AQUATOX Short Course

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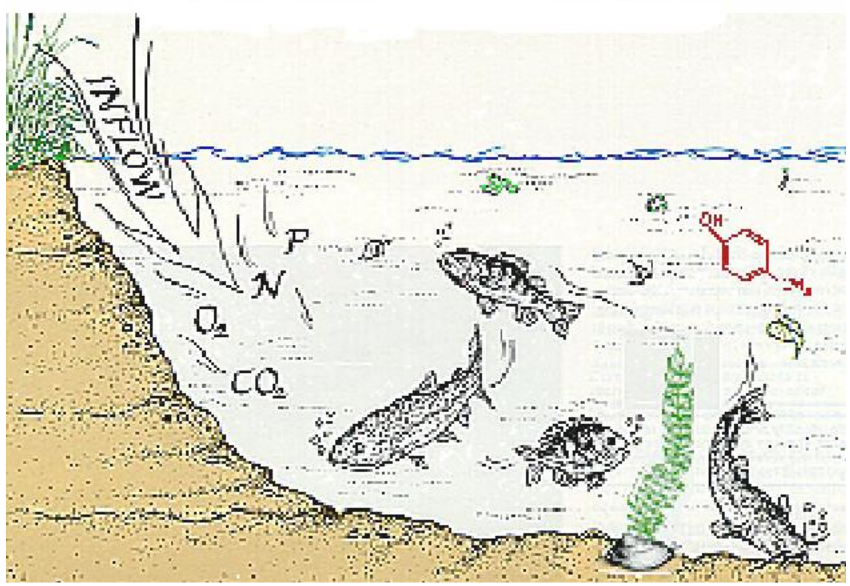


Introduction to Course, Organization

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

Overview: What is AQUATOX?

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

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)
  - "Probably… the most advanced environmental model worldwide. " in review of 17 ecological models (Kianirad et al. 2006)
  - 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
  - WASP7 models total phytoplankton and benthic algae (Wool et al. 2004, Ambrose et al. 2006); zooplankton are just a grazing term; no grazing or sloughing of benthic algae
  - QUAL2K models phytoplankton and "bottom algae" (Chapra and Pelletier 2003); no animals
- 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:
  - What is the most important stressor?
  - Will proposed actions reverse the impairment?
    - restoration of desirable aquatic community and/or designated uses
    - improved chemical water quality
  - Will there be any unintended consequences?
  - How long will recovery take?
  - Uncertainty around predictions

Regulatory Endpoints Modeled

- Nutrient and toxicant concentrations
- Biomass
  - plant, invertebrate, fish
- Chlorophyll a
  - phytoplankton, periphyton, moss
- Biological metrics
- Total suspended solids, Secchi depth
- Dissolved oxygen
  - daily minimum and maximum
- Biochemical oxygen demand
- Bioaccumulation factors
- Half-lives of organic toxicants

Potential Applications *nutrients*

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

Potential Applications of AQUATOX *toxic substances*

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

Potential Applications
aquatic life support

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

Comparison of Dynamic Risk Assessment Models

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

Comparison of Bioaccumulation Models: Biotic State Variables

Table 3.2. Comparison of Bioaccumulation State Variables

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

Imhoff et al. 2004

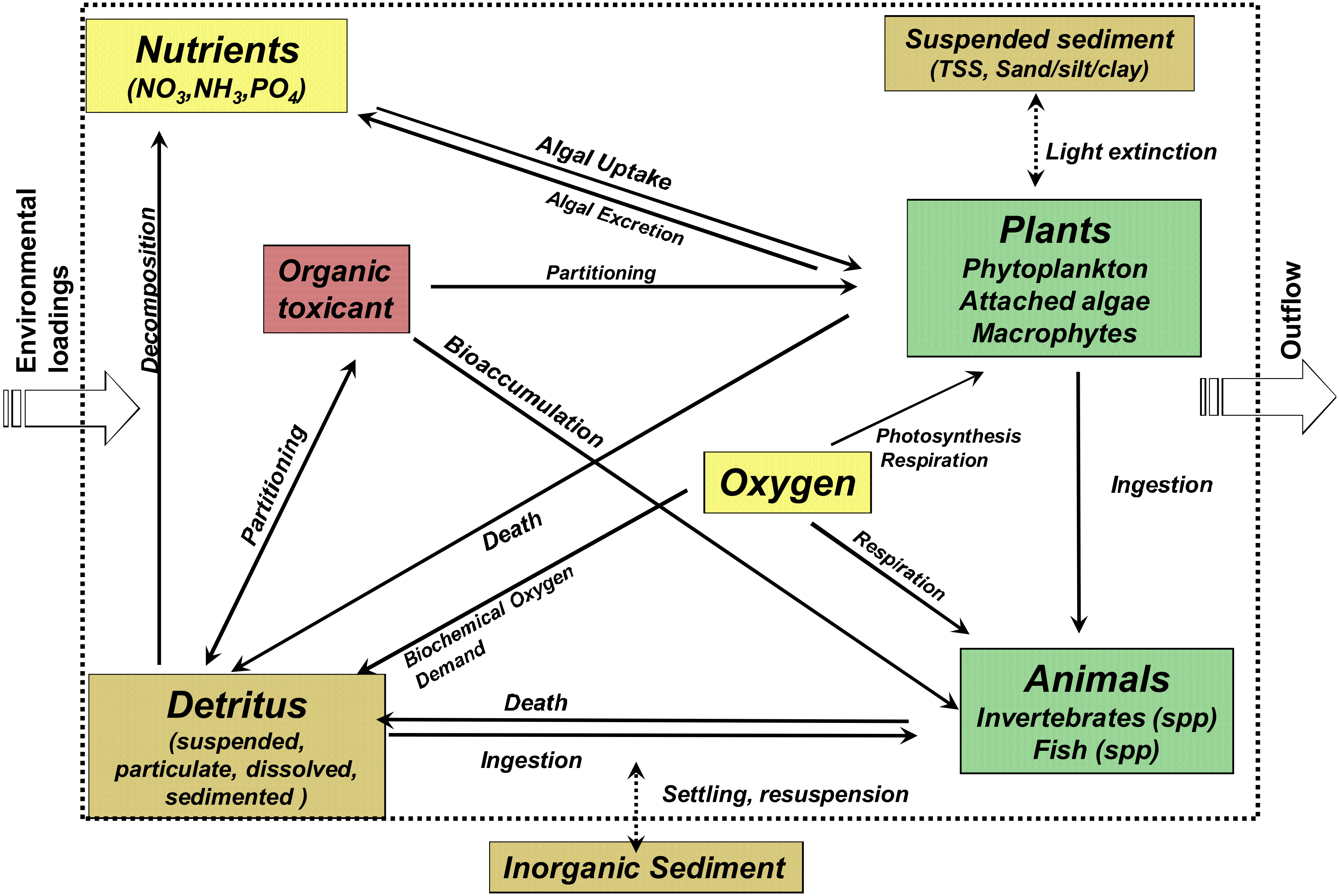
What AQUATOX does *not* do

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

AQUATOX Structure

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

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



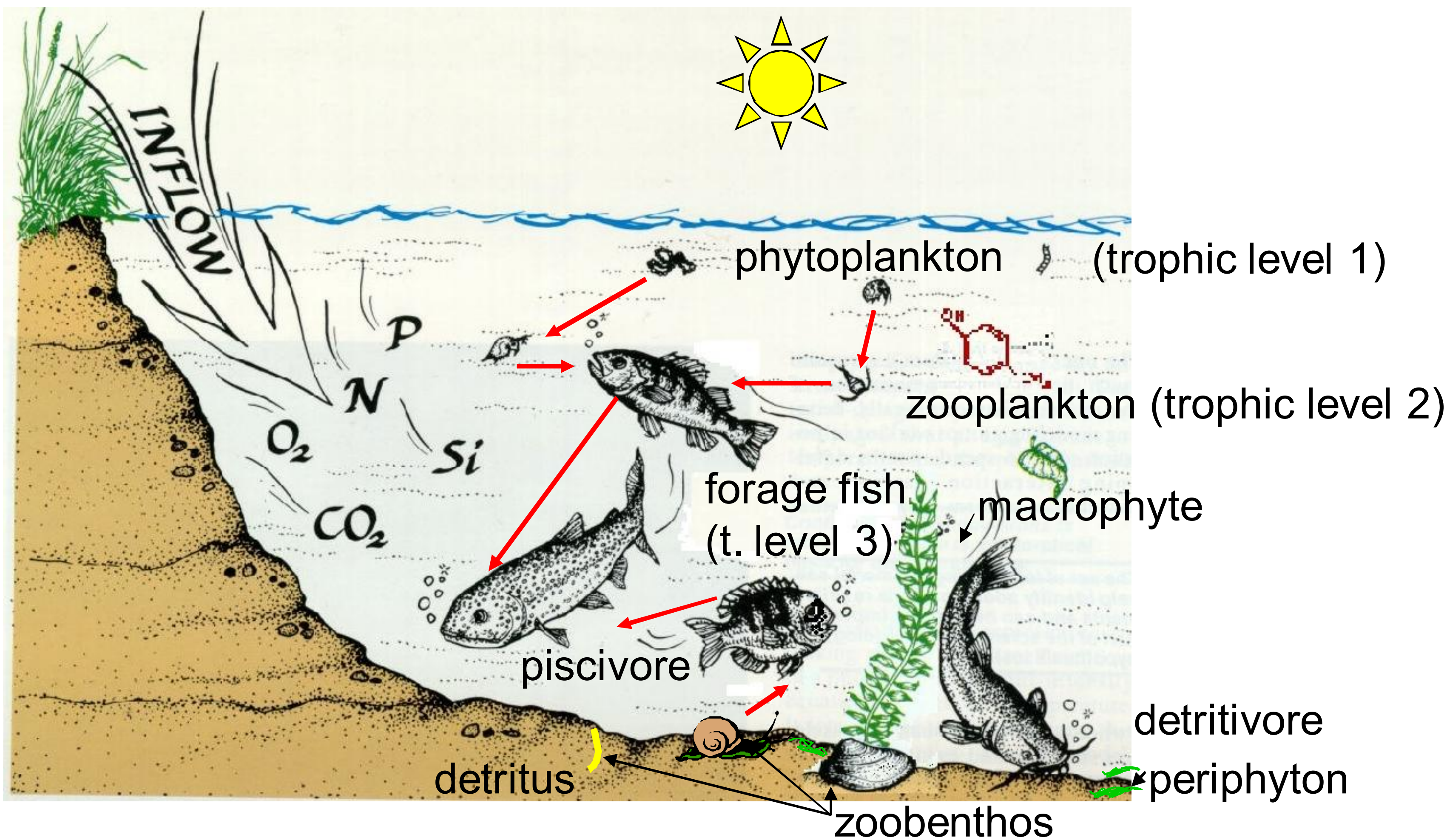
Processes Simulated

- Bioenergetics
  - feeding, assimilation
  - growth, promotion, emergence
  - reproduction
  - mortality
  - trophic relations
  - toxicity (acute & chronic)

- Environmental fate
  - nutrient cycling
  - oxygen dynamics
  - partitioning to water, biota & sediments
  - bioaccumulation
  - chemical transformations
  - biotransformations

- Environmental effects
  - direct & indirect

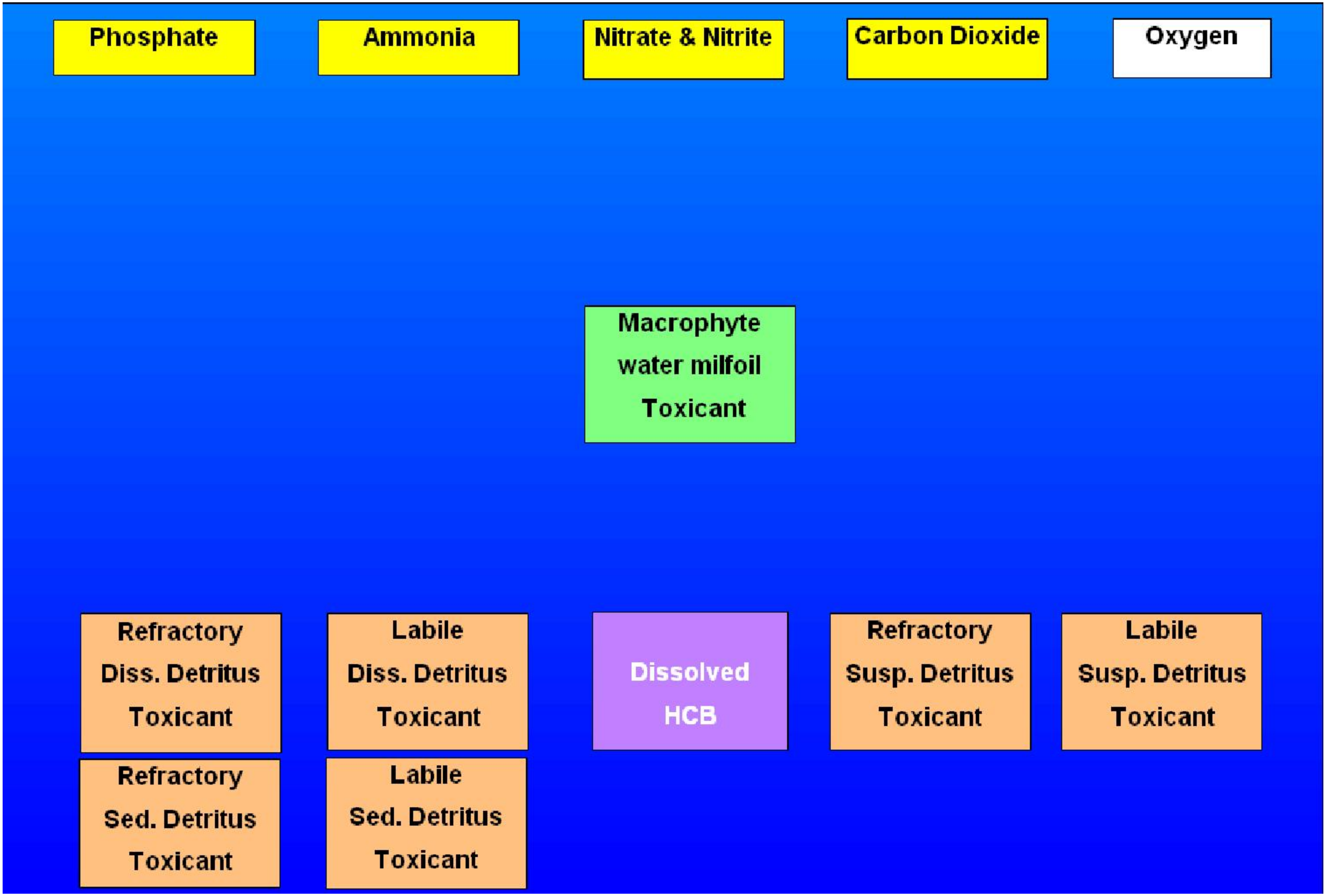
Ecosystem components



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



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

Release 3.1

(Currently in beta release)

- 64-bit-compatible software installer
- Updated ICE toxicity regressions
- Improved uncertainty & sensitivity output
- Additional outputs for diagenesis & bioaccumulation
- Improved database export & search capabilities
- More flexible linkage to HSPF watershed model

- **In progress:**
  - Technical Documentation and interface refinements
  - Testing bioaccumulation refinements.
  - Diagenesis optimization?

Beta available at warrenpinnacle.com AQUATOX page

Demonstration 1

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

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

What are the Analytical Capabilities?

