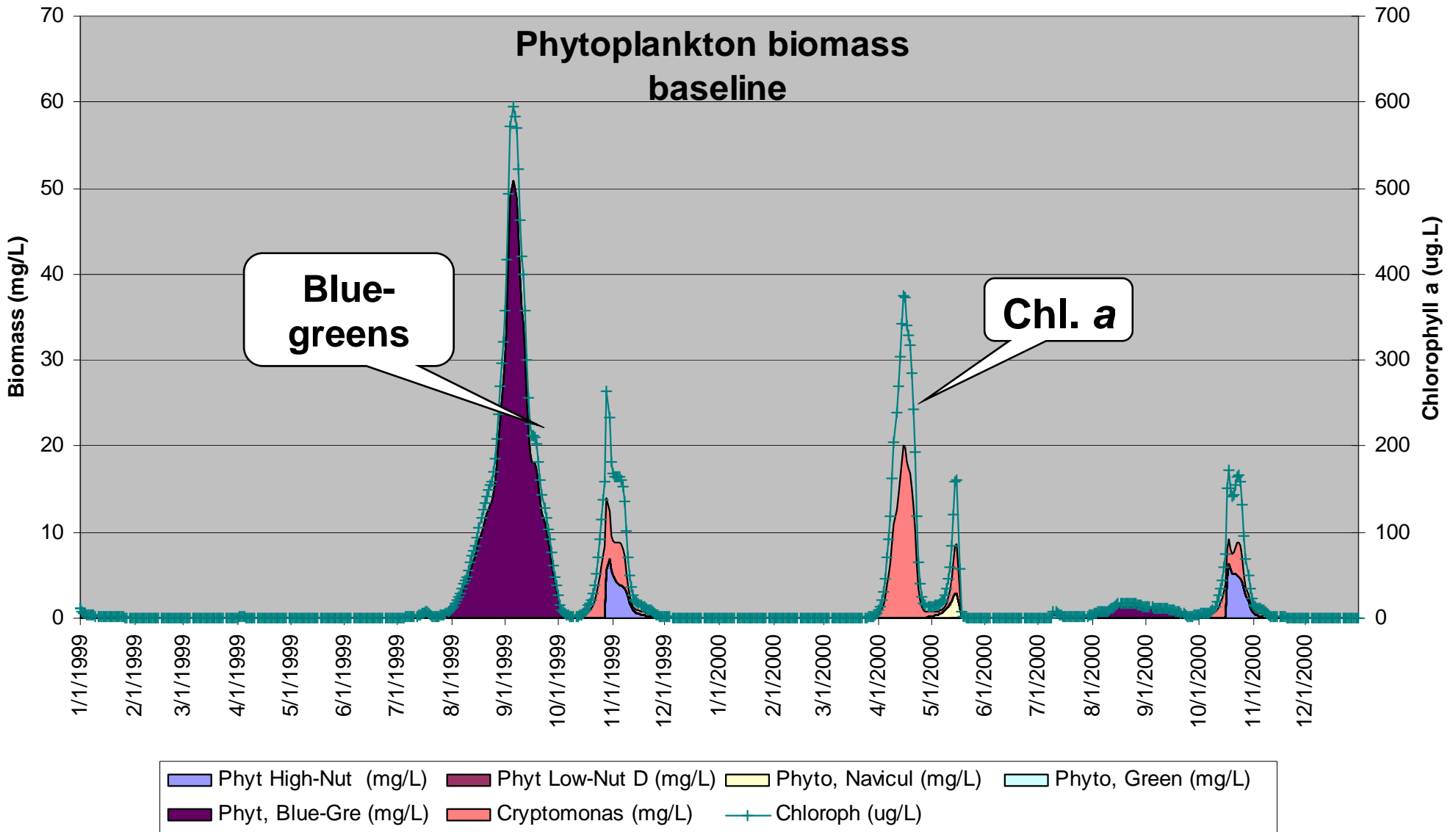


# Target Development

## Method #2

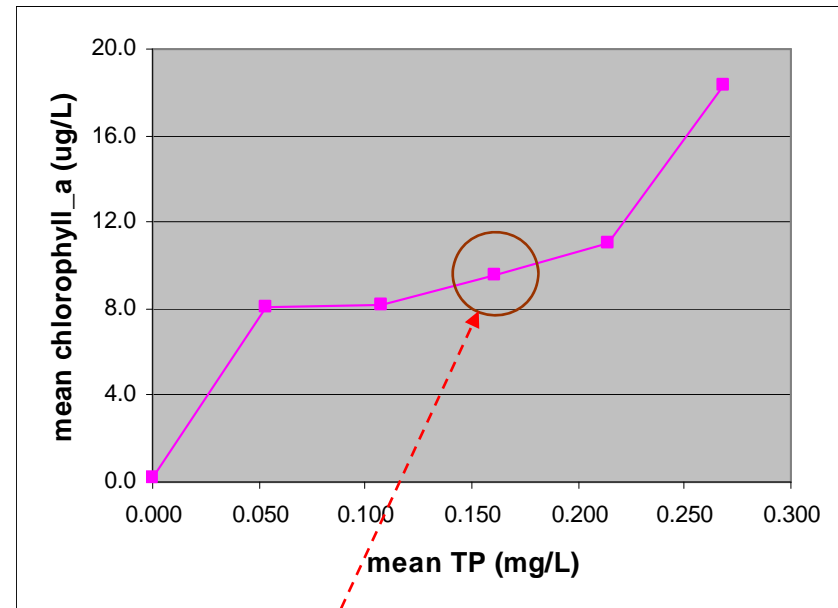
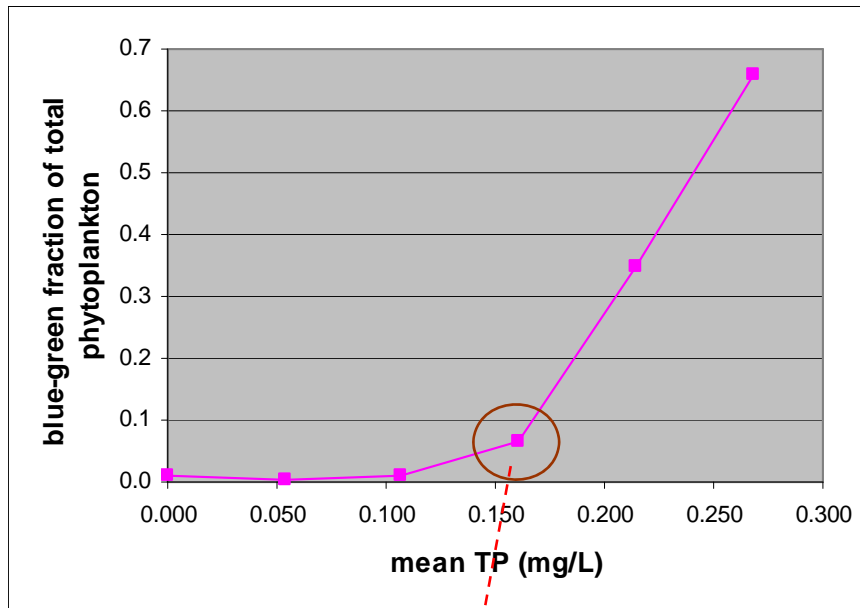
- Focus on specific algal response, not just total chl a
  - Especially blue greens, as blooms can be noxious and cause taste & odor problems
  - At what levels do blue greens reach an “acceptable” proportion of total algae?
- Where do there appear to be shifts in species composition?

# Baseline conditions include large blooms, especially in 1st year



# Target Development

- **Method 2**: Use AQUATOX to estimate chl\_a concentration associated with a shift in dominance between blue-greens and more desirable algae.



**Inflection point** – corresponds with 9.5 ug/L mean chl\_a, 0.161 mg/L TP, and blue-greens <10% of total water column phytoplankton.

**Represents ~40% reduction in TP and TSS.**

## Method #2 Target

- Results suggest that a 40% reduction of TP, if coupled with a corresponding reduction in TSS as well, would result in an algal community with a much reduced proportion of noxious blue green algae

# Summary of Minnesota Analysis

- **Stressor-response linkage**: Algal responses linked quantitatively with TP and TSS concentrations.
- **Criteria development**: Derived alternative hypothetical criteria, one based on ecologically meaningful endpoint (e.g. blue-green fraction of total phytoplankton).
- **Attainability**: Results suggest both 304(a) and hypothetical criteria in Blue Earth river may be very difficult to achieve, even with heavy use of BMPs.

# 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
  - 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



# Animal Parameters

Animal **Mtn. whitefish adult** Species Data Help

Animal Type: **Fish** Toxicity Record: **Trout** Edit All

Taxonomic Type or Guild: **Game Fish**

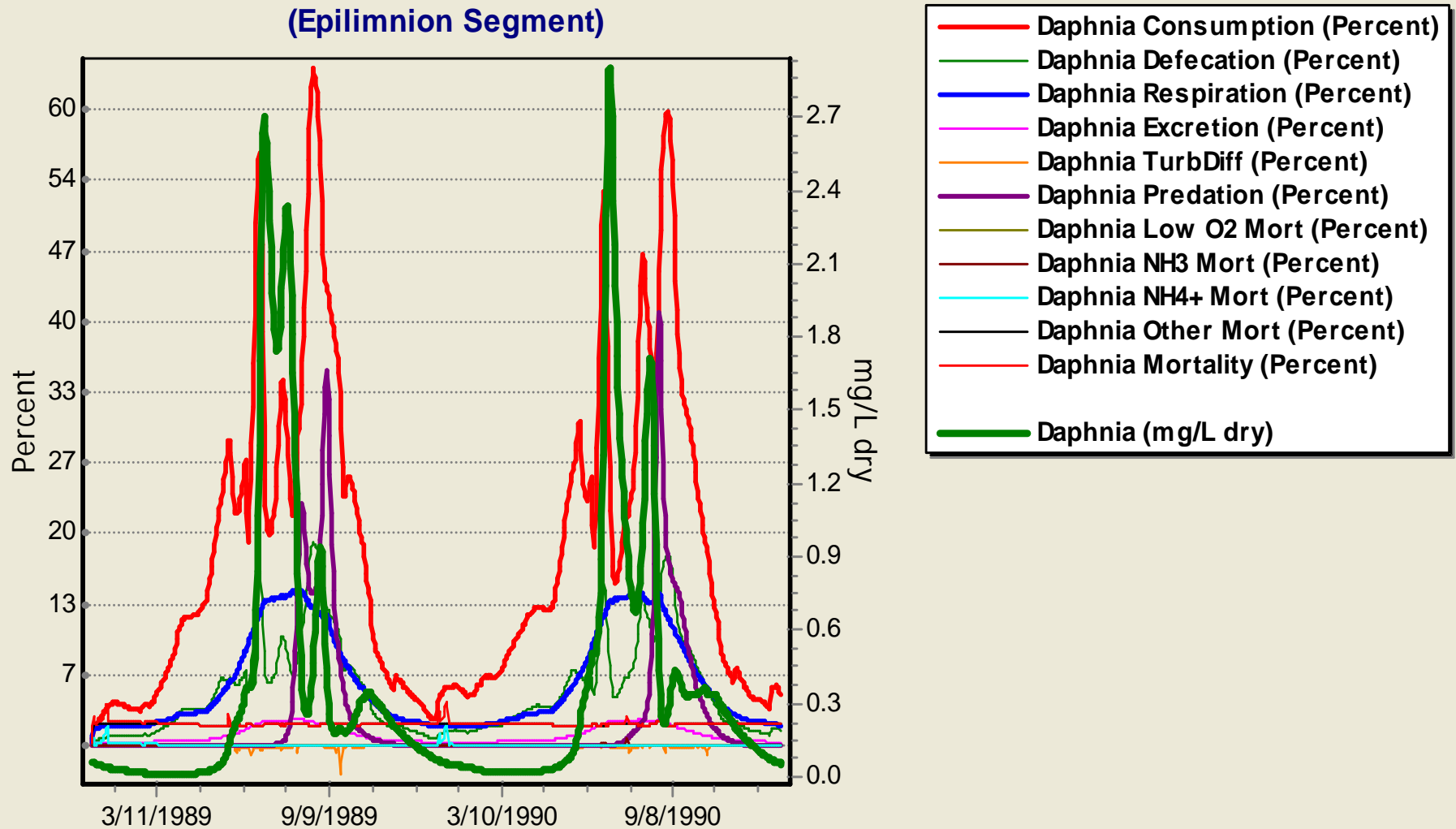
Trophic Interactions

## Animal Data:

			References:
Half Saturation Feeding	<b>0.3</b>	mg / L	<b>Leidy &amp; Jenkins 77 (cf. salmon)</b>
★ Maximum Consumption	<b>0.01</b>	g / g-d	<b>calc. from Hewett &amp; Johnson '92, l. trout</b>
★ Min Prey for Feeding	<b>0.1</b>	g/sq.m	<b>bottom feeder</b>
Temp. Response Slope	<b>2.3</b>		
★ Optimum Temperature	<b>12</b>	°C	<b>Essig, 1998; see also Sauter et al. 2001</b>
Maximum Temperature	<b>23</b>	°C	<b>FishBase</b>
Min Adaptation Temp.	<b>0</b>	°C	<b>Sauter et al. 2001, based on spawning</b>
★ Endogenous Respiration	<b>0.0015</b>	l / d	<b>calc. from Hewett &amp; Johnson '92 prms.</b>
Specific Dynamic Action	<b>0.172</b>	(unitless)	<b>cf. Hewett &amp; Johnson '92</b>
Excretion : Respiration	<b>0.05</b>	ratio	<b>default</b>
N to Organics	<b>0.1</b>	frac. dry	<b>Sterner 2000</b>
P to Organics	<b>0.031</b>	frac. dry	<b>Sterner 2000</b>
Wet to Dry	<b>5</b>	ratio	<b>default</b>

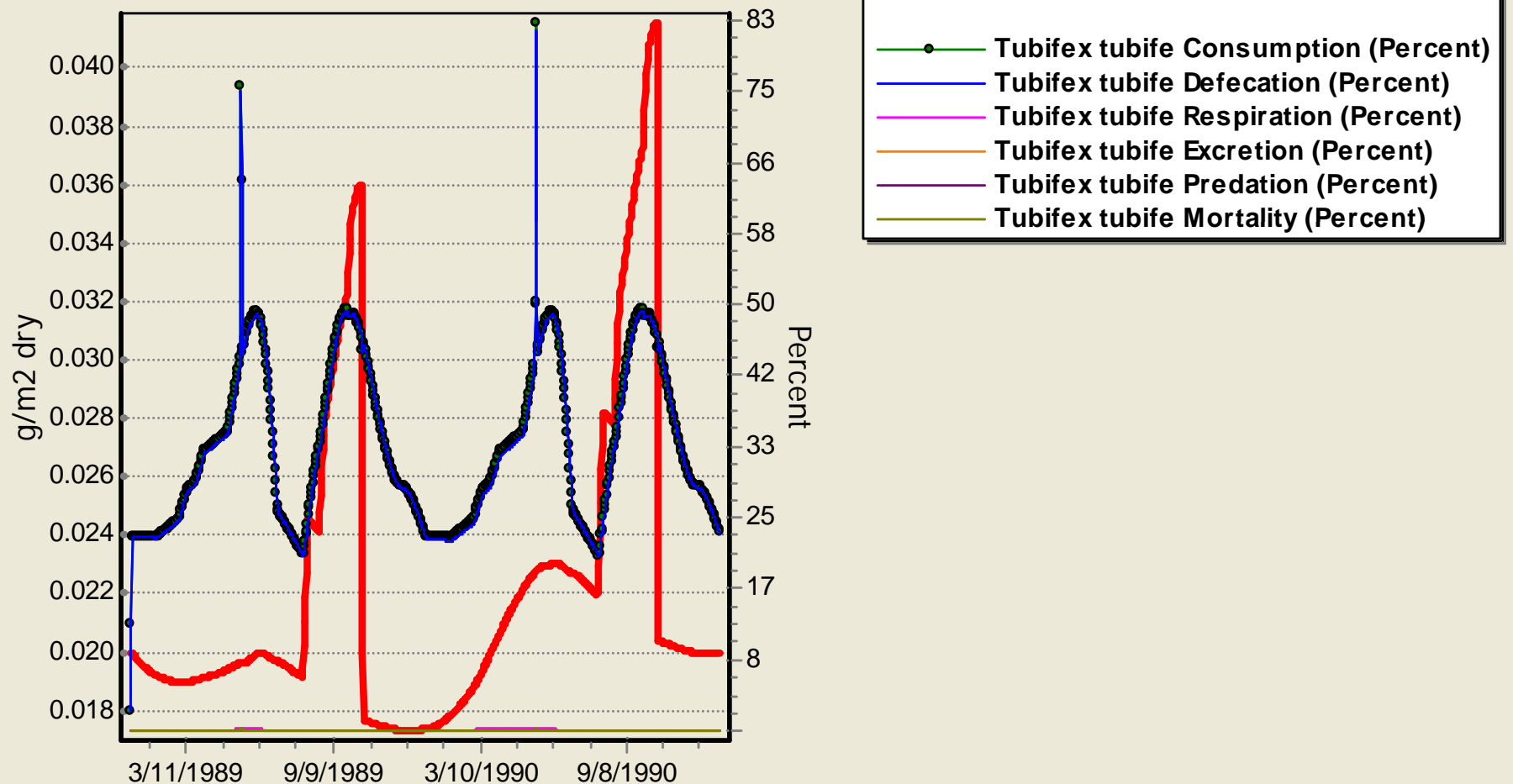
# Zooplankton consumption is tied to phytoplankton productivity

ONONDAGA LAKE, NY (CONTROL) Run on 09-24-08 11:13 AM  
(Epilimnion Segment)



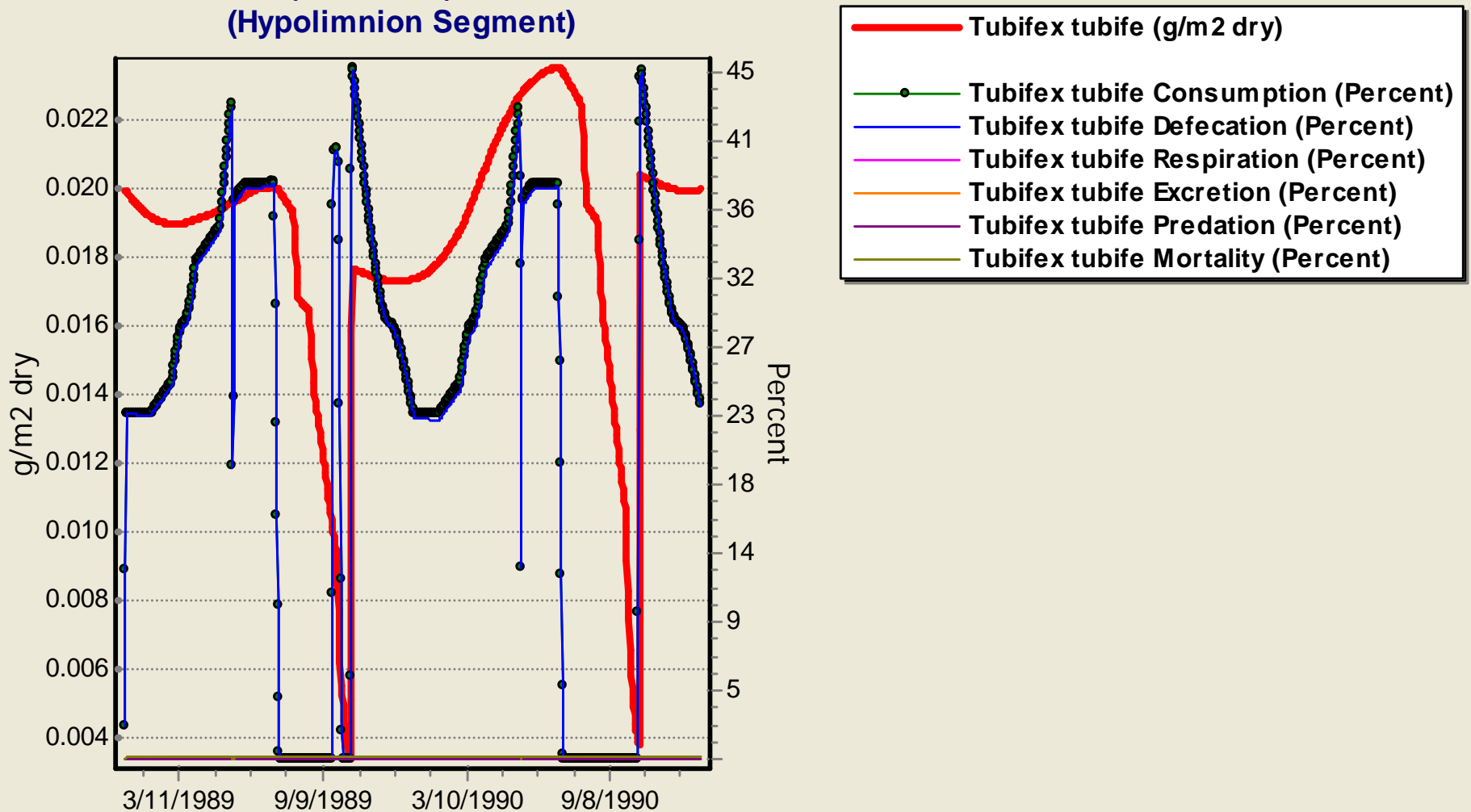
# Benthic invertebrates are also tied to phytoplankton productivity through detritus

ONONDAGA LAKE, NY (CONTROL) Run on 09-24-08 11:13 AM  
(Epilimnion Segment)



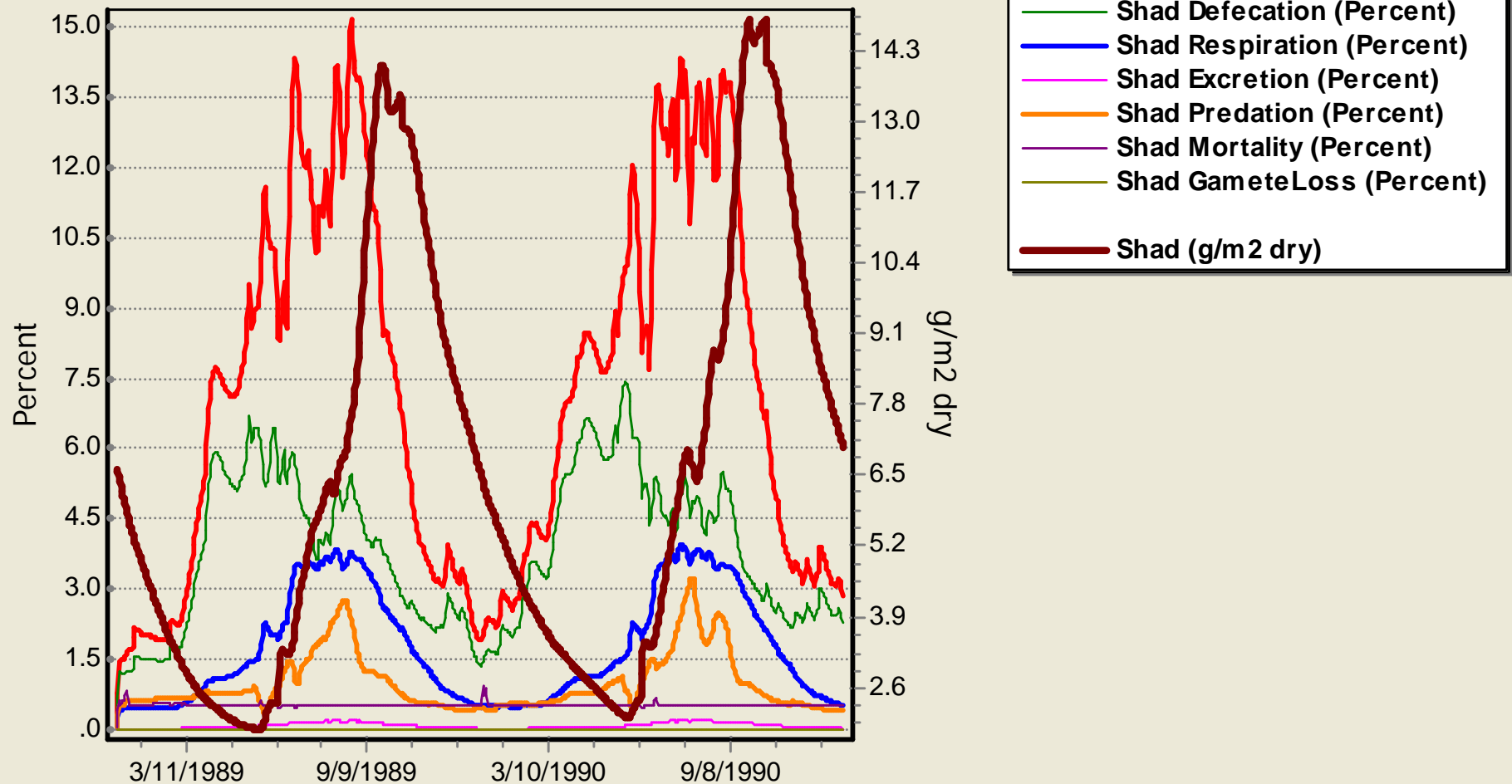
# *Tubifex* in hypolimnion are tolerant of anoxia but stop feeding and slowly decline

ONONDAGA LAKE, NY (CONTROL) Run on 09-24-08 11:13 AM  
(Hypolimnion Segment)



# Fish exhibit seasonal patterns based on food availability and temperature

ONONDAGA LAKE, NY (CONTROL) Run on 10-8-08 8:13 AM  
(Epilimnion Segment)







# Lower Boise River in Boise, Idaho



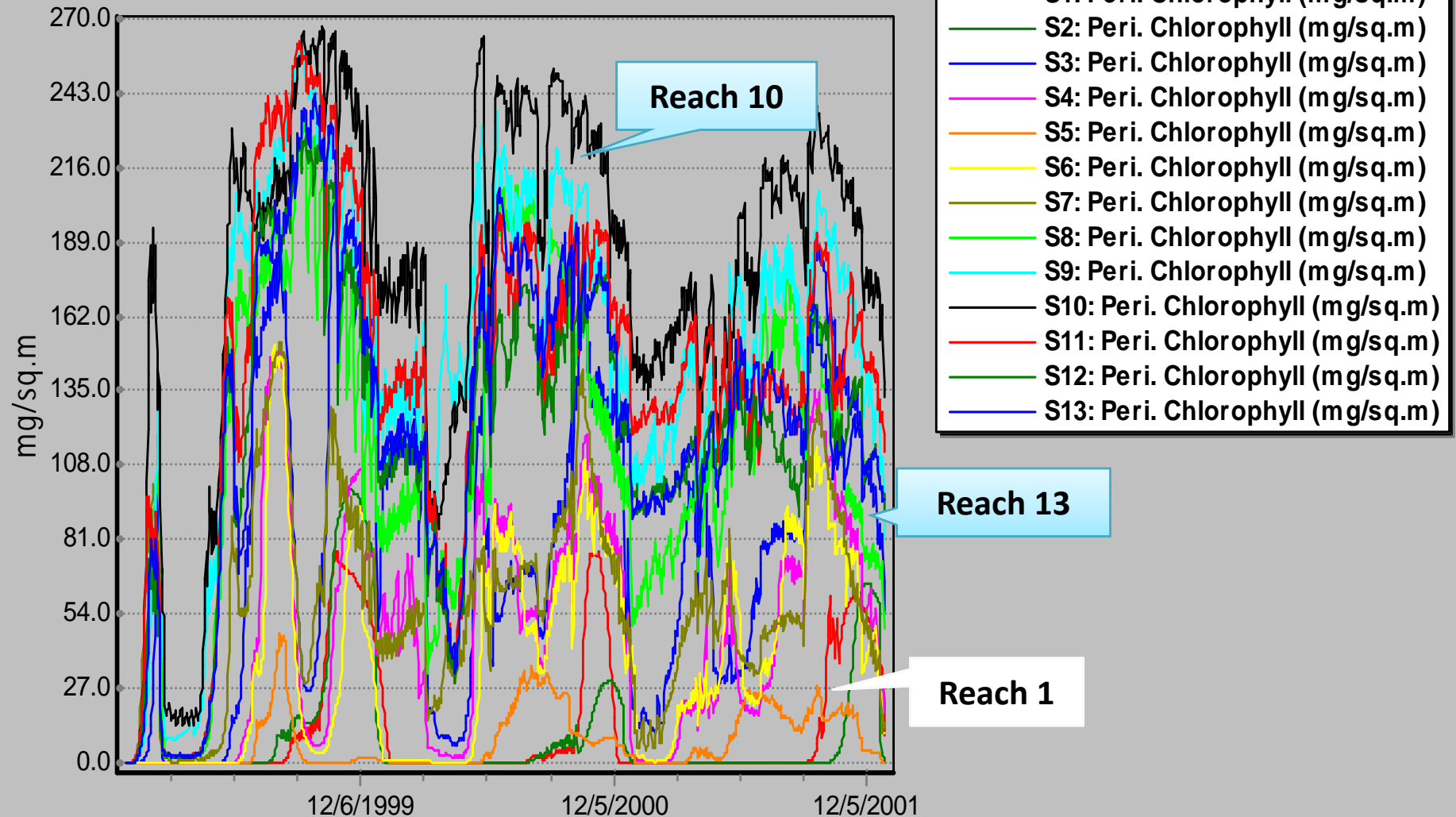


# Complex Linked Model

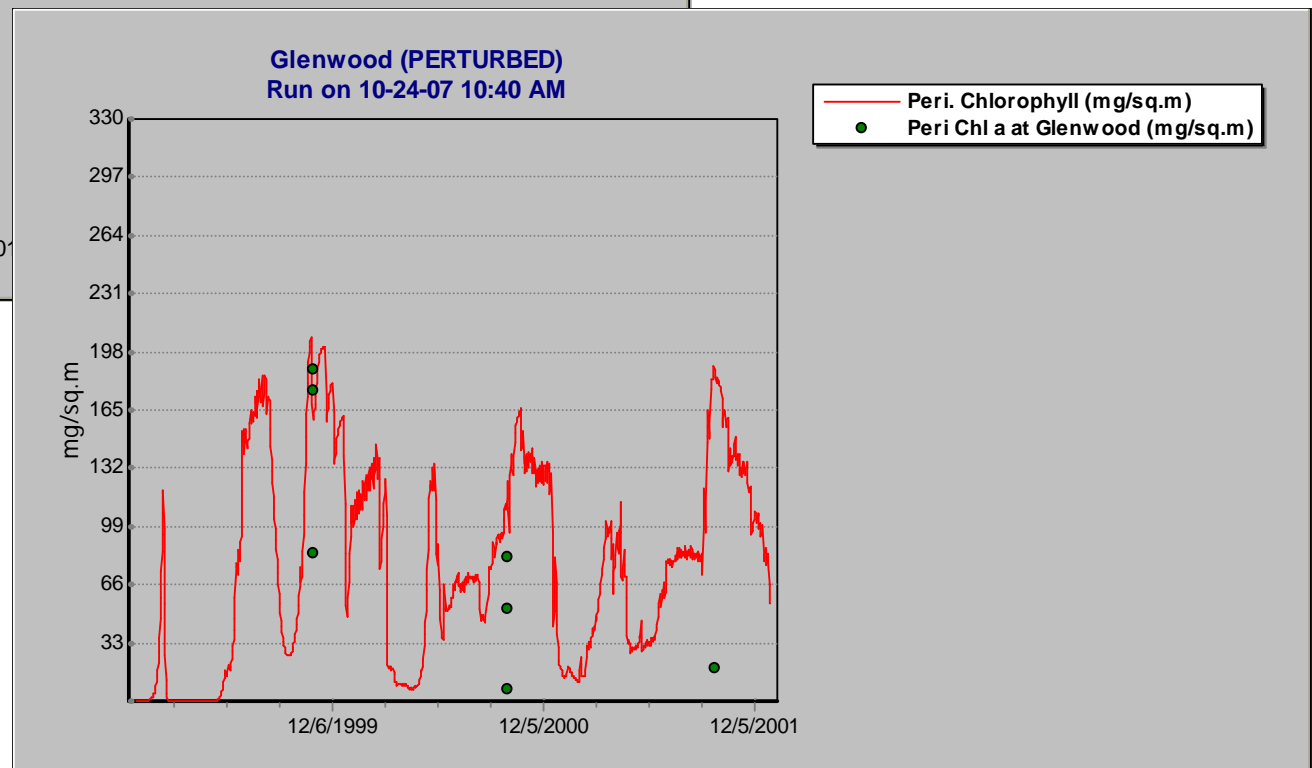
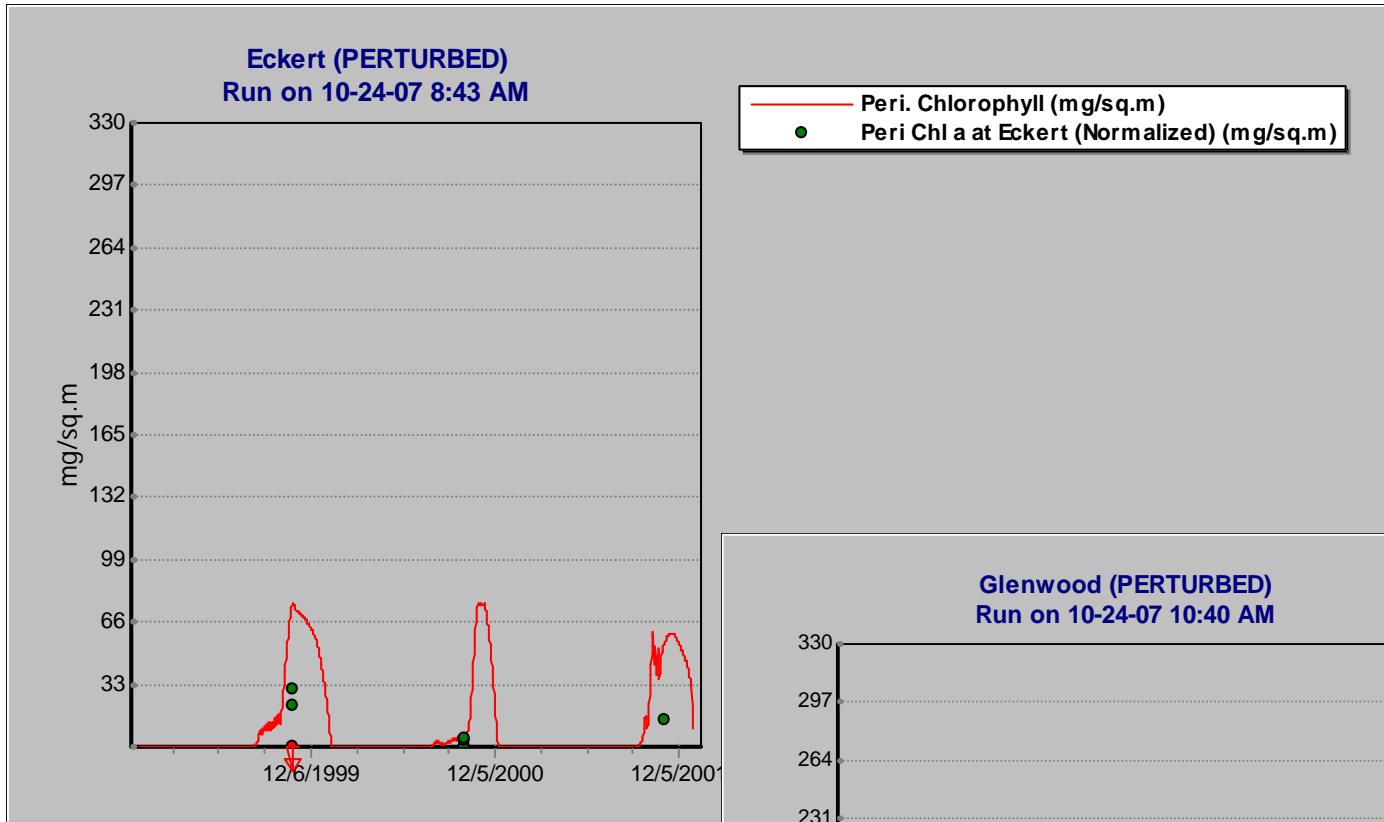
- 13 main-stem segments modeled
- 26 “tributary inputs”
  - Groundwater inputs
  - Waste Water Treatment Facilities
  - Input drains and tributaries
- Extensive water withdrawals
- Complex water-balance model
- Nutrients are integrated within main-stem