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

The Many Types of AQUATOX Output

(in order of output list)

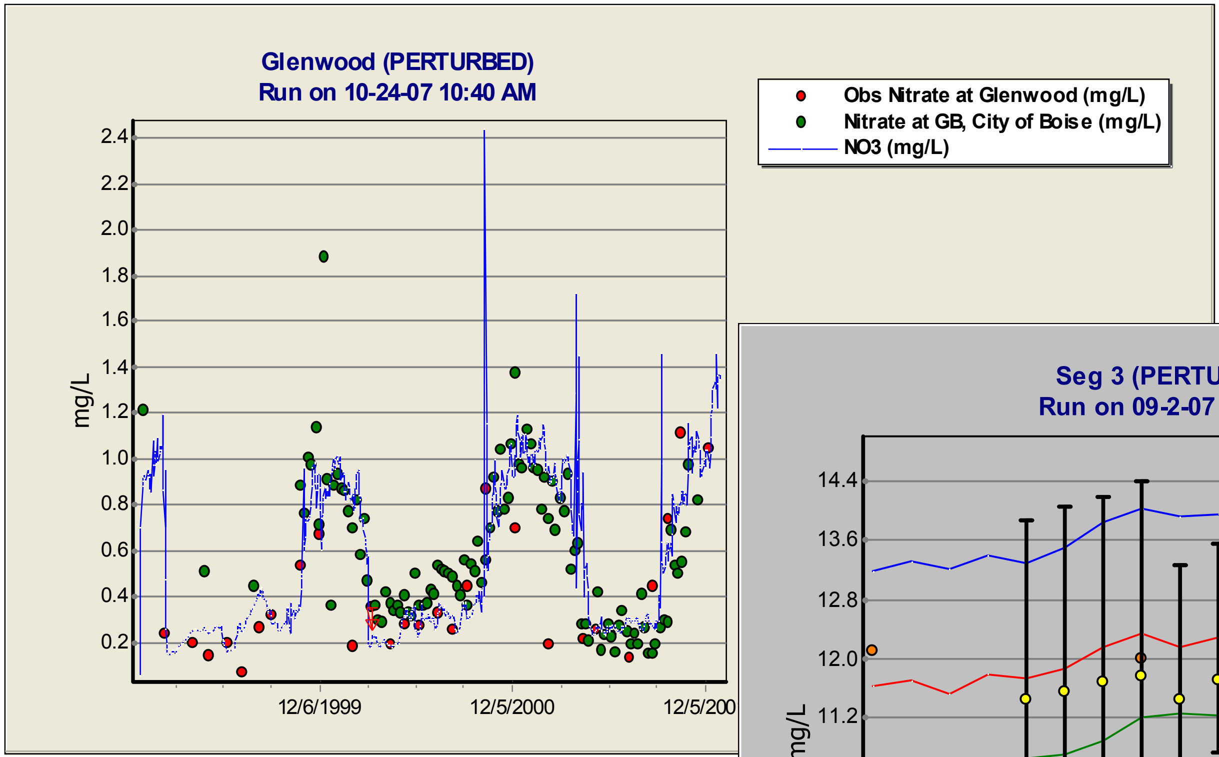
- Concentrations of State Variables
  - toxicants in water
  - nutrients and gasses
  - organic matter, plants, invertebrates, fish
- Physical Characteristic State Variables
  - water volume, temperature, wind, light, pH
- Mass of Toxicants within State Variables (normalized to water volume)
  - T1-T20 in organic matter, plants, invertebrates, and fish
- Additional Model Calculations
  - Secchi depth, chlorophyll *a*, velocity, TN, TP, BOD
- Biological metrics
  - % EPT, Chironomids, Amphipods, % Blue-Greens, Diatoms, Greens, Gross Primary Production, Turnover, Trophic State Indices

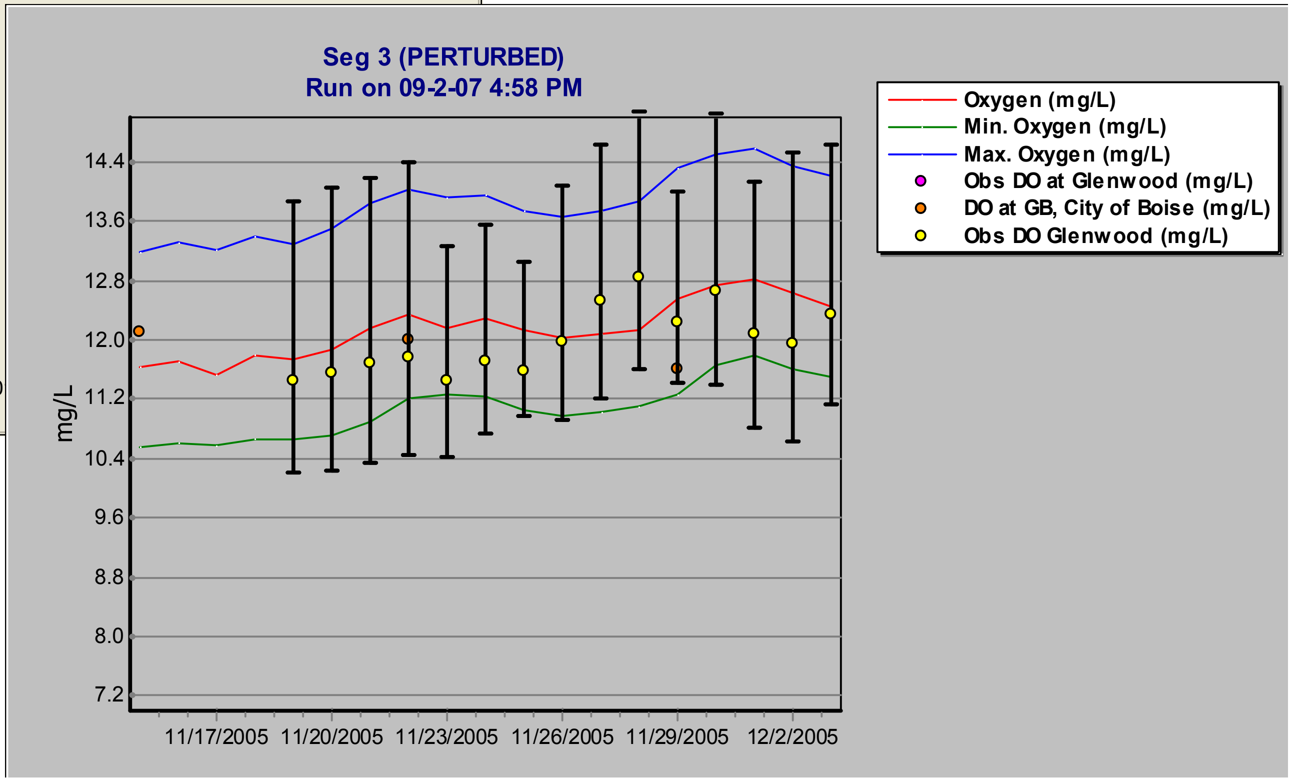
The Many Types of AQUATOX Output
(continued)