# LBR Downstream Periphyton Trend

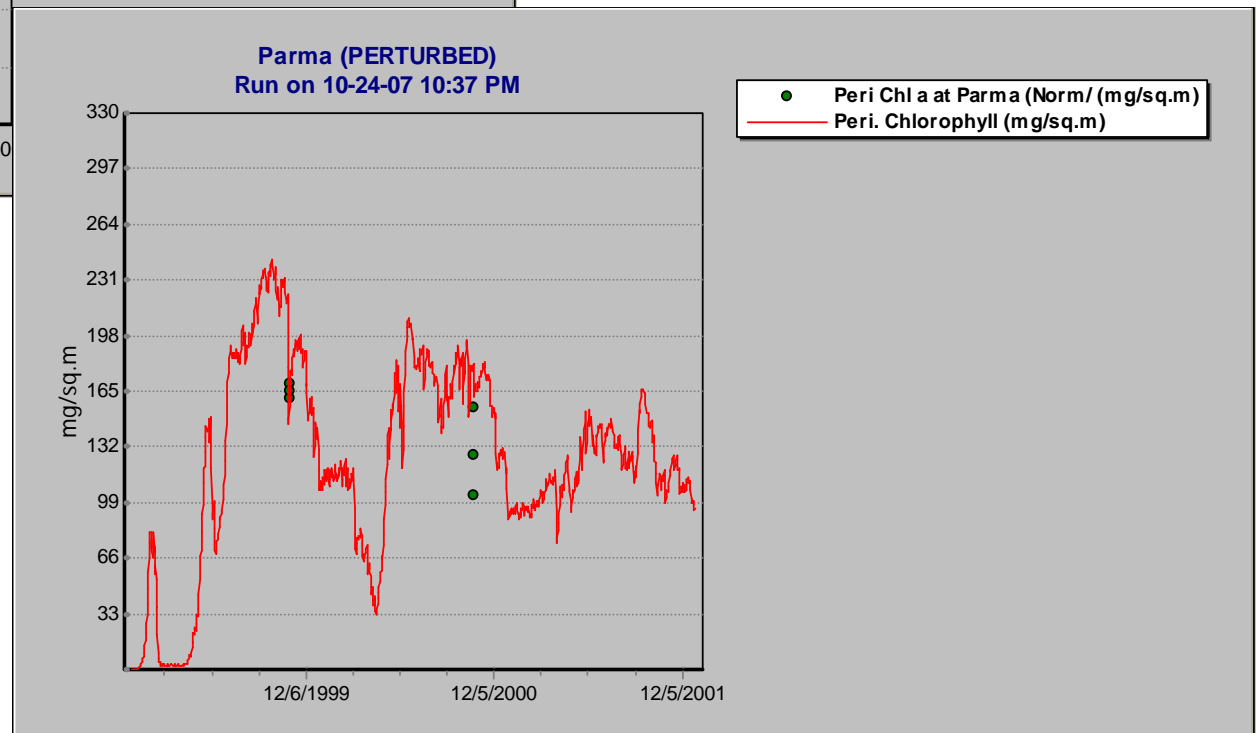
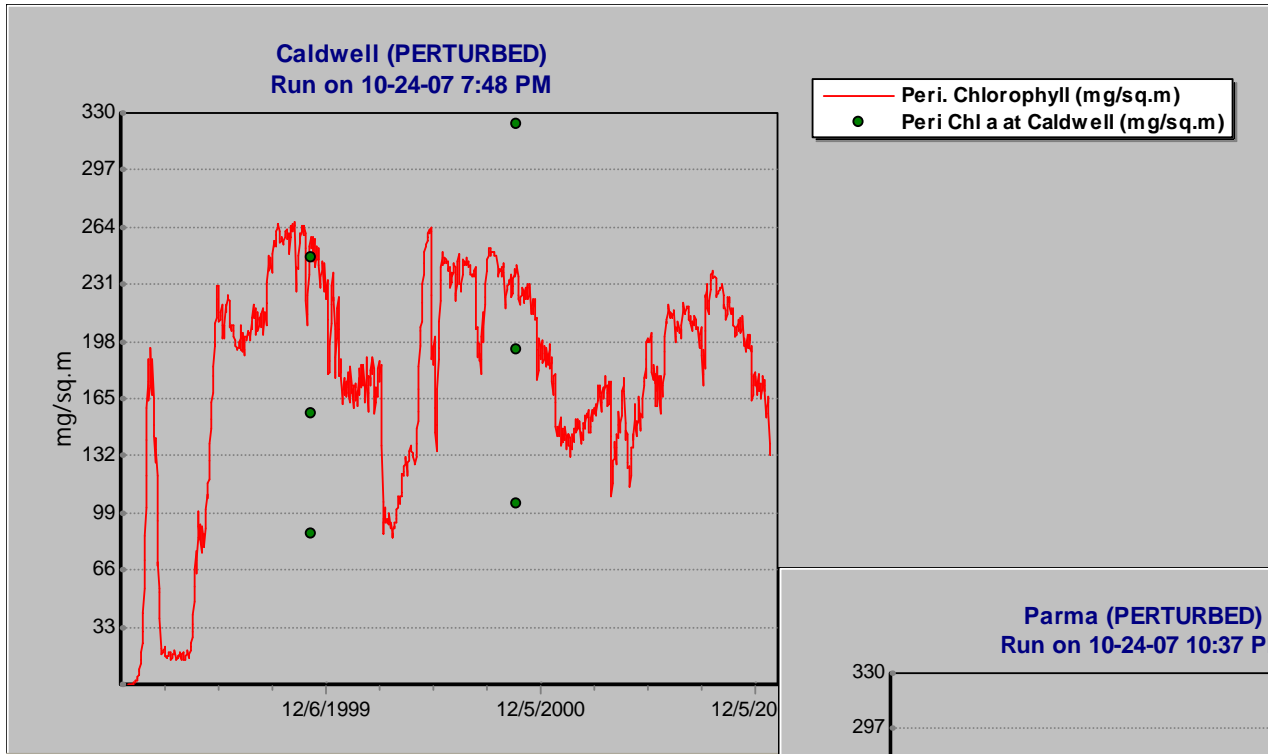
Linked LBR (PERTURBED)  
Run on 10-24-07 10:37 PM



# Periphyton in Reaches 1 and 3, LBR

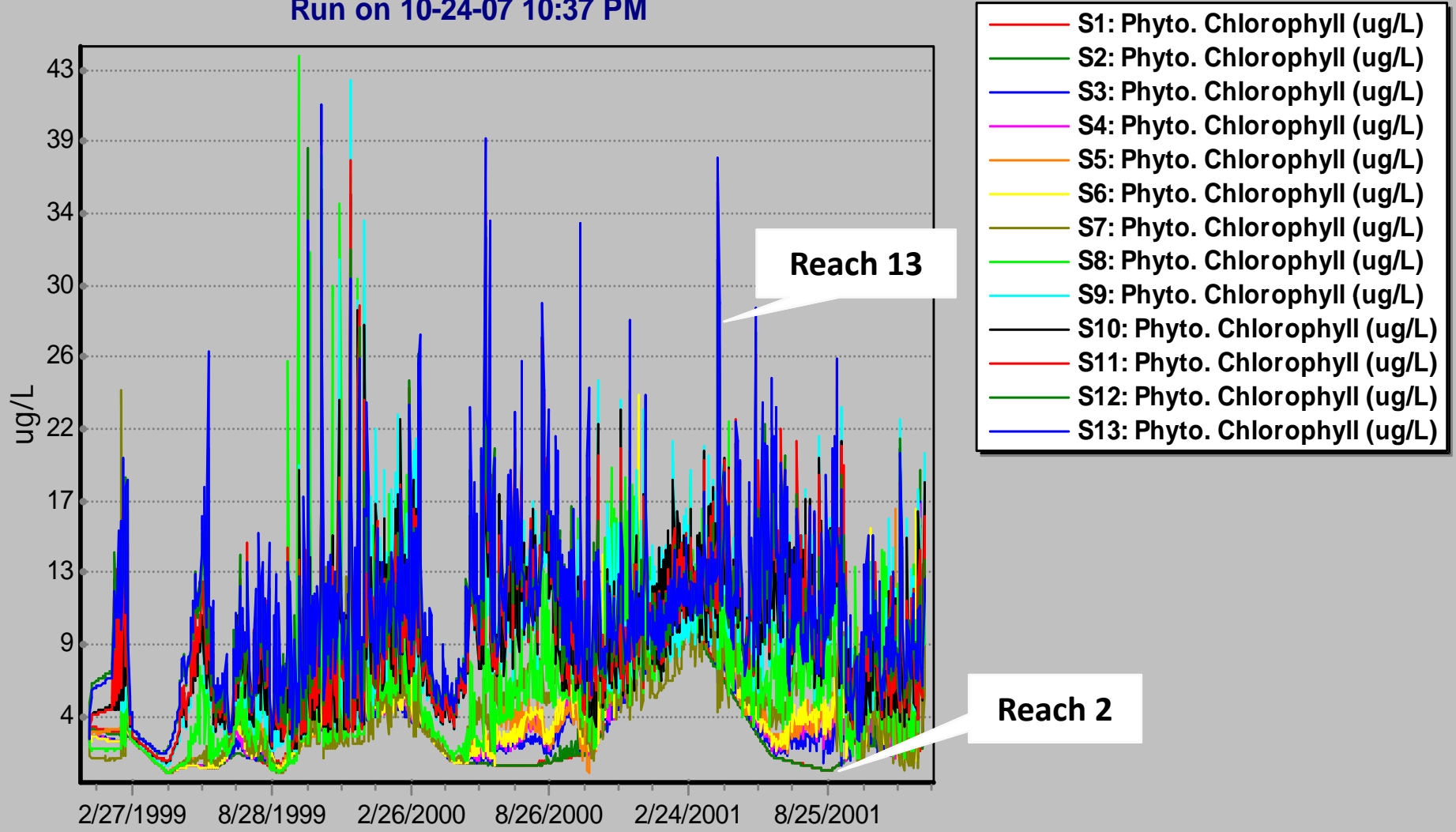


# Periphyton in Reaches 10 and 13, LBR

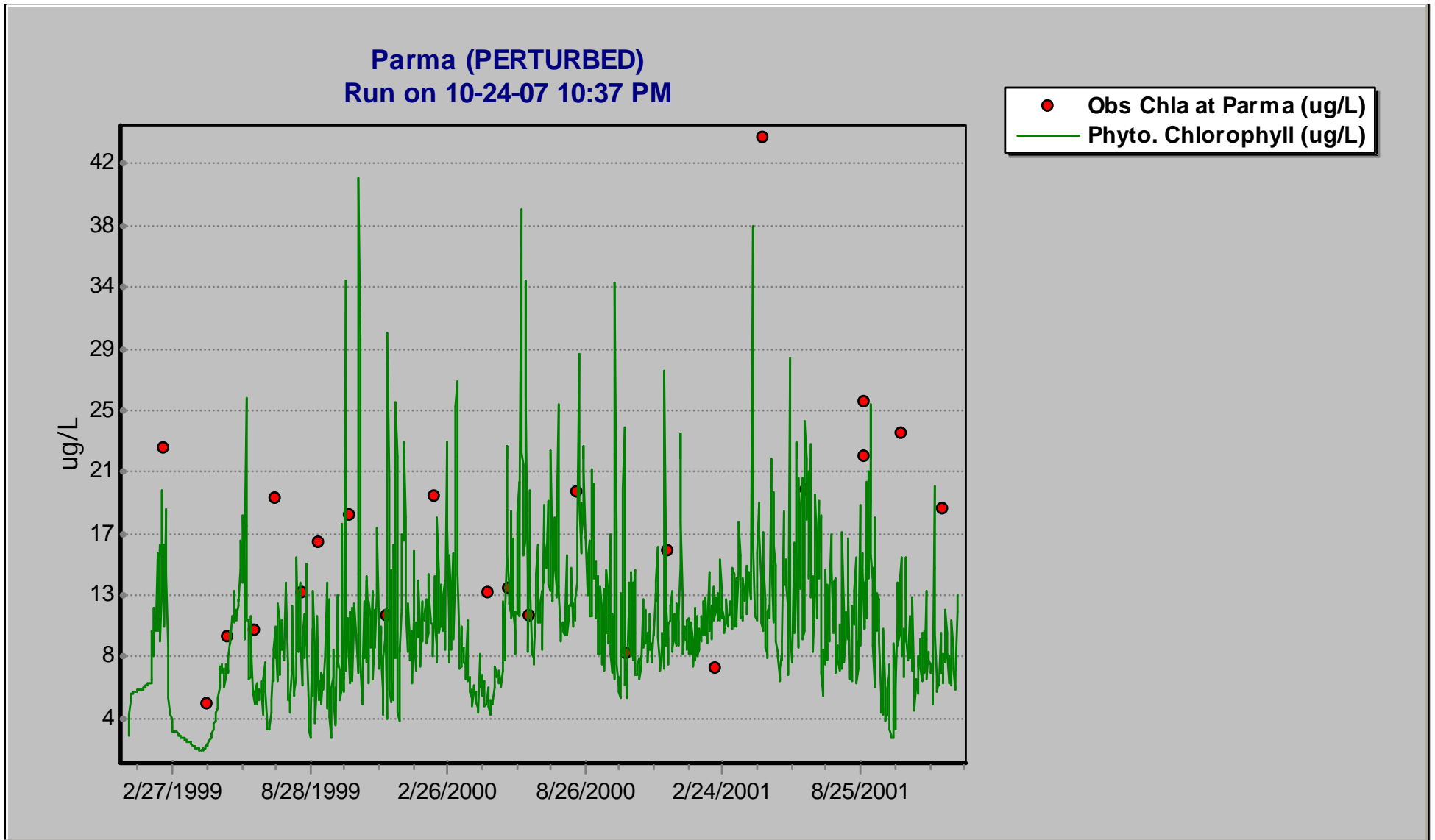


# LBR Downstream Phytoplankton Trend

Linked LBR (PERTURBED)  
Run on 10-24-07 10:37 PM



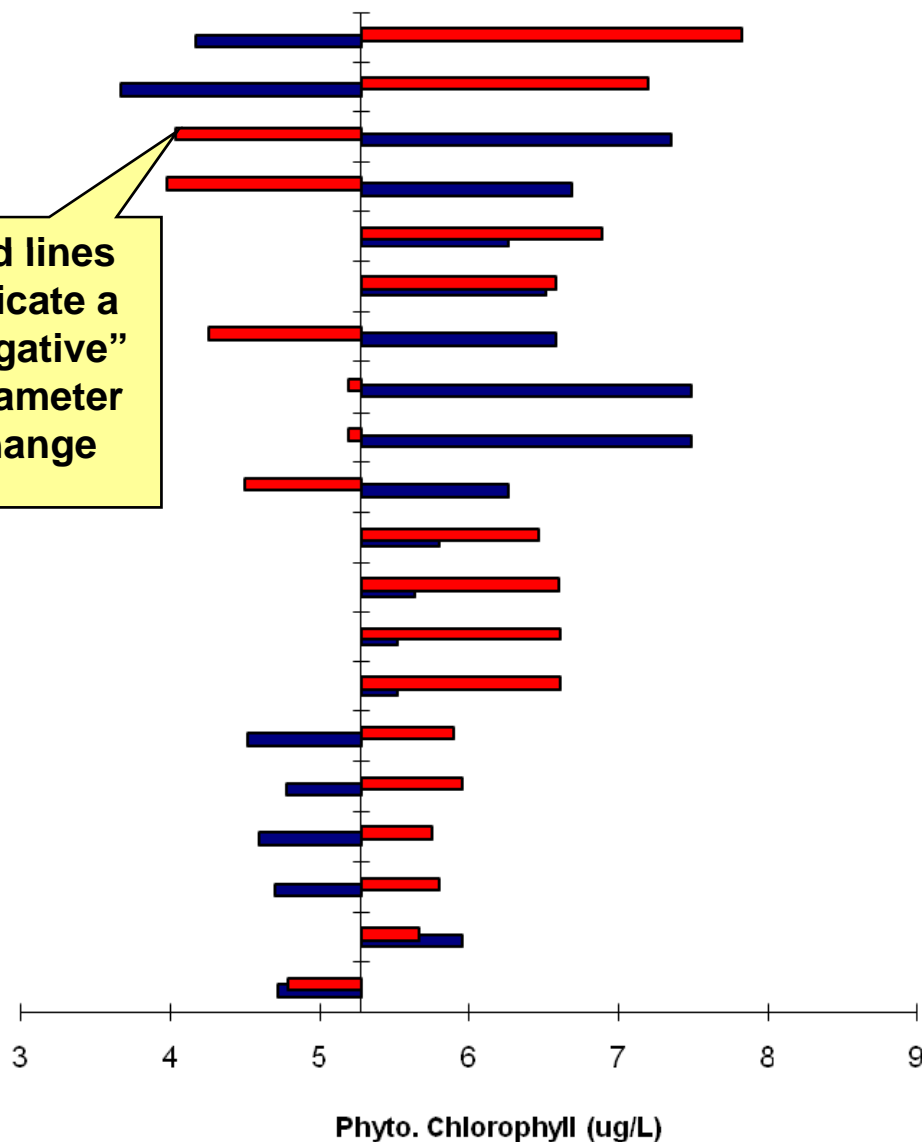
# Sestonic algae at Parma (Reach 13), both upstream loadings and periphyton sloughing



# Phytoplankton Sensitivity, Parma LBR could choose parameters for better fit

Parma: Sensitivity of Phyto. Chlorophyll to 20% Change in Algae & Site Parameters

Red lines indicate a "negative" parameter change



**Sens. Parameter Name**

- 104.9% Phyt High-Nut: Optimal Temperature (deg. C)
- 101.3% Peri High-Nut: Optimal Temperature (deg. C)
- 95.6% Phyt High-Nut: Max Photosynthetic Rate (1/d)
- 78.1% Peri High-Nut: Max Photosynthetic Rate (1/d)
- 74.5% Phyto, Green: Optimal Temperature (deg. C)
- 72.7% Peri, Green: Optimal Temperature (deg. C)
- 66.9% Site: Total Length for Phytoplankton (km)
- 65.8% Peri, Navicula: Optimal Temperature (deg. C)
- 65.8% Phyt Low-Nut D: Optimal Temperature (deg. C)
- 50.4% Peri High-Nut: FCrit, periphyton (newtons)
- 49.0% Peri, Green: Max Photosynthetic Rate (1/d)
- 48.1% Phyto, Green: Max Photosynthetic Rate (1/d)
- 45.0% Peri, Navicula: Max Photosynthetic Rate (1/d)
- 45.0% Phyt Low-Nut D: Max Photosynthetic Rate (1/d)
- 39.6% Peri, Navicula: FCrit, periphyton (newtons)
- 34.0% Peri, Nitzschi: Optimal Temperature (deg. C)
- 33.2% Phyt High-Nut: Exponential Mort. Coefficient: (max / d)
- 31.8% Peri High-Nut: P Half-saturation (mg/L)
- 30.4% Peri Low-Nut D: Optimal Temperature (deg. C)
- 30.4% Cladophora: N Half-saturation (mg/L)

Note: Red bars indicate a negative parameter change and blue bars indicate a positive parameter change

# 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.



# Segmented Version can Represent Dynamically Linked Multiple Segments

The screenshot displays the AQUATOX software interface in "Linked System Mode" for a system named "Linked\_LBR\_10-24-07.als". The interface includes a menu bar (File, View, Library, Study, Segments, Window, Help), a toolbar with various icons, and a main workspace divided into several panels.

**Left Panel: Segment List**

- Radio buttons:  Show Segment Data,  Show Link Data
- Segment list (Model Segment Number):
  - [S1]: Eckert
  - [S2]: Veterans
  - [S3]: Glenwood
  - [S4]: Seg 4
  - [S5]: Seg 5
  - [S6]: Seg 6
  - [S7]: Seg 7
  - [S8]: Middleton
  - [S9]: Seg 9
  - [S10]: Caldwell
  - [S11]: Seg 11
  - [S12]: Seg 12
  - [S13]: Parma
  - [LND]: Lander WWTF
  - [GW4]: S4 Groundwater
  - [GW5]: S5 Groundwater
  - [EAG]: Eagle Drain
  - [GW6]: S6 Groundwater
  - [GW7]: S7 Groundwater
- Buttons: Add, Delete, Edit
- Section: **Data Operations:**
  - Chemicals
  - Setup
  - Notes
  - Help
- Section: **Program Operations:**
  - Perturbed
  - Control
  - Linked Output
  - Export Results

**Right Panel: River Map**

Linked System Name:   
Perturbed: 10-24-07 10:37 PM Control Run: No Ctrl. Run Recorded

R.M. = River Mile

Map features include:

- Major Wastewater Treatment Plants: Lander Street WWTF, Mill, Mason, 15-Mile, Hartley
- Major Tributaries: Eagle Island, Middleton
- Key Locations and Distances:
  - Diversion Dam R.M. 61.2
  - Eckert Road R.M. 58.2
  - Veterans Bridge R.M. 50.1
  - Glenwood Bridge R.M. 47.5
  - Head of Eagle Island R.M. 45.8
  - End of Eagle Island R.M. 38.0
  - Middleton R.M. 31.2
  - R.M. 22.4

Legend:

- Model Segment Number (Hexagon)
- Major Wastewater Treatment Plants (Rectangle)
- Major Tributaries (Wavy Line)

Buttons: Load Map, Clear Map

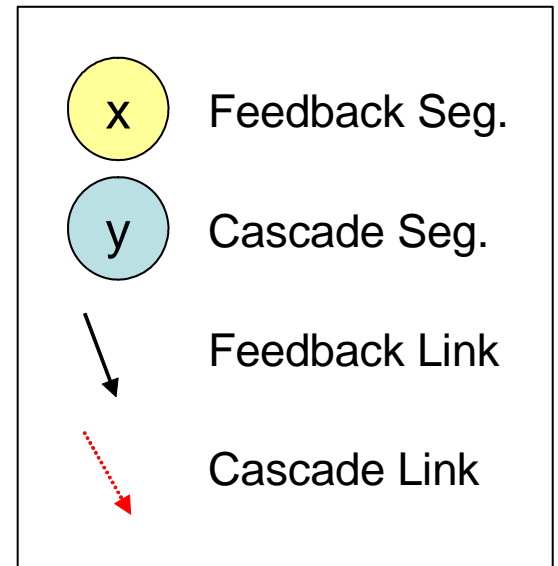
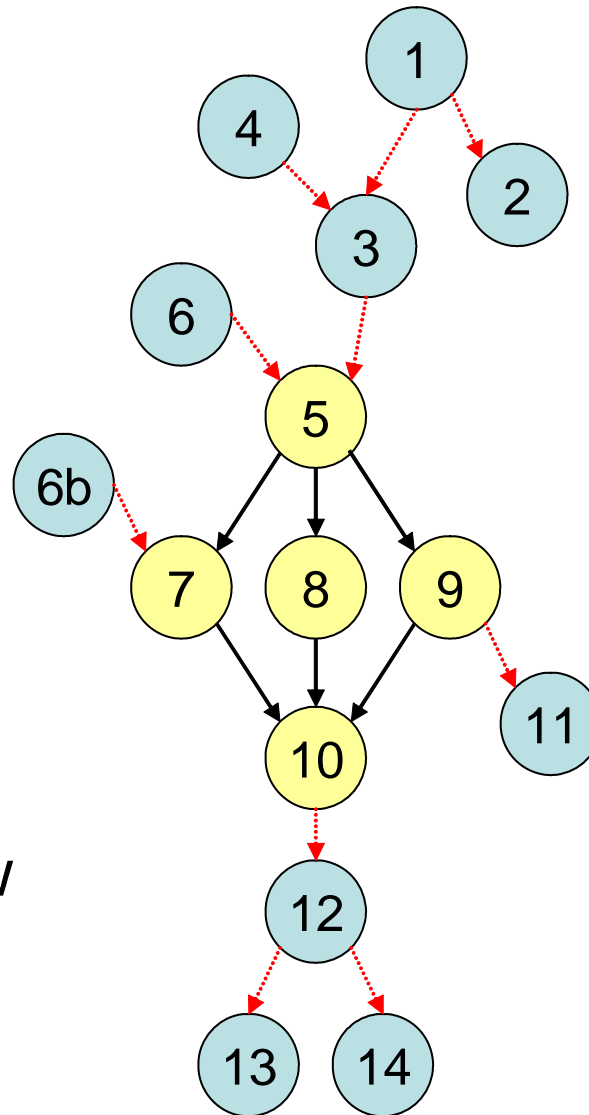
# Cascade & Feedback Linkages

## 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

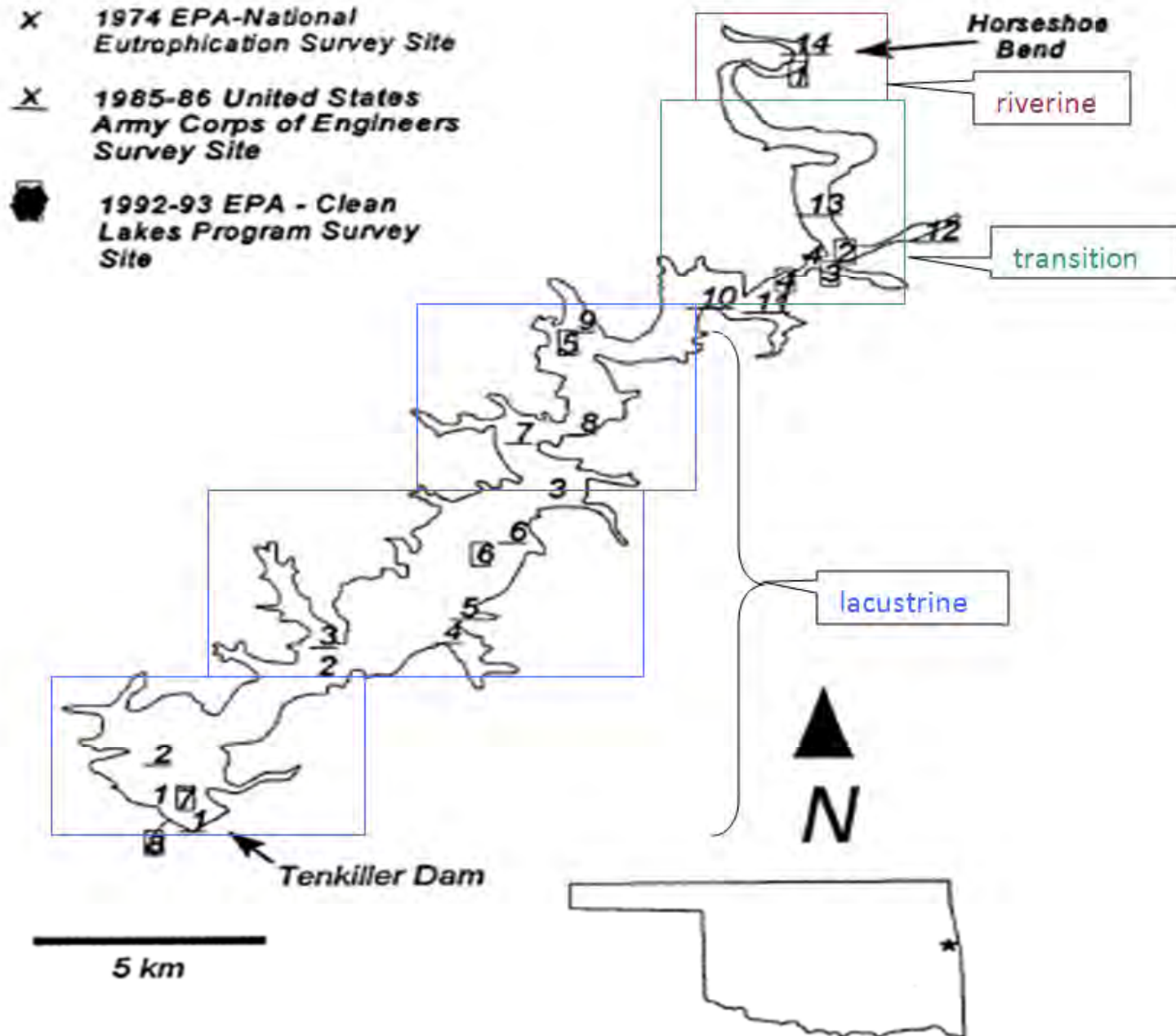


# Linked Segment Model Data Requirements

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

**Interface Demonstration to follow**

# Tenkiller Lake, OK



# 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 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)

# Tenkiller Lake OK

Linked System Mode: "Tenkiller Ferry Lake OK.als"

Linked System Name:

**Perturbed:** 07-27-08 5:15 PM    **Control Run:** 08-21-08 5:26 PM

Show Segment Data     Show Link Data

[R]: Riverine  
[TE]: Trans. Epi.  
[TH]: Trans Hyp  
[LAE]: Lake A Epi.  
[LAH]: Lake A Hyp.  
[LBE]: Lake B Epi.  
[LBH]: Lake B Hyp.  
[LCE]: Lake C Epi.  
[LCH]: Lake C Hyp.  
[TRU]: Trans. Runoff  
[LAR]: Lake A Runoff  
[LBR]: Lake B Runoff  
[LCR]: Lake C Runoff

Hide Tributary-Input Segments

**Data Operations:**

- 
- 
- 
- 

**Program Operations:**

- 
- 
- 
- 

Map details:

- 1974 EPA-National Eutrophication Survey Site
- 1985-86 United States Army Corps of Engineers Survey Site
- 1992-93 EPA - Clean Lakes Program Survey Site
- Horseshoe Bend
- riverine
- transition
- lacustrine
- Tenkiller Dam
- 5 km scale bar
- North arrow

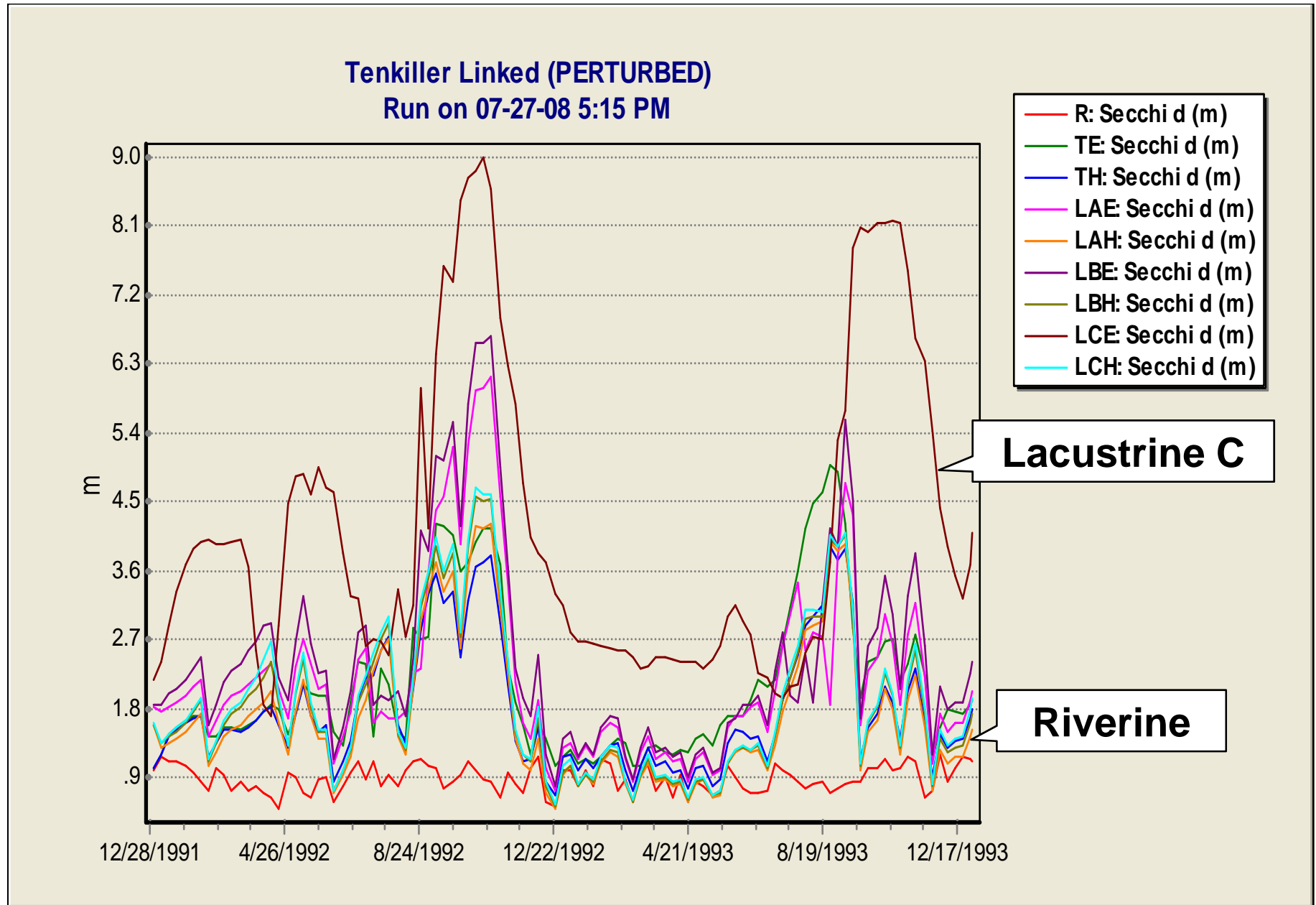
# Storm-water plume, algae-rich riverine segment

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

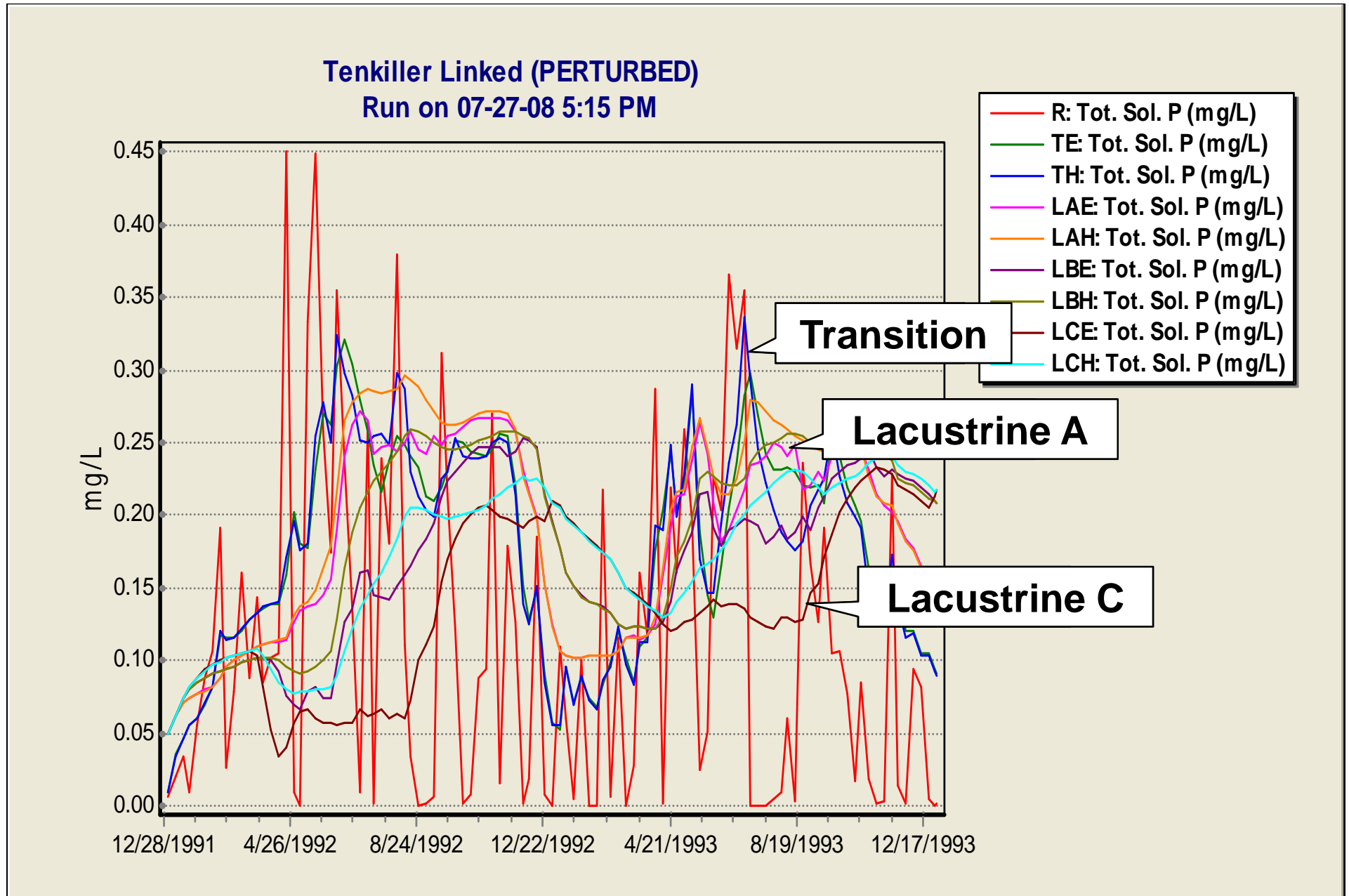




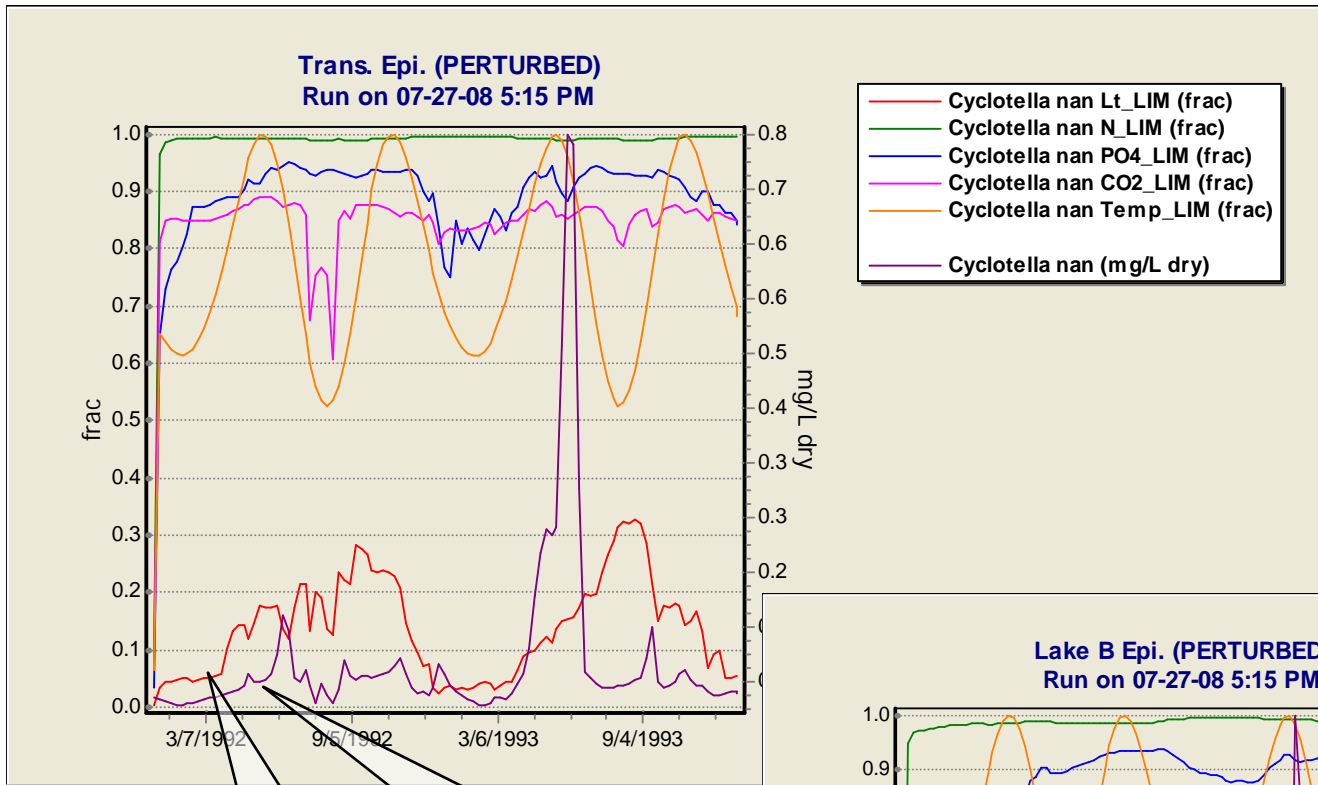
# Known for its clarity, Tenkiller Lake Secchi depth increases down reservoir