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

Graphical Analysis

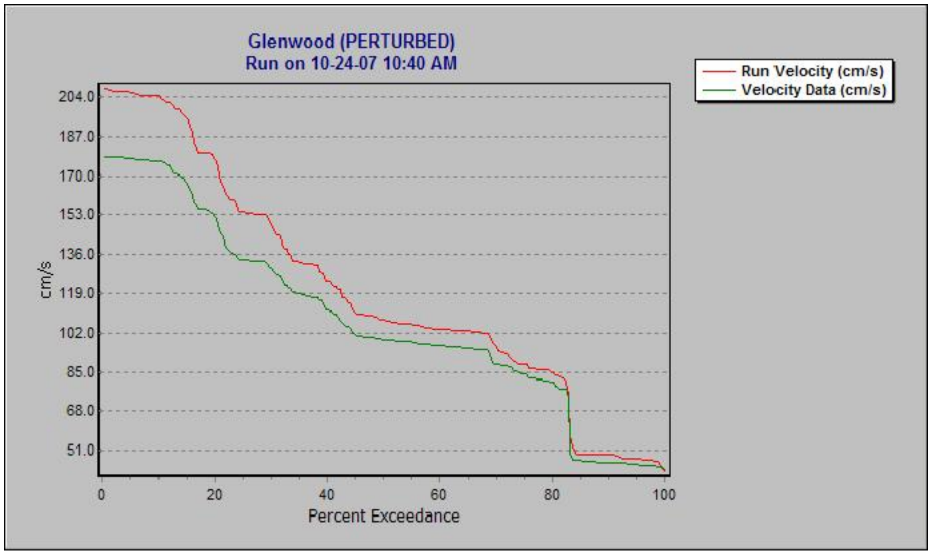
Compare observed data to model output

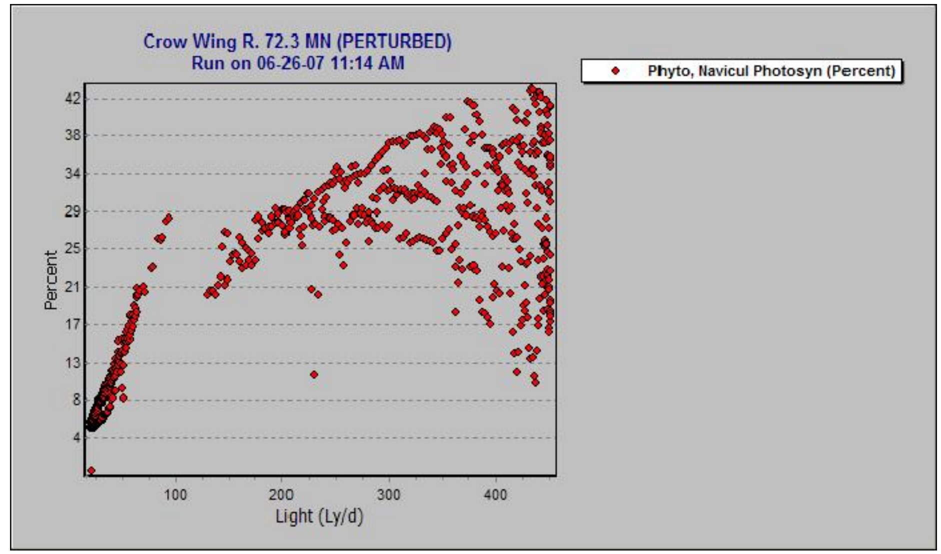




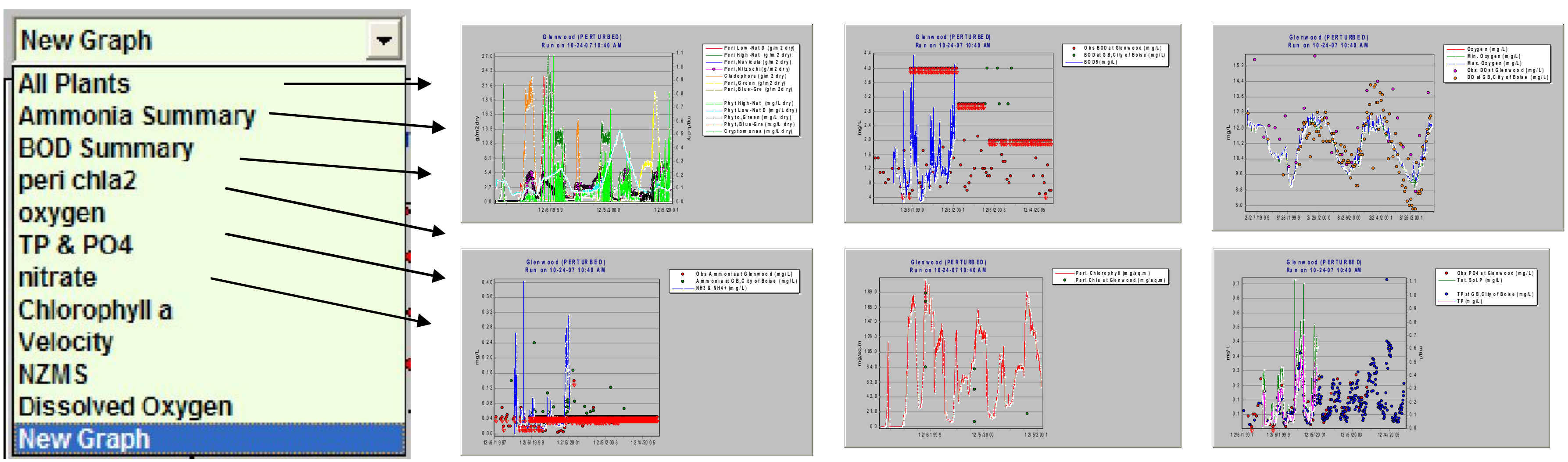
Graphical Analysis

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





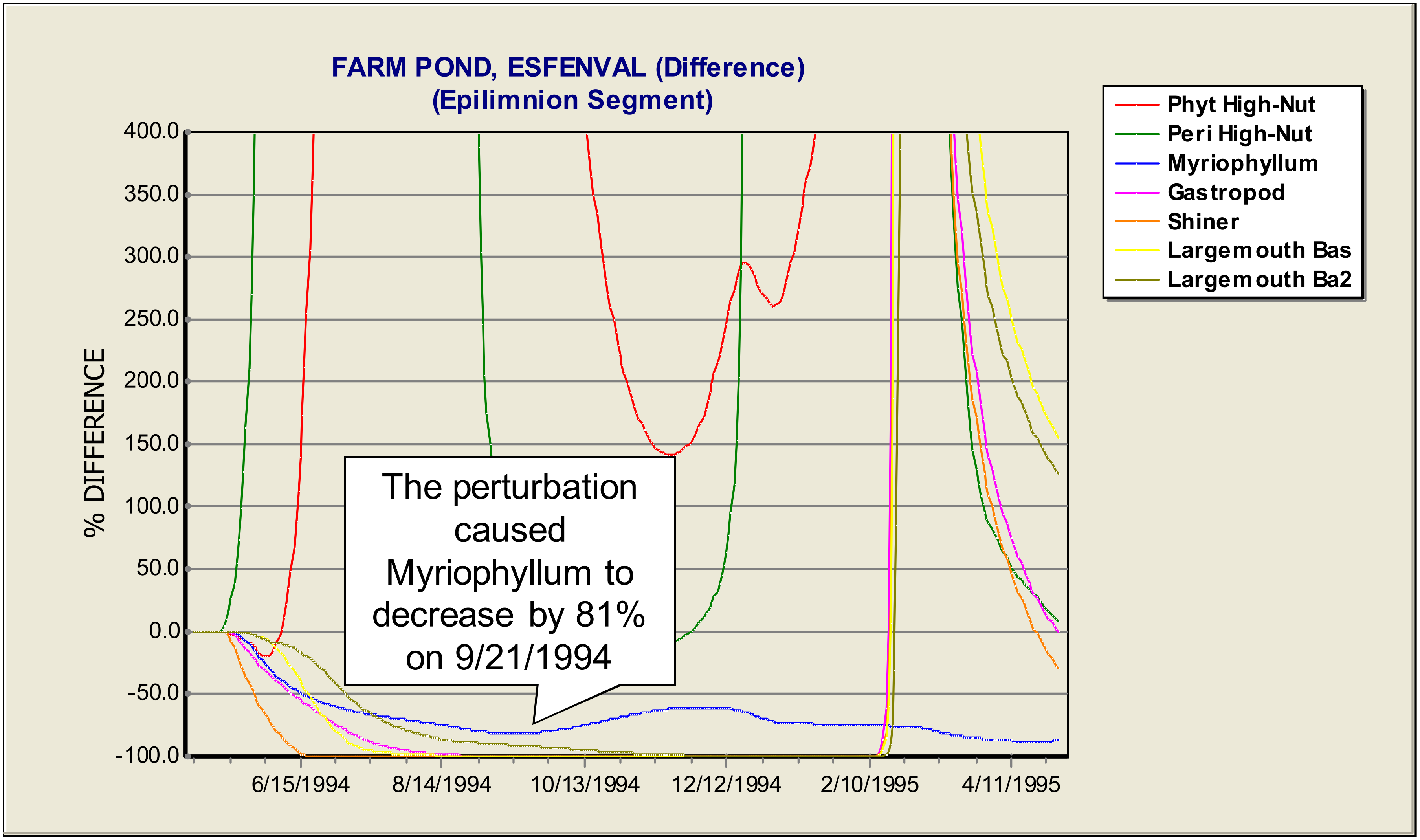
Graph Library saved within simulation



Comparing Scenarios: the "Difference" Graph

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

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



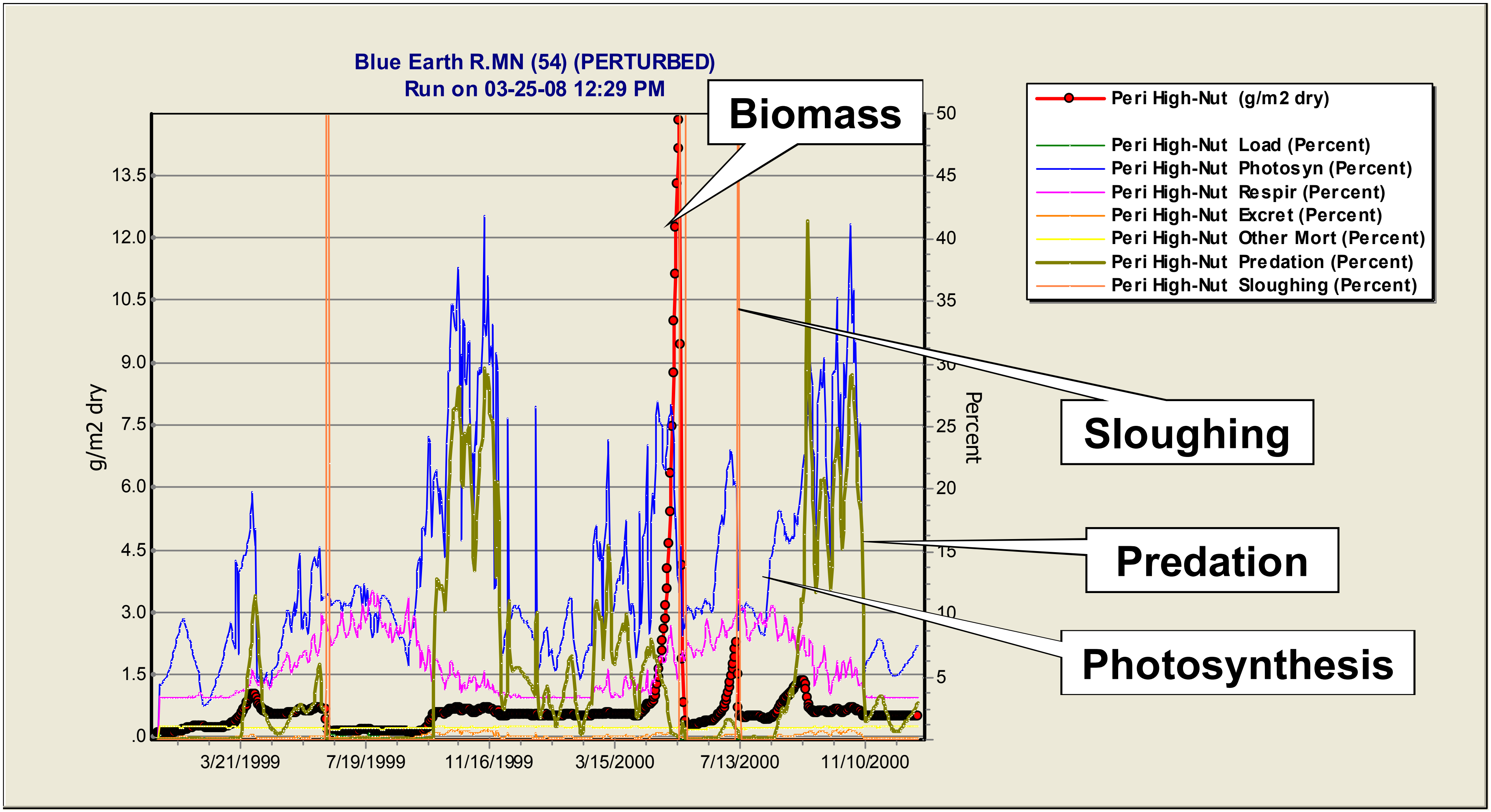
Process Rates

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

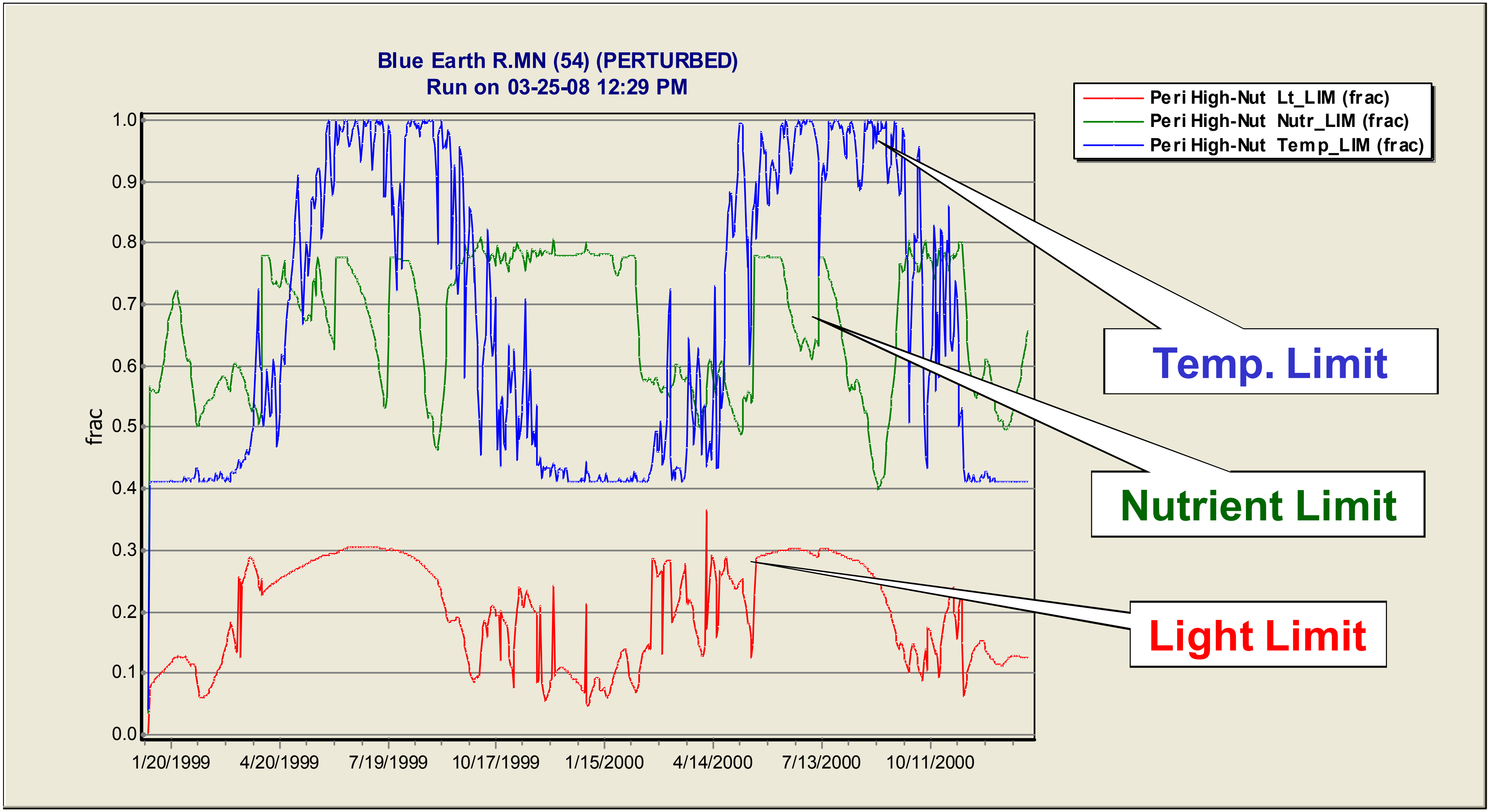
$$\frac{dBiomass_{Peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion$$
$$- Mortality - Predation + Sed_{Peri}$$

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

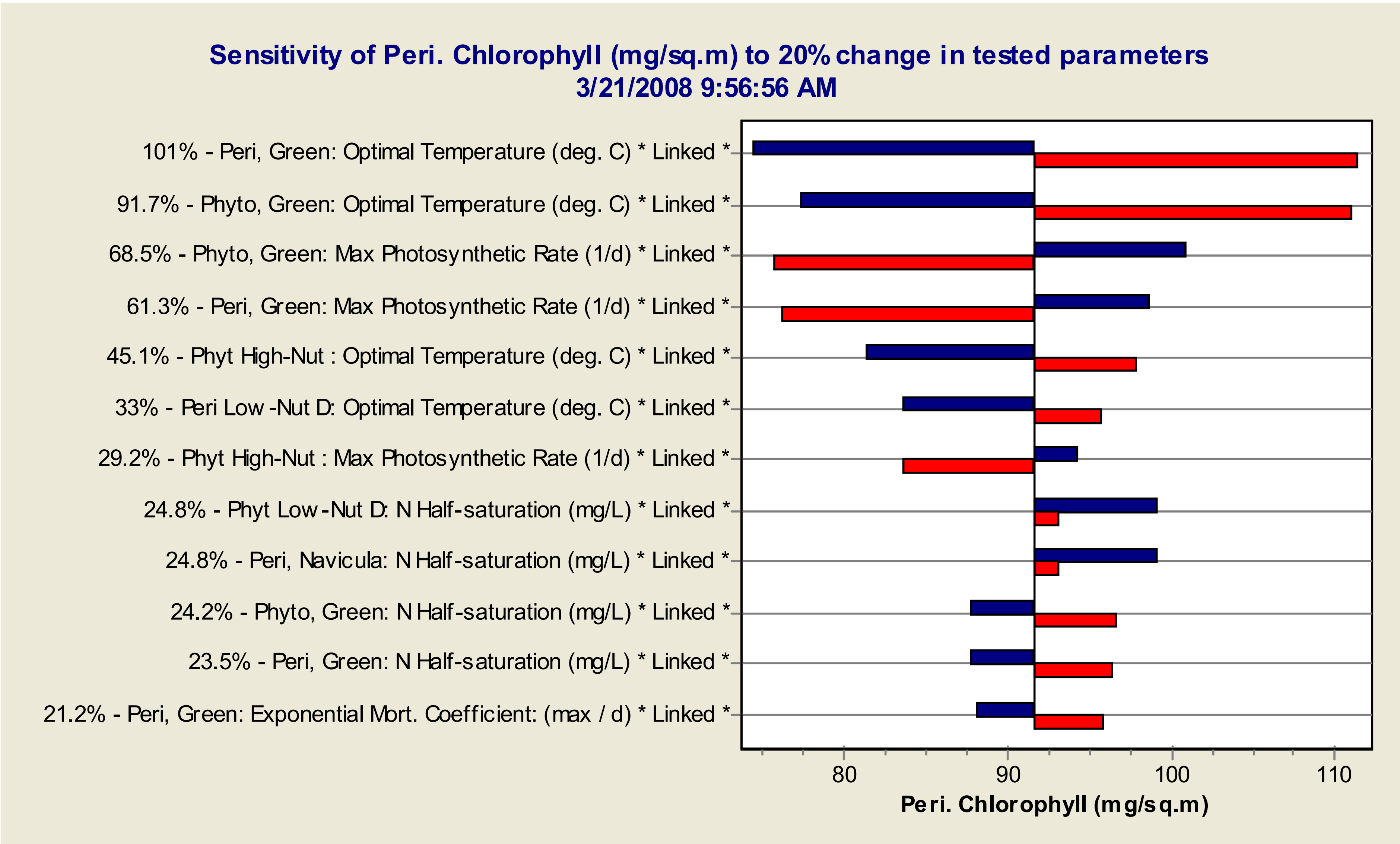
Rates Plot Example: Periphyton



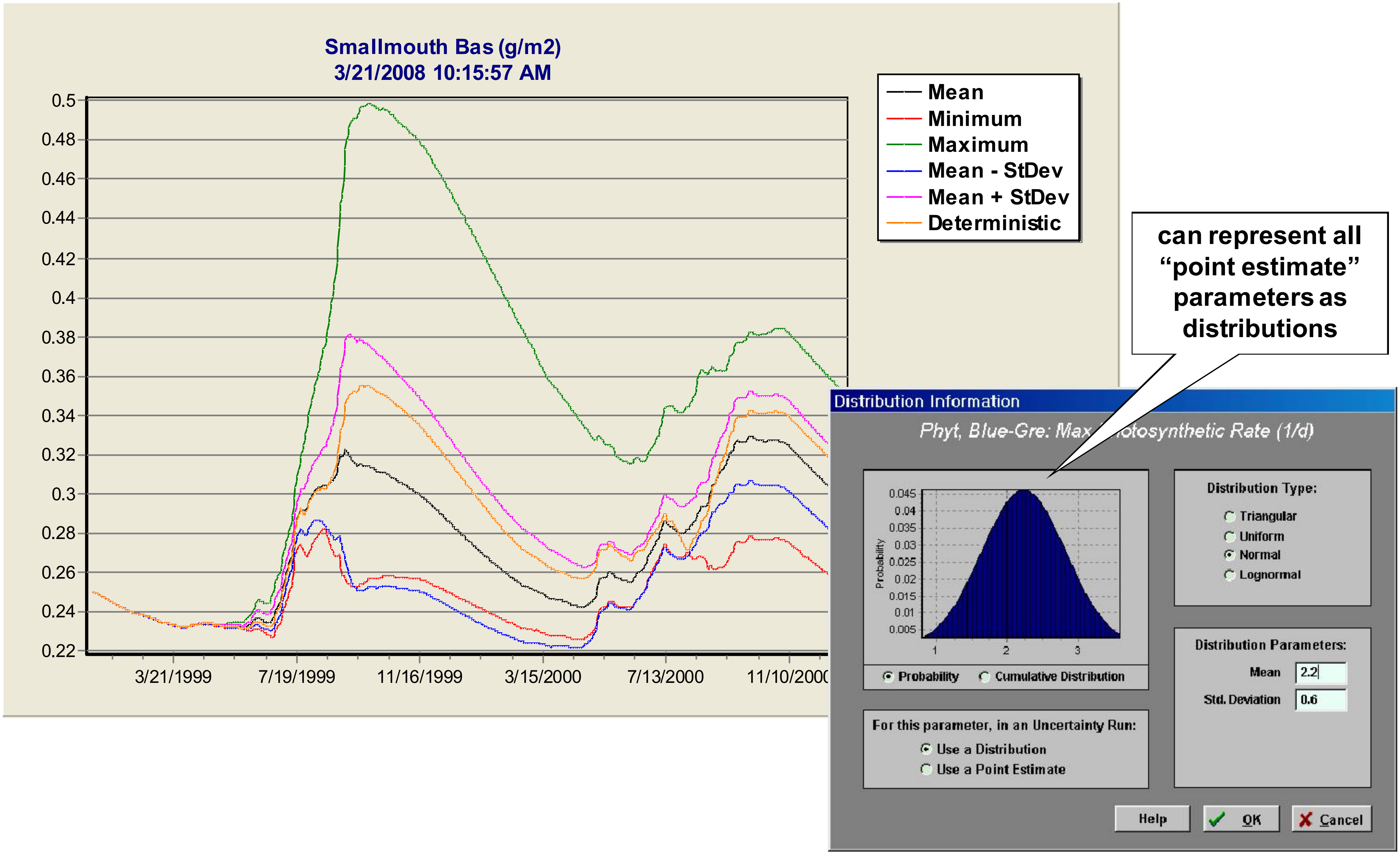
Limitations to Photosynthesis May also be Graphed