# Peak phosphorus decreases down reservoir

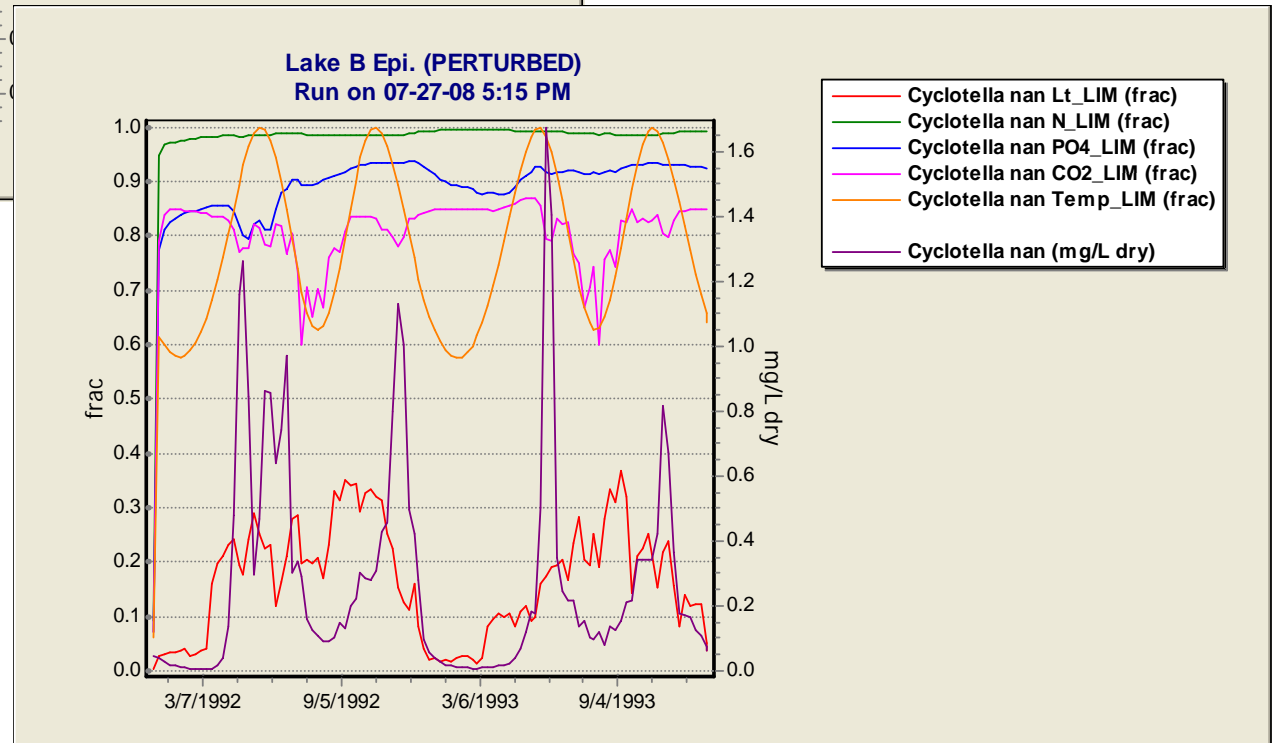


# Transition diatoms suppressed by turbidity

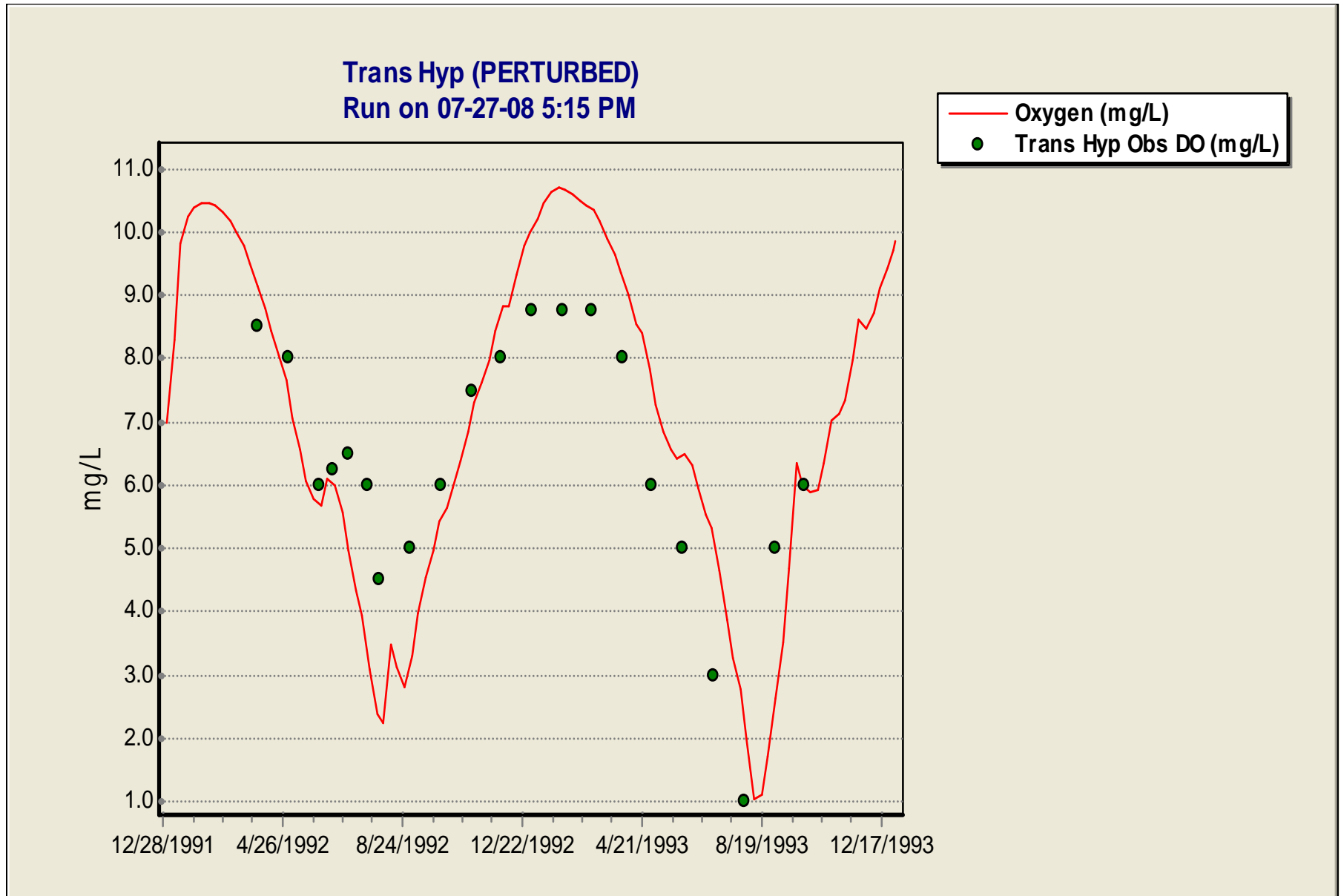


Diatom biomass

Light limitation



# Transition hypolimnion exhibits hypoxia



# AQUATOX– Chemical Fate Overview

- Can model up to twenty chemicals simultaneously
- Fate processes:
  - ionization
  - volatilization
  - hydrolysis
  - photolysis
  - sorption
  - microbial degradation
- Biotransformation—can model daughter products
- Bioaccumulation

# Chemical fate clarified using half-Lives and DT95

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

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

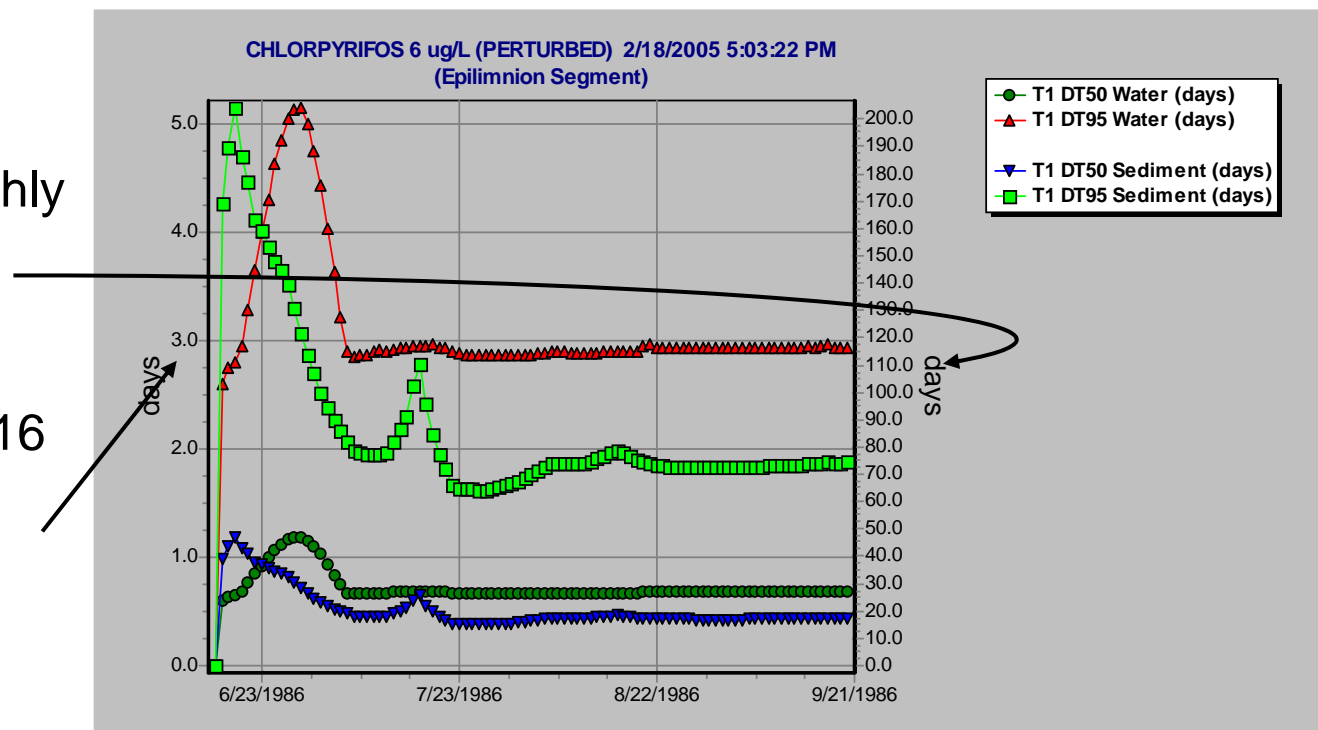
$$Loss_{Sed} = \frac{Microbial_{Sed} + Hydrolysis_{Sed} + Desorption}{Mass_{Sed}}$$

For this Chlorpyrifos Study:

Half-life in Sediment of roughly  
20 days

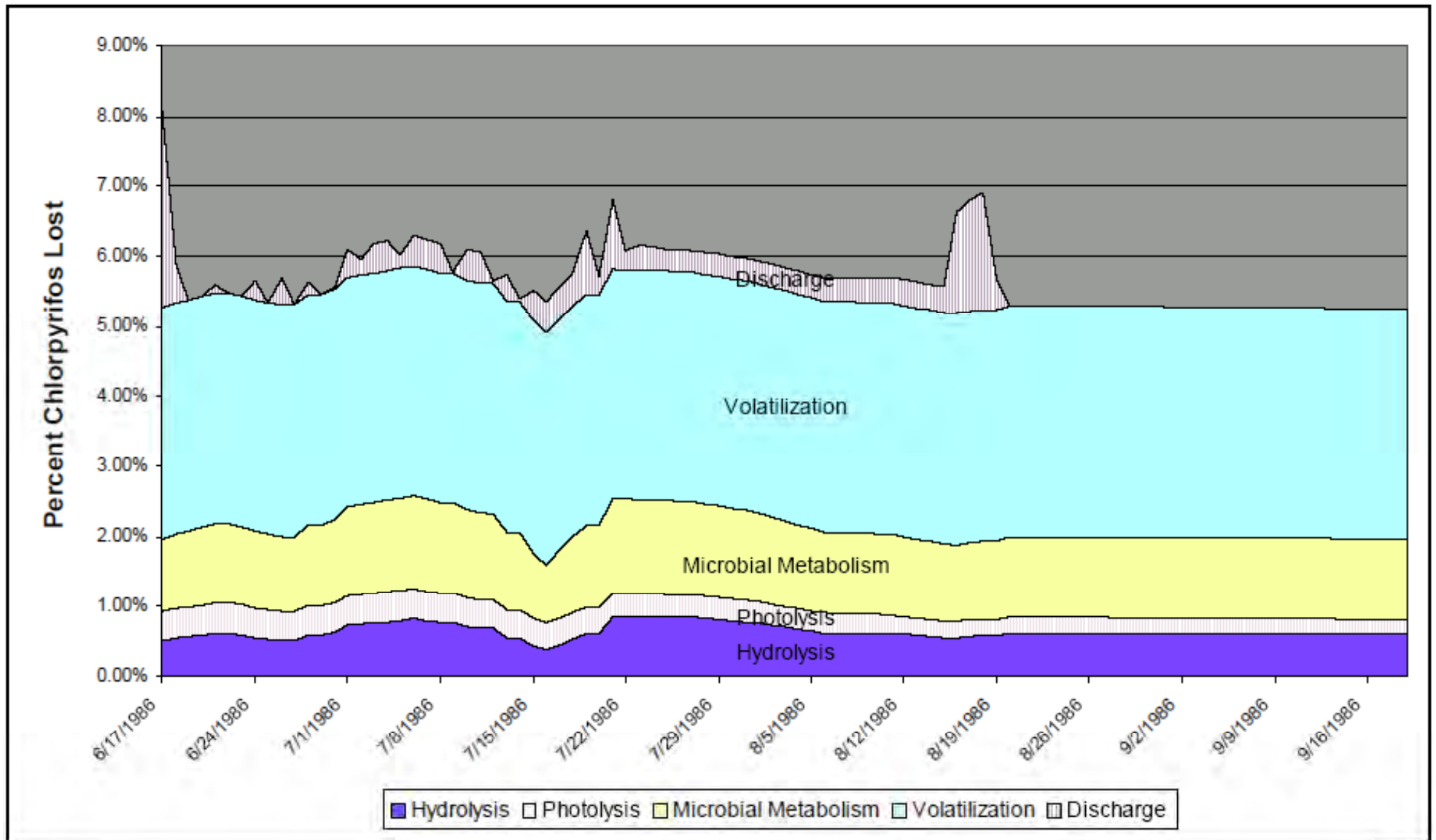
DT95 of roughly 75 days

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



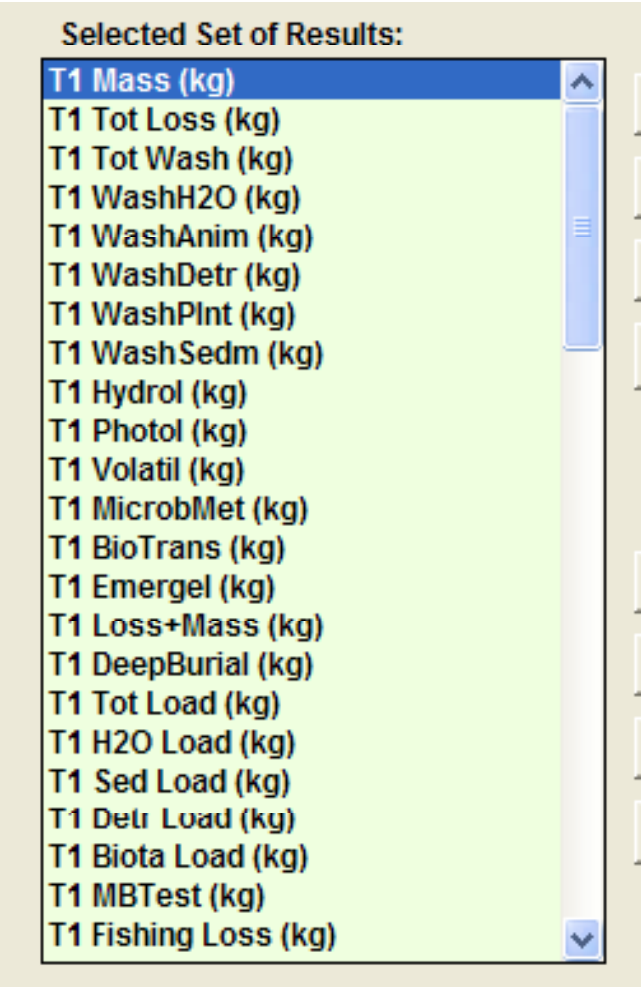
# Chemical rates may be tracked

Predicted In-situ Degradation Rates for Chlorpyrifos in Pond



# 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



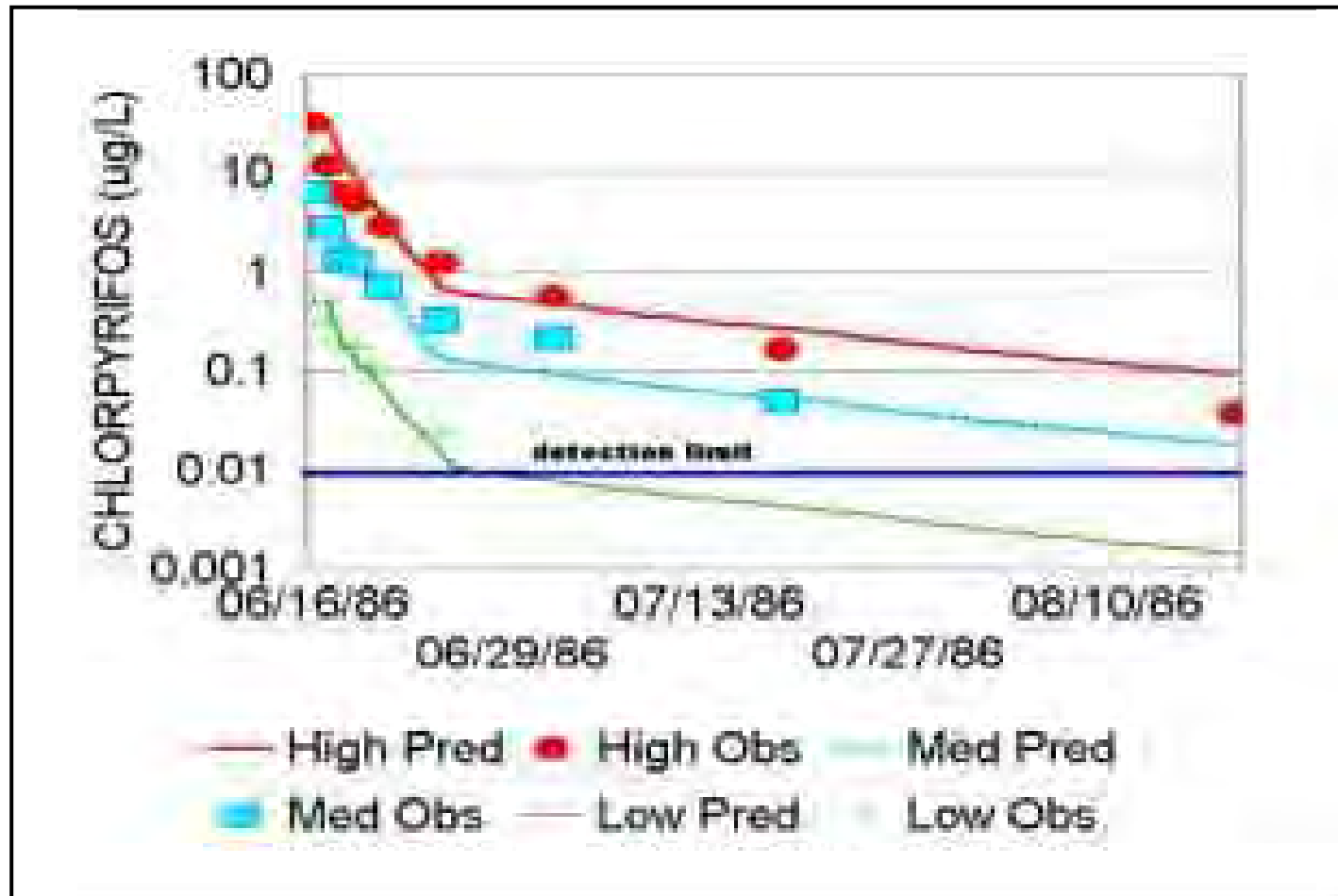
Selected Set of Results:

T1 Mass (kg)
T1 Tot Loss (kg)
T1 Tot Wash (kg)
T1 WashH2O (kg)
T1 WashAnim (kg)
T1 WashDetr (kg)
T1 WashPInt (kg)
T1 WashSedm (kg)
T1 Hydrol (kg)
T1 Photol (kg)
T1 Volatil (kg)
T1 MicrobMet (kg)
T1 BioTrans (kg)
T1 Emergel (kg)
T1 Loss+Mass (kg)
T1 DeepBurial (kg)
T1 Tot Load (kg)
T1 H2O Load (kg)
T1 Sed Load (kg)
T1 Detr Load (kg)
T1 Biota Load (kg)
T1 MBTest (kg)
T1 Fishing Loss (kg)



# Fate of Chlorpyrifos in the Duluth MN Pond was Predicted Successfully

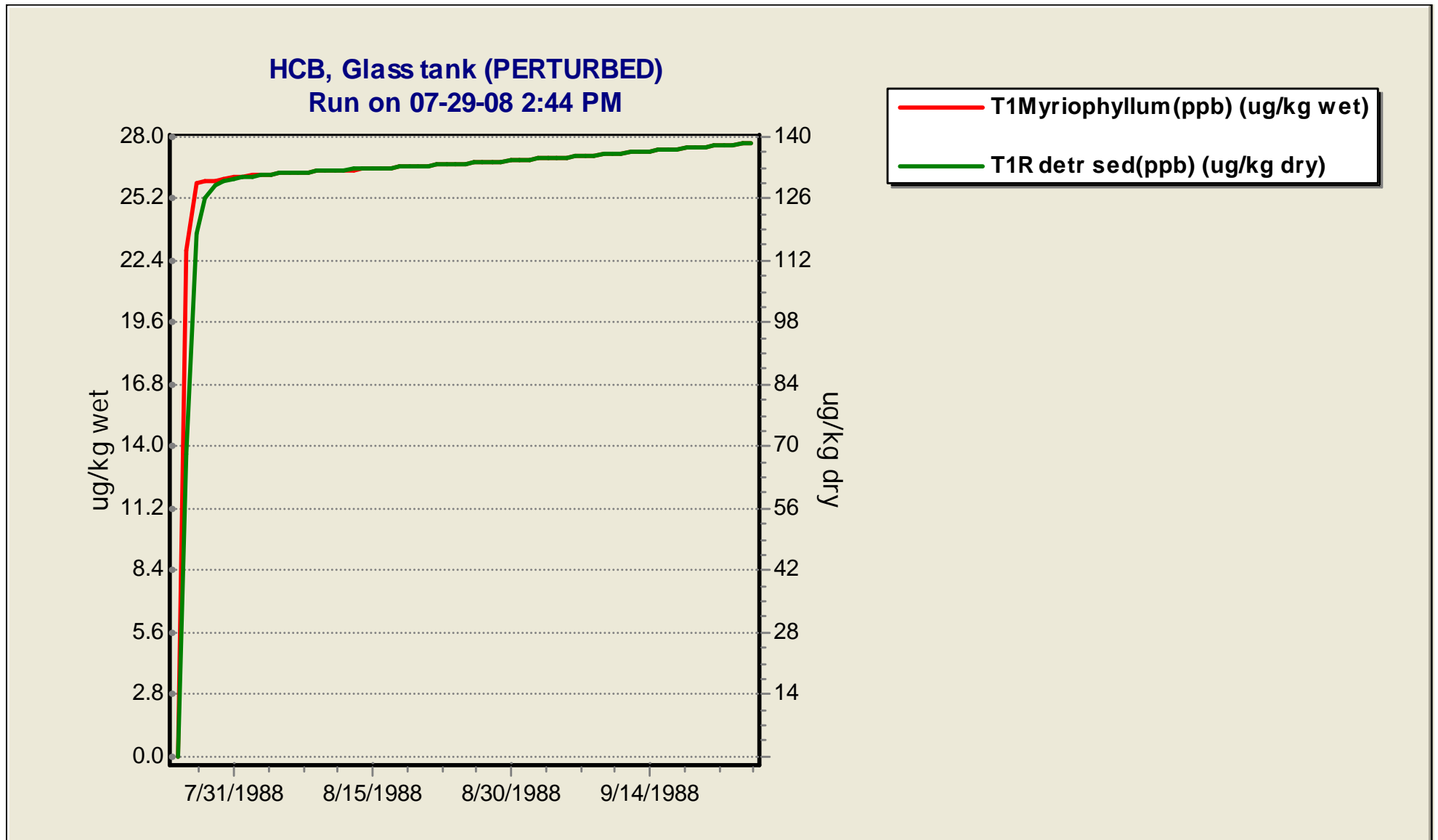
Multiple Dosing Levels



# HCB in tank

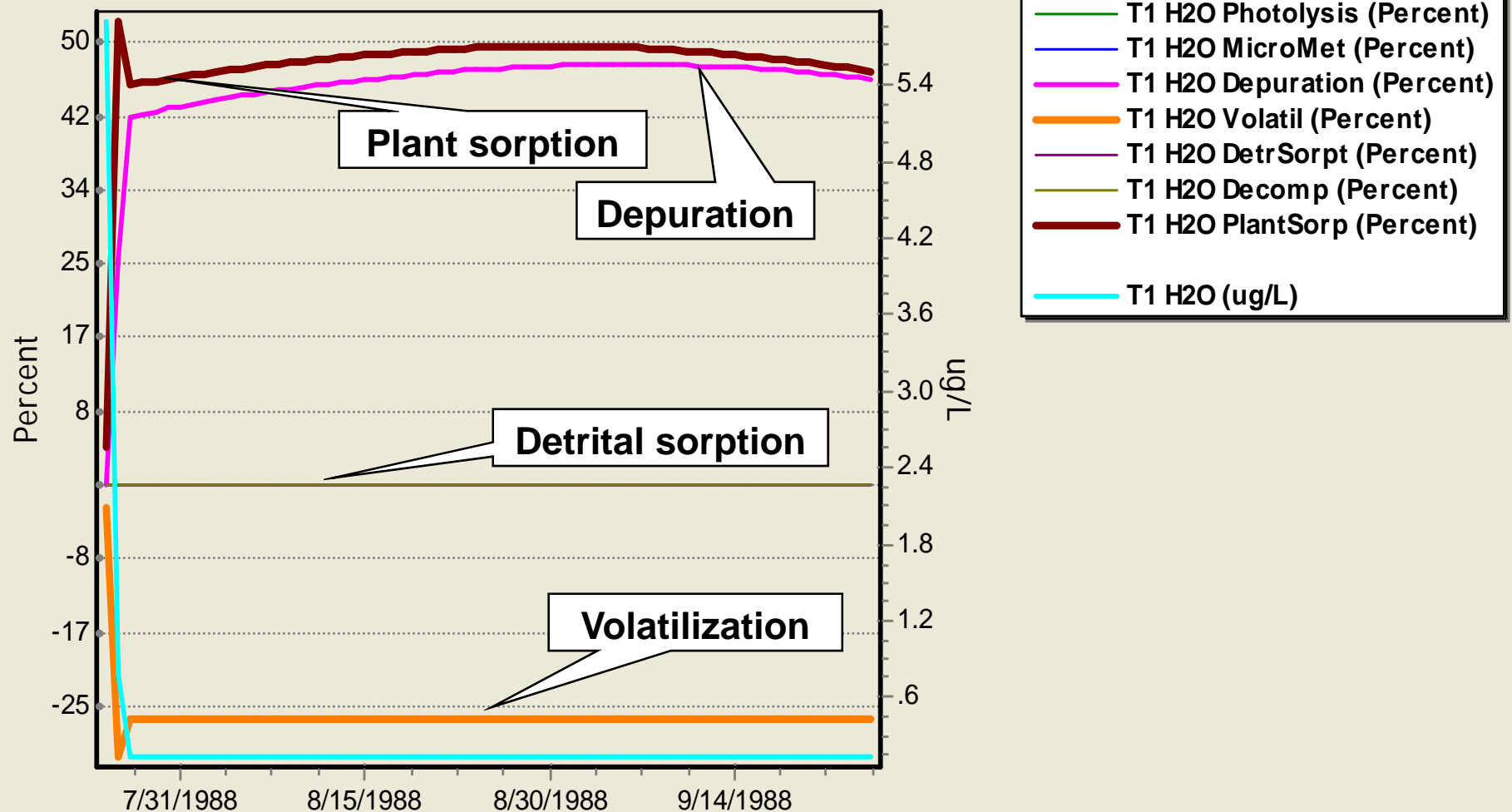
- Reproduces experimental results (Gobas) in which macrophytes are enclosed in an aquarium tank
- A single dose of hexachlorobenzene is applied at the beginning of the simulation
- Simplest type of AQUATOX model setup

# HCB is taken up rapidly by macrophyte and by organic sediments



# HCB loss rates can be plotted, showing that sorption to detritus is negligible (due to mass)

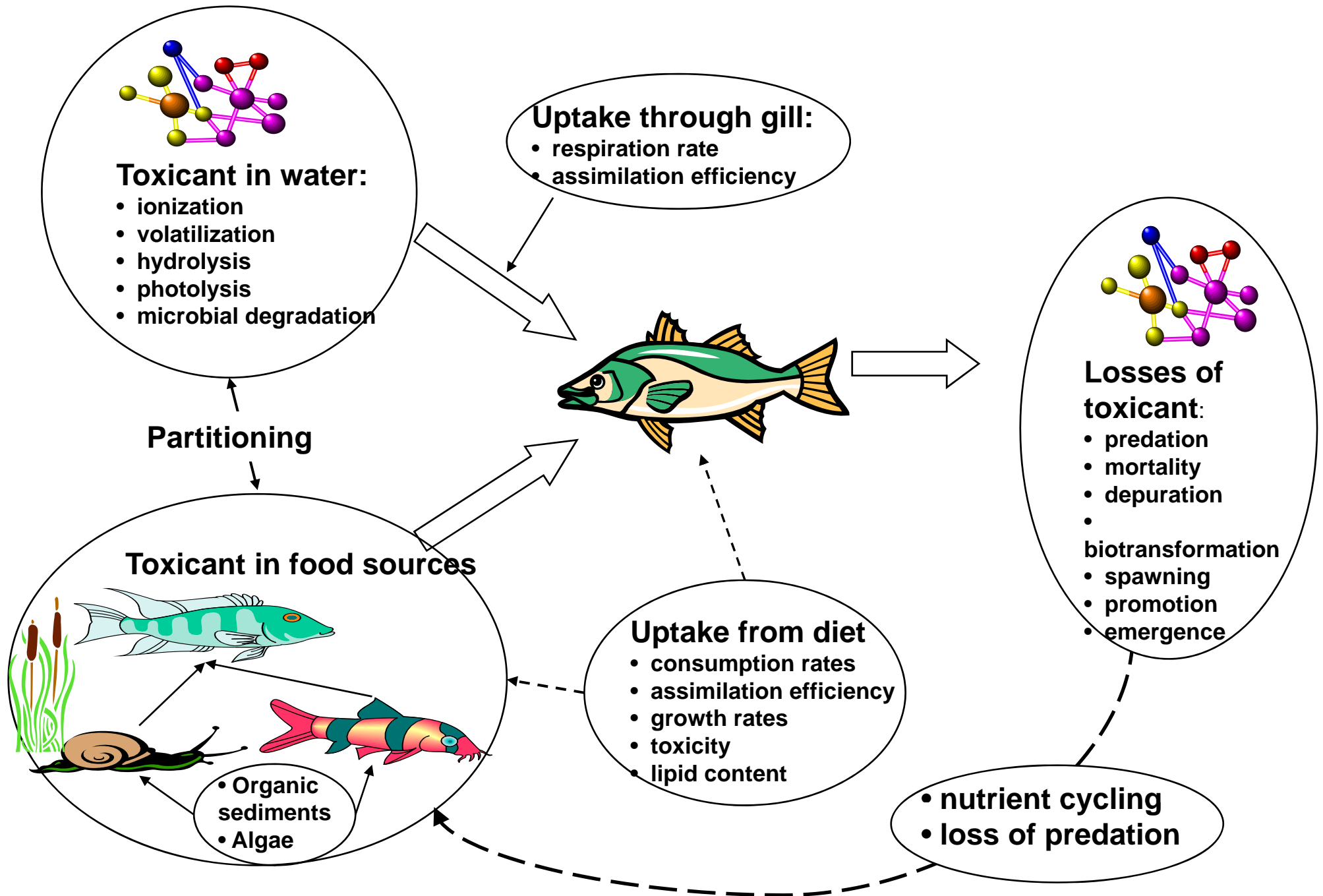
HCB, Glass tank (PERTURBED)  
Run on 07-29-08 2:44 PM



# Chemical Bioaccumulation Overview

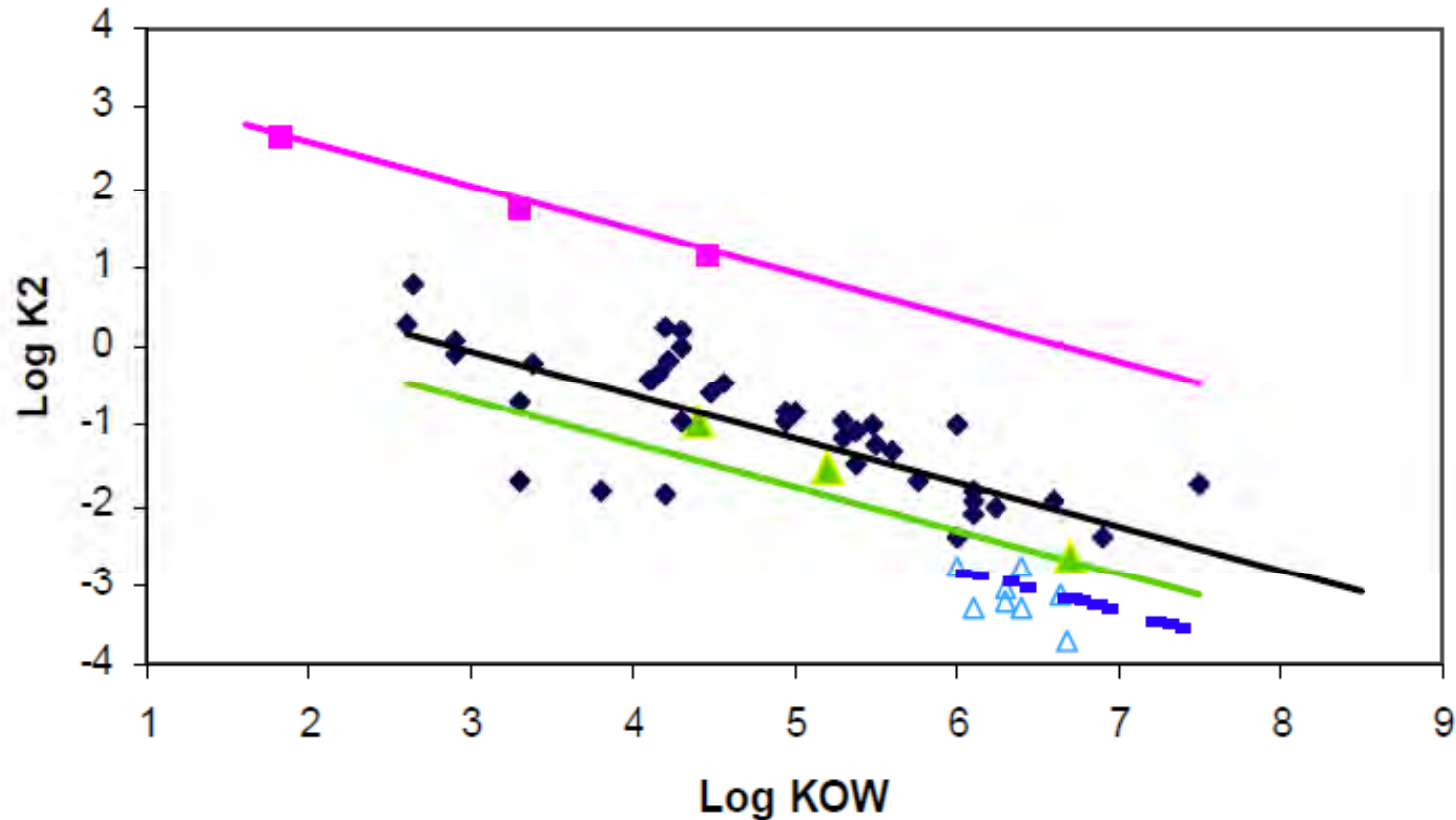
- Kinetic model of uptake and depuration
  - Uptake through gill
  - Uptake through diet
    - Consumption rate
    - Assimilation efficiency
  - Loss through depuration, biotransformation, growth dilution (implicit)
- Alternative (simple) BCF model available

# Bioaccumulation in AQUATOX



# Depuration Rate Constants for Invertebrates and Fish

## K2 for Various Animals



# Alternative Chemical Uptake Model

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

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

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

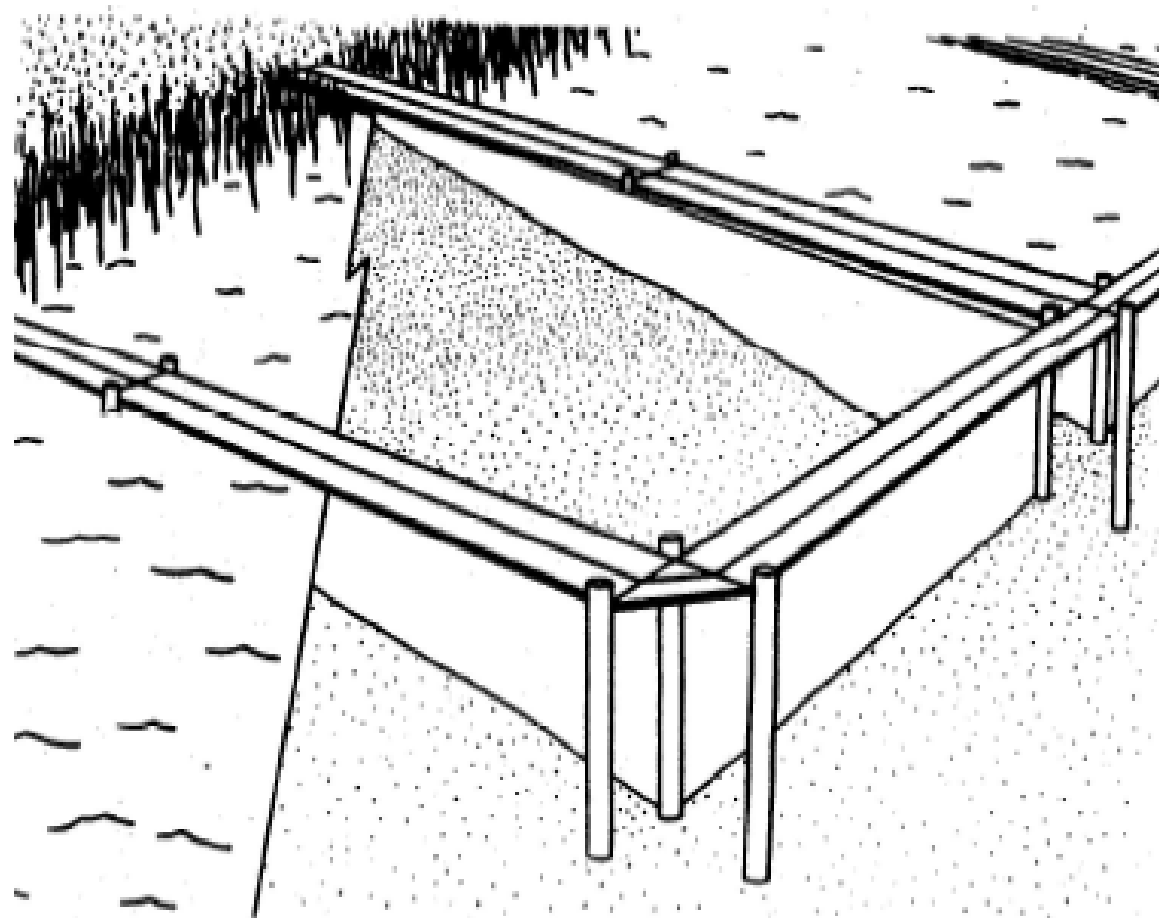
Dietary uptake of chemicals by animals is not affected by this alternative parameterization.