Integrated Nominal Range Sensitivity Analysis with Graphics

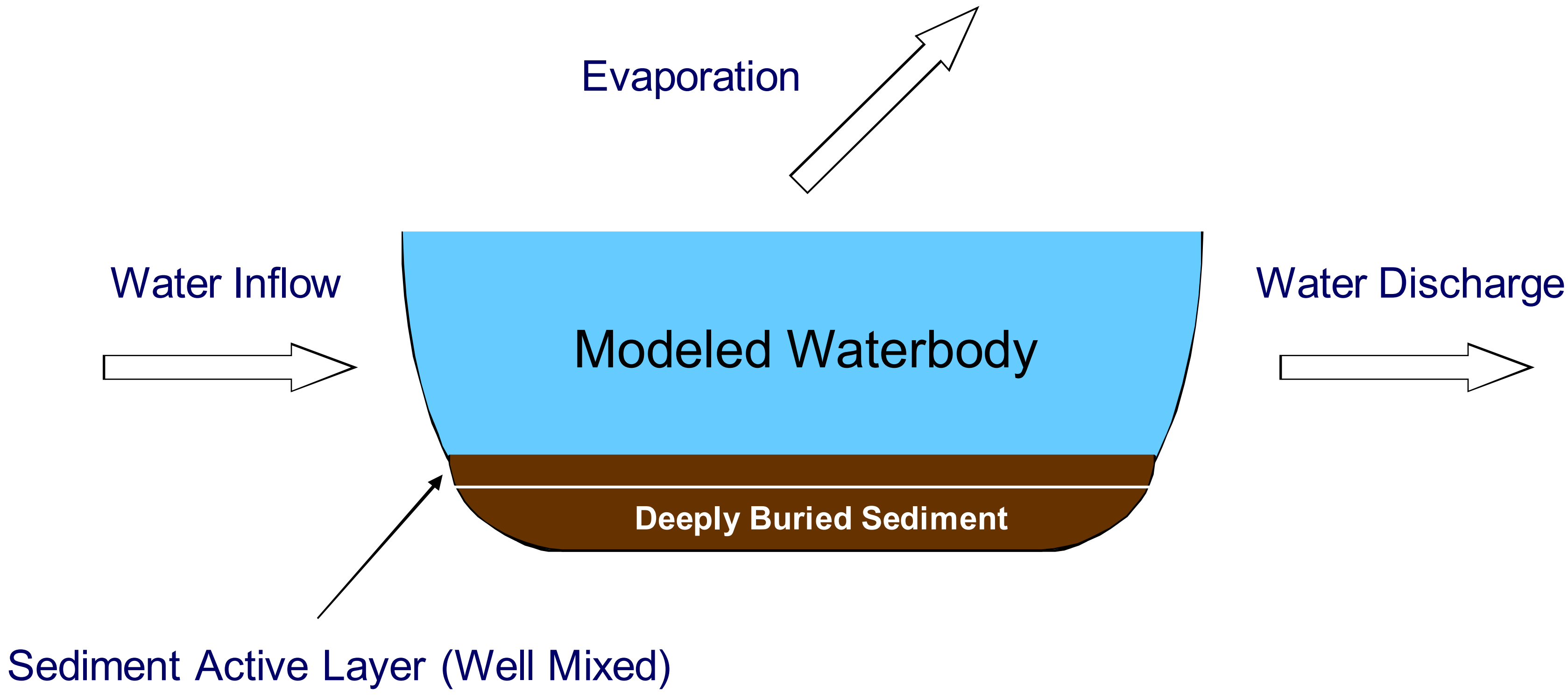


Integrated Latin Hypercube Uncertainty Analysis with Graphics

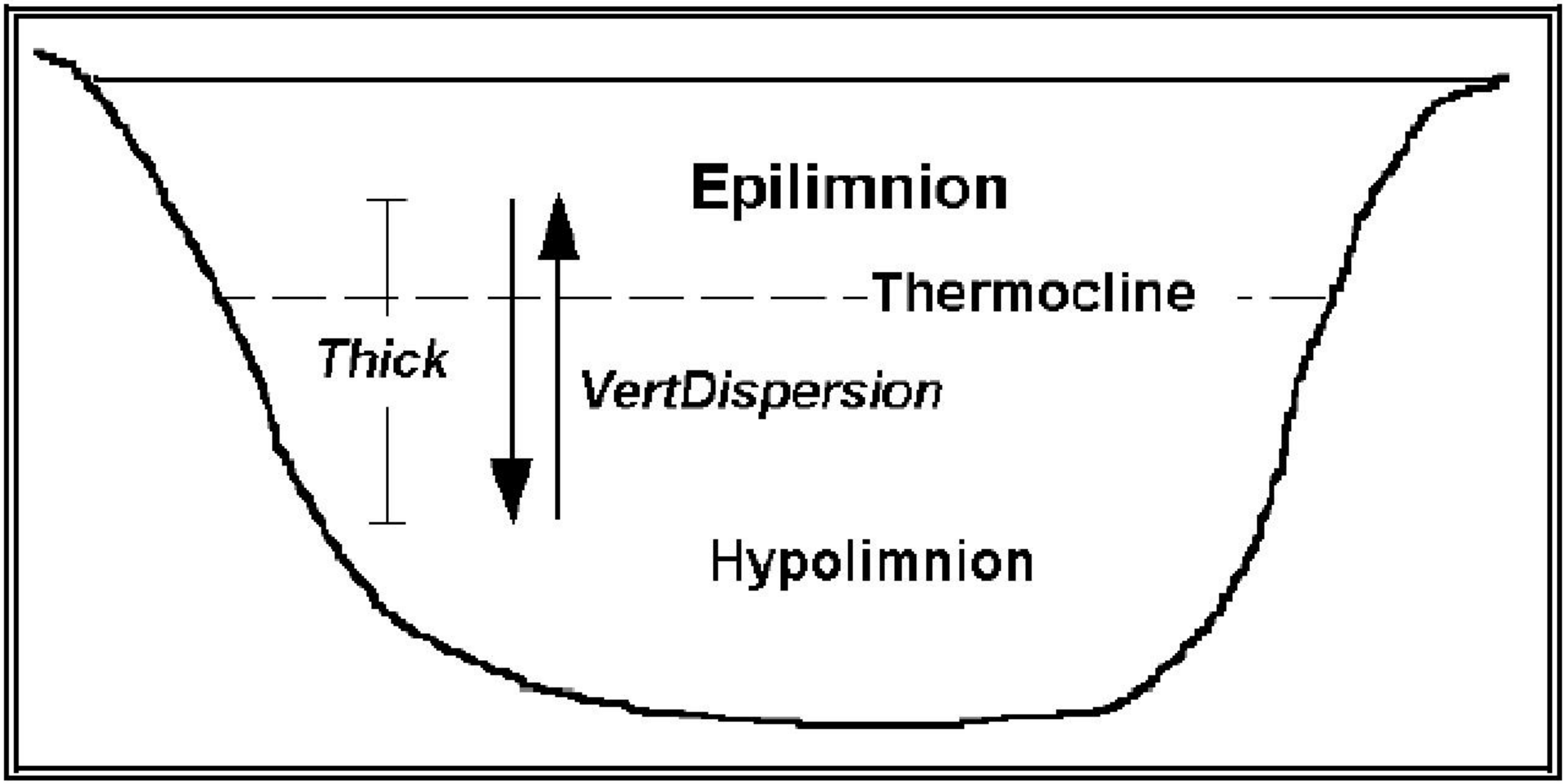


Physical Characteristics of a Site

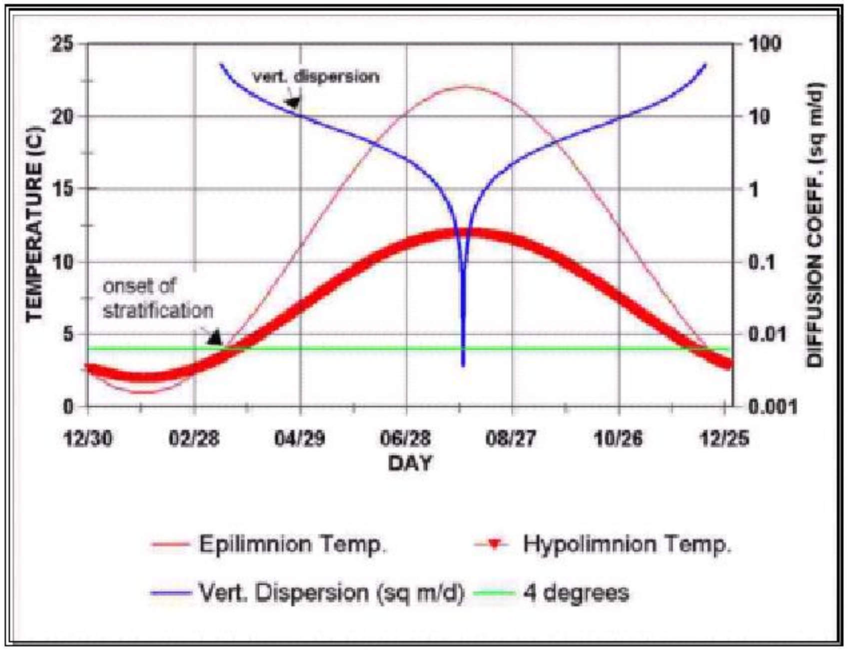
Water Balance and Sediment Structure



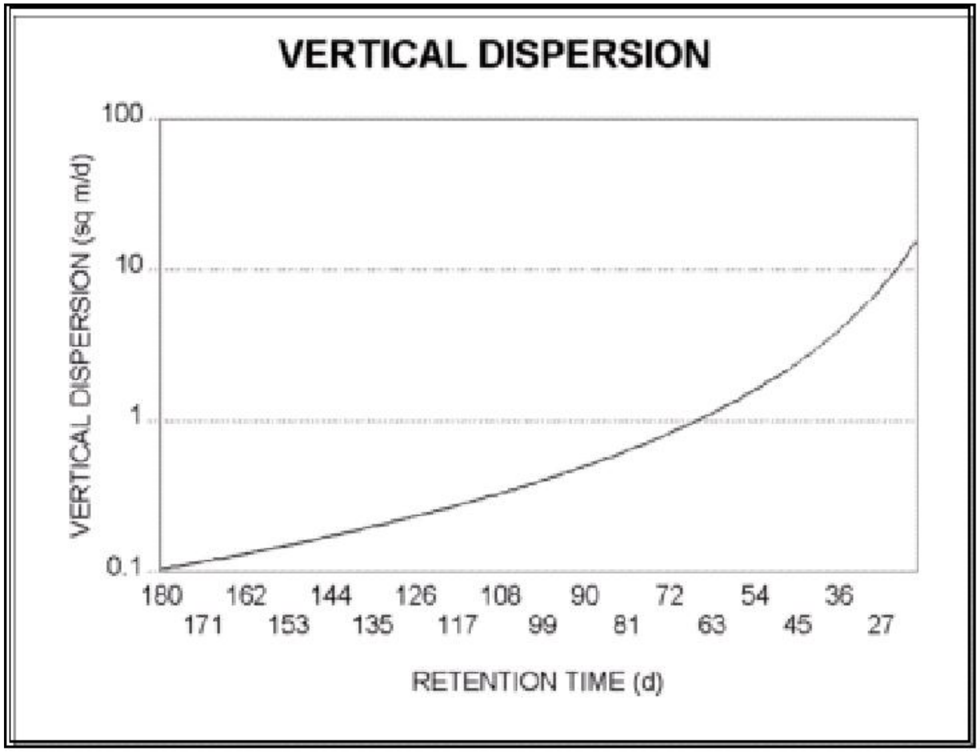
Thermal Stratification in a Lake



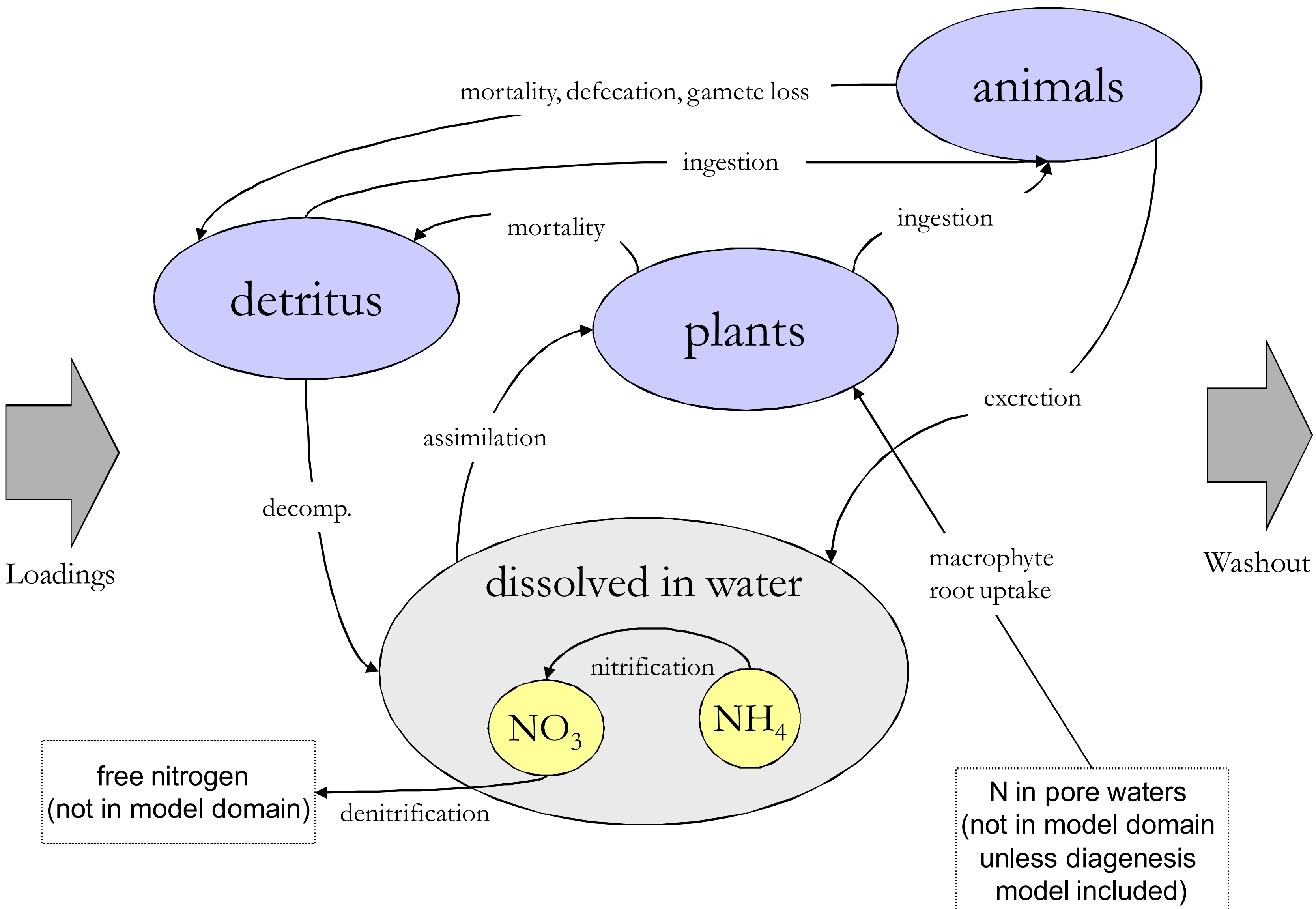
Stratification is a function of temperature differences



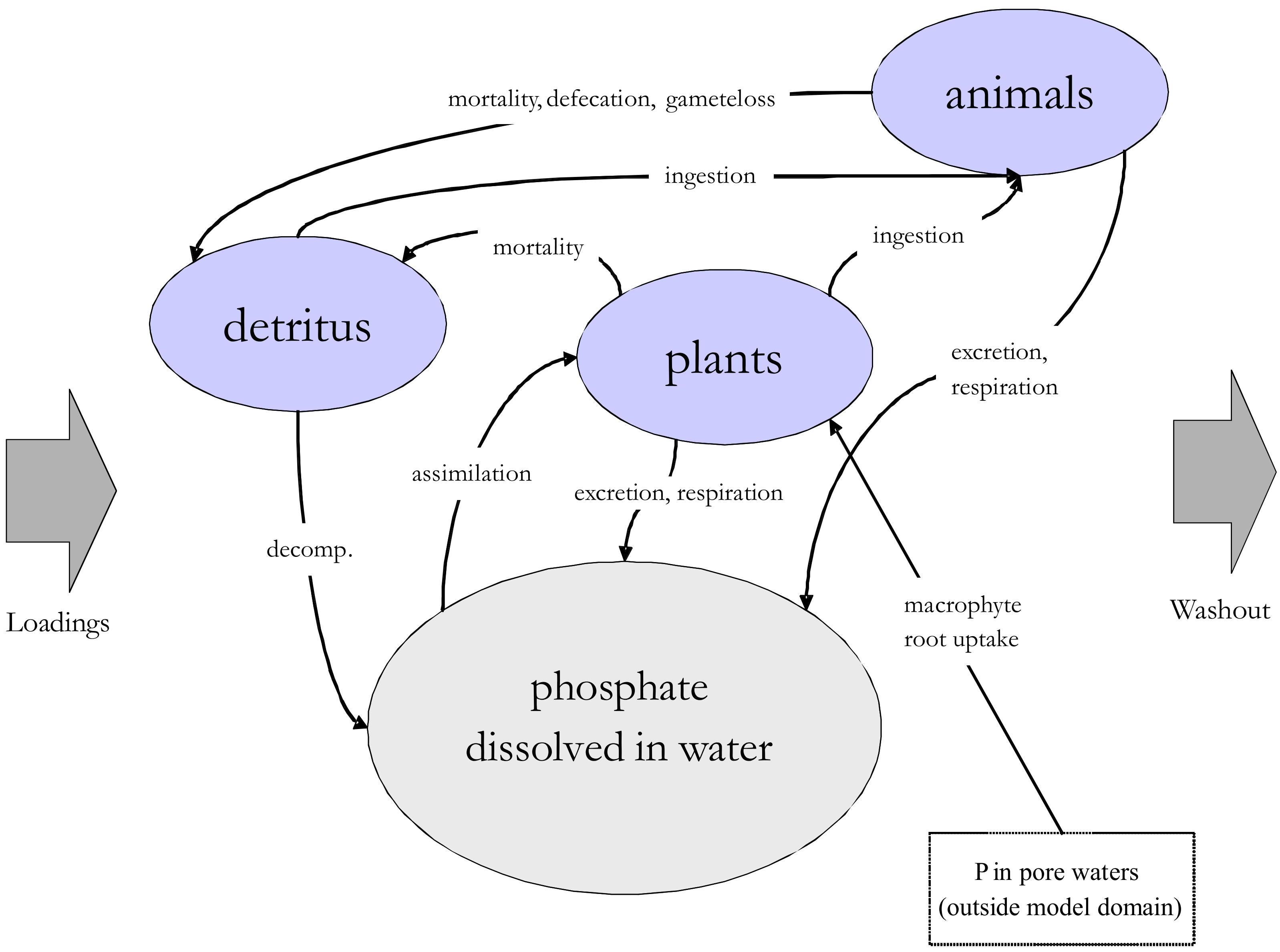
Increased mixing is also a function of discharge



Nutrient Cycle in AQUATOX (Nitrogen)

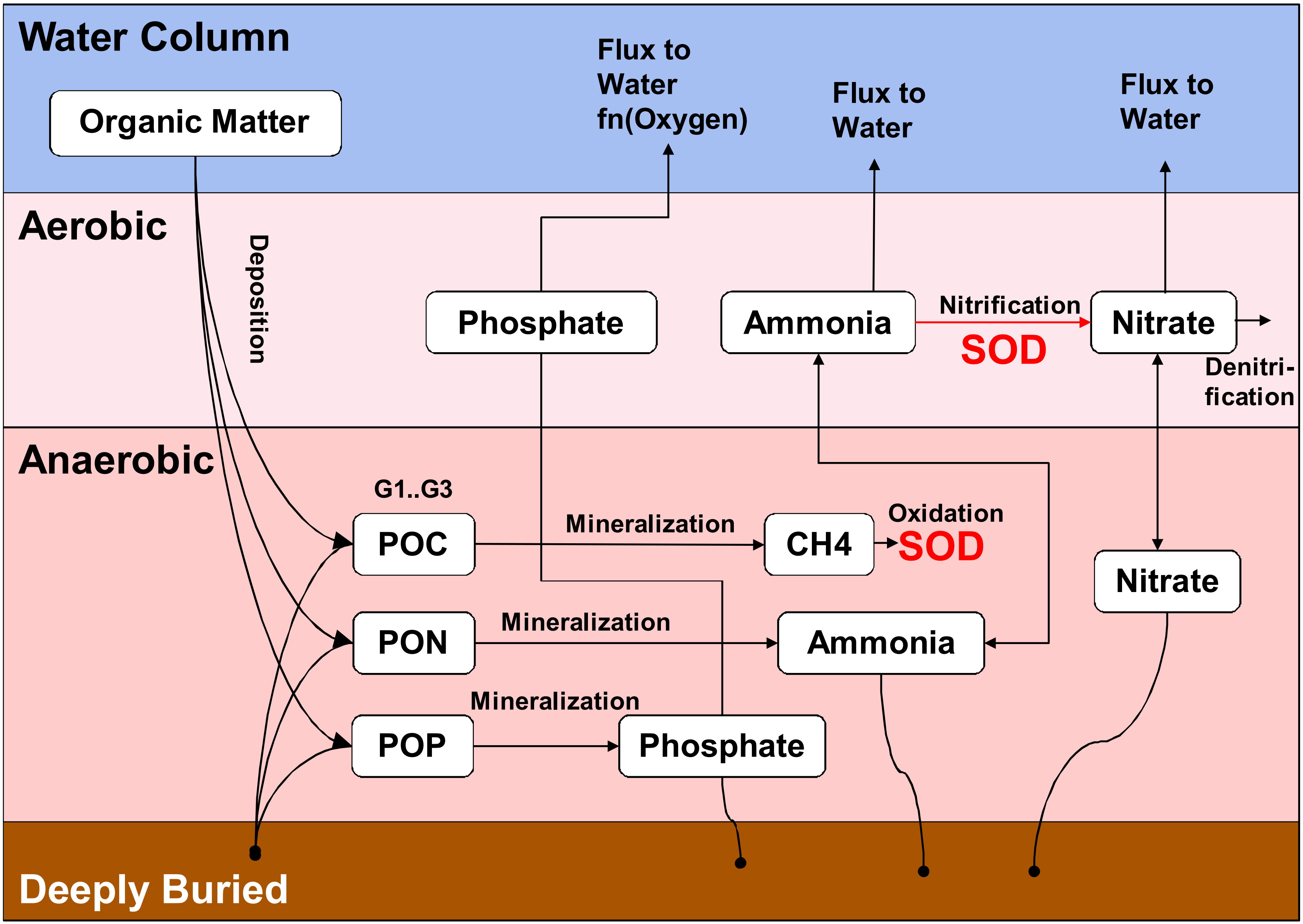


Nutrient Cycle in AQUATOX (Phosphorus)



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) is a function of specific chemical reactions following the decomposition of organic matter
  - methane or sulfide production
  - nitrification of ammonia

Nutrient Effects on Simulations

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

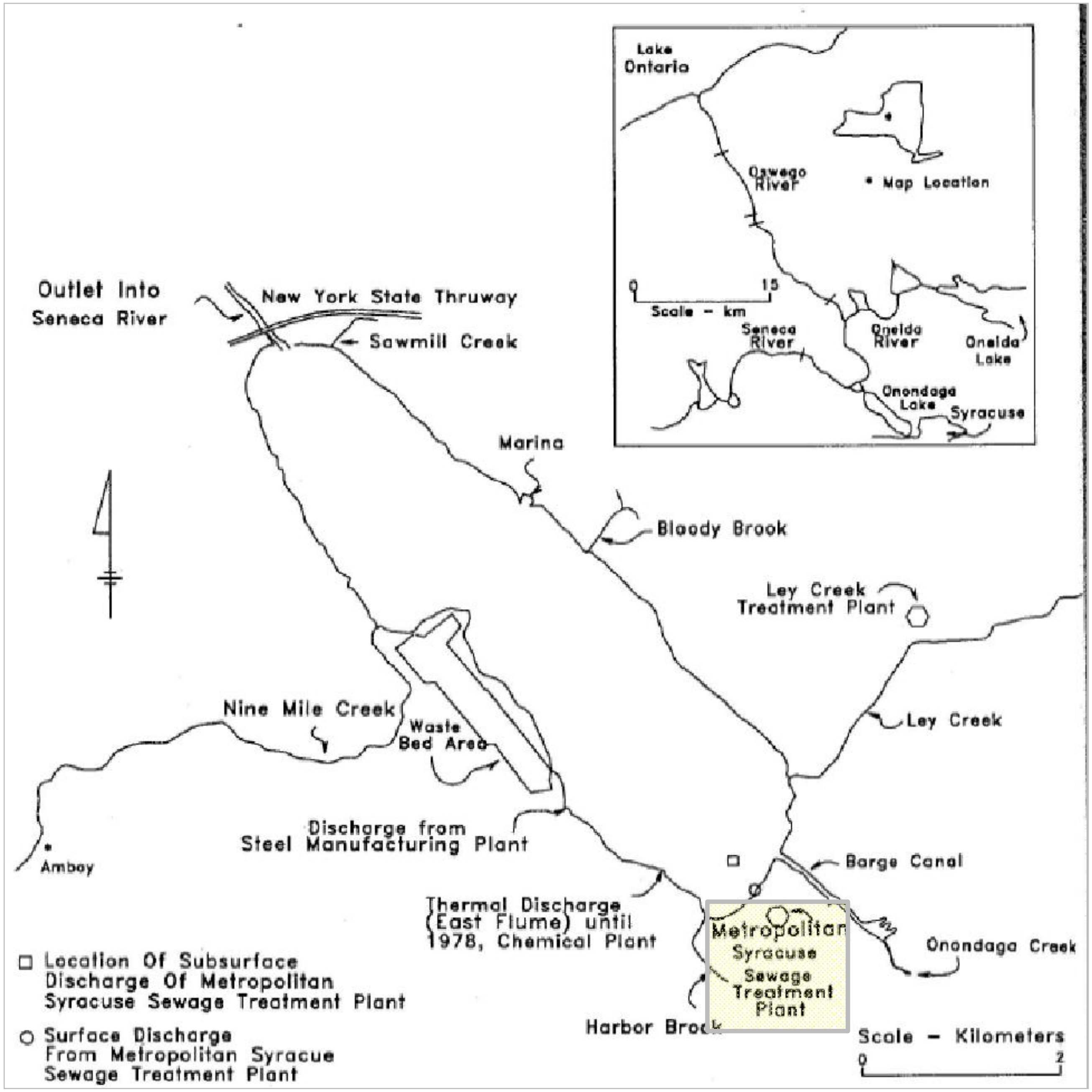
Applications in Nutrient Analysis

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

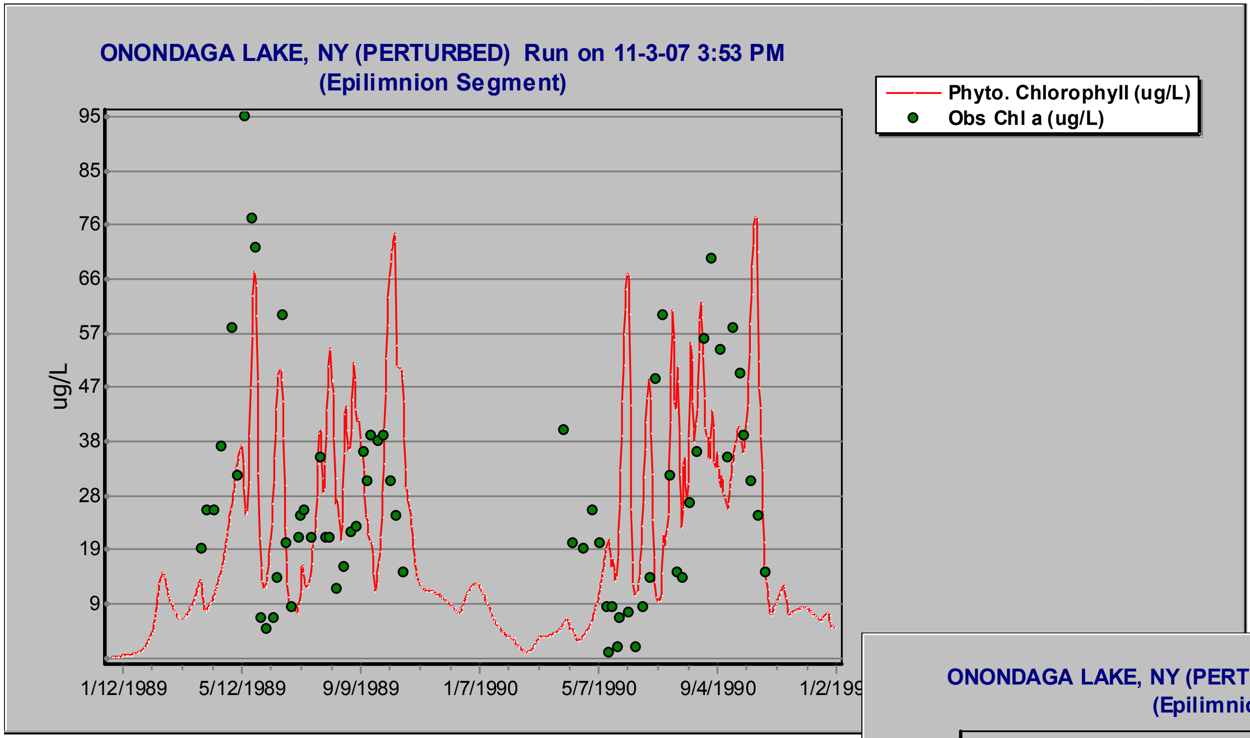
Lake Onondaga, NY

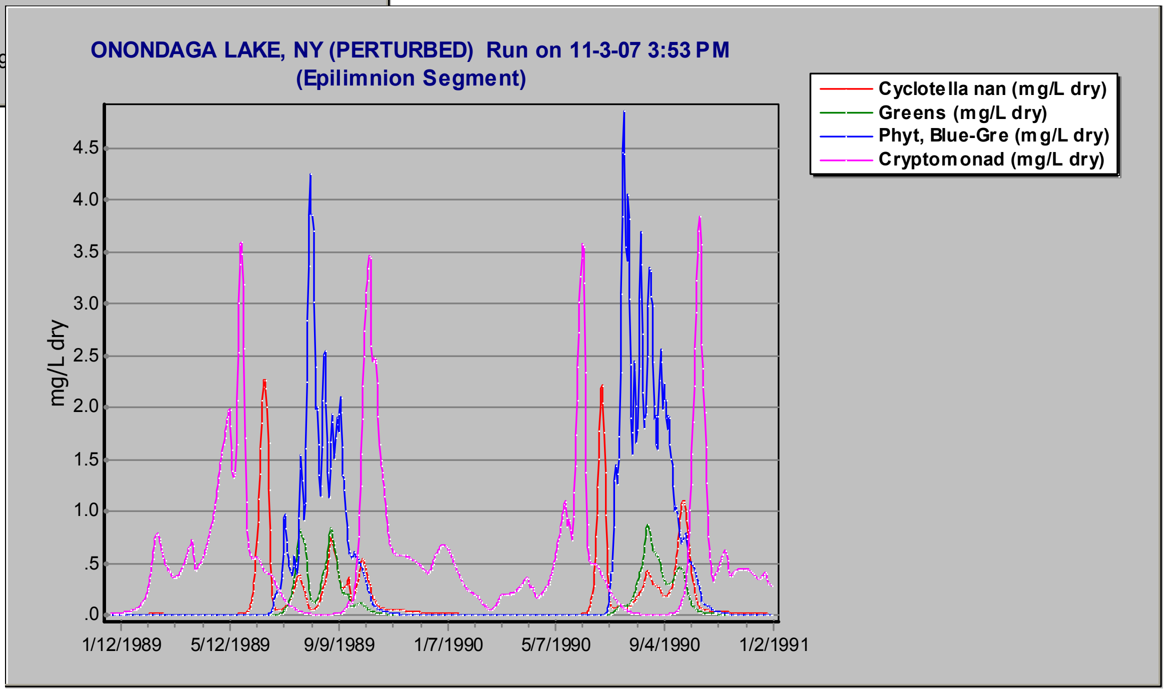
- AQUATOX Validation Site for Release 1
- Was called "Most polluted lake in U.S."
  - nutrient inputs from wastewater treatment plant ("Metro") & combined sewers
  - successive algal blooms
  - hypoxia in hypolimnion
  - build-up of organic sediments in bottom
  - high mercury levels (not modeled at present)
  - high salinity affects stratification
- *Many problems in lake have been corrected*
  - *recent implementation was recalibrated*