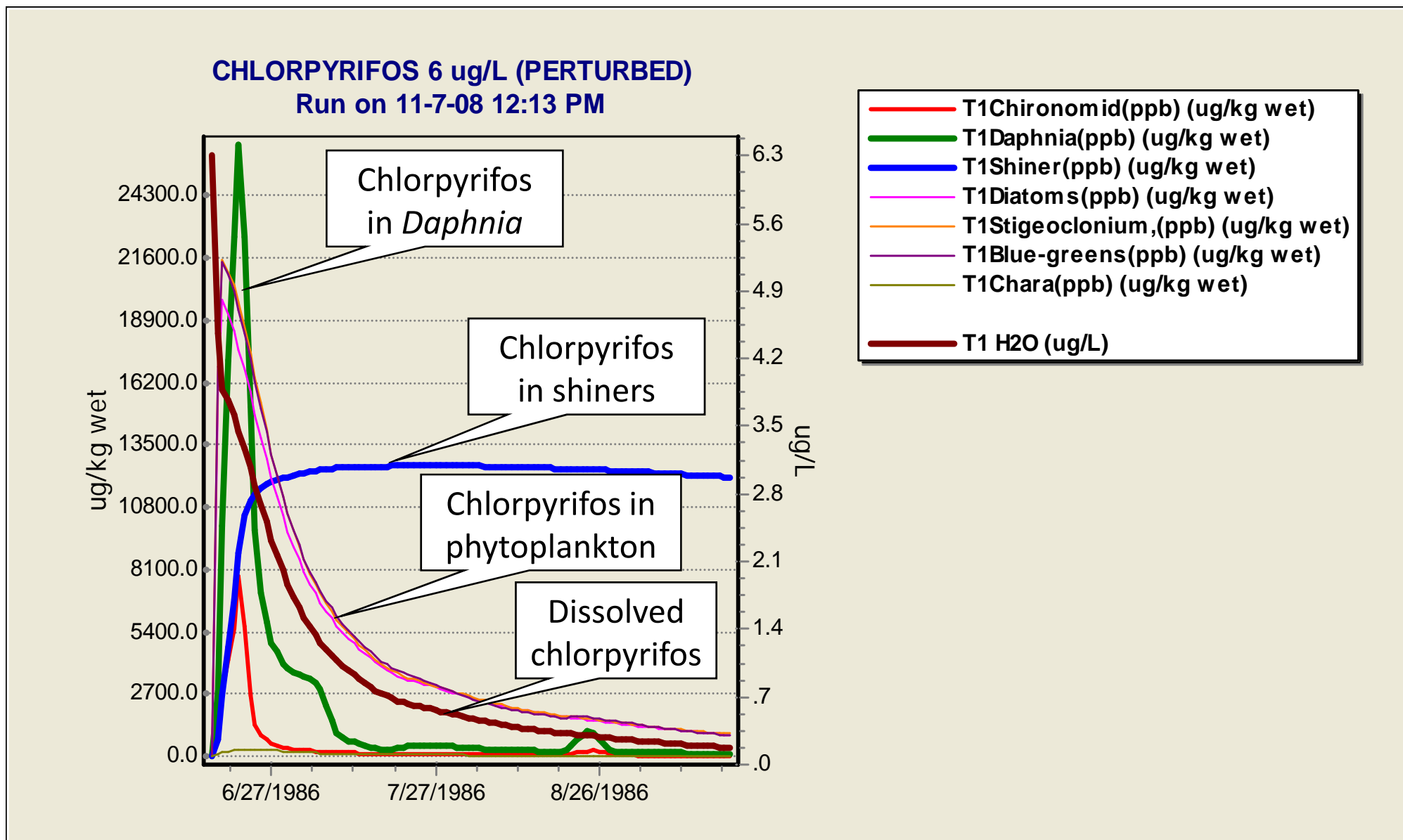
# Chlorpyrifos in Pond

- 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

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

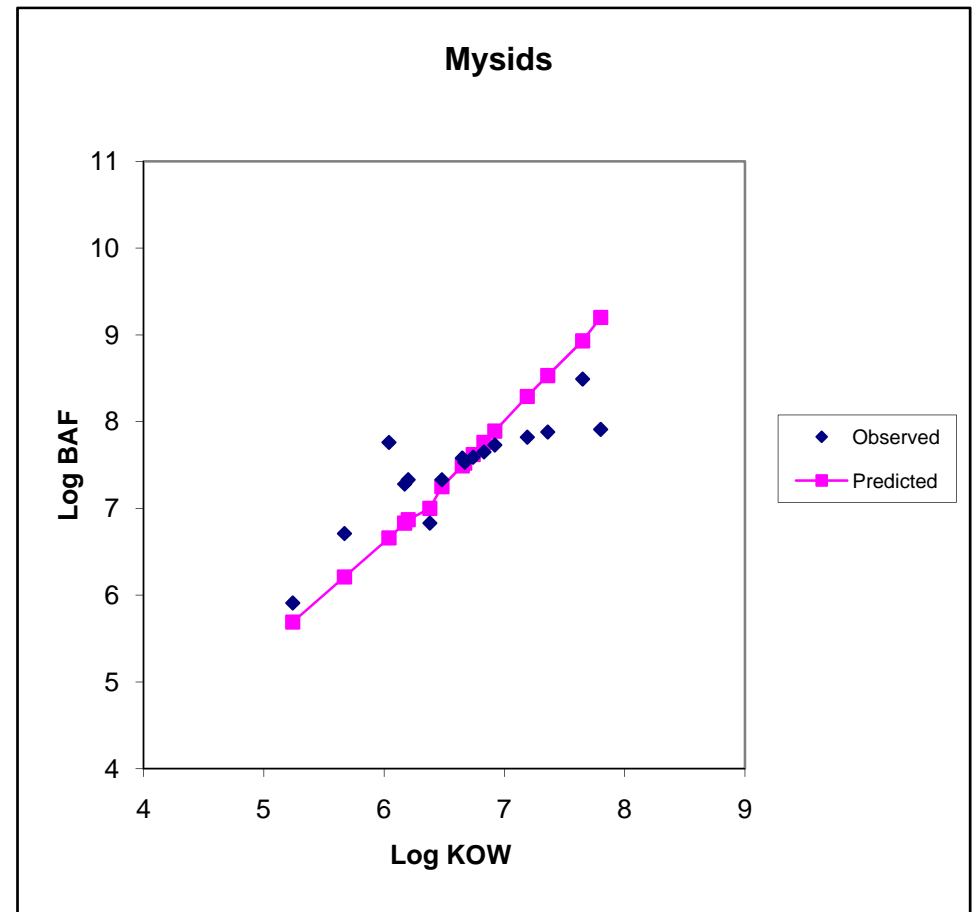
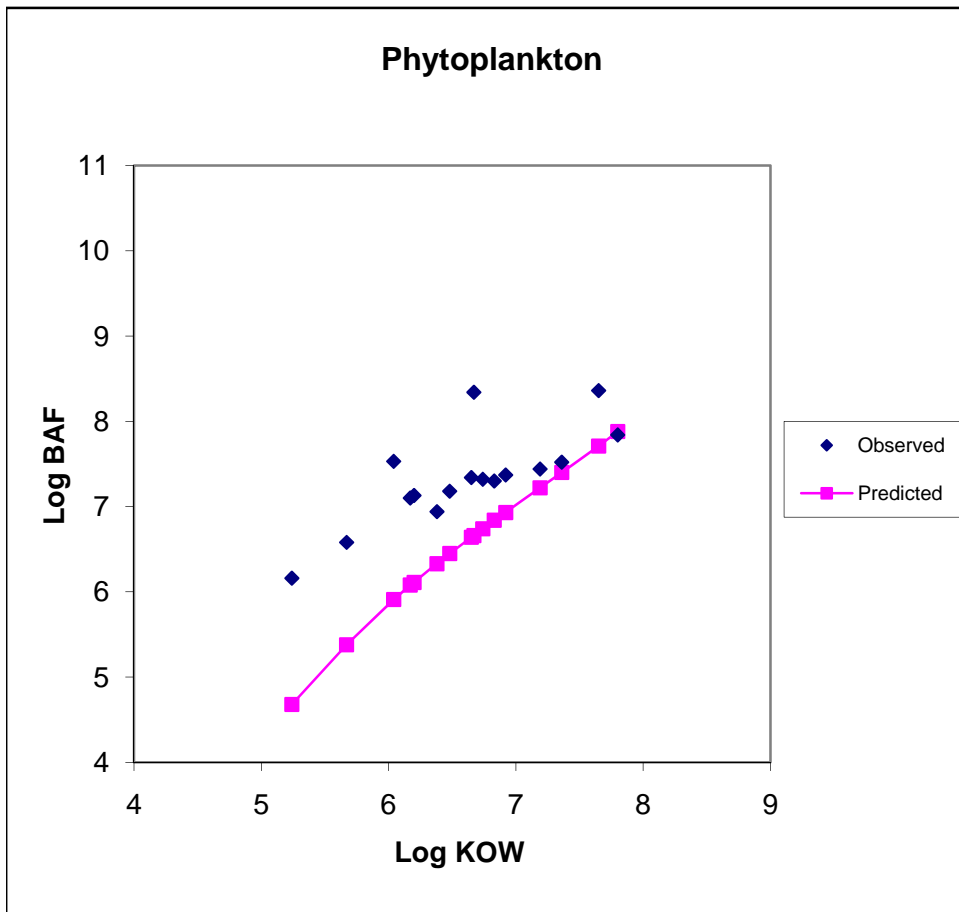


# Can trace how the toxicant is partitioned in the biota



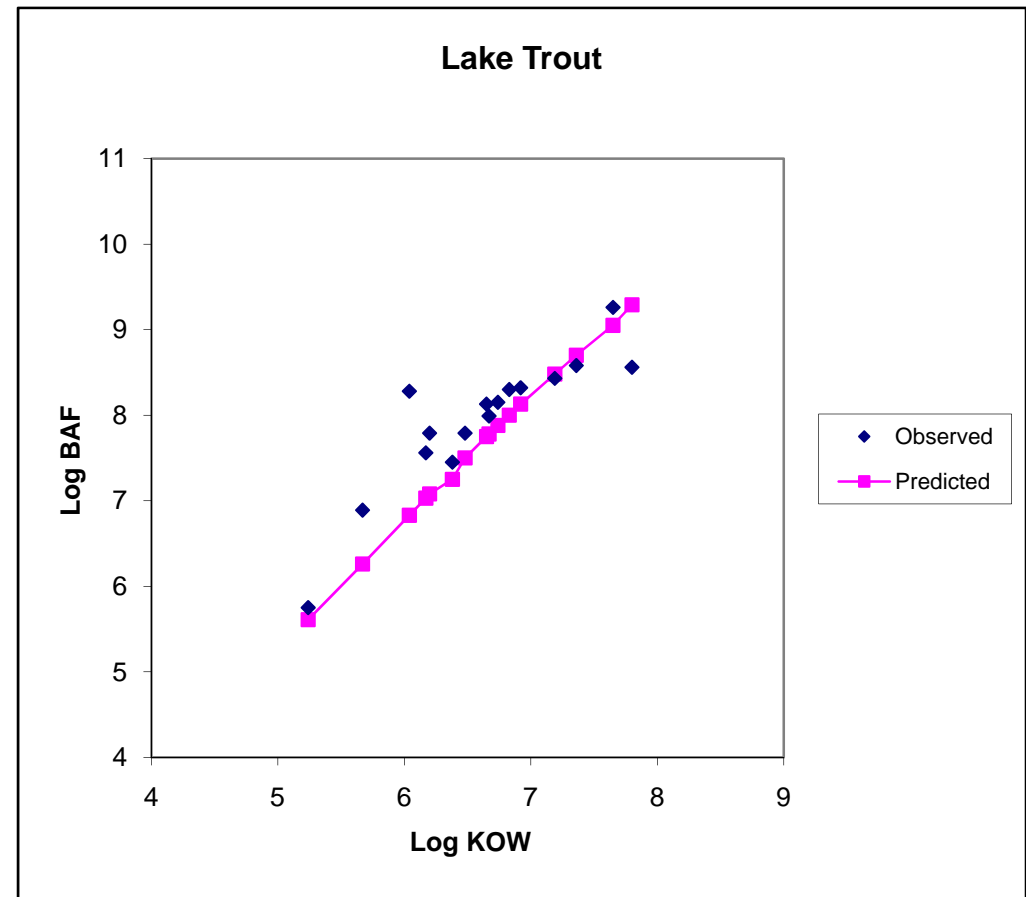
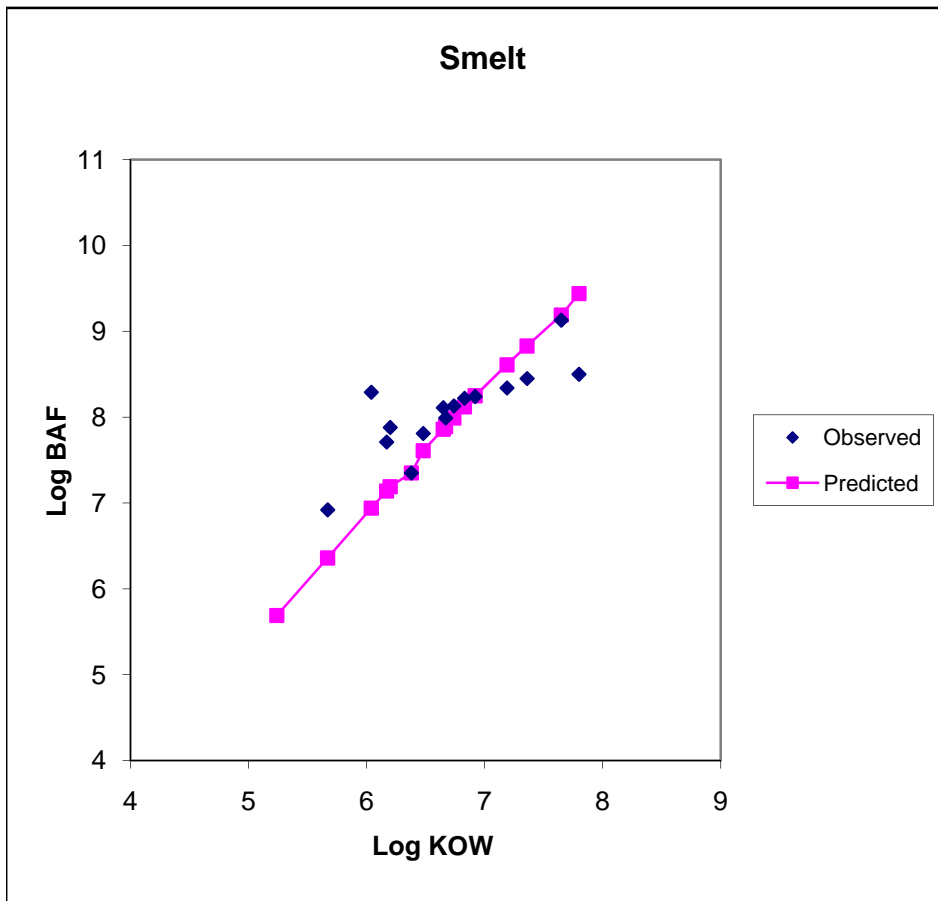
# Lake Ontario Bioaccumulation

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

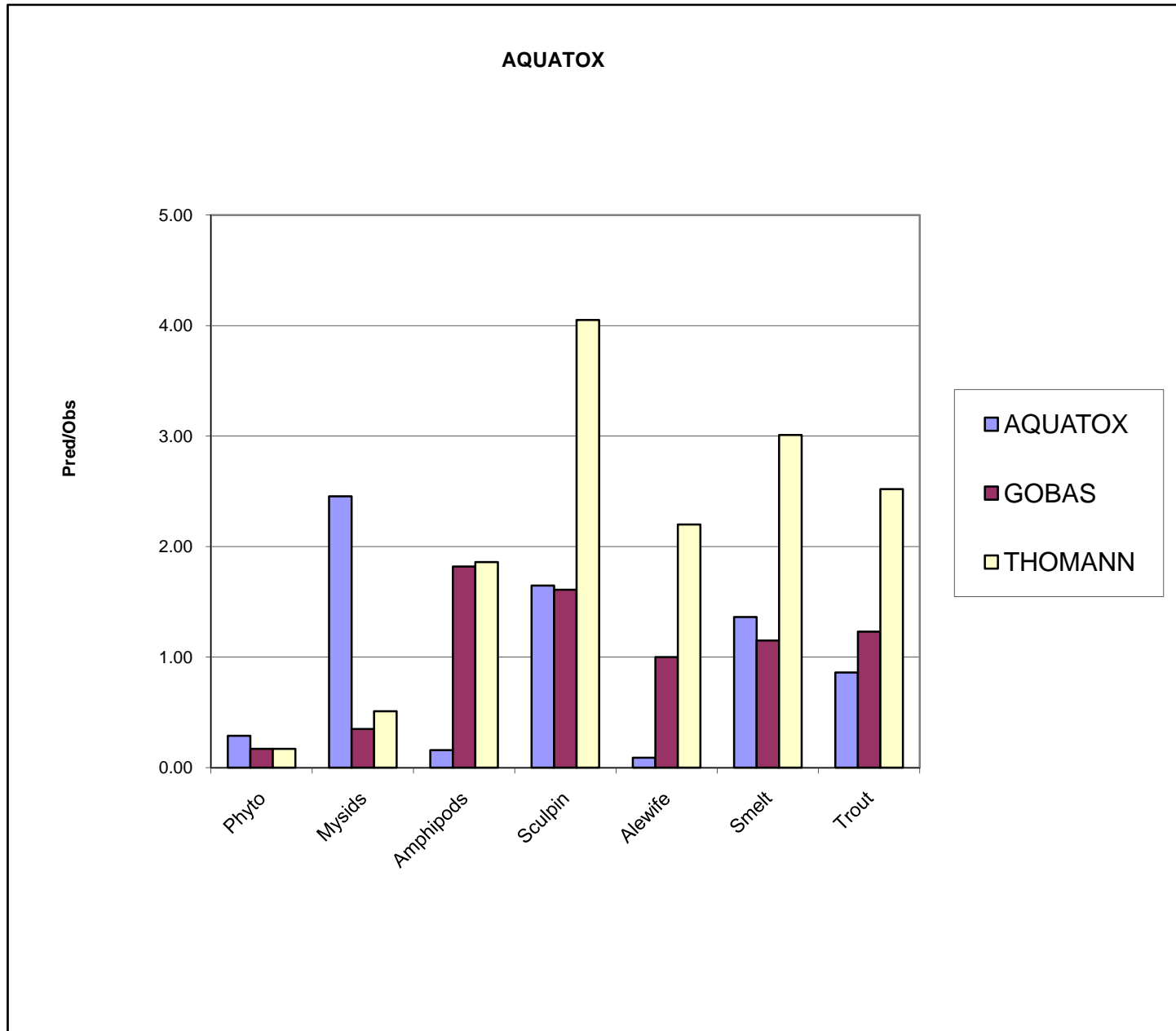


# Lake Ontario Bioaccumulation

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



# Lake Ontario BAF model comparison

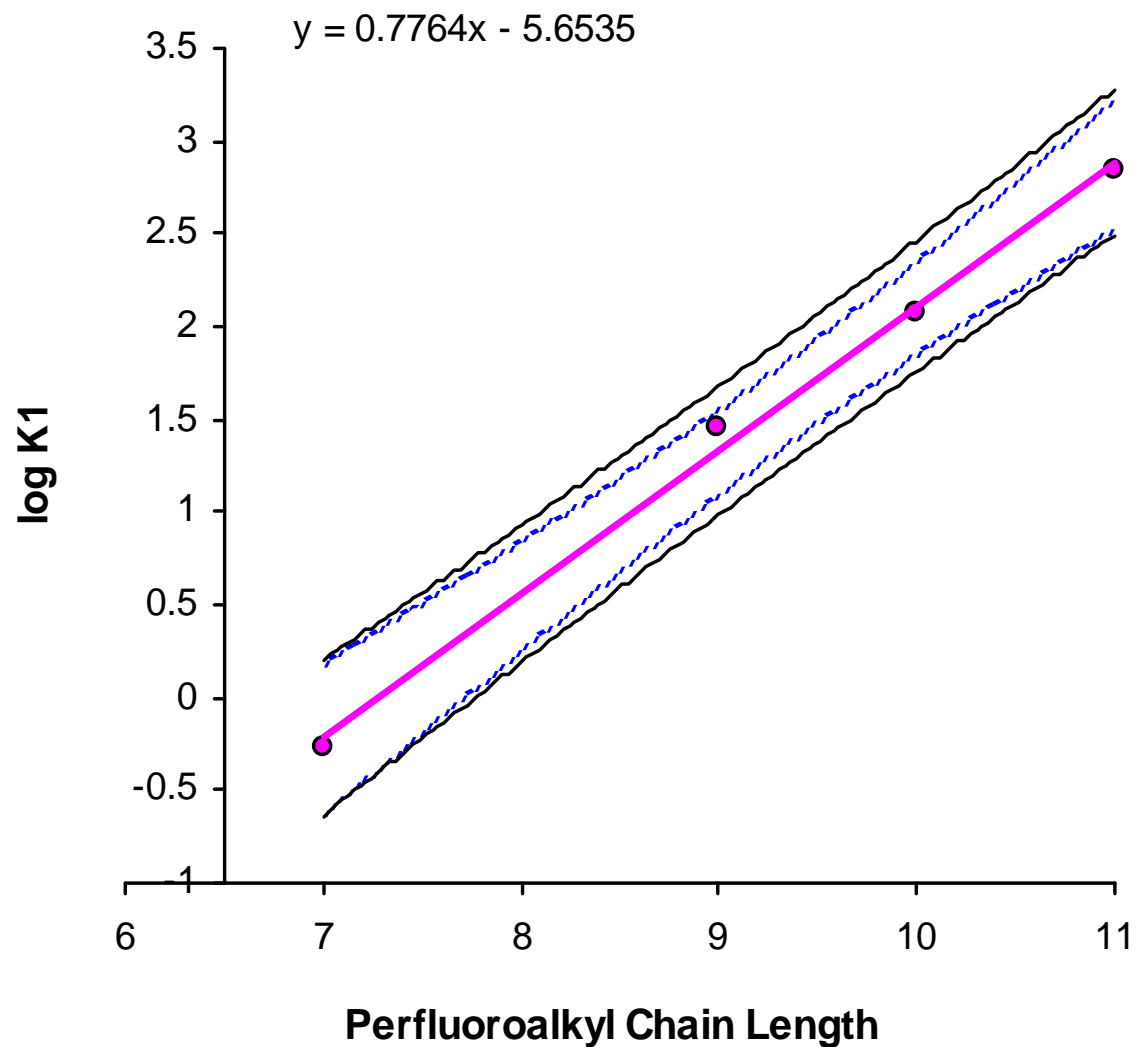


# Perfluorinated Surfactants (PFAs)

- 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

# Uptake of carboxylates can be predicted by chain length

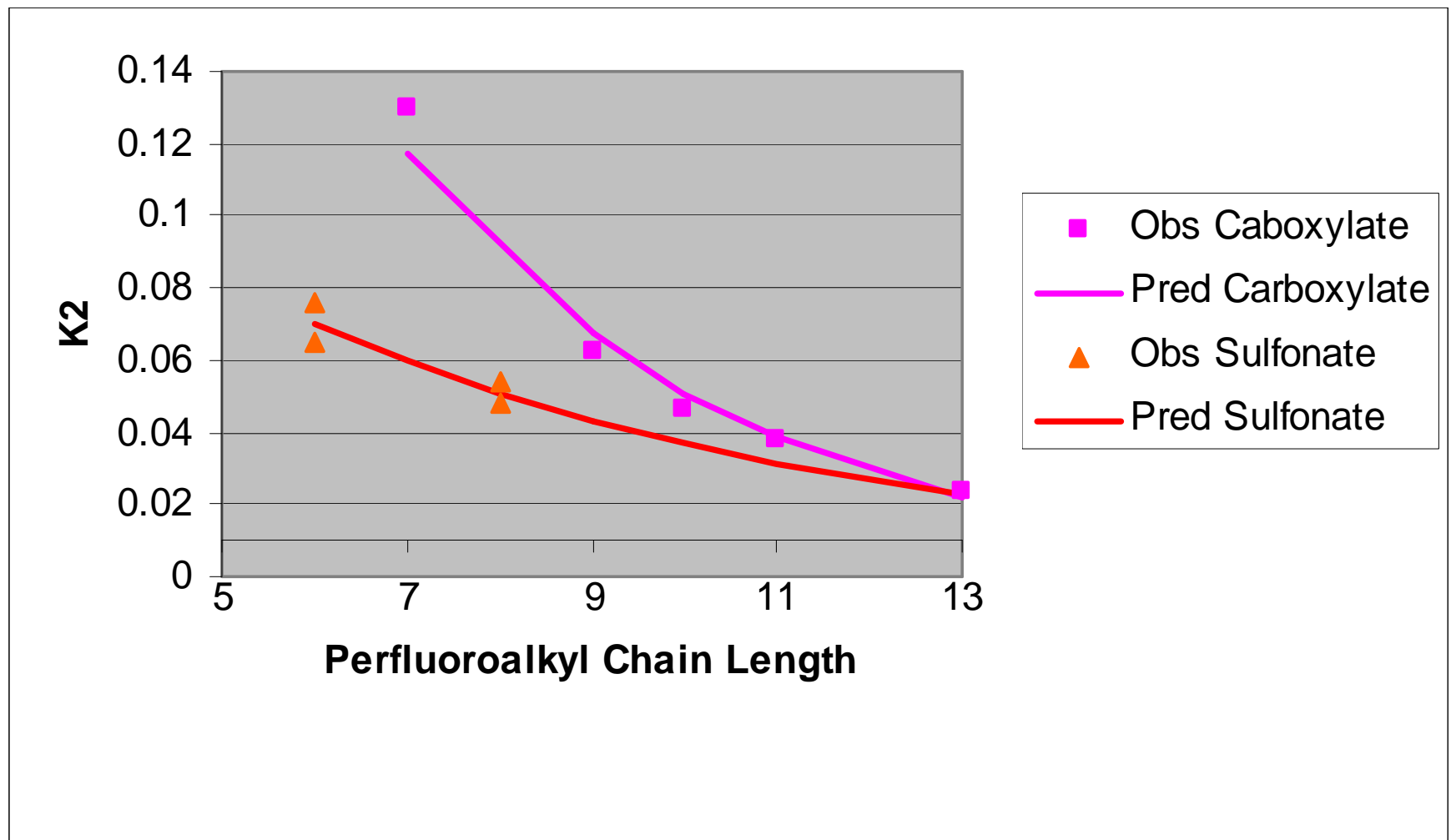
*data from Martin et al., 2003*





# Depuration rate is also a function of chain length

*data from Martin et al., 2003*



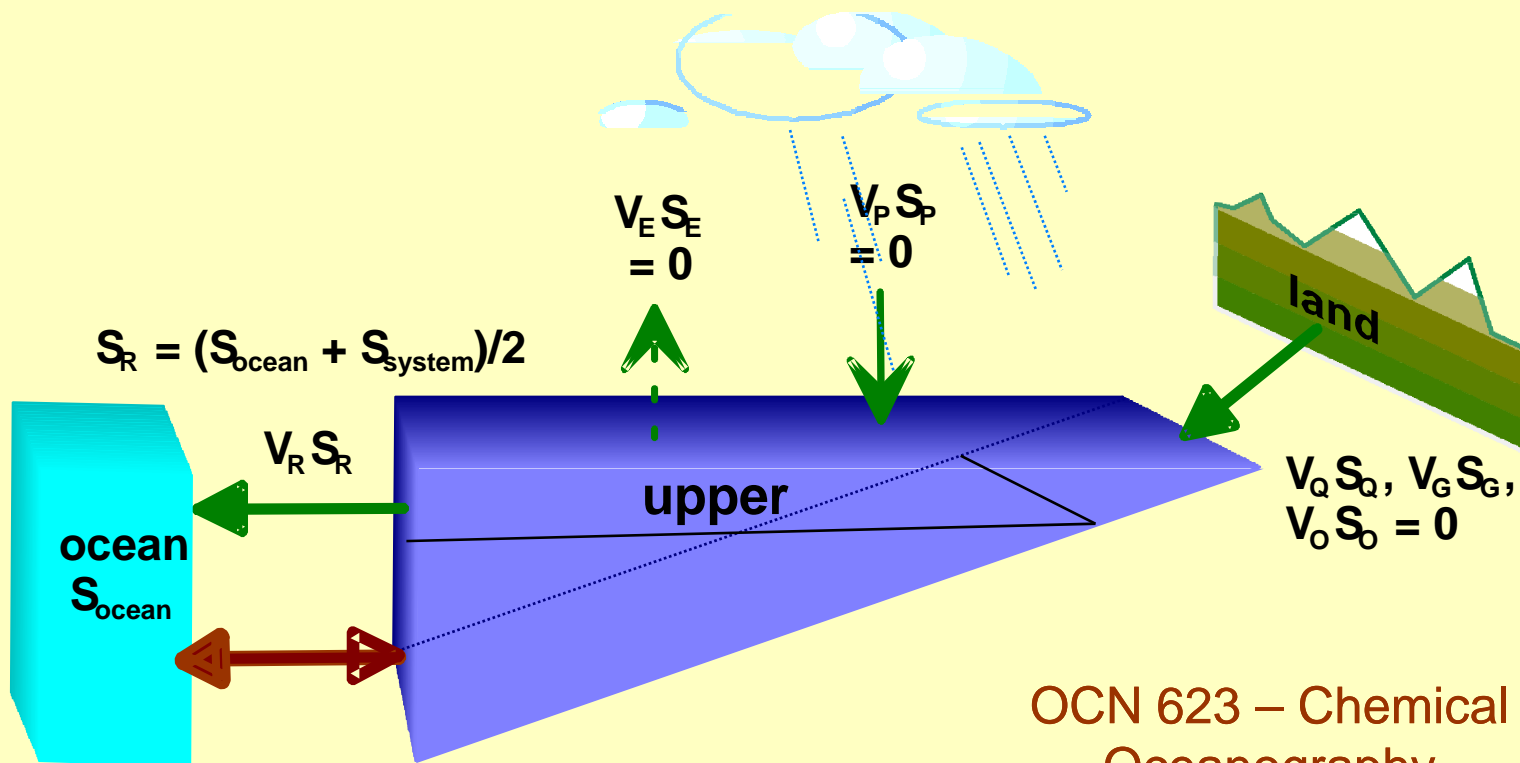
# Estuarine version applied to Galveston Bay, Texas, to evaluate toxicants



Photo Courtesy NASA Johnson Space Center

# Estuarine Features

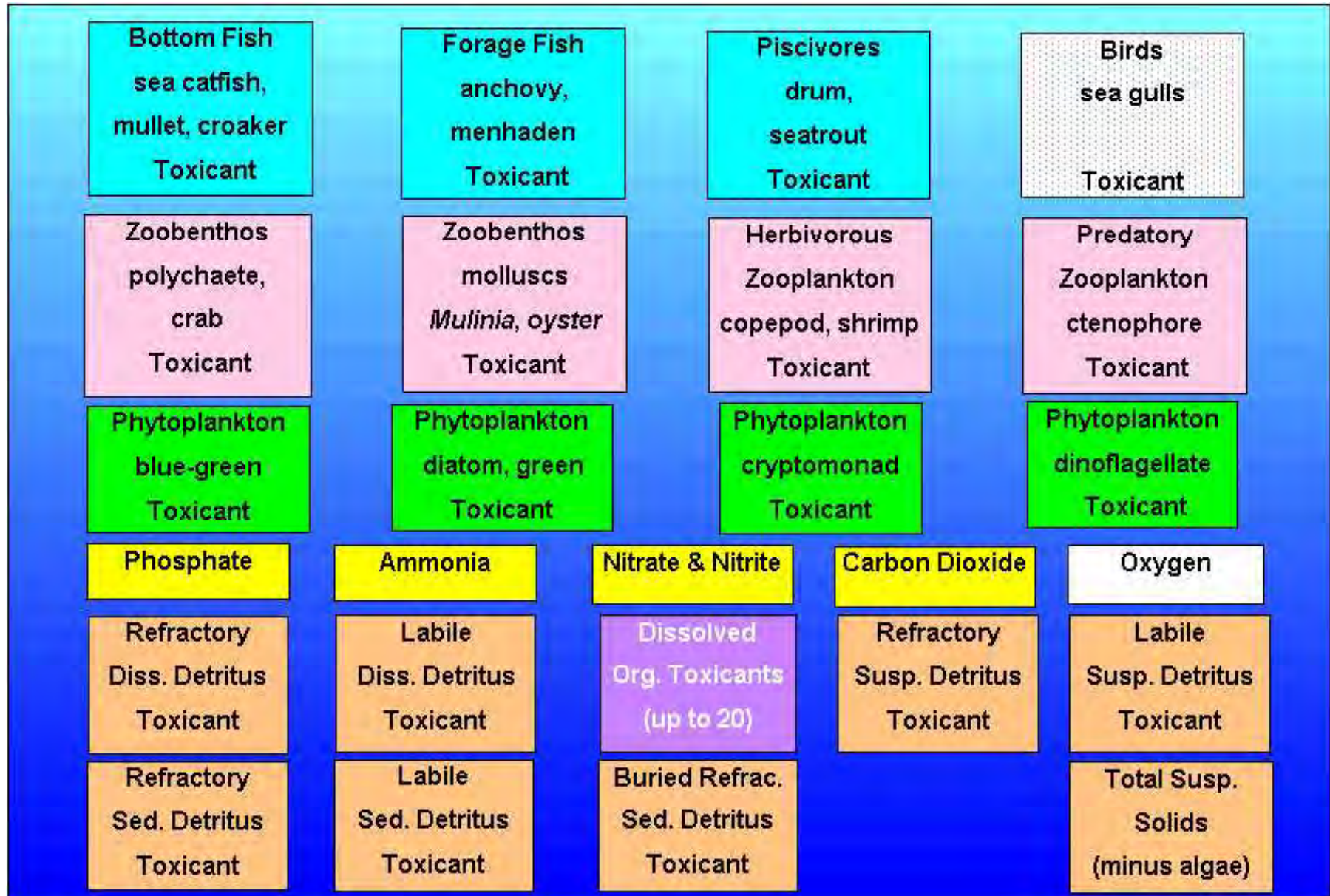
- Stratification – salt wedge
- Water Balance – salt balance approach
- Entrainment Process – lower to upper layers