Lake Onondaga NY, heavily polluted

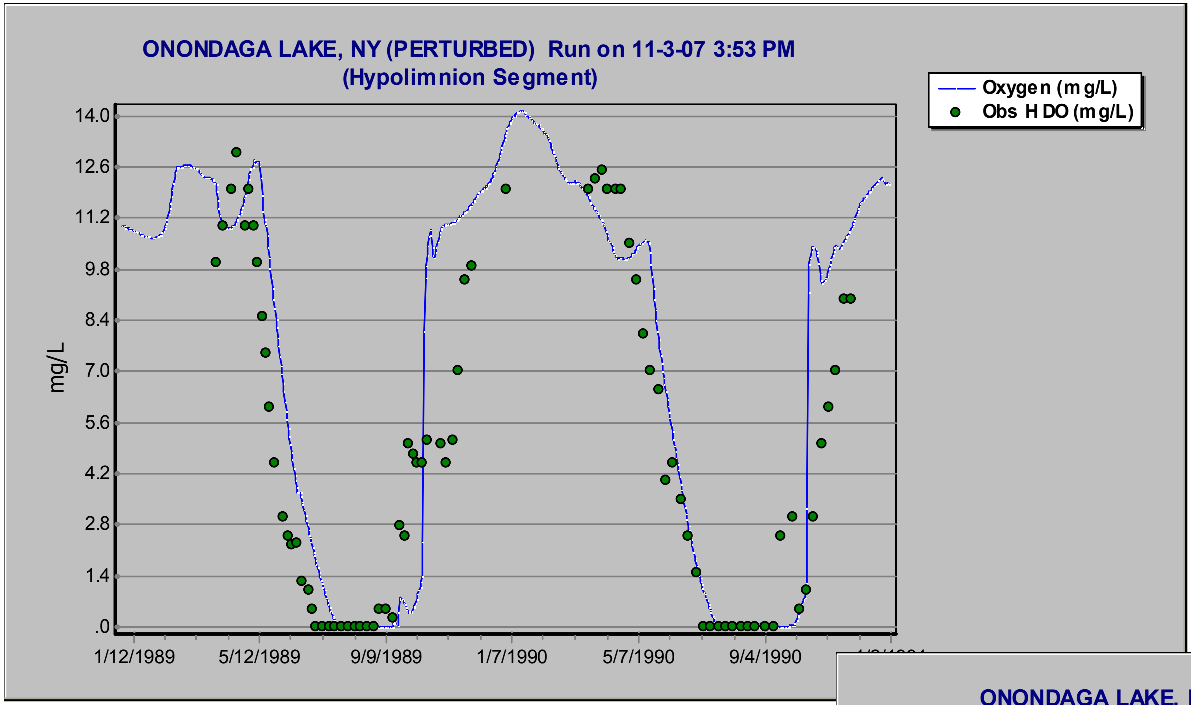


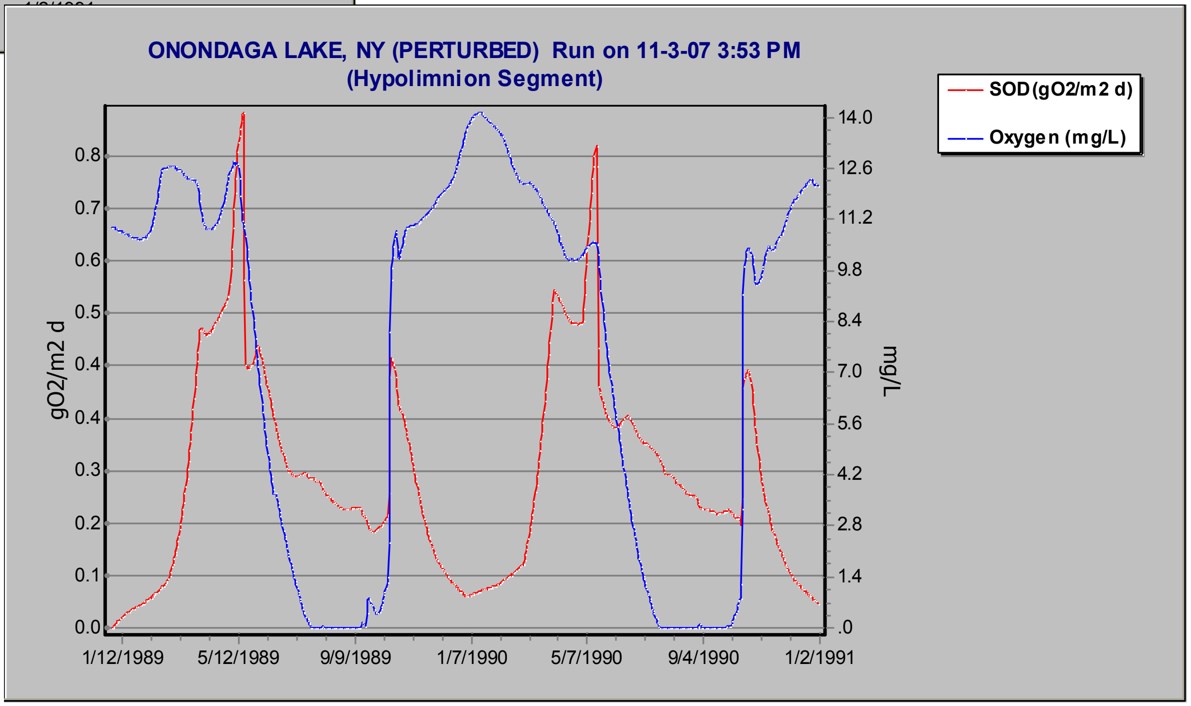
Lake Onondaga was very productive with succession of algal groups



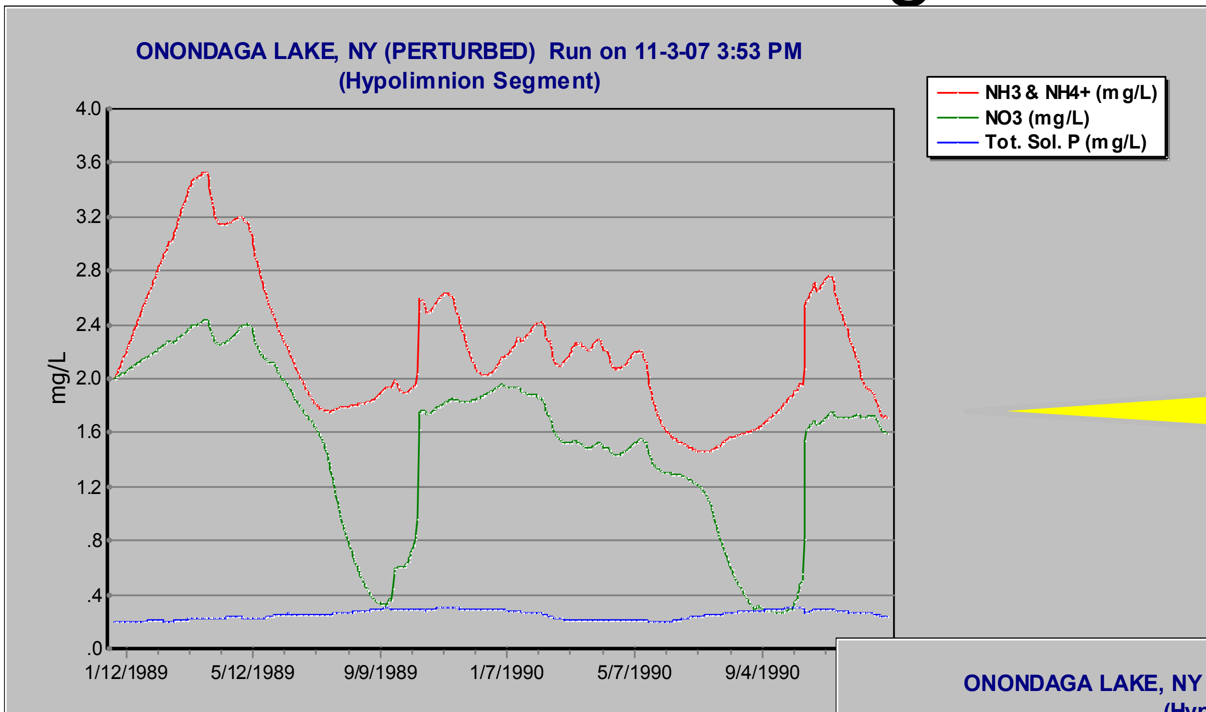


Hypolimnion goes anoxic with high SOD

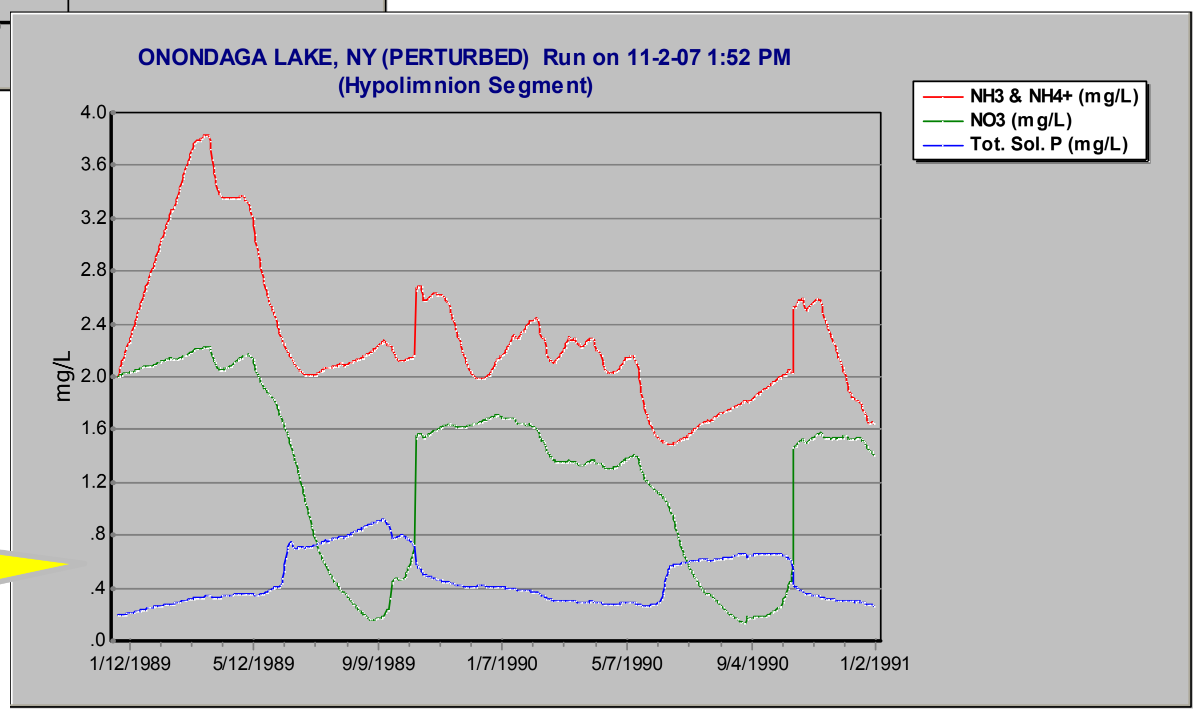




Hypolimnion phosphorus is better modeled by sediment diagenesis submodel

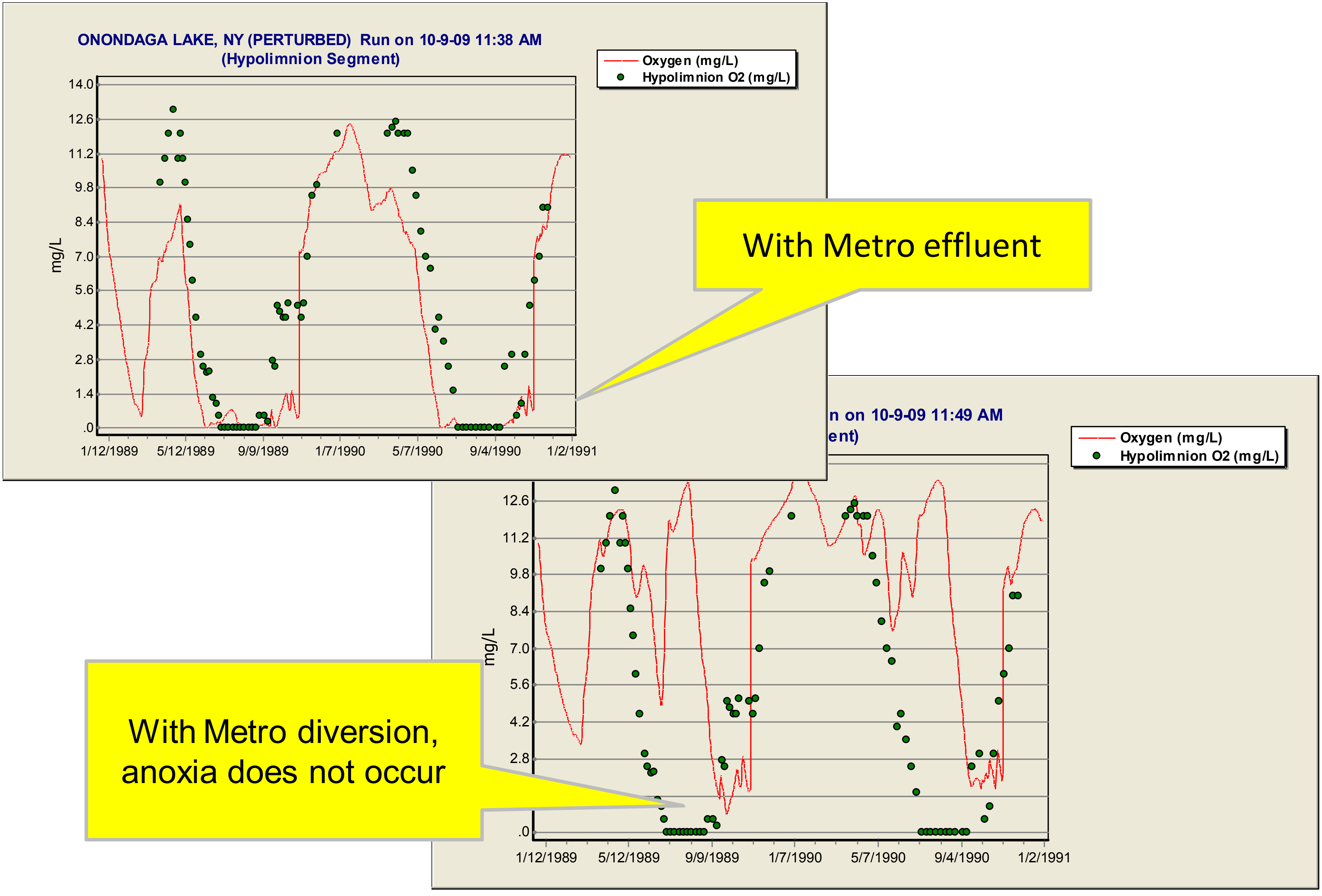


“Classic” AQUATOX model (P is blue)

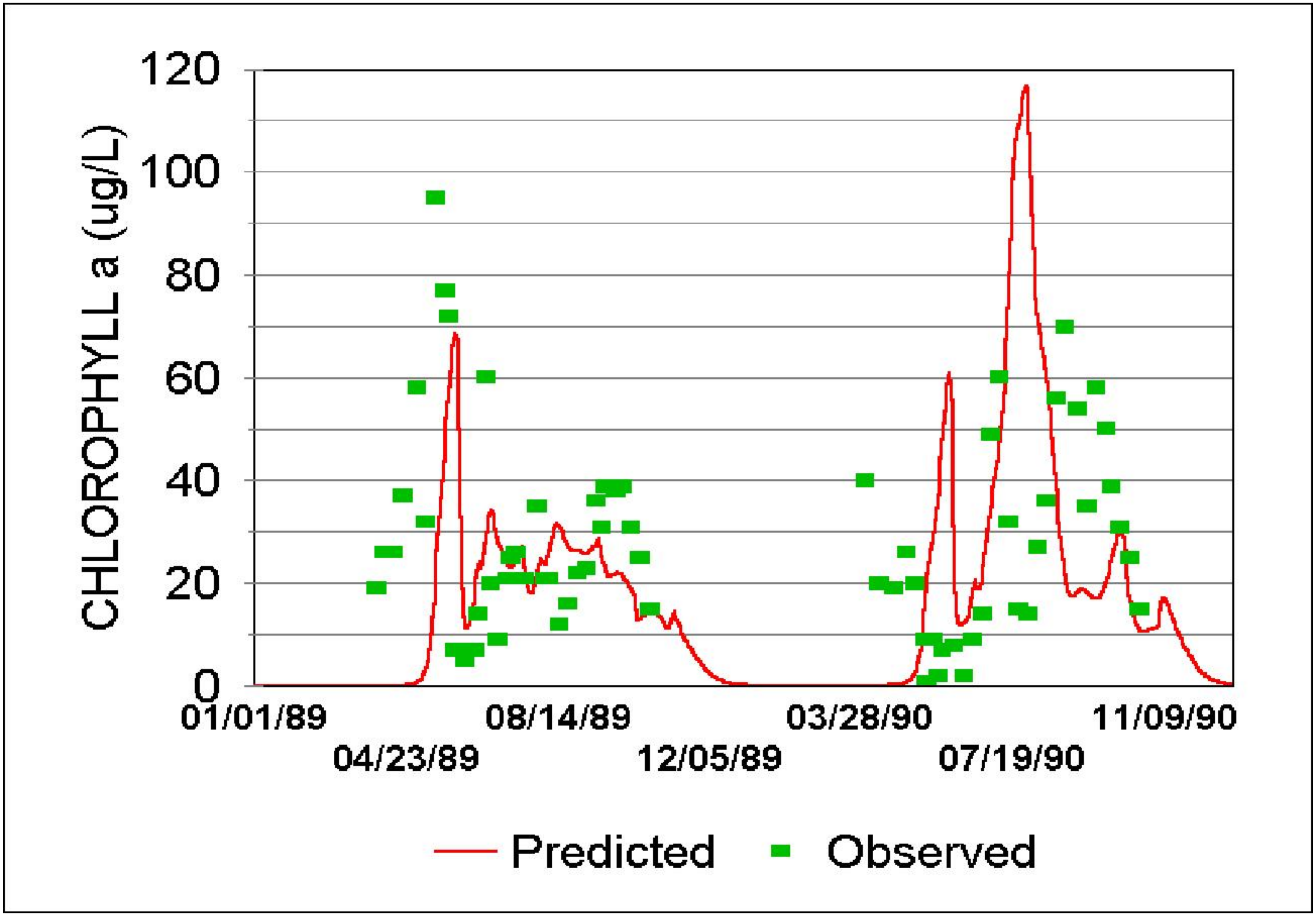


Sediment diagenesis model (note >P release)