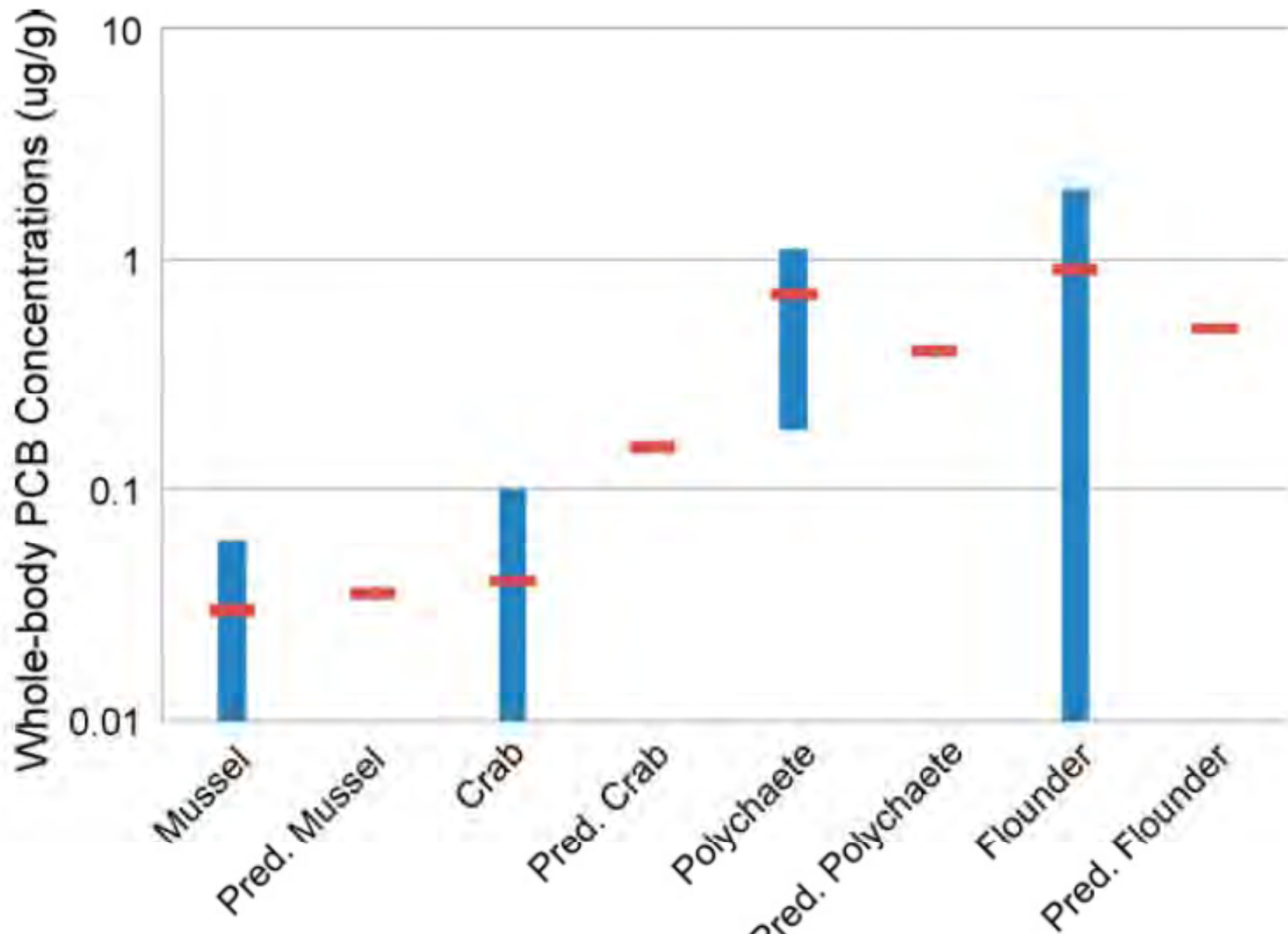
# Estuary Model Data Requirements

- 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

# Galveston Bay, Texas, compartments

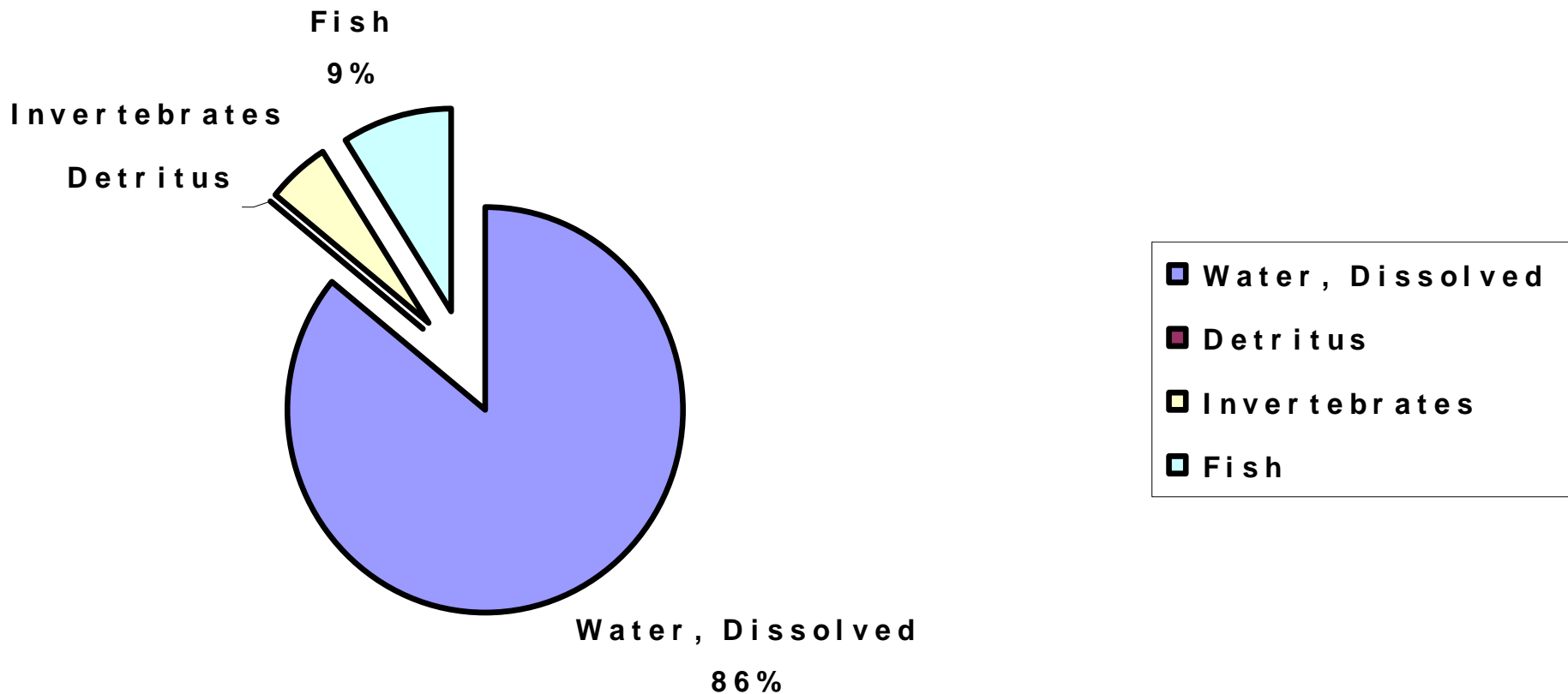


# Validation: New Bedford Harbor MA, observed & predicted PCB values are comparable



Park et. al, 2008, Figure 7, data from Connolly, 1991

# Predicted distribution of PFOS among major compartments in Galveston Bay at end of year



# 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)



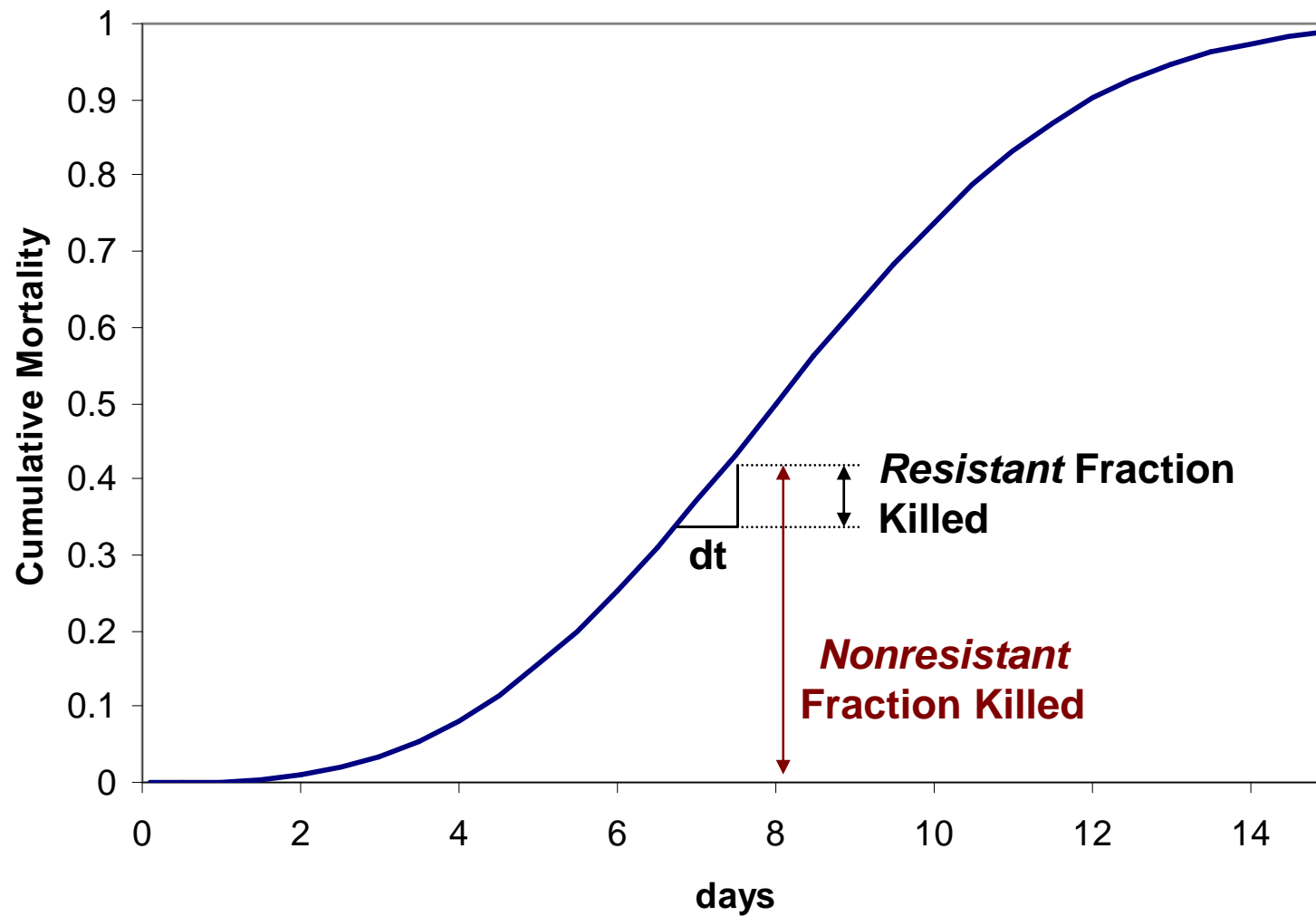
# Toxicity Models within Bioaccumulation Models

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	★			★

# Steps Taken to Estimate Toxicity

- Enter  $LC_{50}$  and  $EC_{50}$  values
  - $LC_{50}$  estimators are available for species
- Compute internal  $LC_{50}$
- Compute infinite  $LC_{50}$  (time-independent)
- Compute t-varying internal lethal concentration
- Compute cumulative mortality
- Compute biomass lost per day by disaggregating cumulative mortality
- Sublethal toxicity is related to lethal toxicity through an application factor
- Option has been added to use external concentration.

# Disaggregation of Cumulative Mortality



# New Option to Model with External Concentrations

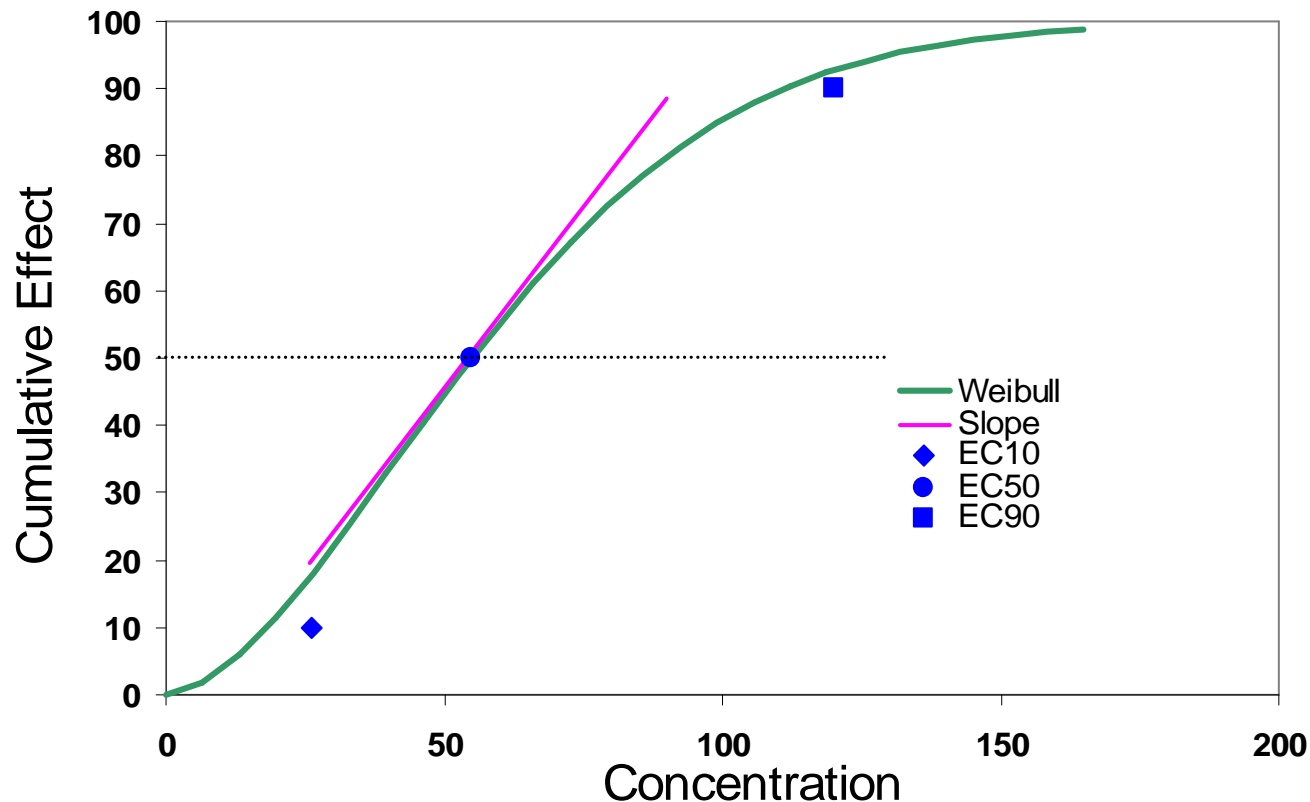
Two-parameter Weibull distribution as in Christensen and Nyholm (1984)

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

Two Required Parameters:

LC50 (or EC50)

“Slope Factor” = Slope at LC50 multiplied by LC50

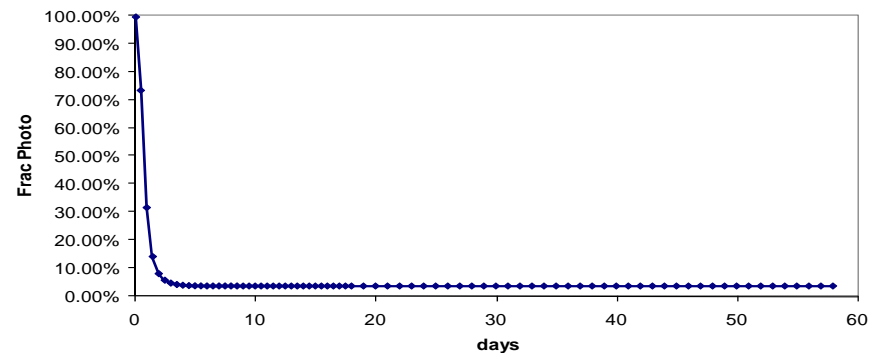
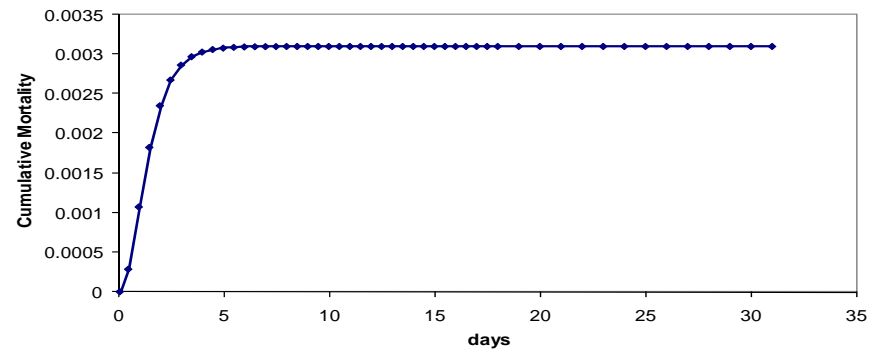
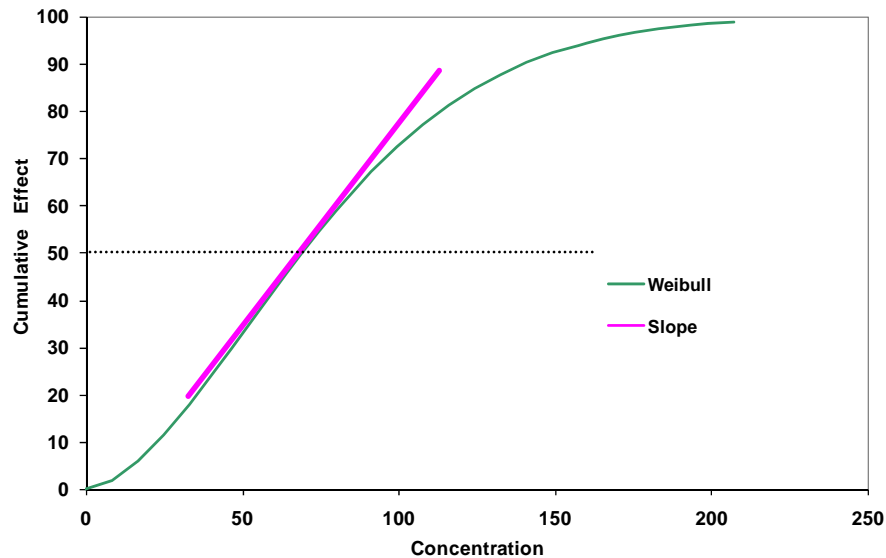


# Spreadsheet Demo

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

## AQUATOX\_Internal\_Toxicity\_Model.xls

## AQUATOX\_External\_Toxicity\_Model.xls



# Chemical Toxicity Screen

## Chemical Toxicity Parameters -- Chlorpyrifos

Animal Toxicity Data

Add Animal Toxicity Record

Export Grid to Excel (to print)

To delete a record,  
press <Ctrl> <Del>

Drift Threshold only  
relevant to zoobenthos

Animal name	LC50 (ug/L)	LC50 exp. time (h)	LC50 comment	K2 Elim. rate const (1/d)	K1 Uptake const (L/kg d)	BCF (L/kg)	Biotransfm. rate (1/d)	EC50 growth (ug/L)	Gro
▶ Trout	8.701	96	Regression on Bluegill	1.9E-03			0	0.71	
Bluegill	2.4	96	EPA Duluth '88, p. 124	7.6E-03			0	0.17	
Bass	9.849	96	Regression on Bluegill	3.3E-03			0	1.2439	
Catfish	387.174	96	Regression on Bluegill	3.7E-03			0	28	
Minnow	203	96	Holcombe et al., 1982	1.85E-02			0	20.3	
Daphnia	0.17	24	EPA '87, p. 42 (Duluth)	9.15E-02			0	0.09	
Chironomid	1.416	24	Regression on Daphnia	5.32E-02			0	0.5798	
Stonefly	10	96	Mayer & Ellersieck, 1982	4.03E-02			0	1	
Ostracod	2.055	24	Regression on Daphnia	6.93E-02			0	0.5776	
Amphipod	0.29	48	EPA '87, p. 42 (Duluth)	6.93E-02			0	0.011	
Other	0	96		0E+00			0	0	

Enter or Estimate K2, Calculate K1 and BCF (default behavior)
  Enter K1 and K2, Calculate BCF
  Enter K1 and BCF, Calculate K2
  Enter K2 and BCF, Calculate K1

Plant Toxicity Data

Add Plant Toxicity Record

Export Grid to Excel (to print)

Plant name	EC50 photo (ug/L)	EC50 exp. time (h)	EC50 dislodge (ug/L)	EC50 comment	K2 Elim. rate const (1/d)	K1 Uptake Const (L/kg d)	BCF (L/kg)	Biotransfm. rate (1/d)
▶ Greens	0	96	0		2.4			
Diatoms	0	96	0		2.4			
Bluegreens	0	96	0		2.4			
Macrophytes	0	96	0		0.3247			

Enter or Estimate K2, Calculate K1 and BCF (default behavior)
  Enter K1 and K2, Calculate BCF
  Enter K1 and BCF, Calculate K2
  Enter K2 and BCF, Calculate K1

K1, BCF entered on a dry weight basis; lipid frac. is wet wt.

Estimate Animal K2s using Kow

Estimate Plant K2s using Kow

Interspecies Toxicity Correlation Models

Estimate plant LC50s using EC50 to LC50 ratio

Estimate animal EC50s using LC50 to EC50 ratio

Help

✓ O.K.

# Release 3: Additional Toxicity Features

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

**Interspecies Toxicity Correlation Interface**

**Available Interspecies Toxicity Correlation Models:**

Step 1: Choose a database  
ICE Aquatic Species Common Names

Step 2: Choose a surrogate species  
Brown shrimp(Penaeus aztecus)  
Brown trout(Salmo trutta)  
Bryozoa(Lophopodella carteri)  
Bryozoa(Pectinatella magnifica)  
Bryozoa(Plumatella emarginata)  
Cape Fear shiner(Notropis mekistocholas)  
**Channel catfish(Ictalurus punctatus)**  
Chinook salmon(Oncorhynchus tshawytscha)  
Coho salmon(Oncorhynchus kisutch)  
Colorado squawfish(Ptychocheilus lucius)  
Common carp(Cyprinus carpio)  
Common rangia(Rangia cuneata)  
Common starfish(Asterias forbesii)  
Copepod(Acartia clausi)  
Copepod(Acartia tonsa)  
Copepod(Eurytemora affinis)  
Copepod(Nitocra spinipes)

Step 3: Choose a predicted taxa  
Atlantic silverside(Menidia menidia)  
Black bullhead(Ameiurus melas)  
Black crappie(Pomoxis nigromaculatus)  
Bluegill sunfish(Lepomis macrochirus)  
Bonytail chub(Gila elegans)  
Brook trout(Salvelinus fontinalis)  
**Brown trout(Salmo trutta)**  
Cape Fear shiner(Notropis mekistocholas)  
Chinook salmon(Oncorhynchus tshawytscha)

Step 4: Evaluate / examine model

**Log Scale:** Confidence Interval **0.95** XMin **0** (log) XMax **6** (log)

**Surrogate:**  
Channel catfish(Ictalurus punctatus)

**Predicted:**  
Brown trout(Salmo trutta)

**Sample Size:**  
16

**Intercept (a):**  
0.5162406726

**Regression Coefficient (slope b):**  
0.6172946138

**Average Value of Predicted Taxa:**  
2.095636

**Error Mean Square (EMS):**  
1.03186928

**Standard Error of Slope (SEB):**  
0.18635262

**Correlation Coefficient:**  
0.6628634852

**Probability (Pr) that slope <> 0:**  
0.0051

Click on the regression line for more information.

Step 5: Apply Model to AQUATOX Toxicity Parameters

**The Selected Surrogate Species:**  
Channel catfish(Ictalurus punctatus)

**The Selected Predicted Species:**  
Brown trout(Salmo trutta)

**Selected Model:**  
Based on Catfish with LC50 of 7600 ug/L  
Trout LC50 will be set to 816.293 ug/L

**Is represented by the AQUATOX toxicity record:**  
Catfish

**Is represented by the AQUATOX toxicity record:**  
Trout

Execute Model

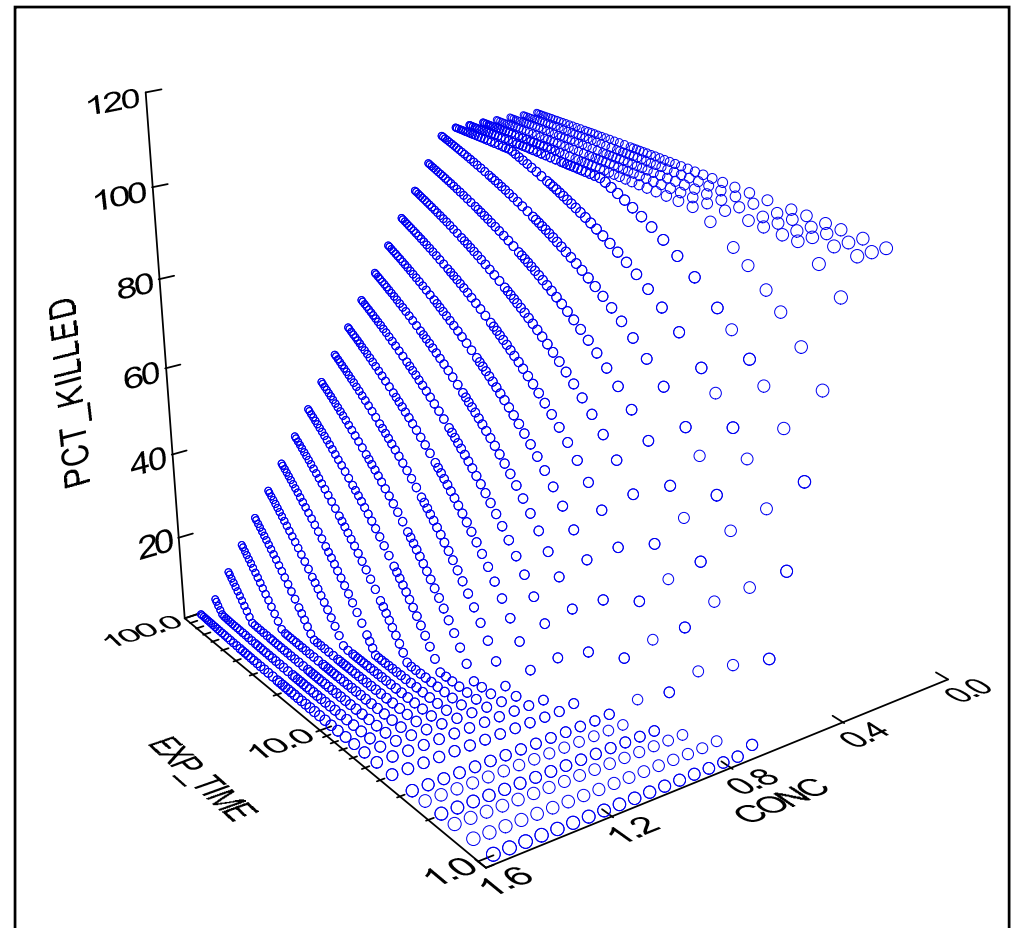
Help  
Cancel  
OK

# Release 3: Additional Toxicity Features

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

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

Includes non-lethal effects on consumption and reproduction



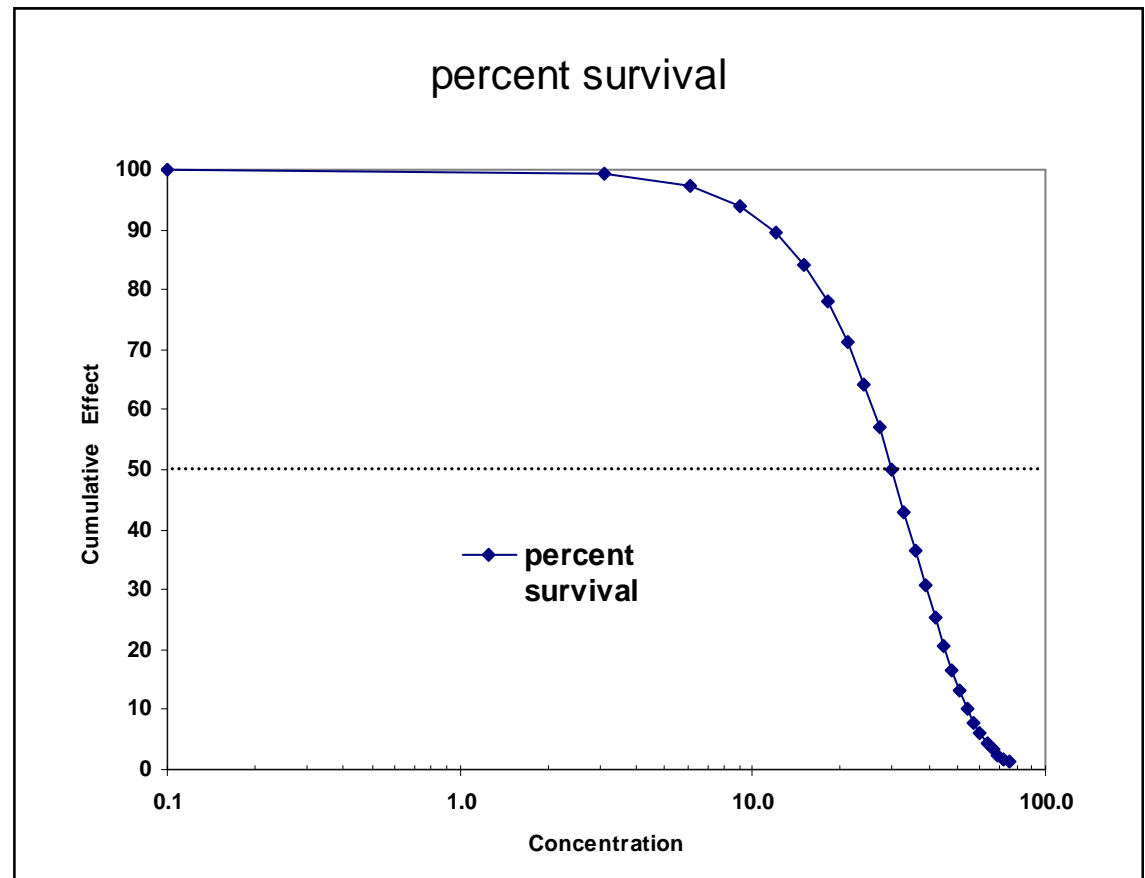


# Release 3: Additional Toxicity Features

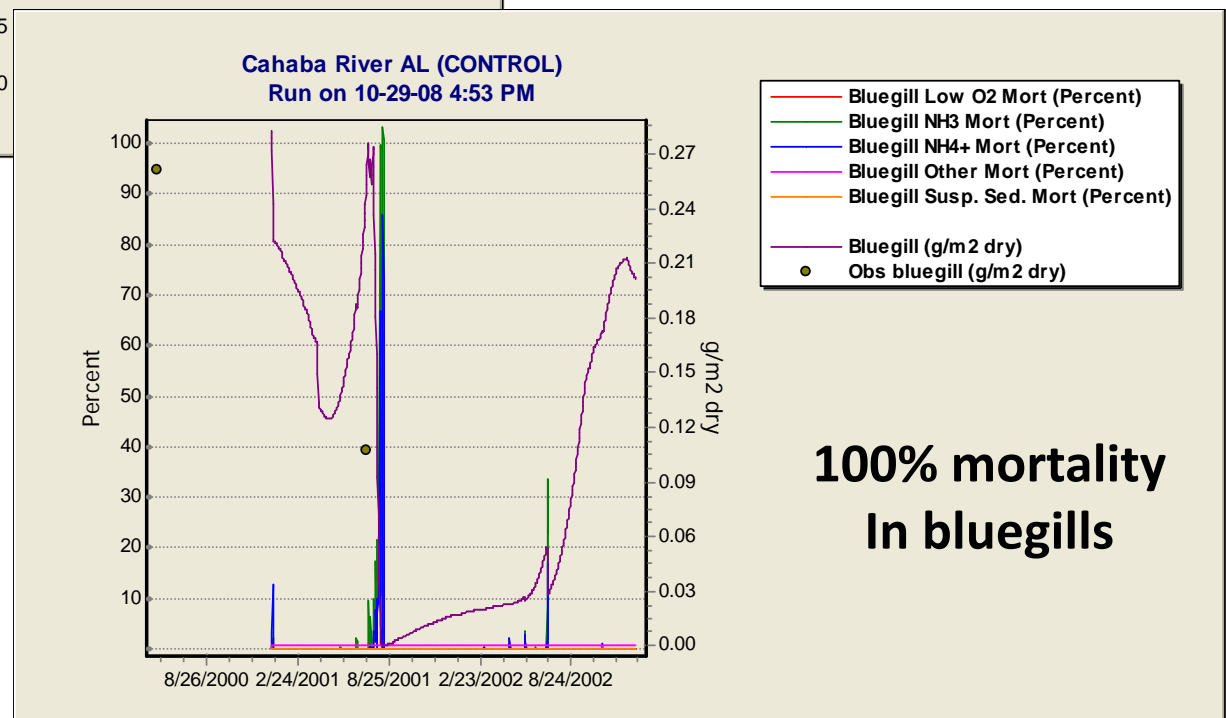
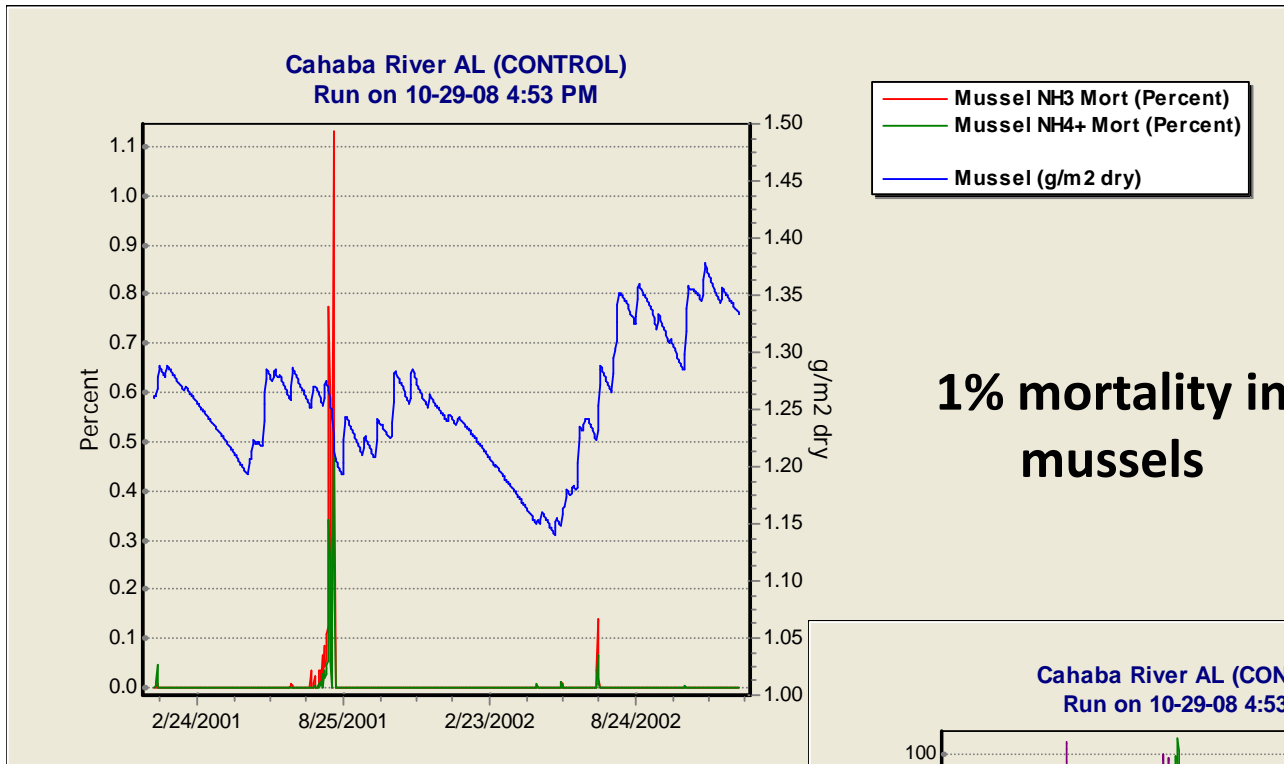
- Integration with ICE: a large EPA database of toxicity regressions
- DO effects
- Ammonia effects

External Toxicity Model Utilized

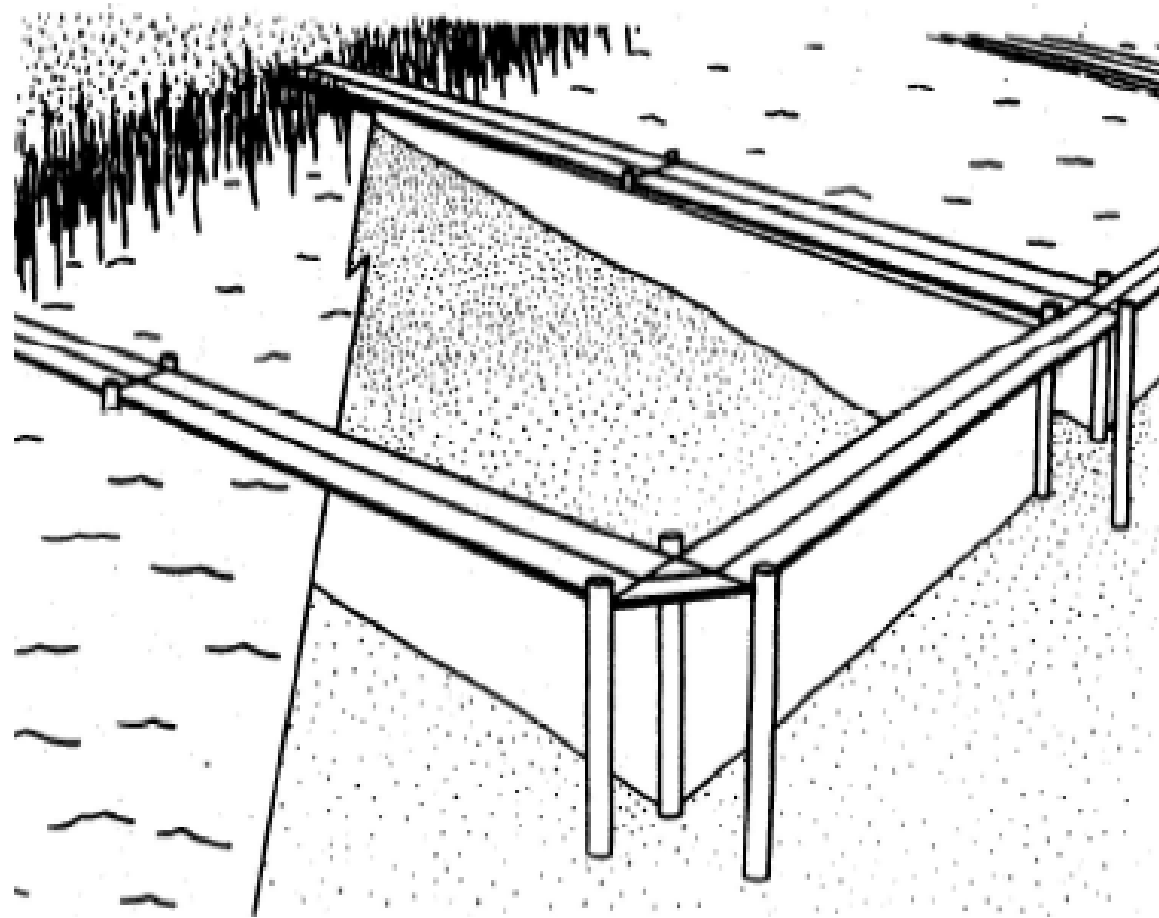
Effects from un-ionized and ionized ammonia are additive



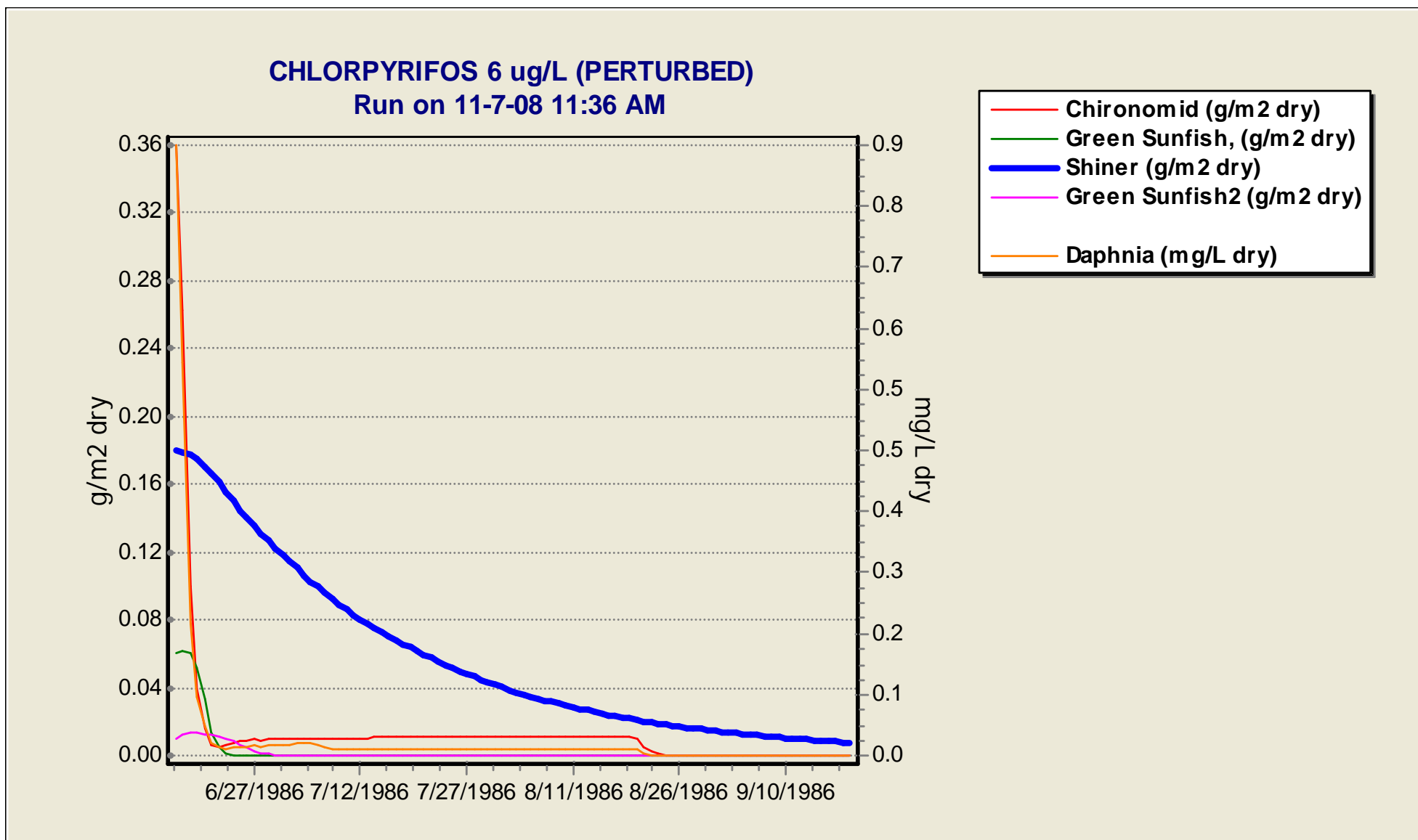
# Predicted ammonia toxicity in Cahaba River AL



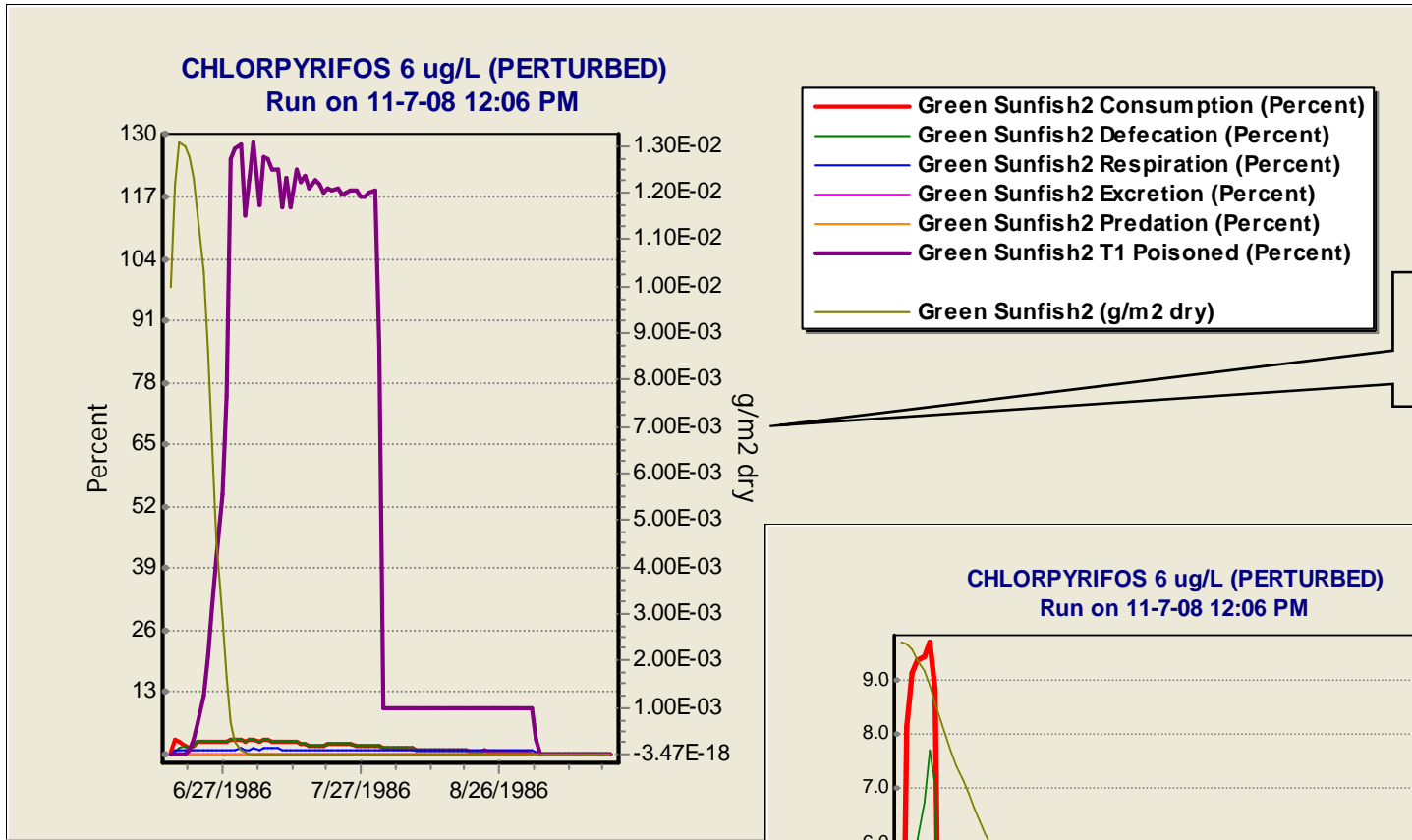
# Returning to the Limnocorral in Duluth MN . . .



# Animals all decline at varying rates following a single initial dose of chlorpyrifos

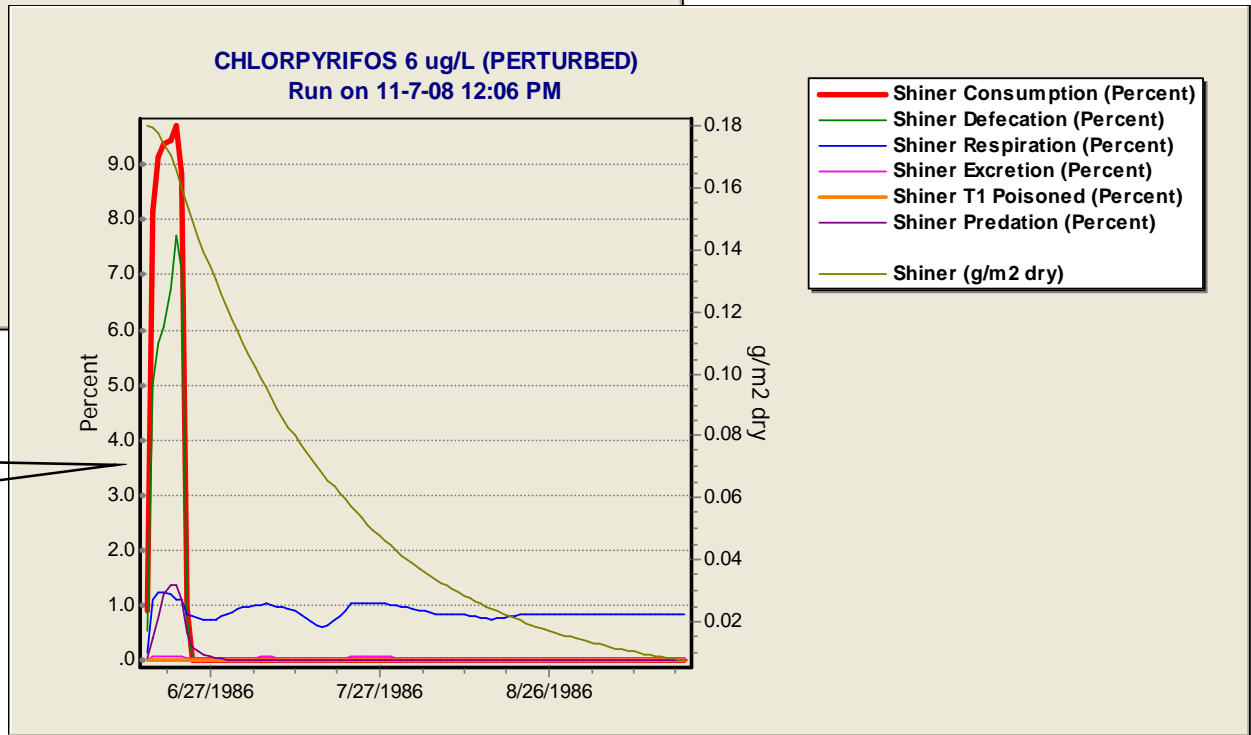


# Sunfish have acute toxicity, shiners have chronic toxicity to chlorpyrifos

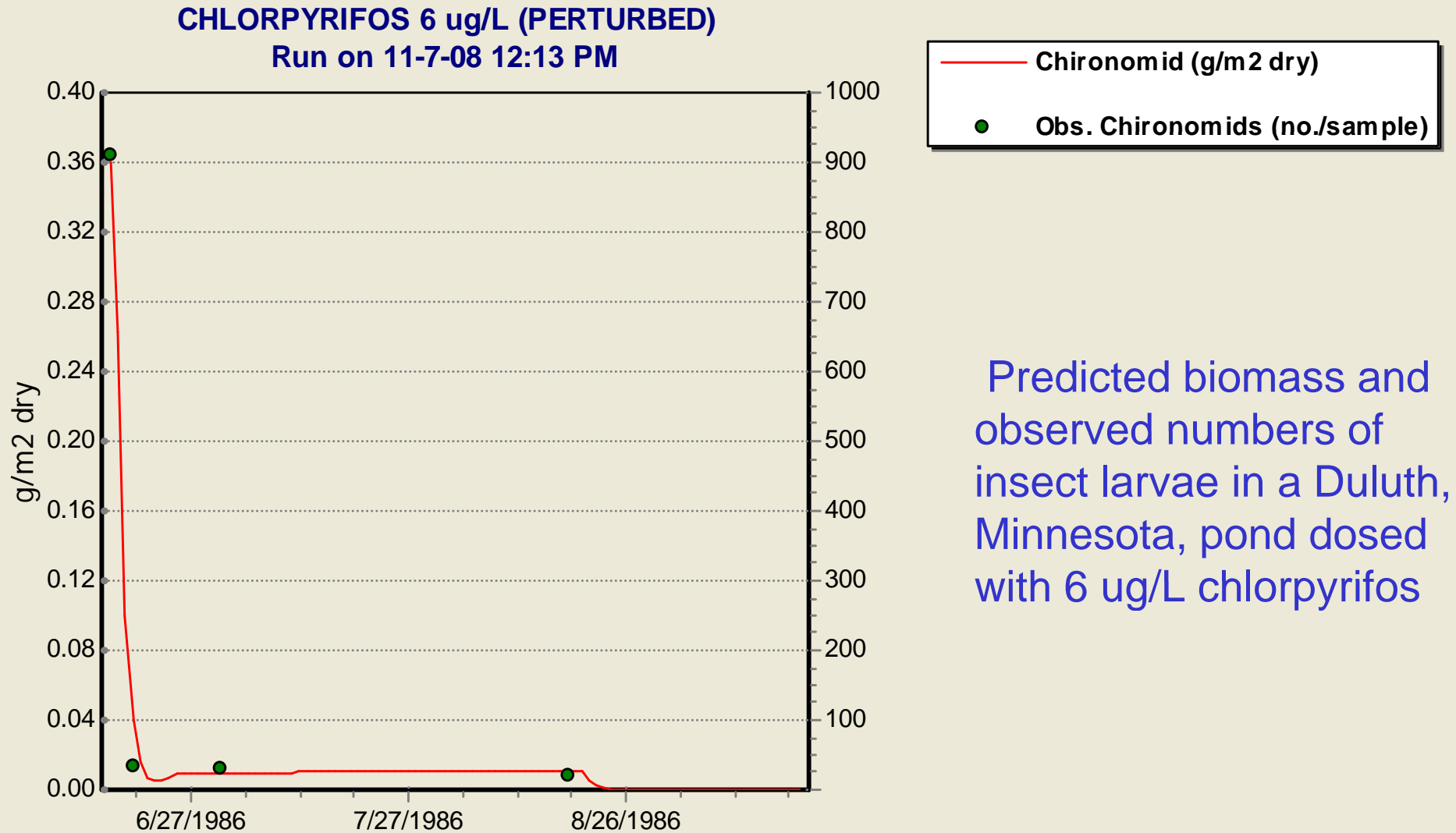


Sunfish with acute toxicity

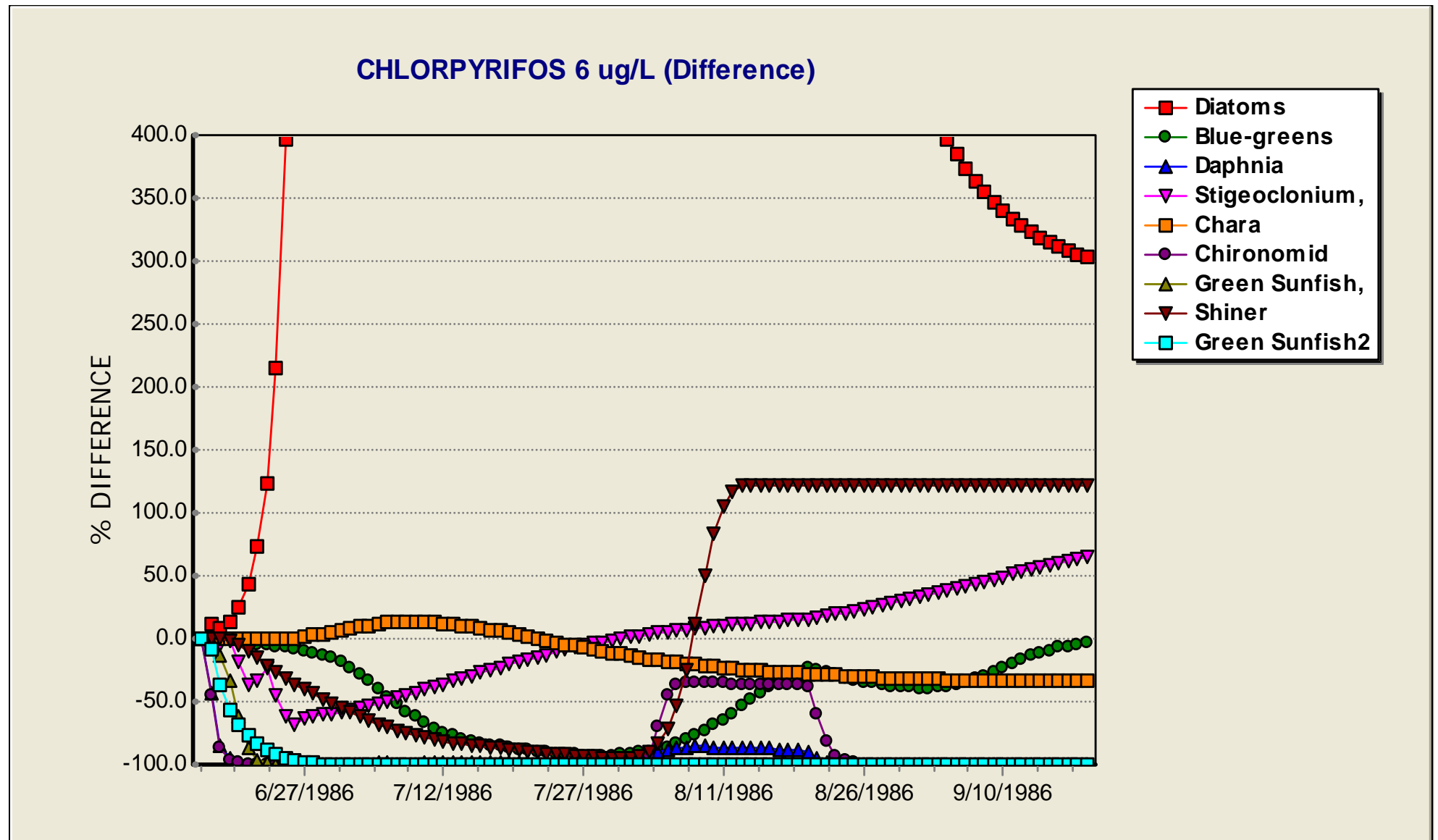
Shiner with chronic toxicity only



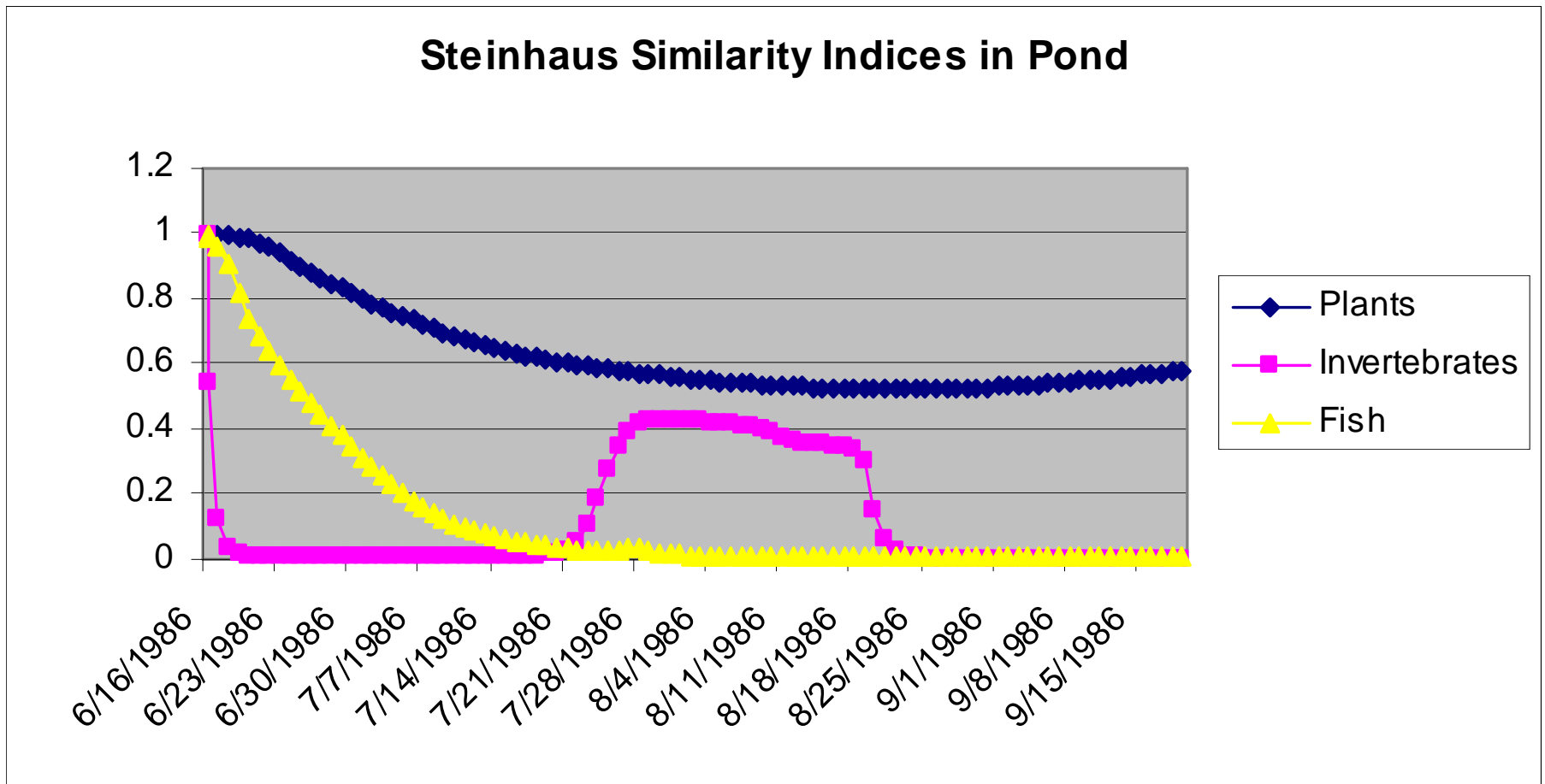
# Toxic effects of Chlorpyrifos in Duluth pond



# % Difference Graph shows differences in species response to toxicant



# Steinhaus Indices show ecosystem impacts predicted by the model



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



# 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)

# Set exposure to a constant in Study Setup

Set “Control Setup” to omit toxicants from “control” results

**Simulation Setup**

First Day Of Simulation  Last Day

Relative Error  Min. Stepsize **1E-10**

Daily Simulation  Hourly Simulation

**Biota Modeling Options:**

Disable Dynamic Lipid Calculations for Fish

Run model in Spin-up Mode (Initial Conditions set at end)

**Toxicant Modeling Options:**

Track Toxicant Mass Balance (Default)

Keep Freely Dissolved Toxicant Constant

When calculating toxic effects...

Use Internal Concs  Use External Concentrations

When calculating toxicant uptake in organisms...

Calculate Normally  Estimate Using BCF  
(gill / dietary uptake and depuration) (will speed up Low Kow simulations)

Include Complexed Tox. in BAF Calculations

**Output Options**

Data Storage Step (avg. period)   Days  Hours

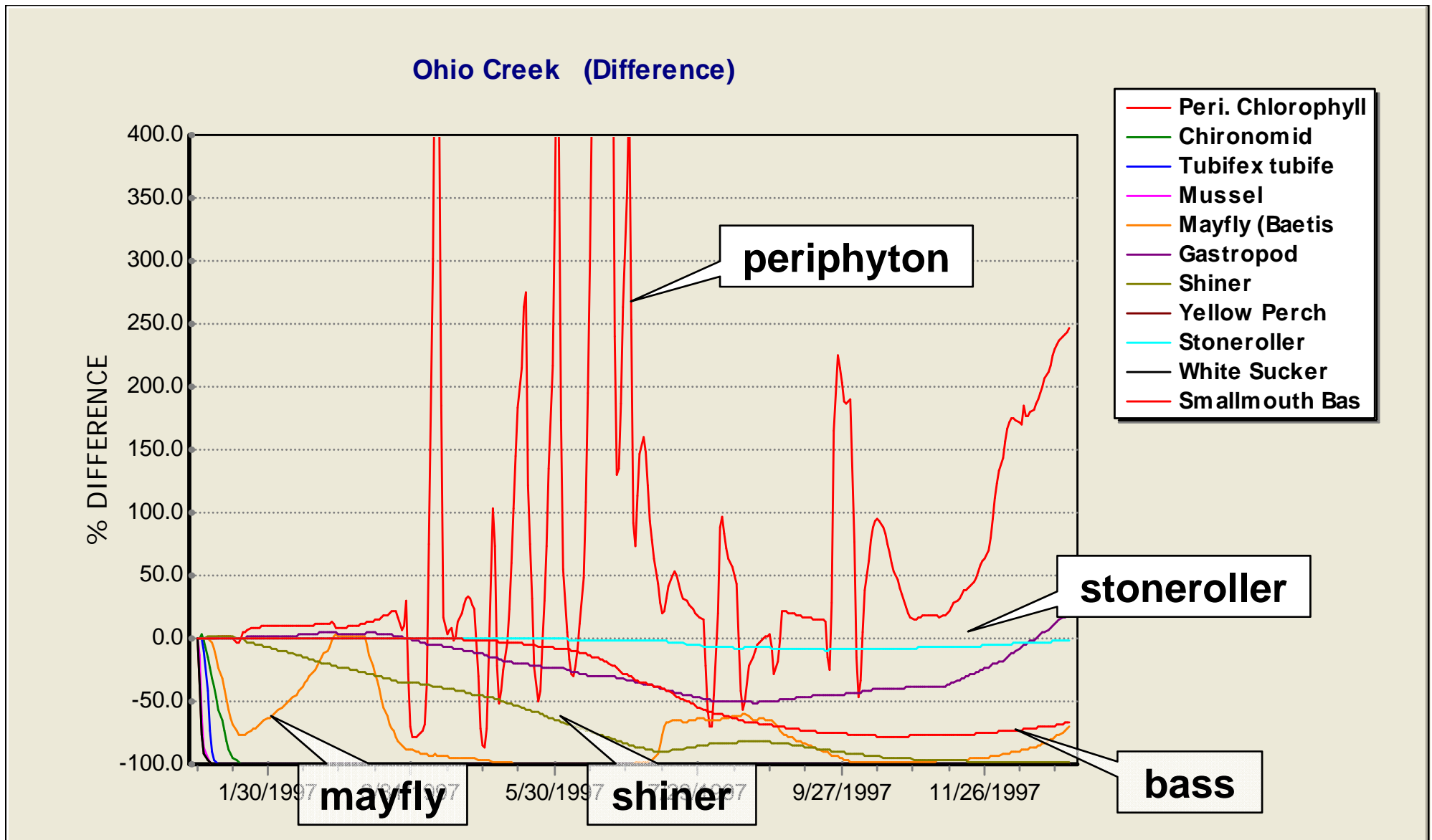
Write Hypolim. Data When System not Stratified

Show Integration Info  Don't Show Integration

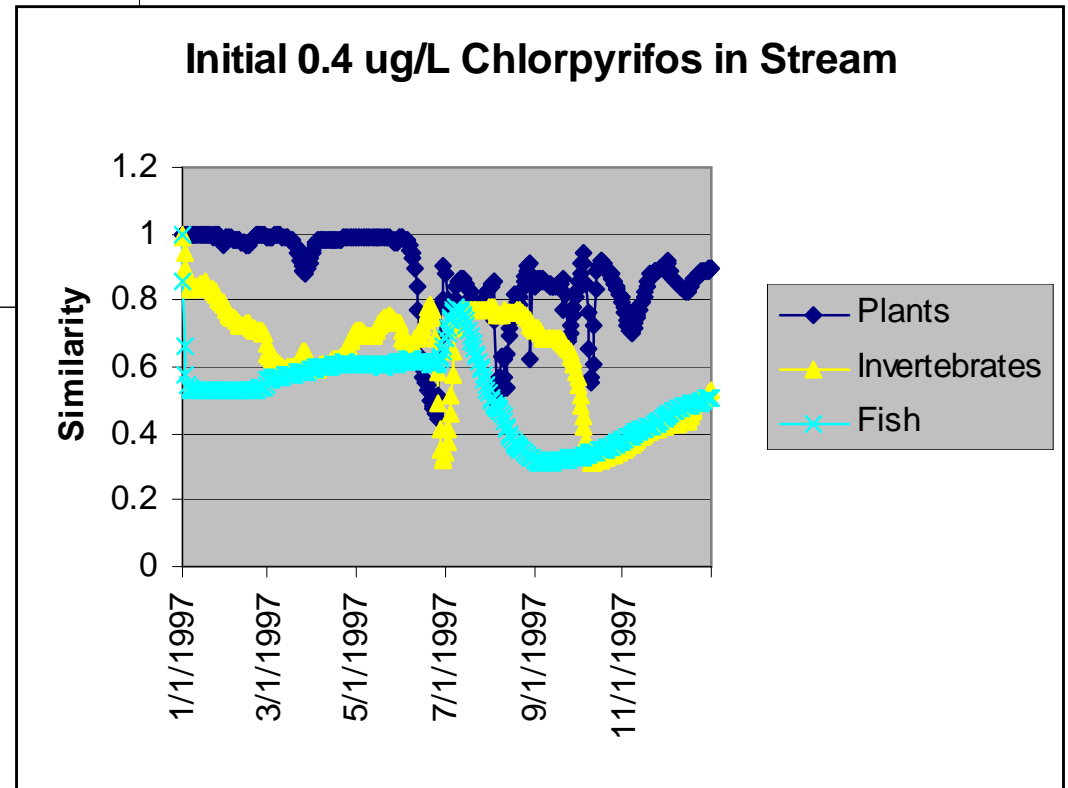
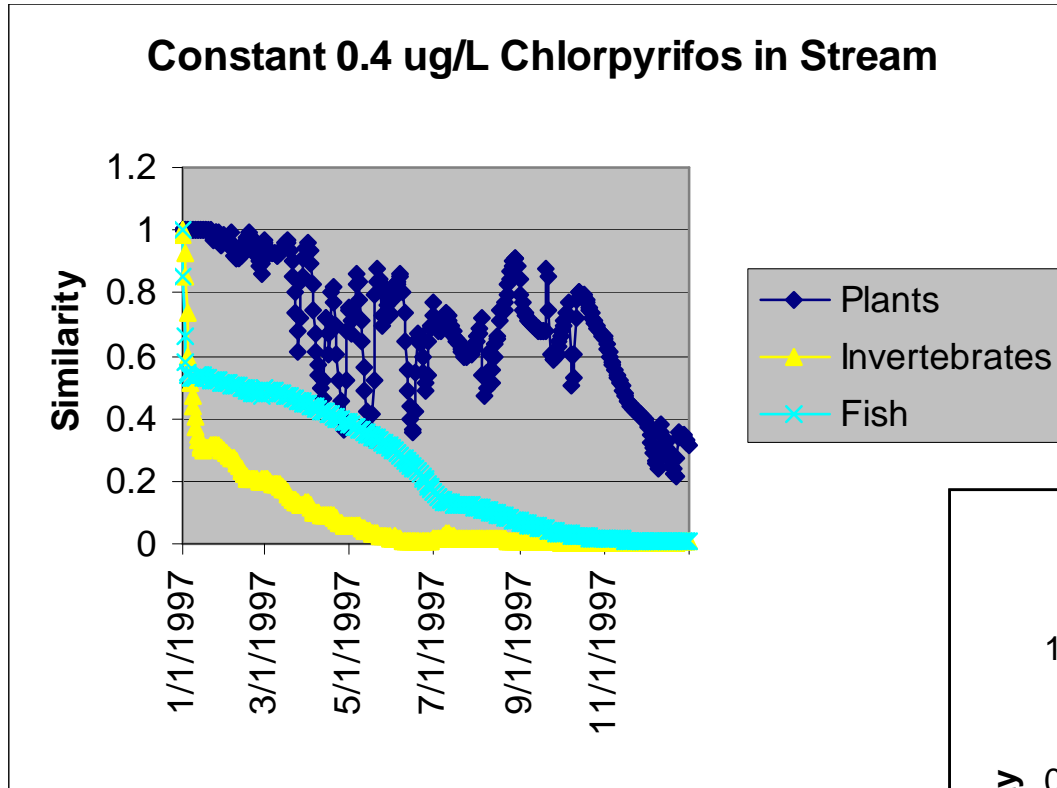
Trapezoidally Integrate Results  Output Instantaneous Concs.

check  
box

Impacts of constant chlorpyrifos are dramatic:  
animals decline, algae increase (less herbivory)



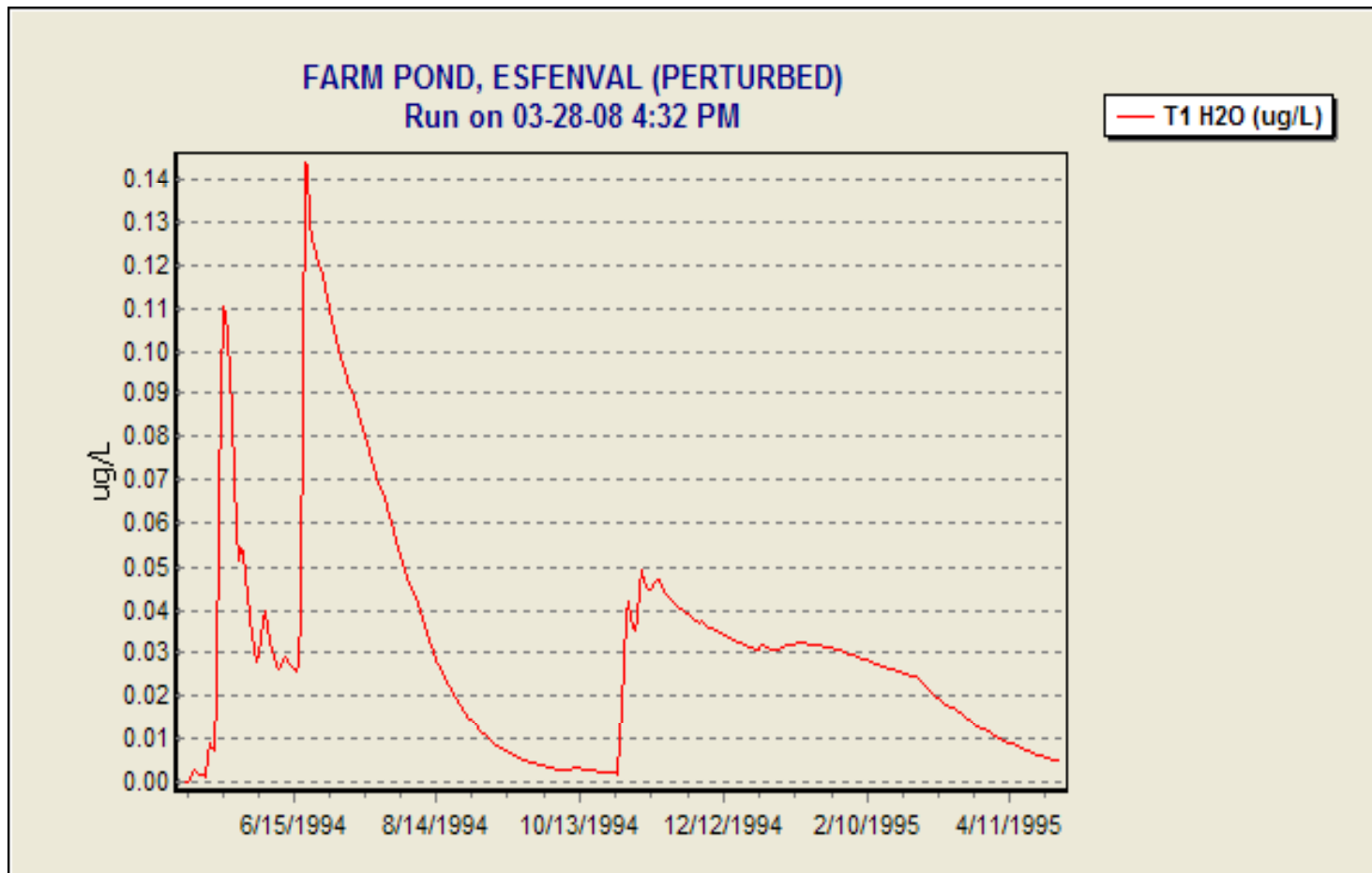
# Plot of Steinhaus indices shows lasting impacts predicted by the model



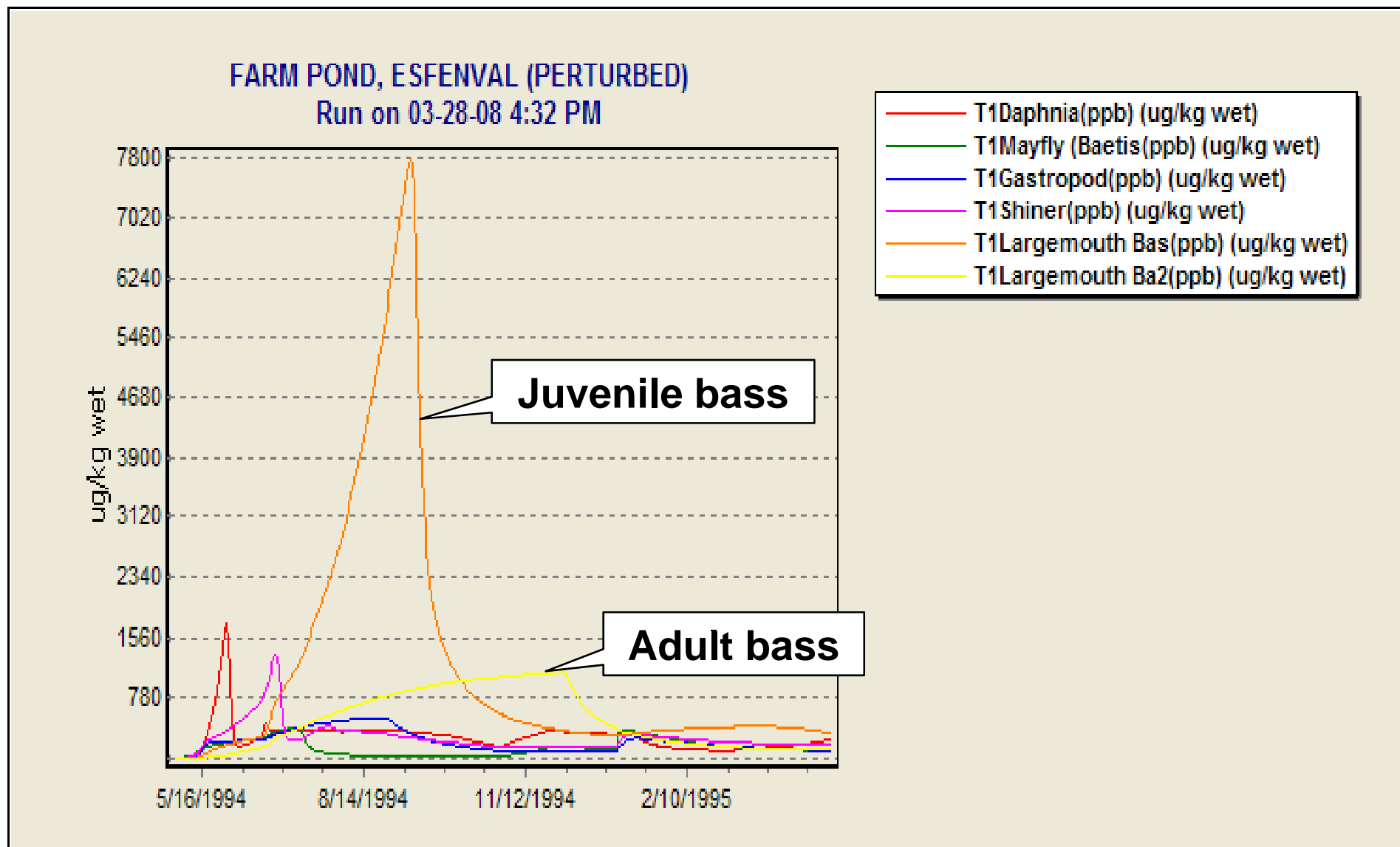
$$S = \frac{2 * \sum_{k=1}^n \text{Min}(a_{1,k}, a_{2,k})}{\sum_{k=1}^n a_{1,k} + \sum_{k=1}^n a_{2,k}}$$

# Farm Pond MO, Esfenvalerate

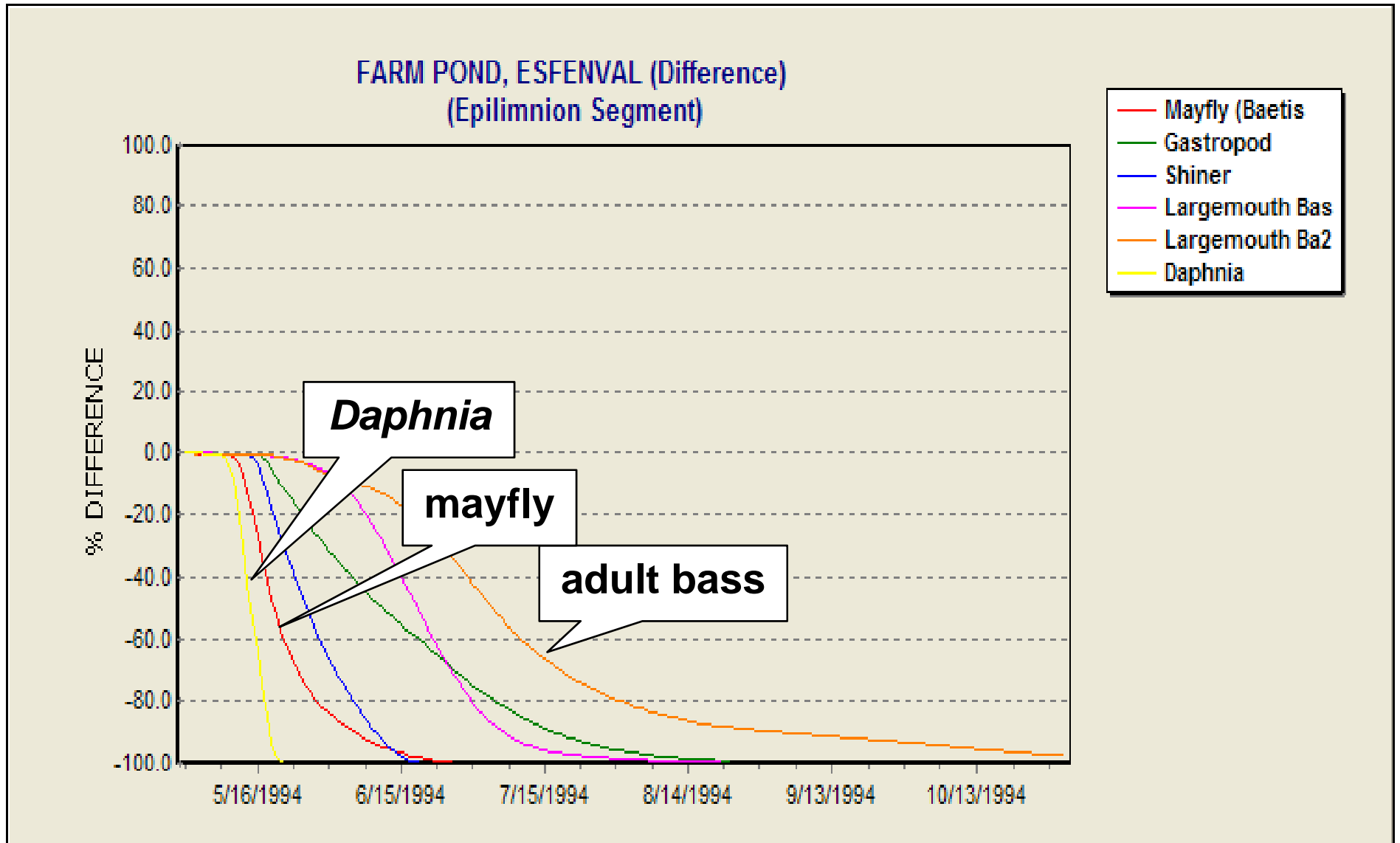
- Loadings from PRIZM for adjacent cornfield
- 20% of worst case scenario for runoff of pesticide predicted by PRZM



# Farm Pond, Esfenvalerate Chemical Uptake in animals



# Farm Pond, Esfenvalerate Difference Graph



# Fluridone (Sonar) used to eradicate *Hydrilla* in Clear Lake CA

- Six doses
  - 20 ppb dose
- What is impact on non-target organisms?
- What is recovery of Clear Lake ecosystem?
- Impact on DO from death of large *Hydrilla* biomass?