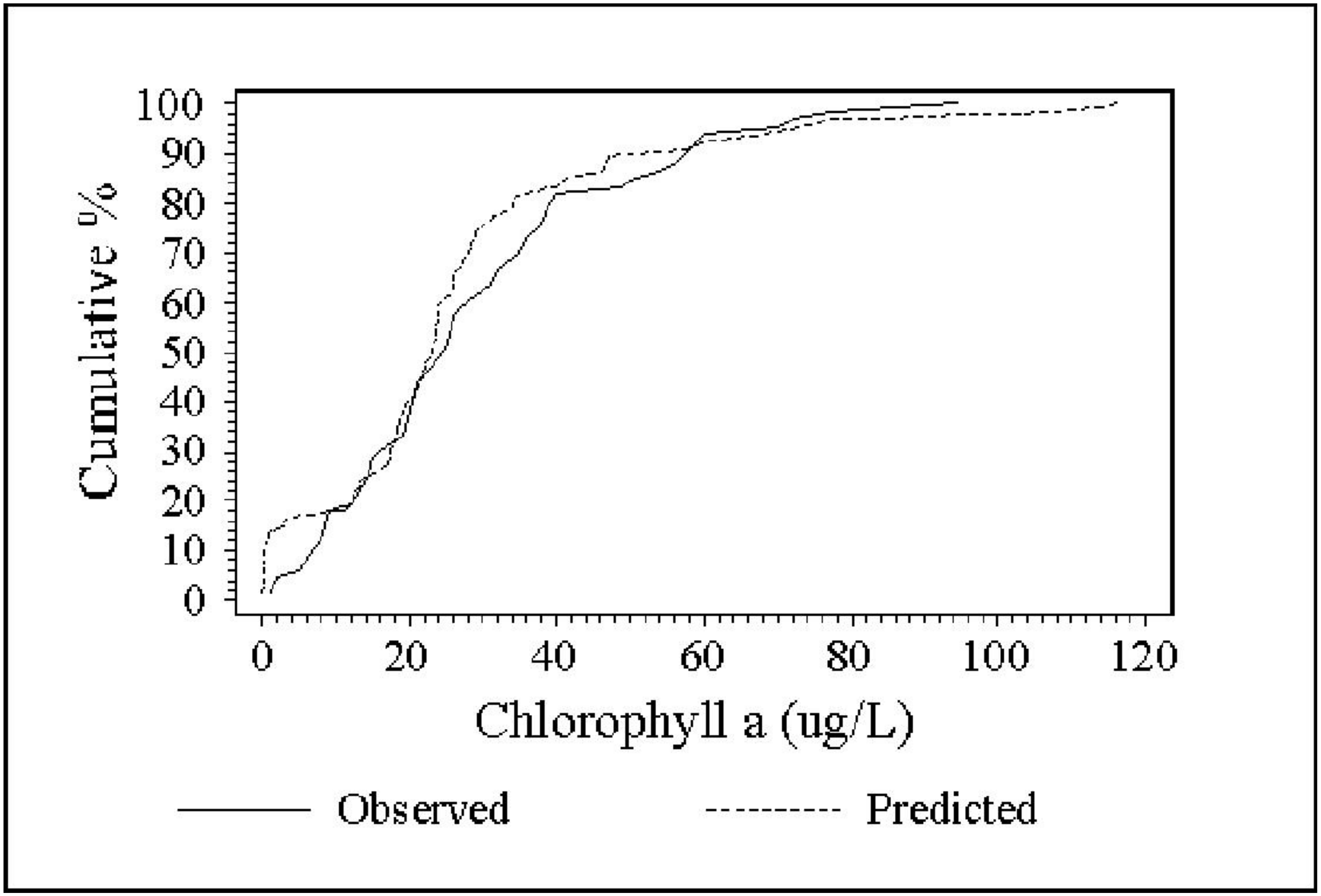
What if Metro WWTP effluent were diverted?



Validation of AQUATOX with Lake Onondaga Data—visual test



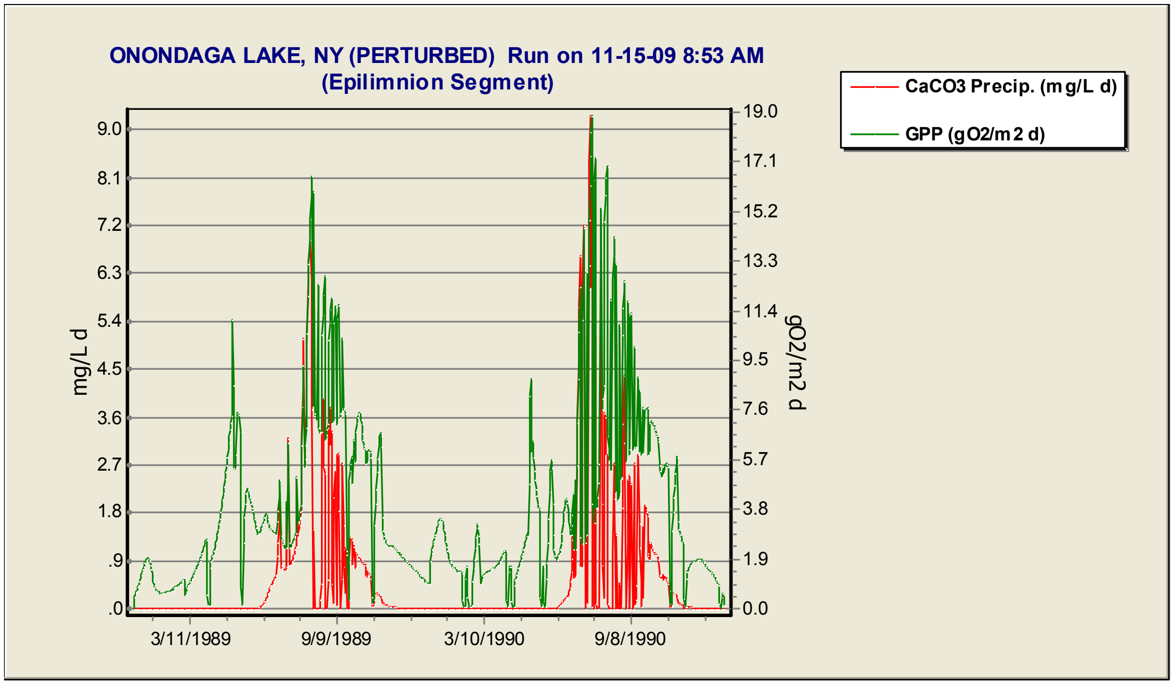
Validation with chlorophyll a in Lake Onondaga, NY



Kolmogorov-Smirnov p statistic = 0.319 (not significantly different)

Release 3 Addition: Calcium Carbonate Precipitation

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



Modeling Phytoplankton

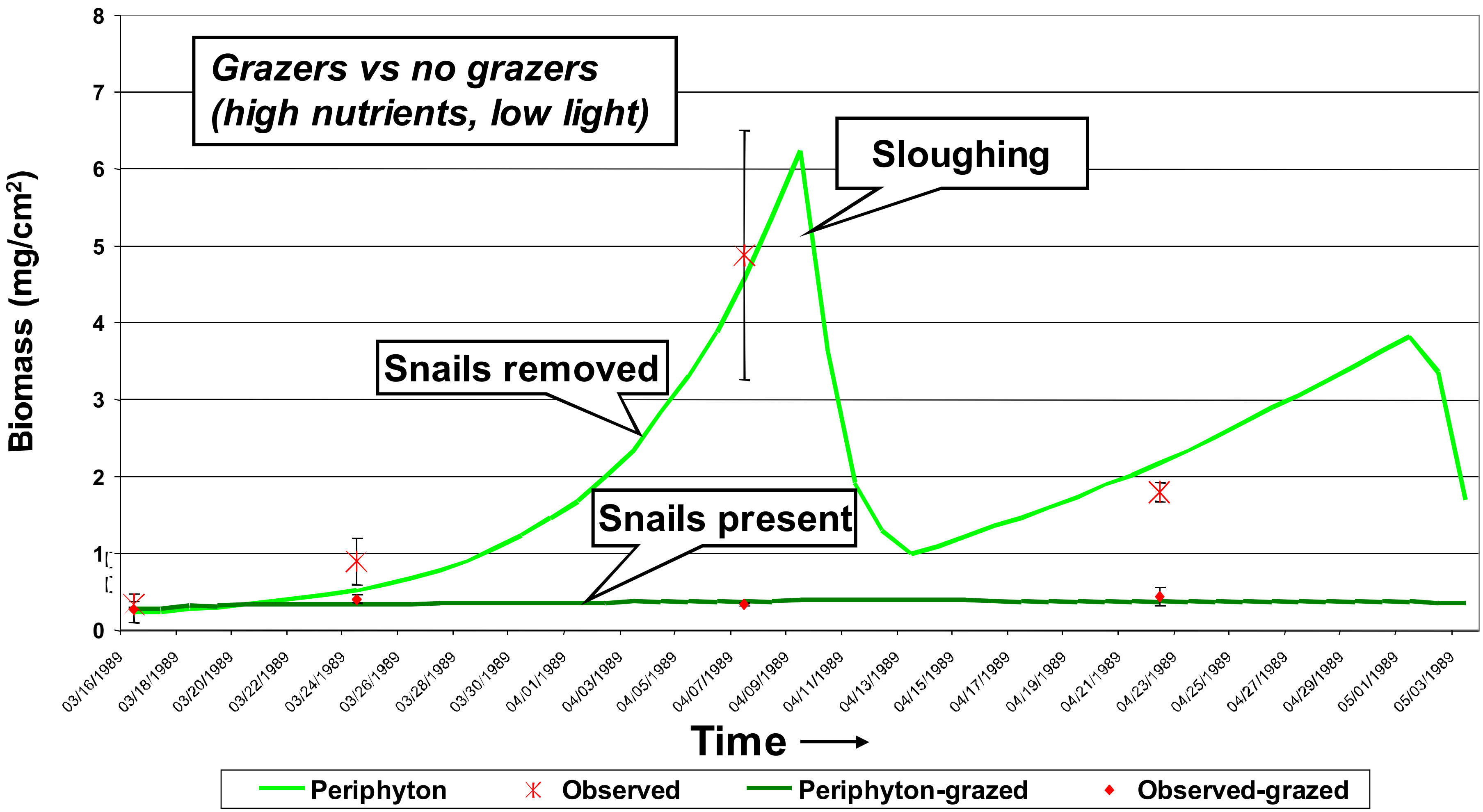
- Phytoplankton may be greens, blue-greens, diatoms or "other algae"
- Subject to sedimentation, washout, and turbulent diffusion
- In stream simulations, assumptions about flow and upstream production are important

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, Two Illustrated by Separate Simulations