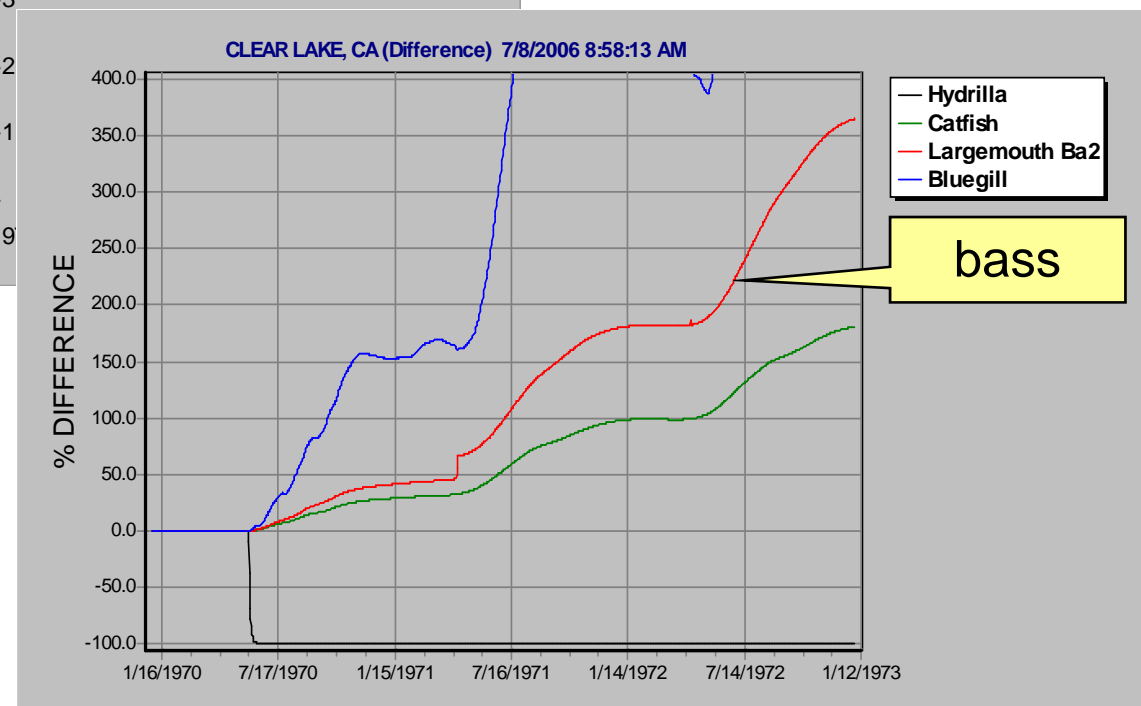
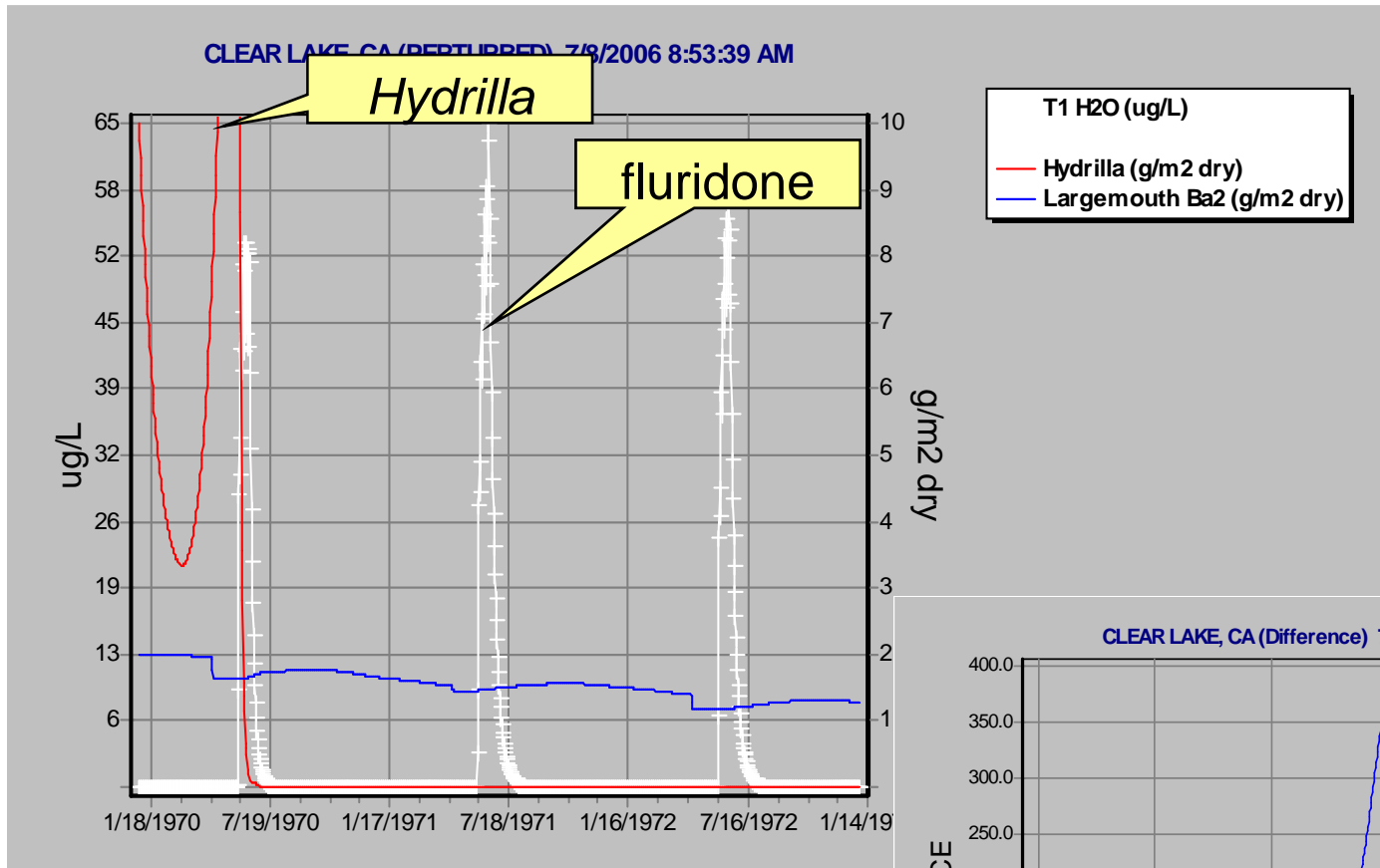


## Clear Lake Project

- Sonar SRP label
  - “Where FasTEST has determined that concentrations are less than 10 parts per billion”
    - “no irrigation precautions for irrigating established tree crops, ... row crops or turf”
  - “do not use ... treated water if concentration ... greater than 5 ppb.”
    - tobacco, tomatoes, peppers...newly seeded grasses

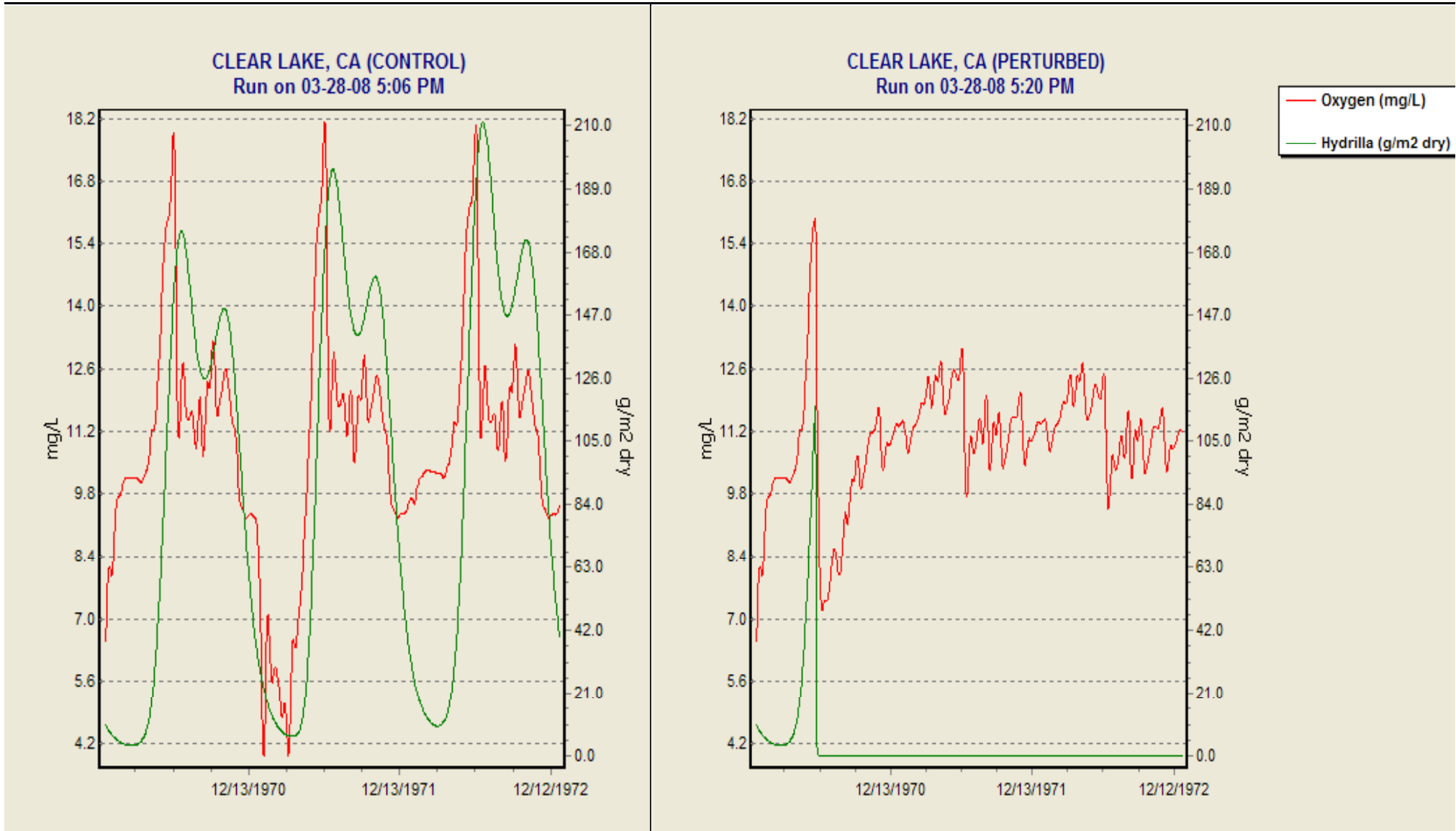


# Addition of Fluridone causes dramatic response of Clear Lake ecosystem



# Indirect Effects Captured

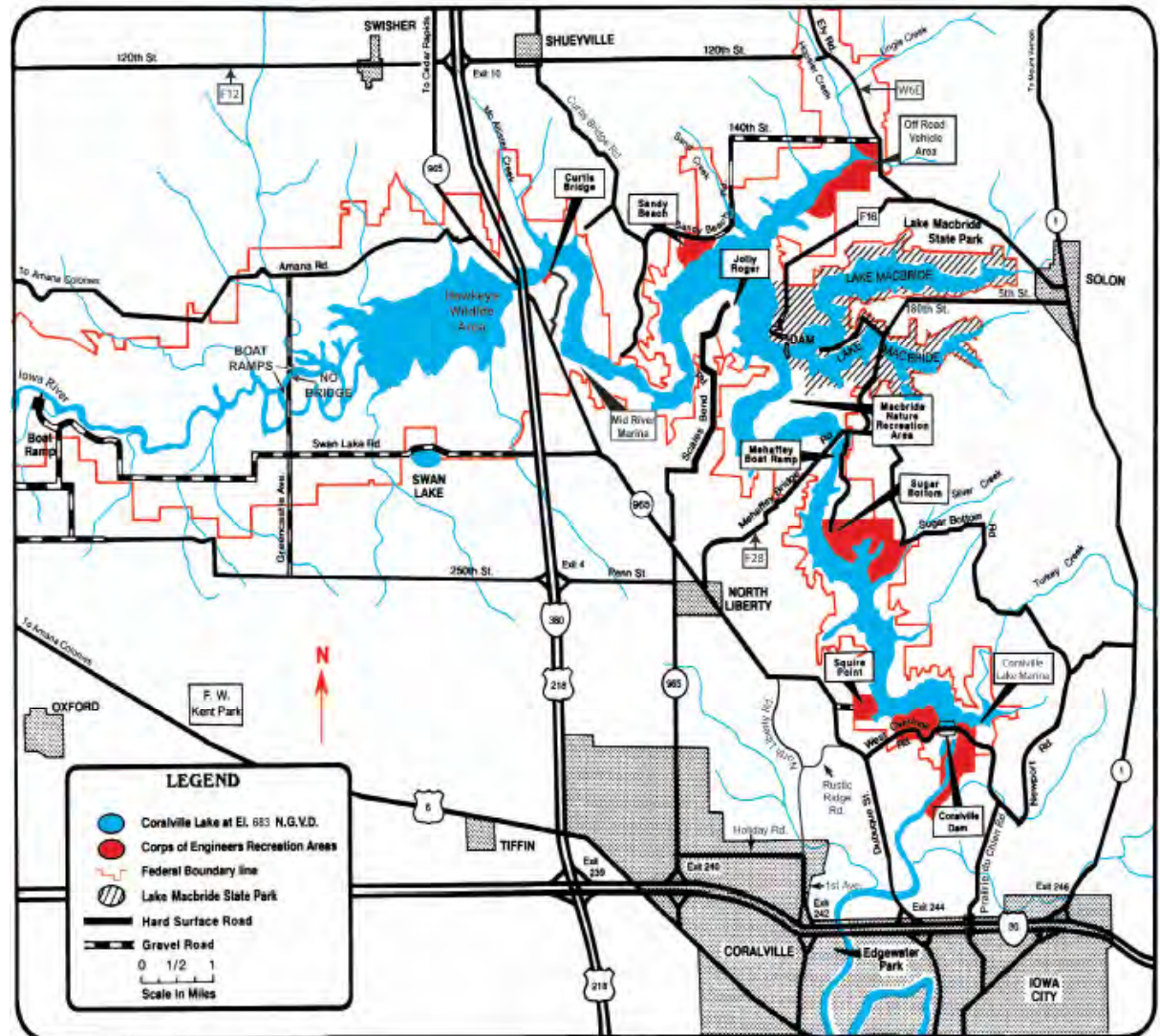
e.g. Impact on DO levels is negligible



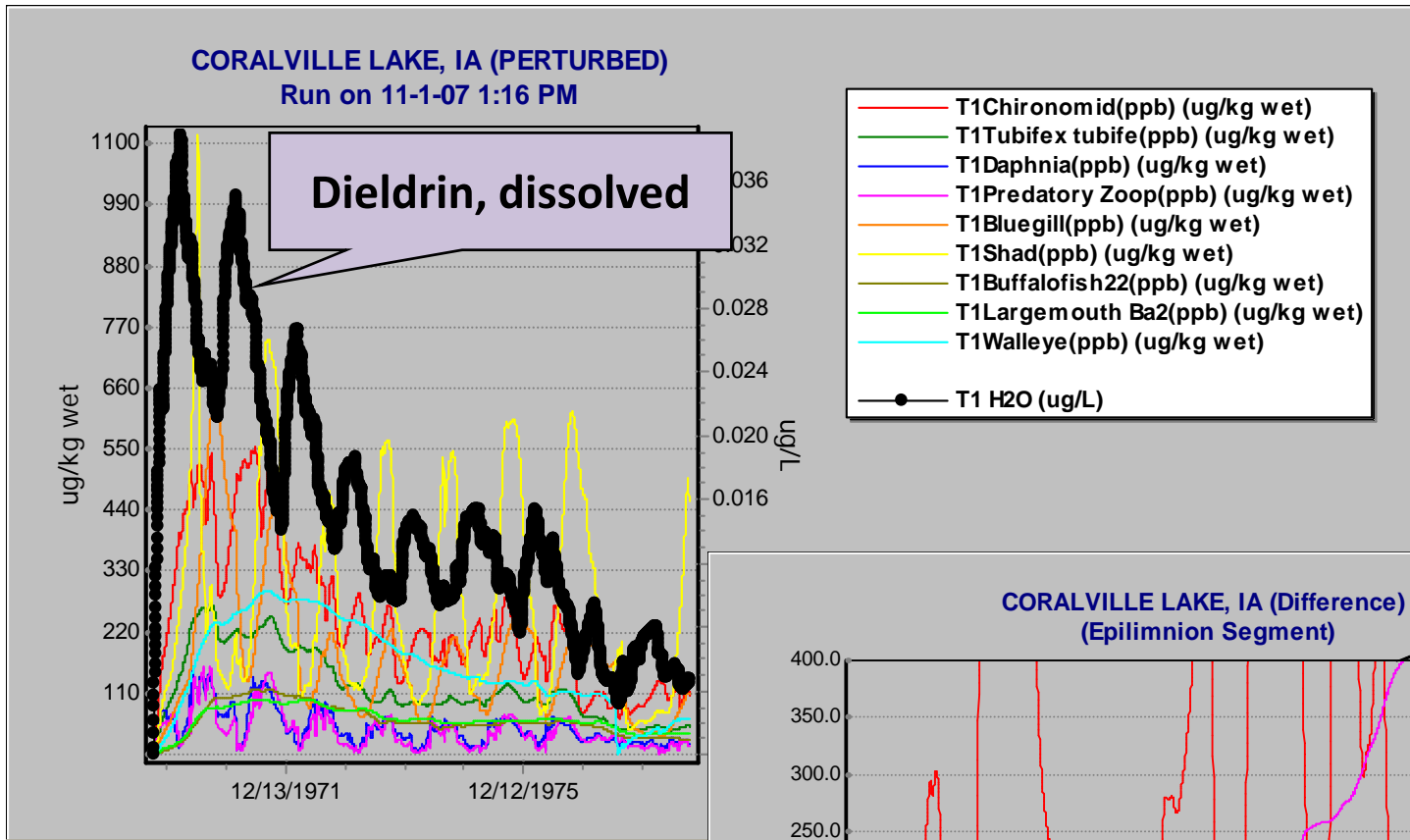
# Coralville Reservoir Iowa

## long-term contamination with dieldrin

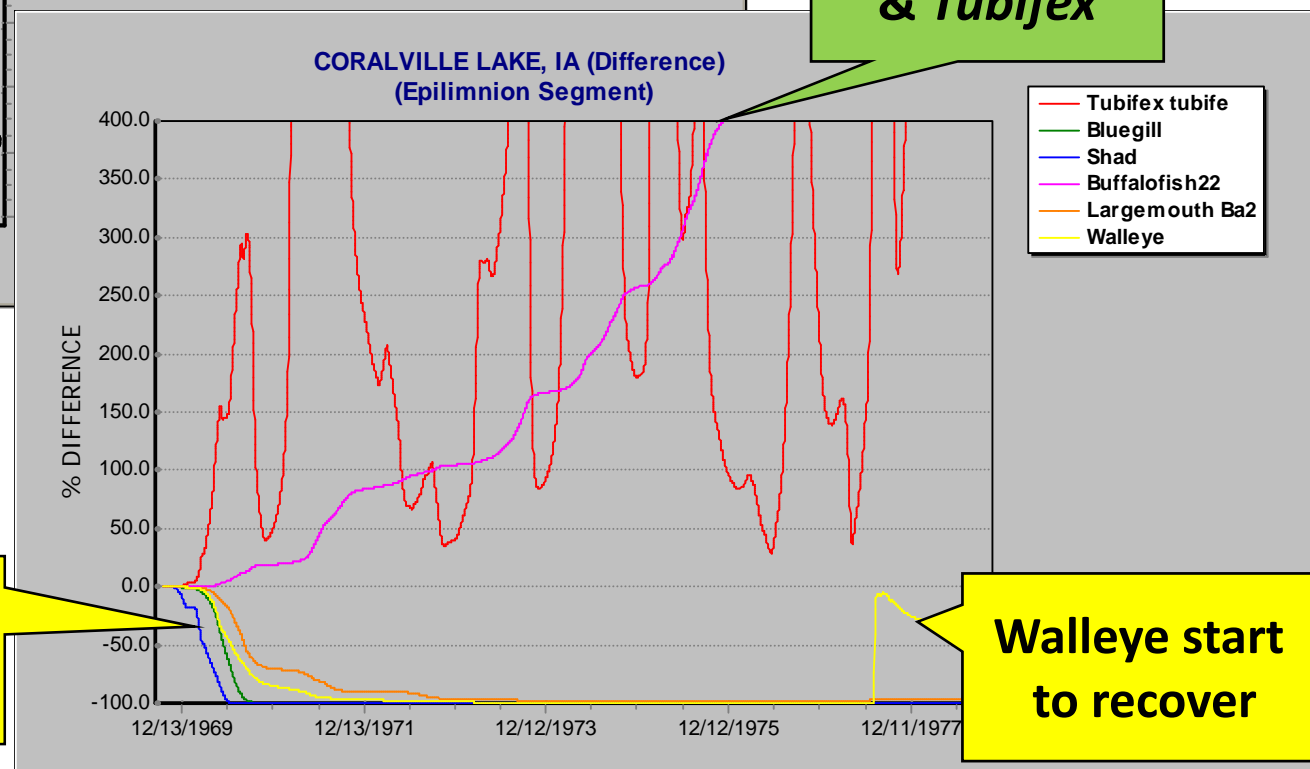
- Run-of-river
- Flood control
- 90% of basin in agriculture
  - Nutrients
  - Pesticides
  - Sediment



# Dieldrin bioaccumulates & declines over 20 years with fish mortality, but tolerant buffalofish, *Tubifex* prosper



**Buffalofish & Tubifex**

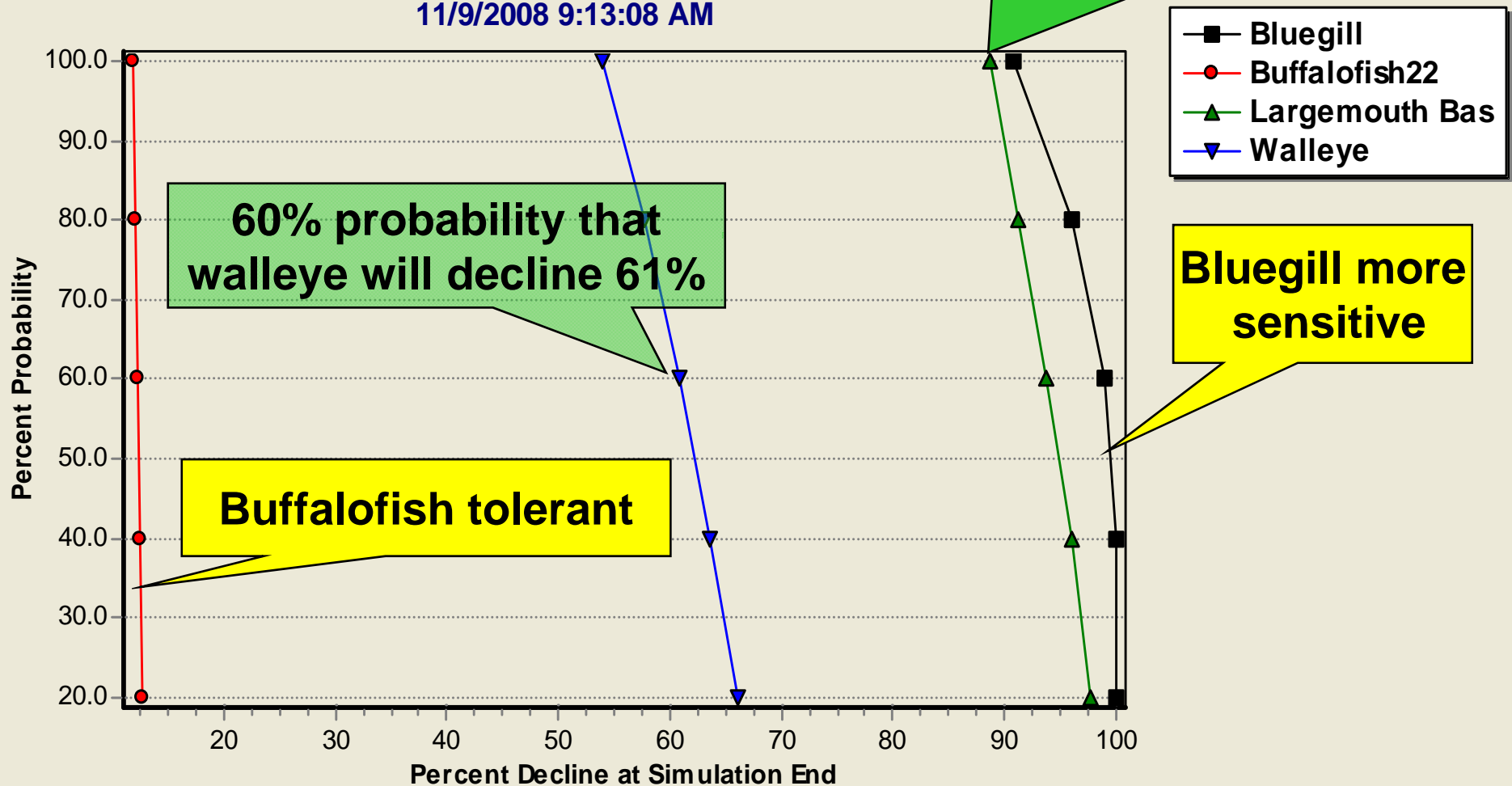


**Shad, bluegill, walleye, bass die off**

**Walleye start to recover**

# Probability of decline in biomass (end of 1<sup>st</sup> year) can be estimated based on uncertainty

Biomass Risk Graph  
11/9/2008 9:13:08 AM



# Uncertainty and Sensitivity Analysis

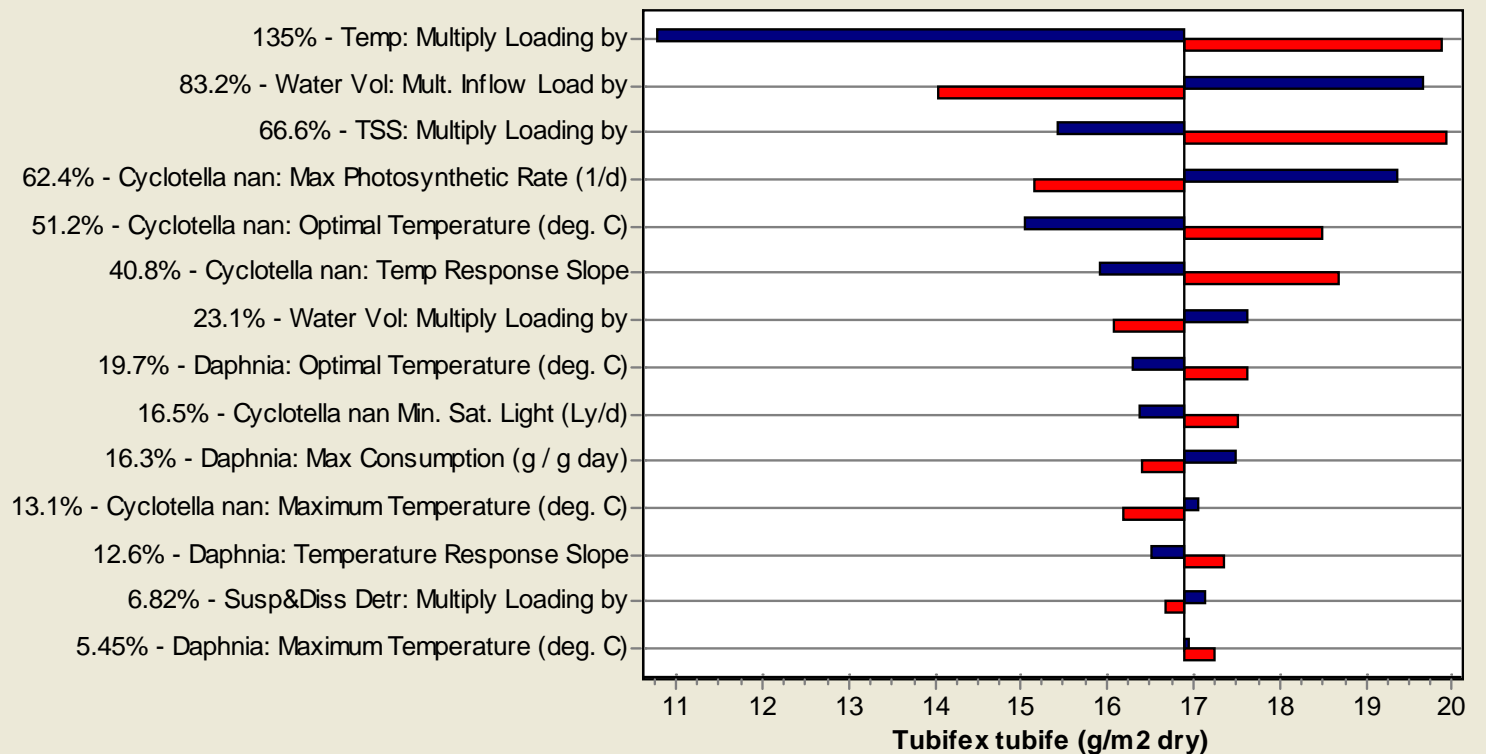
- “Sensitivity” refers to the variation in output of a mathematical model with respect to changes in the values of the model inputs (Saltelli, 2001).
- Sensitivity analysis provides a ranking of the model input assumptions with respect to their relative contribution to model output variability or uncertainty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

# Coralville Sensitivity Analysis Demo

## Demonstration of inputs and outputs from Coralville analysis



**Sensitivity of Tubifex tubife (g/m2 dry) to 20% change in tested parameters**  
3/28/2008 3:31:16 PM



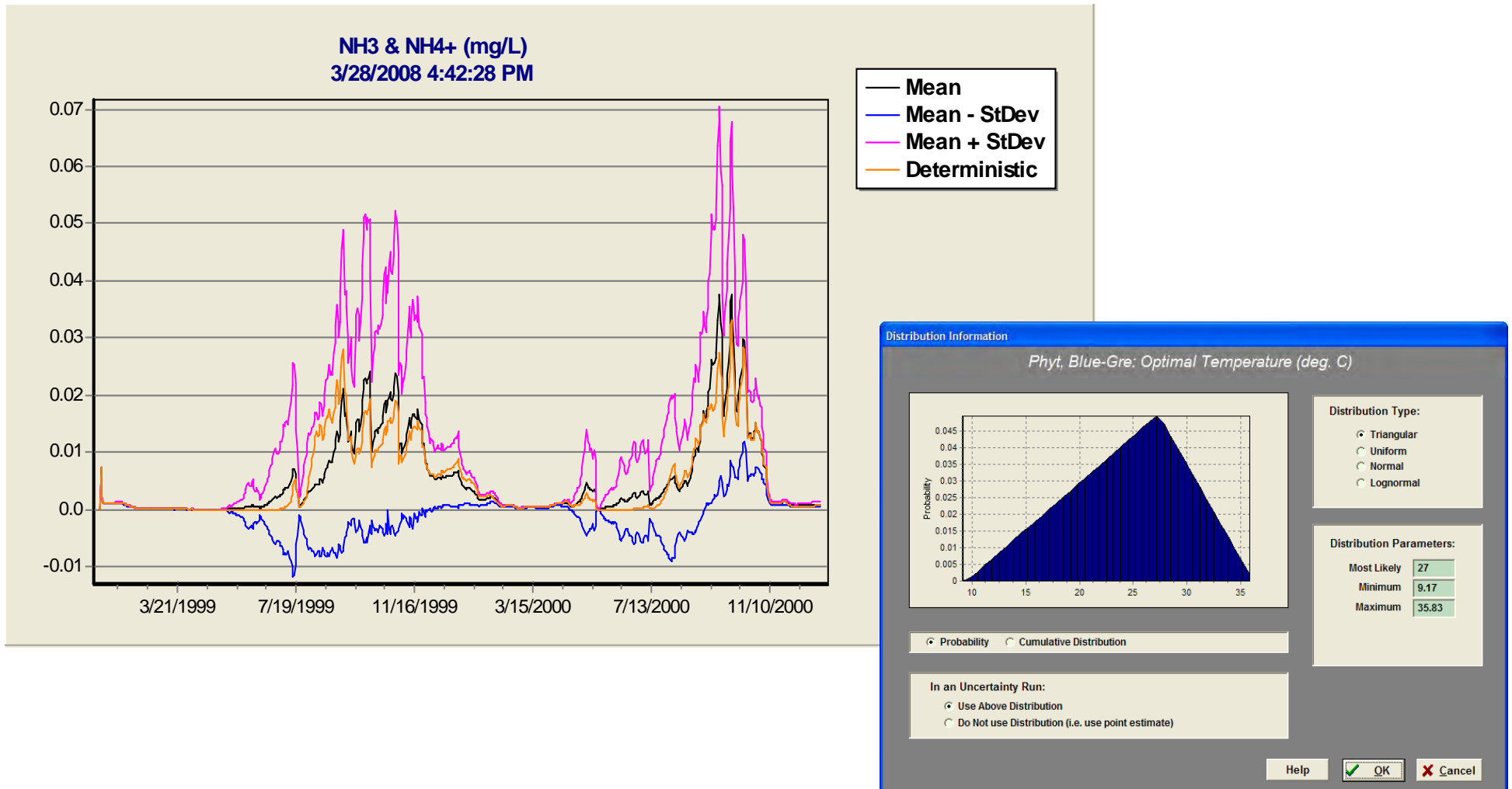
# Uncertainty Analysis

- Uncertainty analyses describe sources of uncertainty and variability
- There are many sources of uncertainty e.g.
  - parameter uncertainty
  - model uncertainty due to necessary simplification of real-world processes
- Monte Carlo analysis is a statistical sampling technique that allows us to obtain a probabilistic approximation to the effects of parameter uncertainty
- AQUATOX Utilizes Monte Carlo analysis with efficient “Latin Hypercube Sampling” (reduces required iterations)



# Blue Earth Uncertainty Analysis Demo

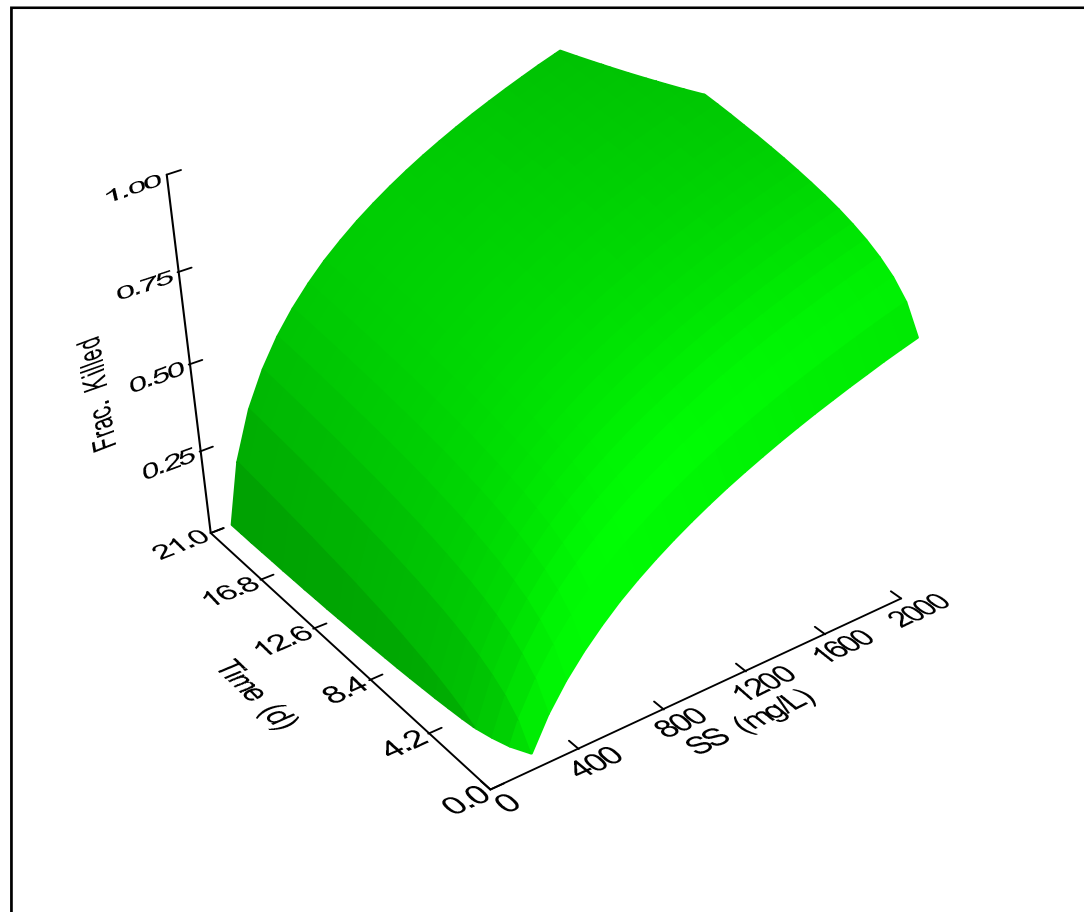
## Demonstration of inputs and outputs from Blue Earth River, MN



# Sediment Effects Overview

- Suspended and bedded sediment effects
  - Mortality

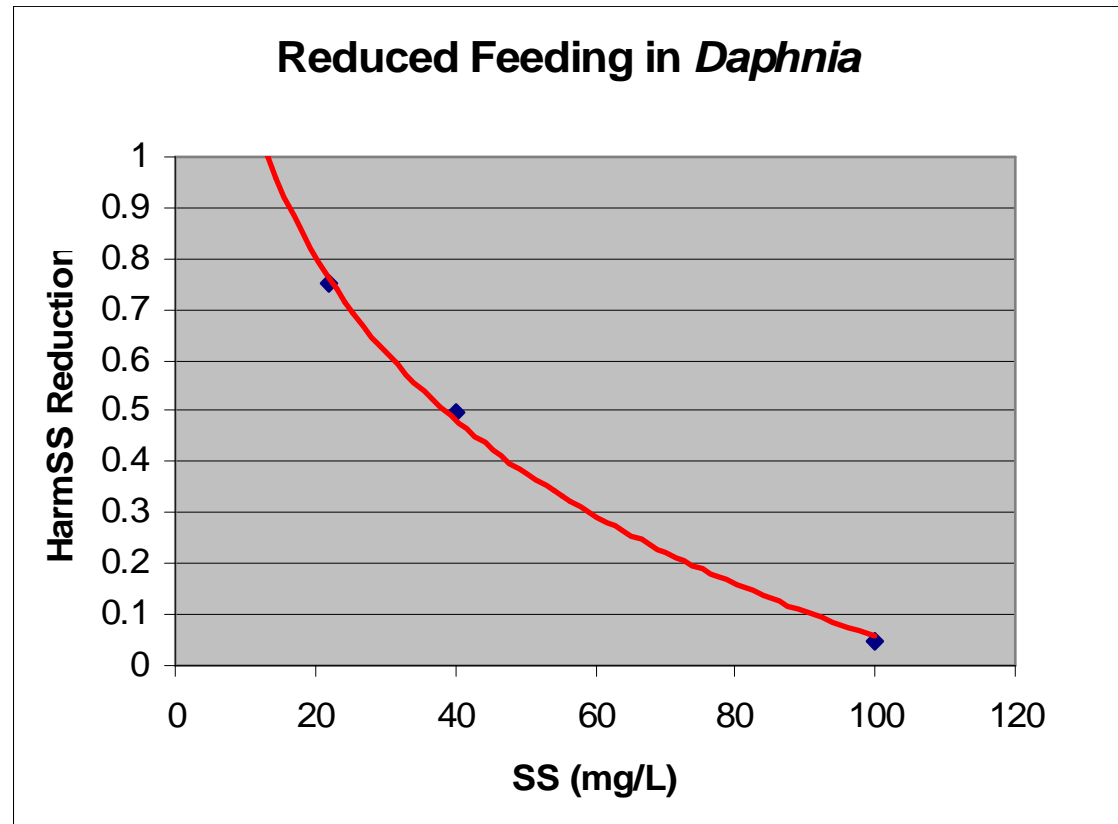
- Highly Sensitive
- Sensitive
- Tolerant
- Intolerant



# Sediment Effects Overview

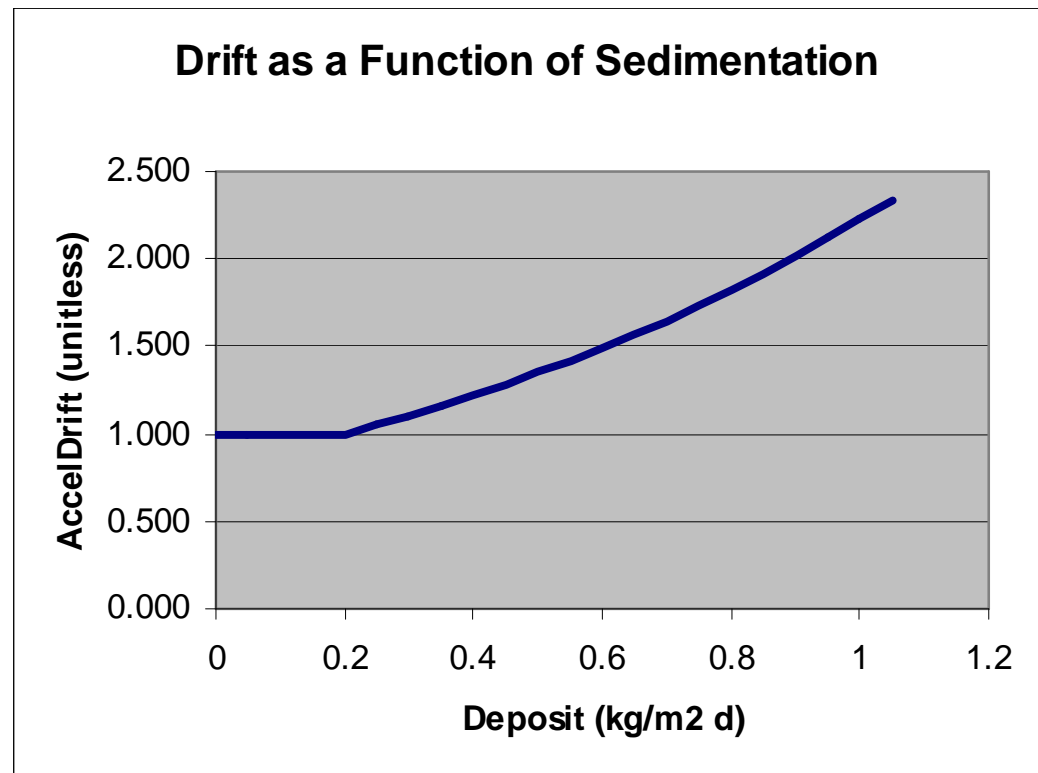
- Suspended and bedded sediment effects
  - Mortality
  - Reduced Feeding

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



# Sediment Effects Overview

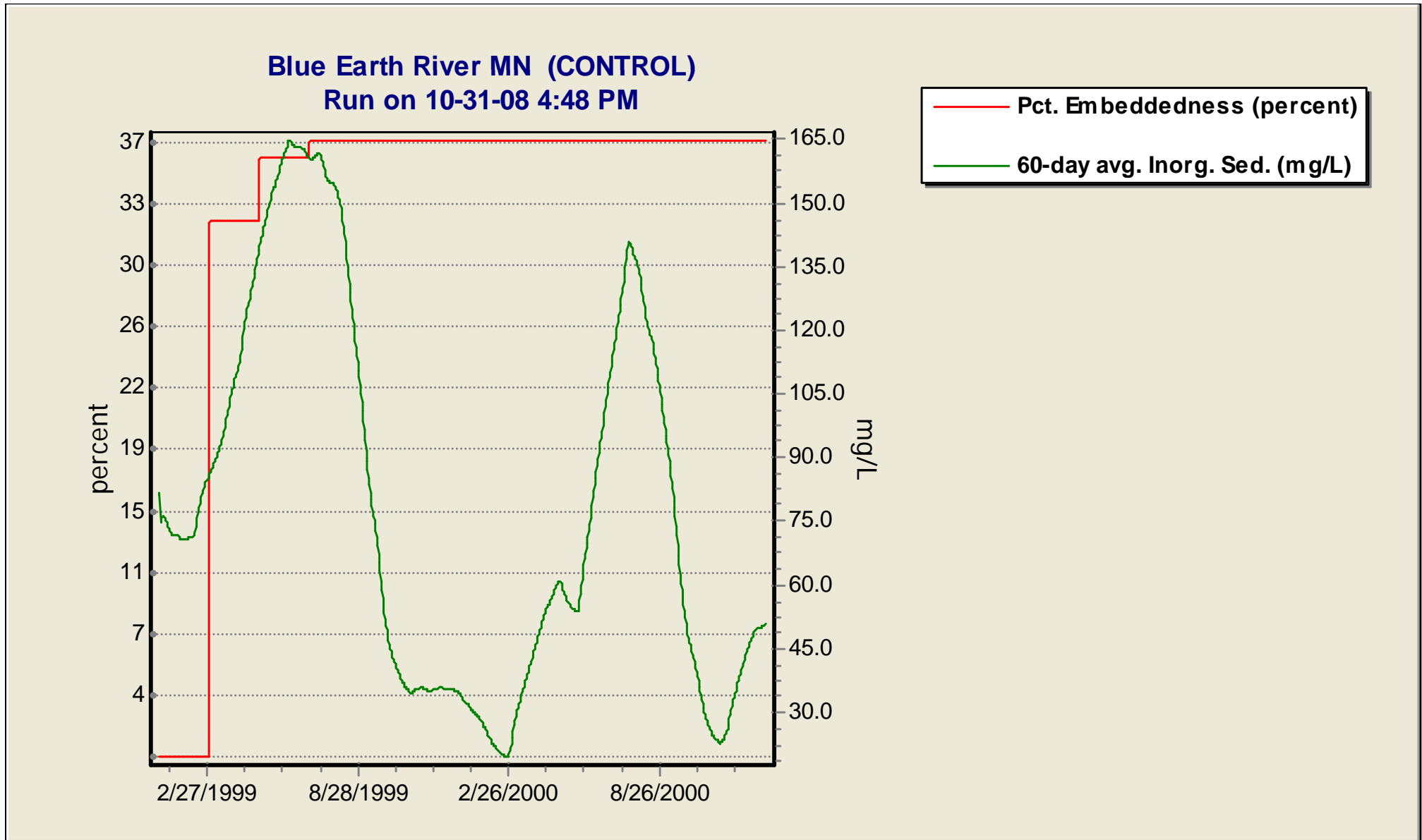
- Suspended and bedded sediment effects
  - Mortality
  - Reduced Feeding
  - Increased drift of grazers due to sedimentation



# Sediment Effects Overview

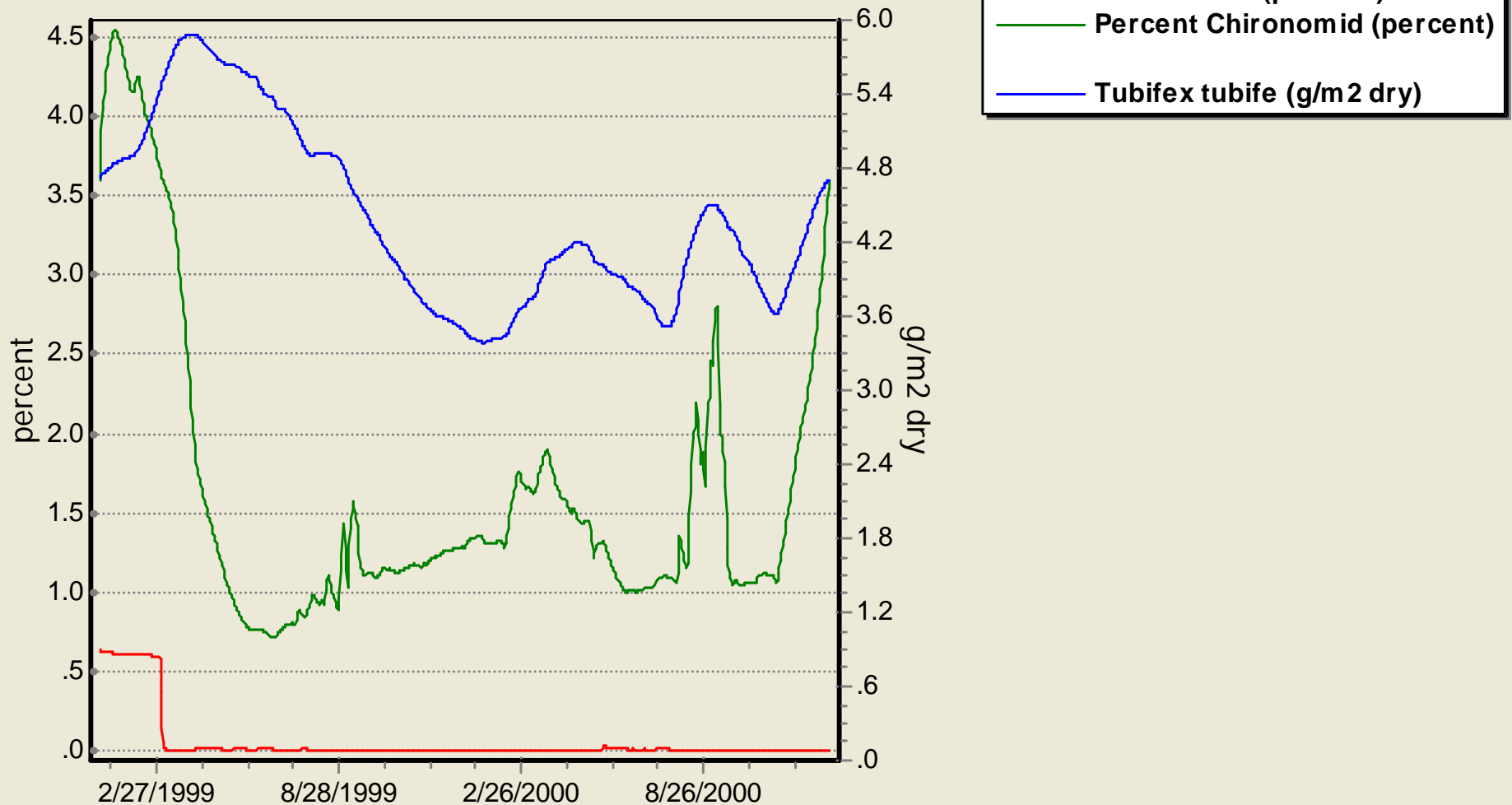
- Suspended and bedded sediment effects
  - Mortality
  - Reduced Feeding
  - Increased drifting of grazers due to sedimentation
  - Deposition of fines and affect on invertebrates and salmonid reproduction
    - Percent Embeddedness calculated as a function of 60-day average TSS

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

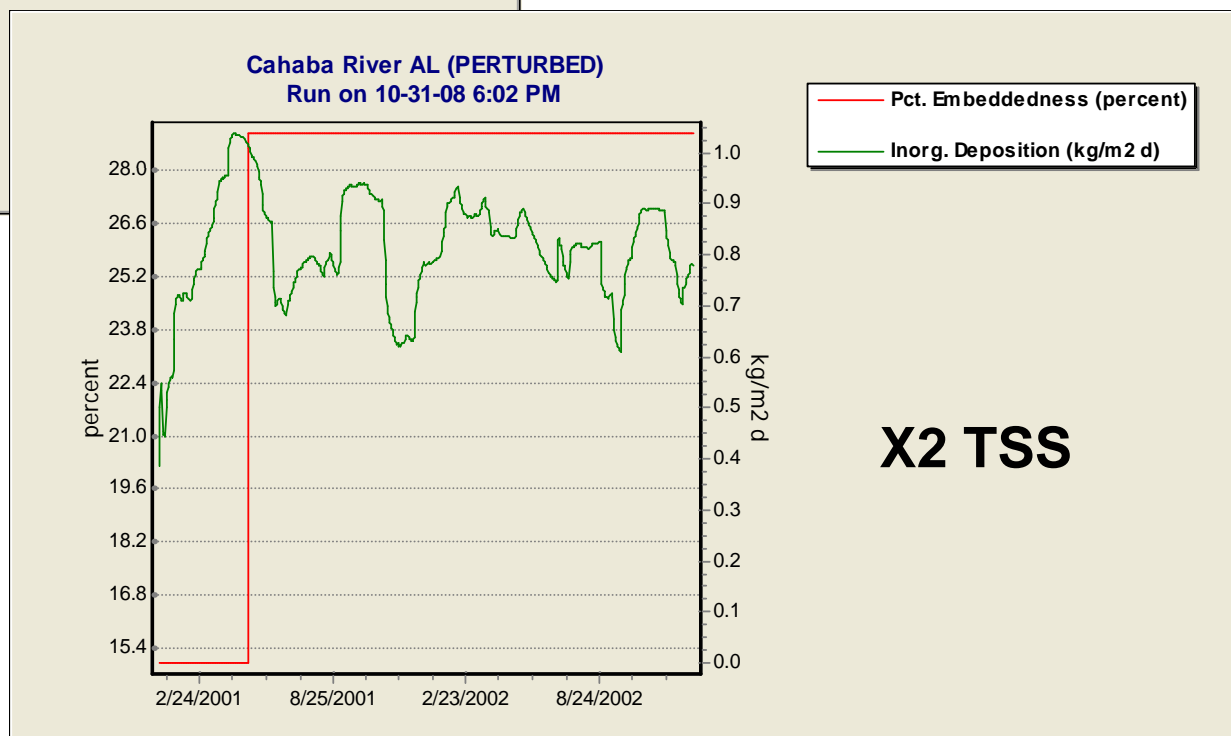
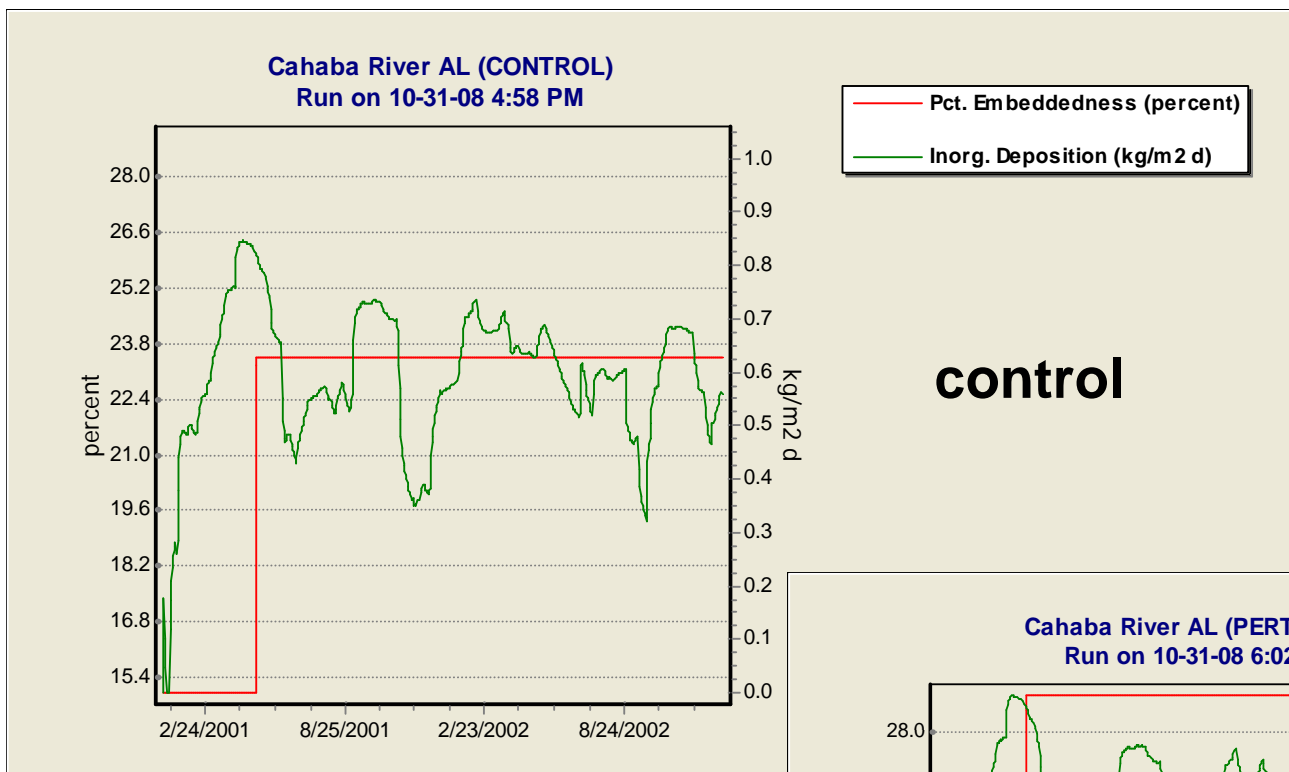


Mayflies, stoneflies, & caddisflies (EPT) are sensitive to embeddedness, chironomids aren't

Blue Earth River MN (CONTROL)  
Run on 10-31-08 4:48 PM

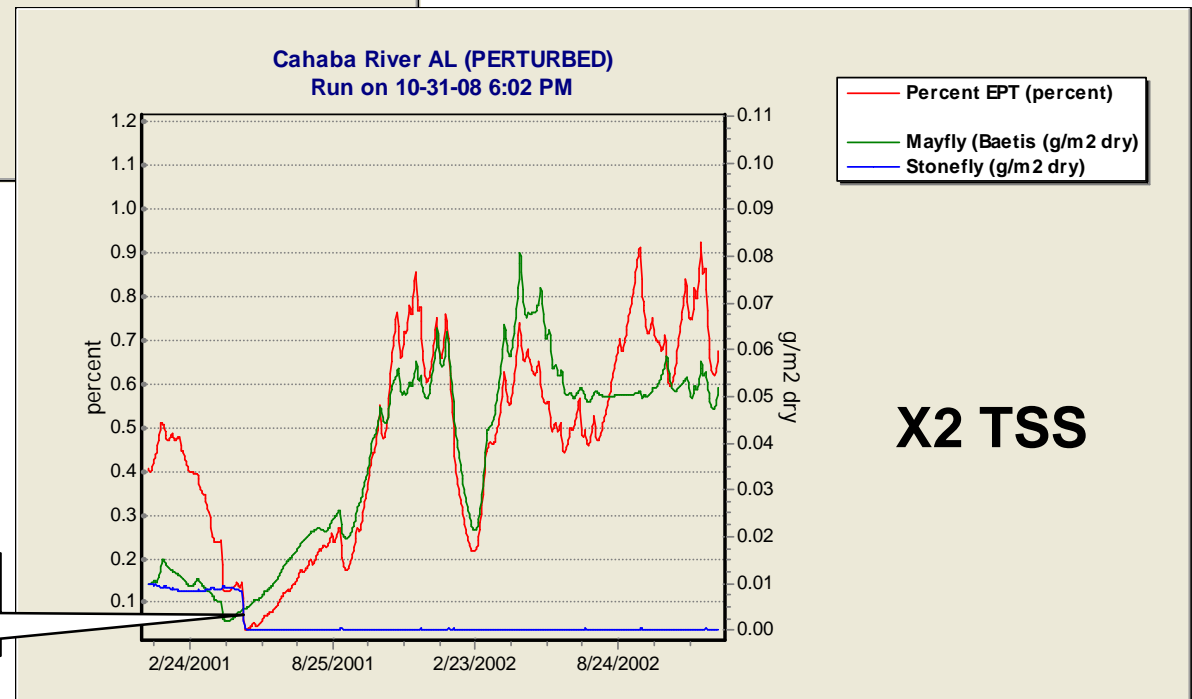
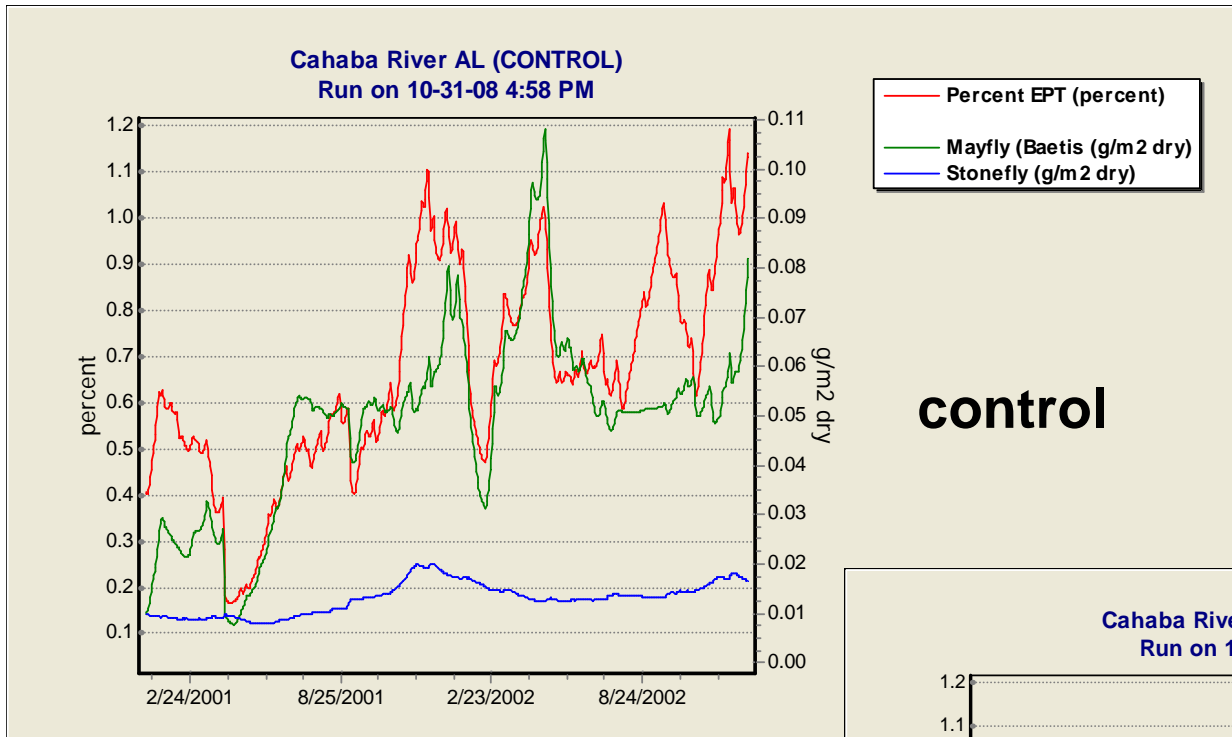


# Doubling TSS increases embeddedness in Cahaba River, AL





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



**stoneflies crash**

# Closure

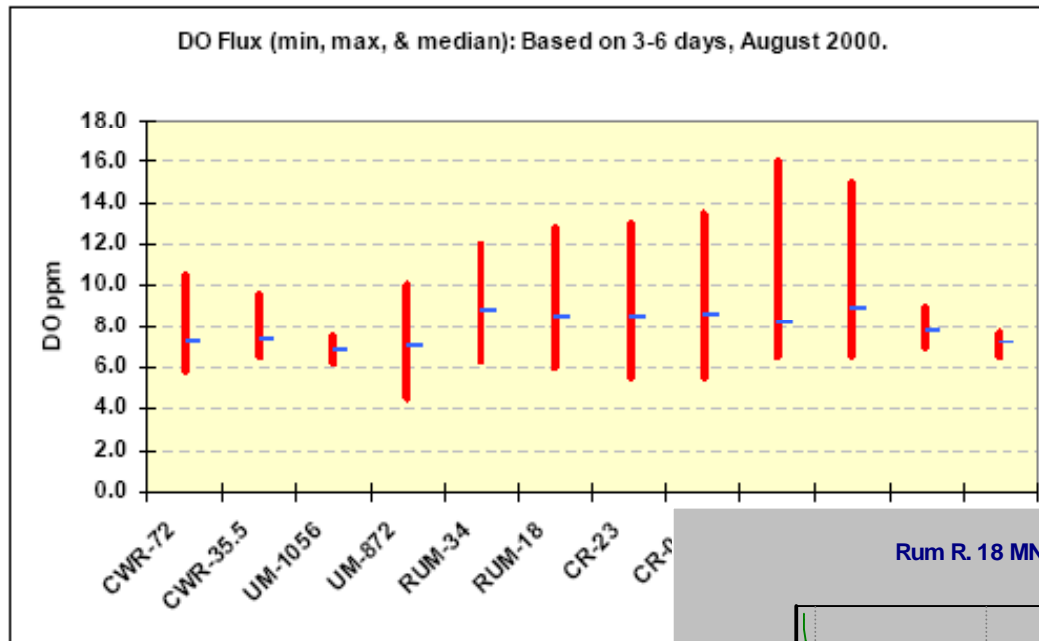
- Topics not yet covered (time-permitting)
  - Diel Oxygen
  - Sand-Silt-Clay model
  - Multi-layer sediment model
- Final Q&A

# 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://epa.gov/ost/models/aquatox/>

# Diel Oxygen, Light; Hourly time-step

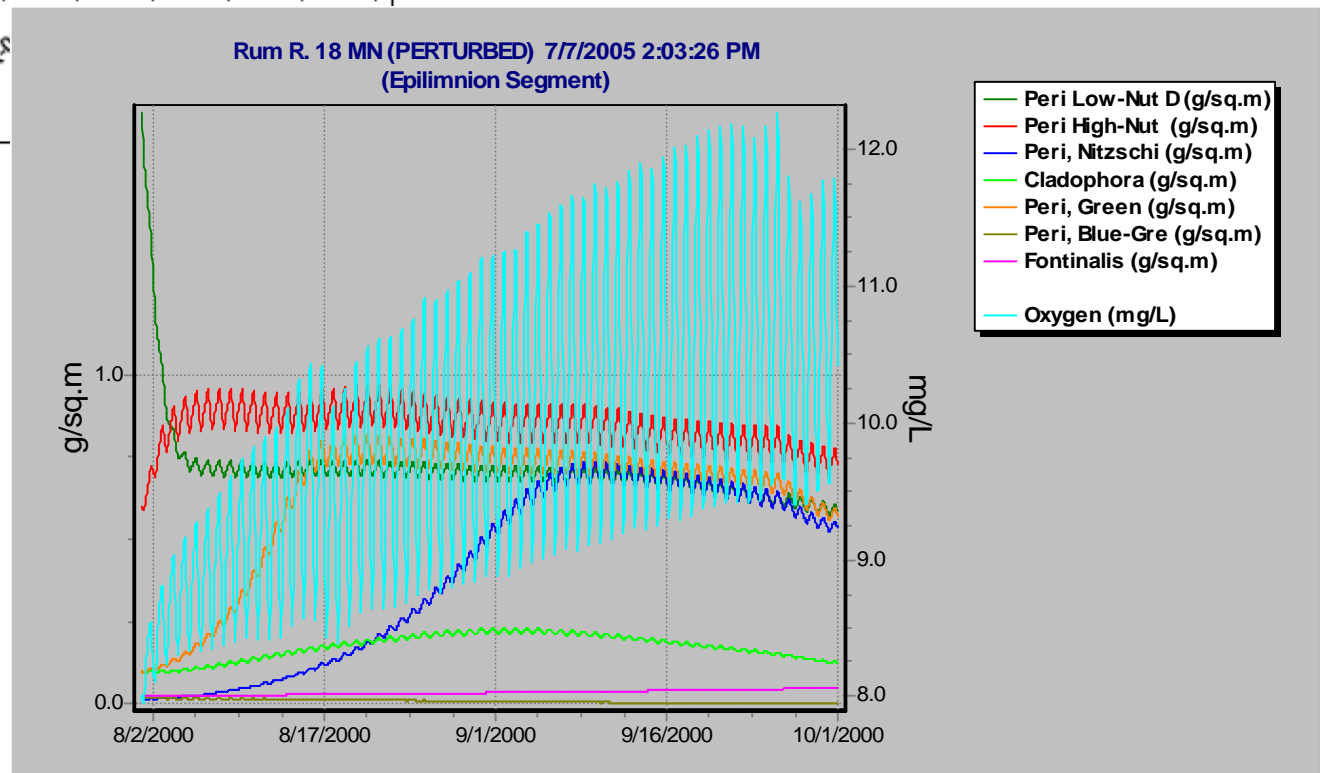
Figure 4. Dissolved oxygen flux based on continuous measurement.



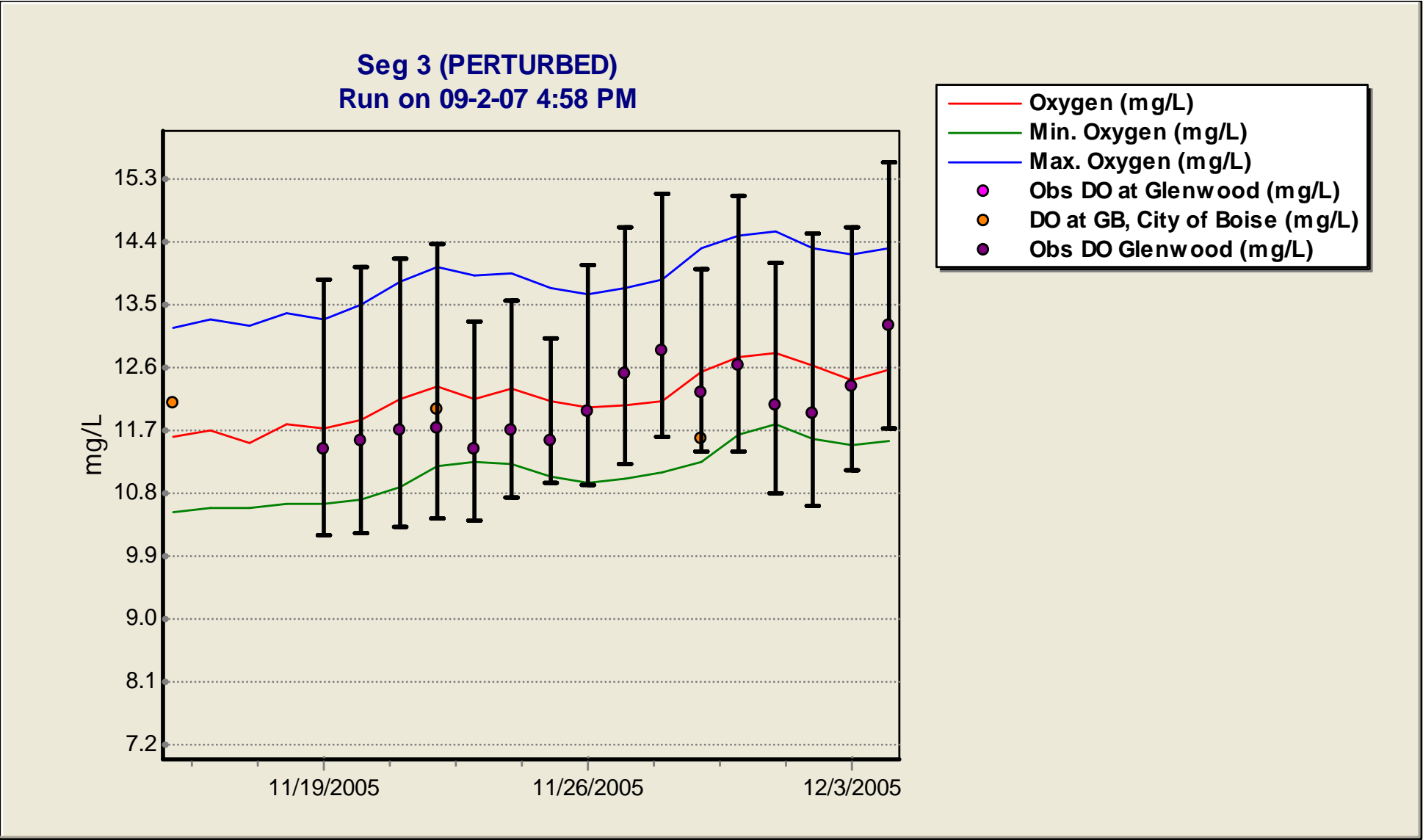
AQUATOX can now run with an hourly time-step including hourly light inputs. This results in a simulation of oxygen concentrations on an hourly basis



Monitoring data indicate that oxygen levels fluctuate daily



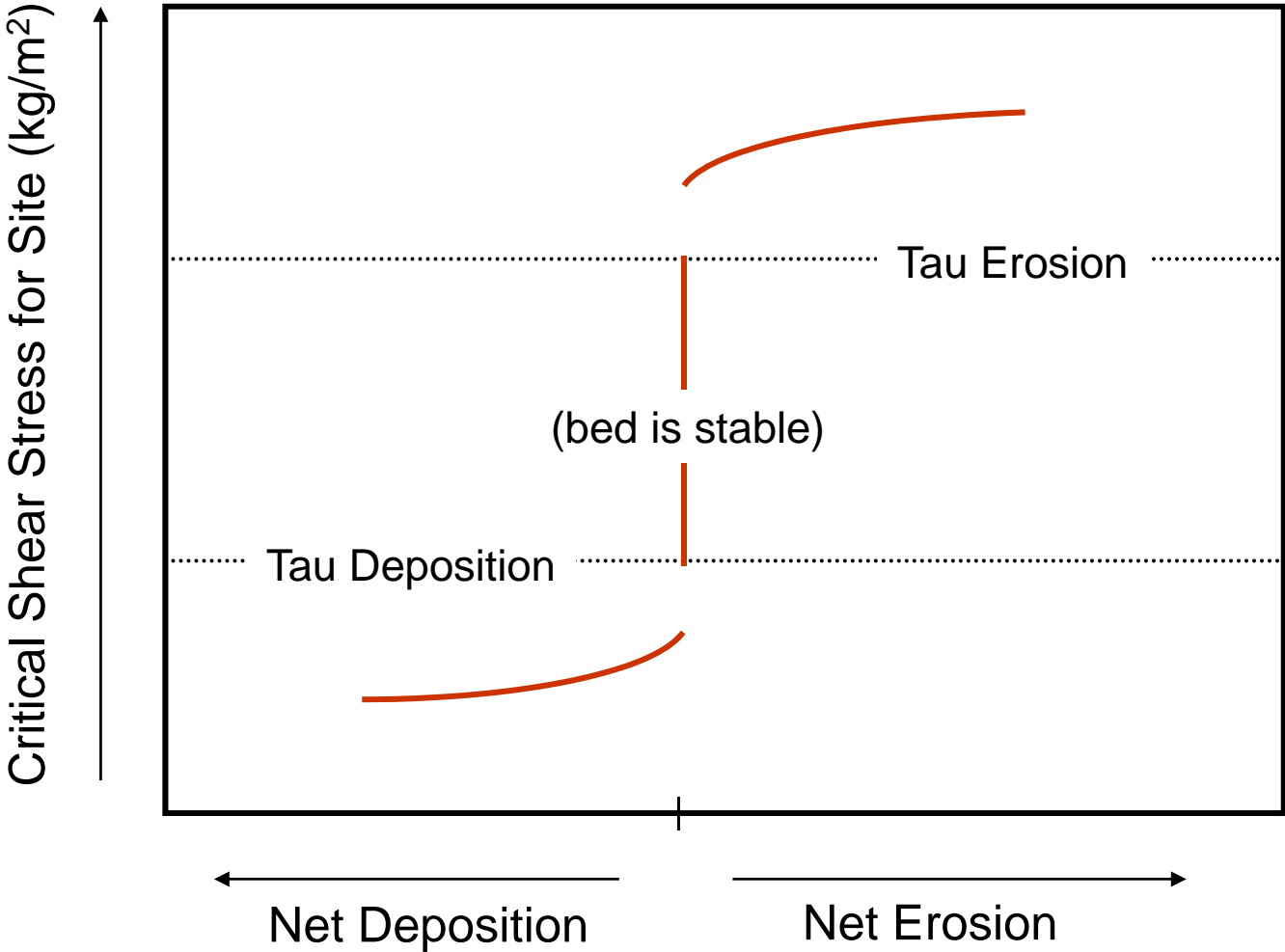
# Diel Oxygen, Light; Hourly time-step



# 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

# Critical Shear Stress for Erosion and Deposition Key Parameters



# AQUATOX Multi-Layer Sediment Model based on the IPX module (Velleux et al. 2000)