One important factor is grazing by snails another is sloughing



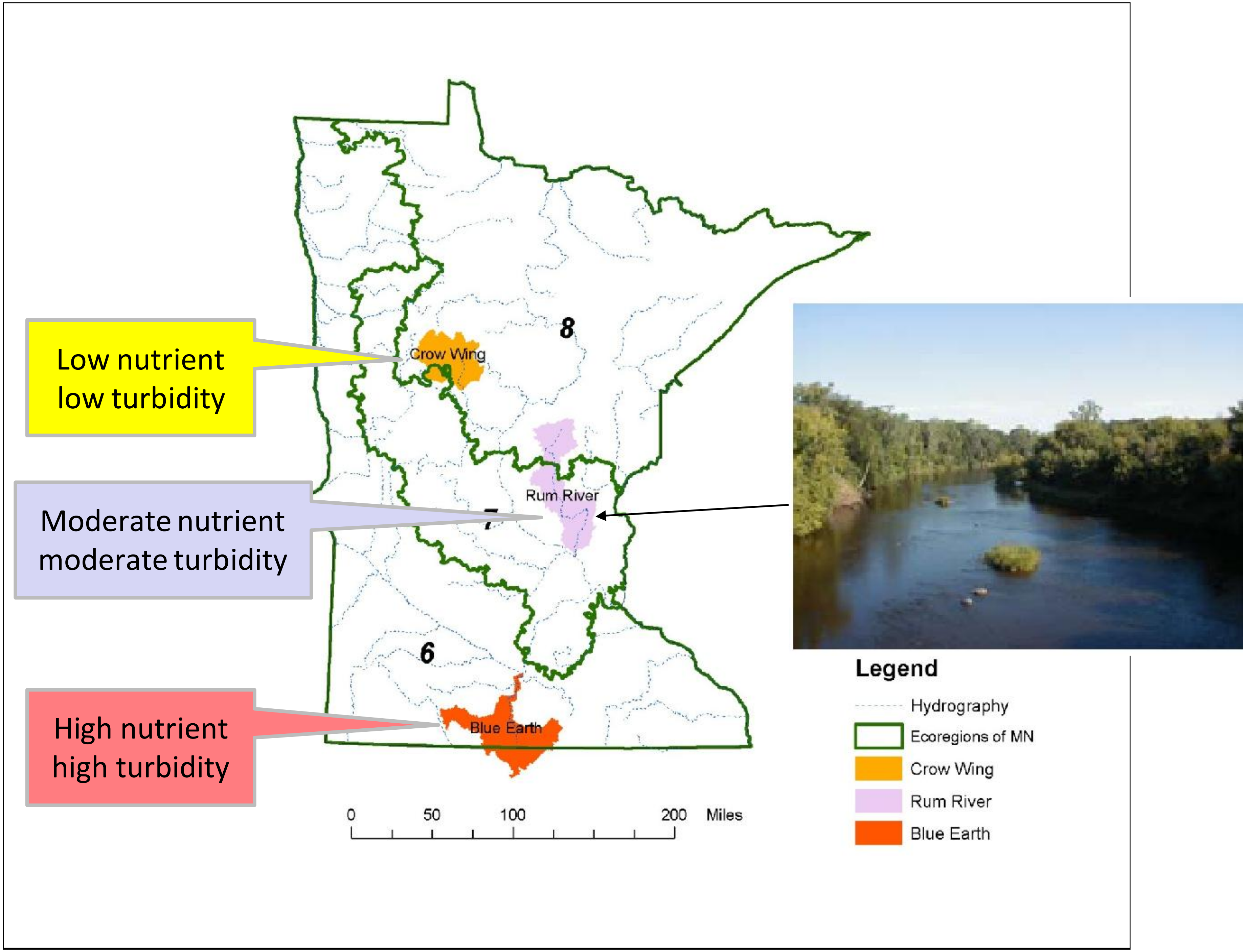
Modeling Macrophytes

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

Calibration of Plants

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

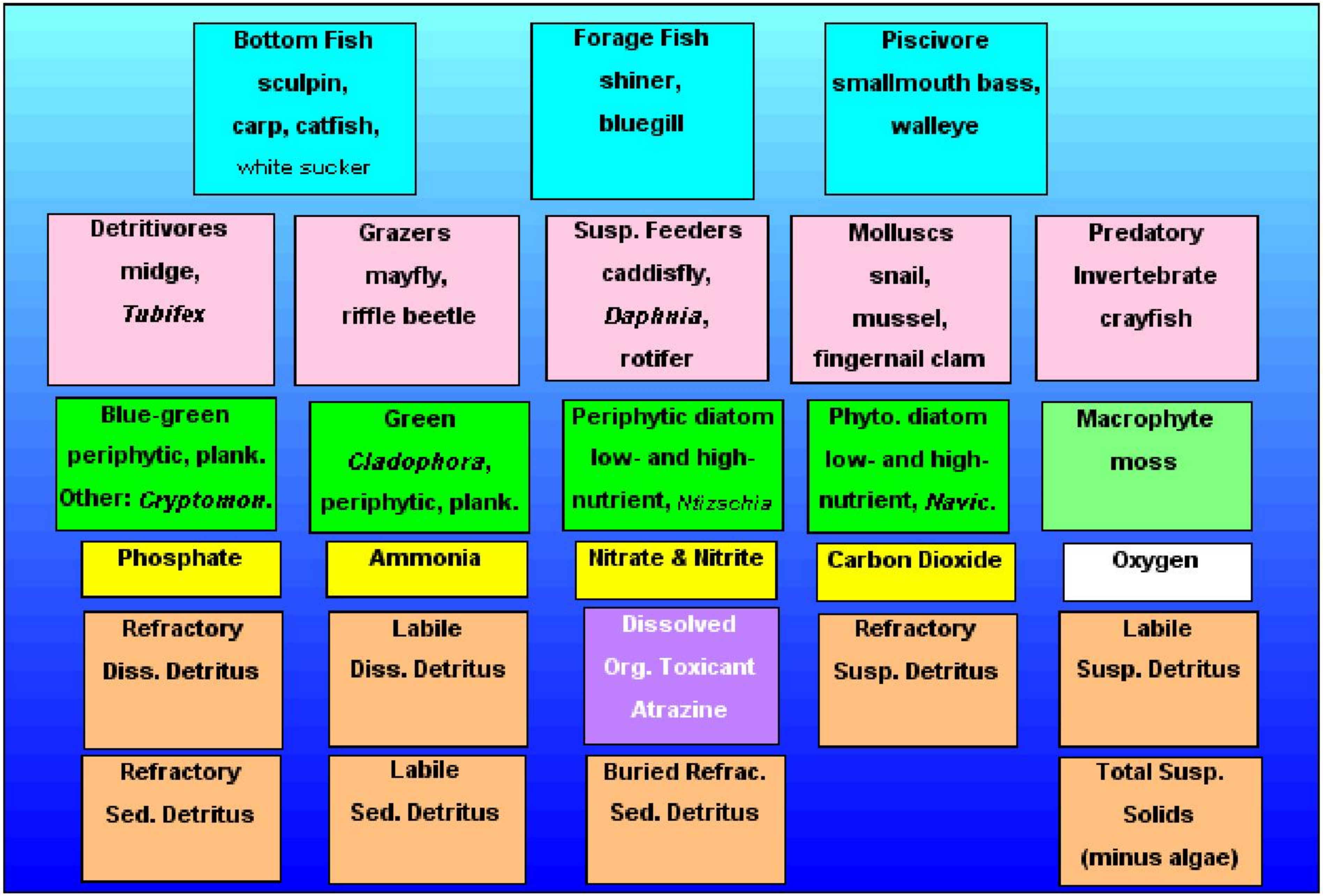
Minnesota Streams Project



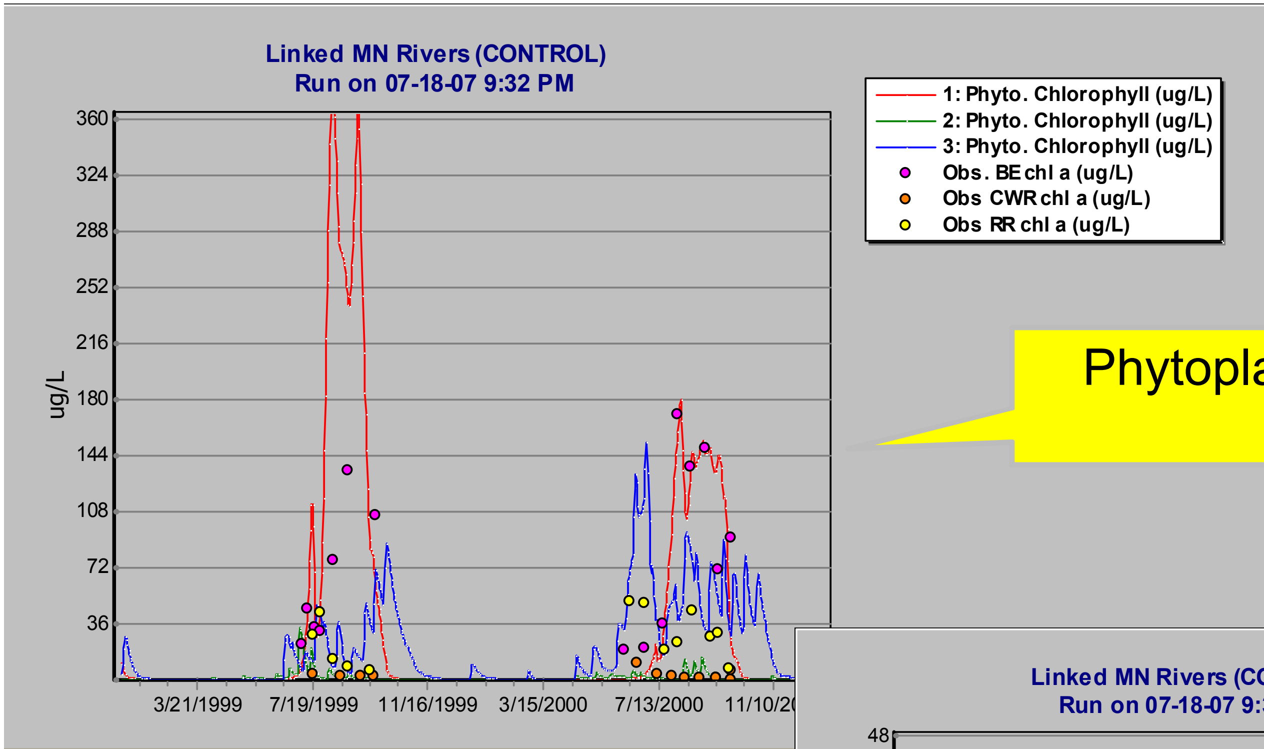
Calibration Strategy for Minnesota Rivers

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

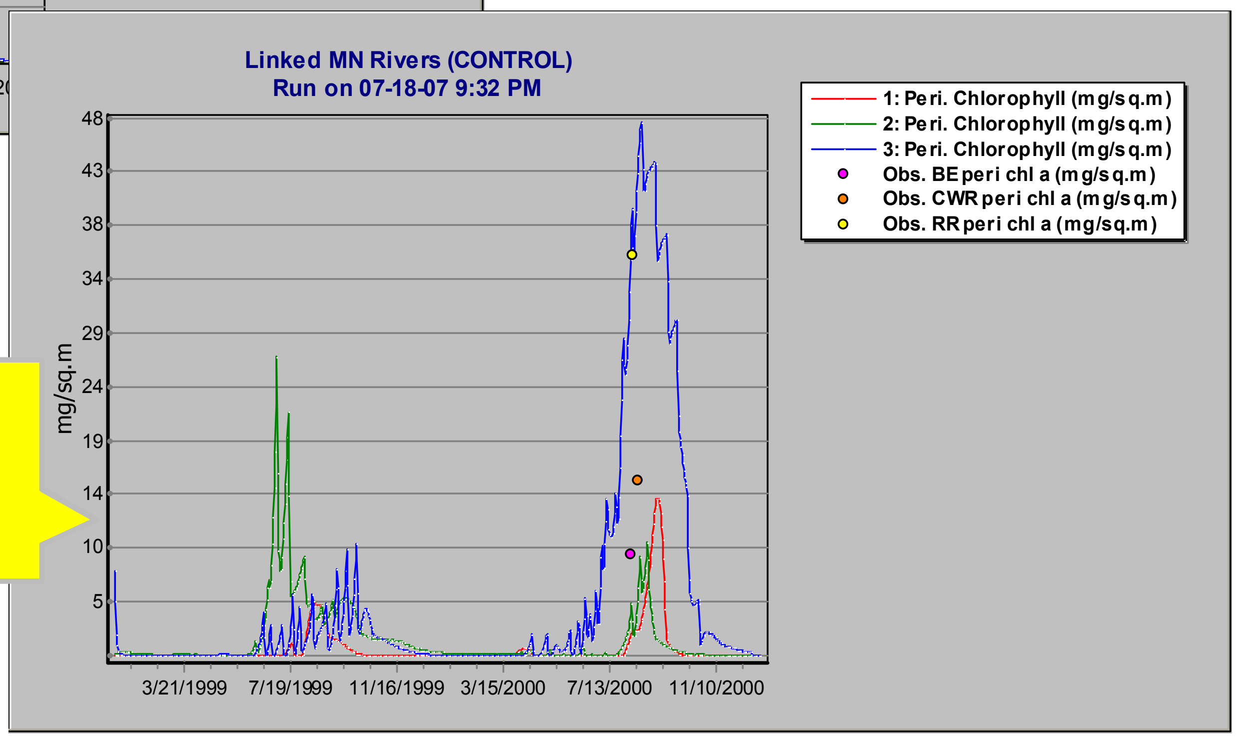
State variables in MN rivers simulations



Chlorophyll *a* Trends in MN Rivers

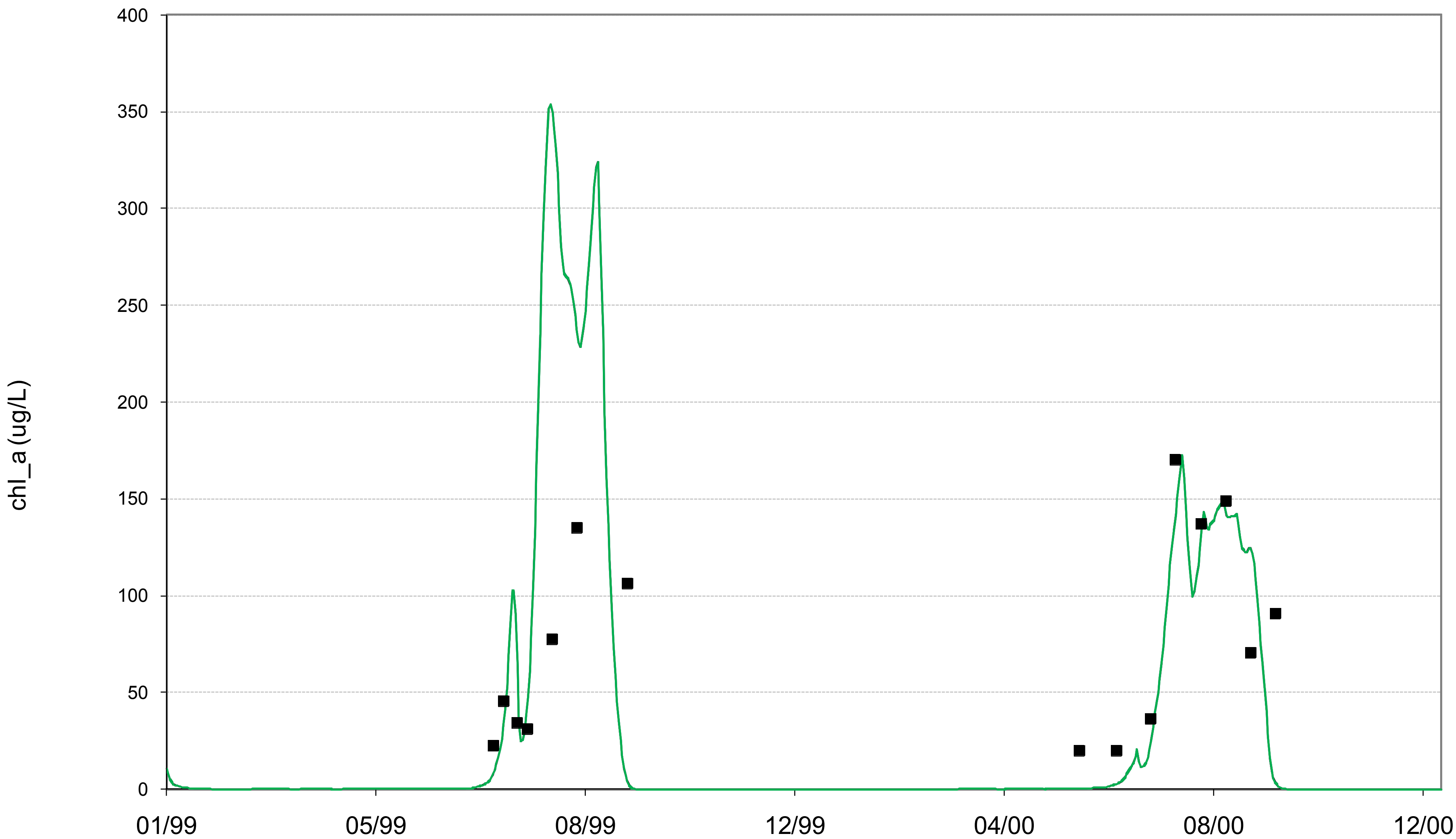


Phytoplankton follow nutrient trend

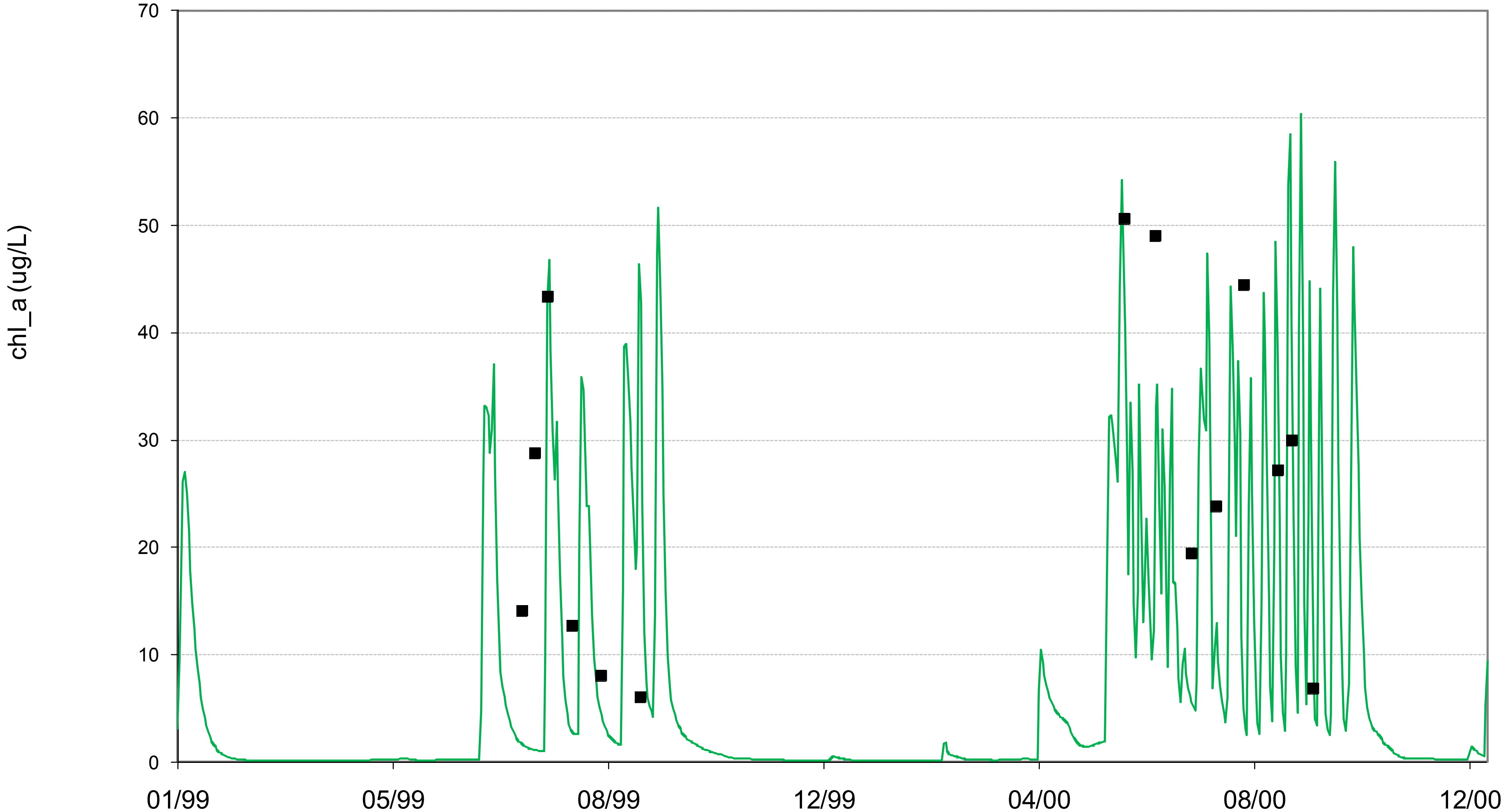


Periphyton reach maximum in Rum River with moderate nutrients and turbidity

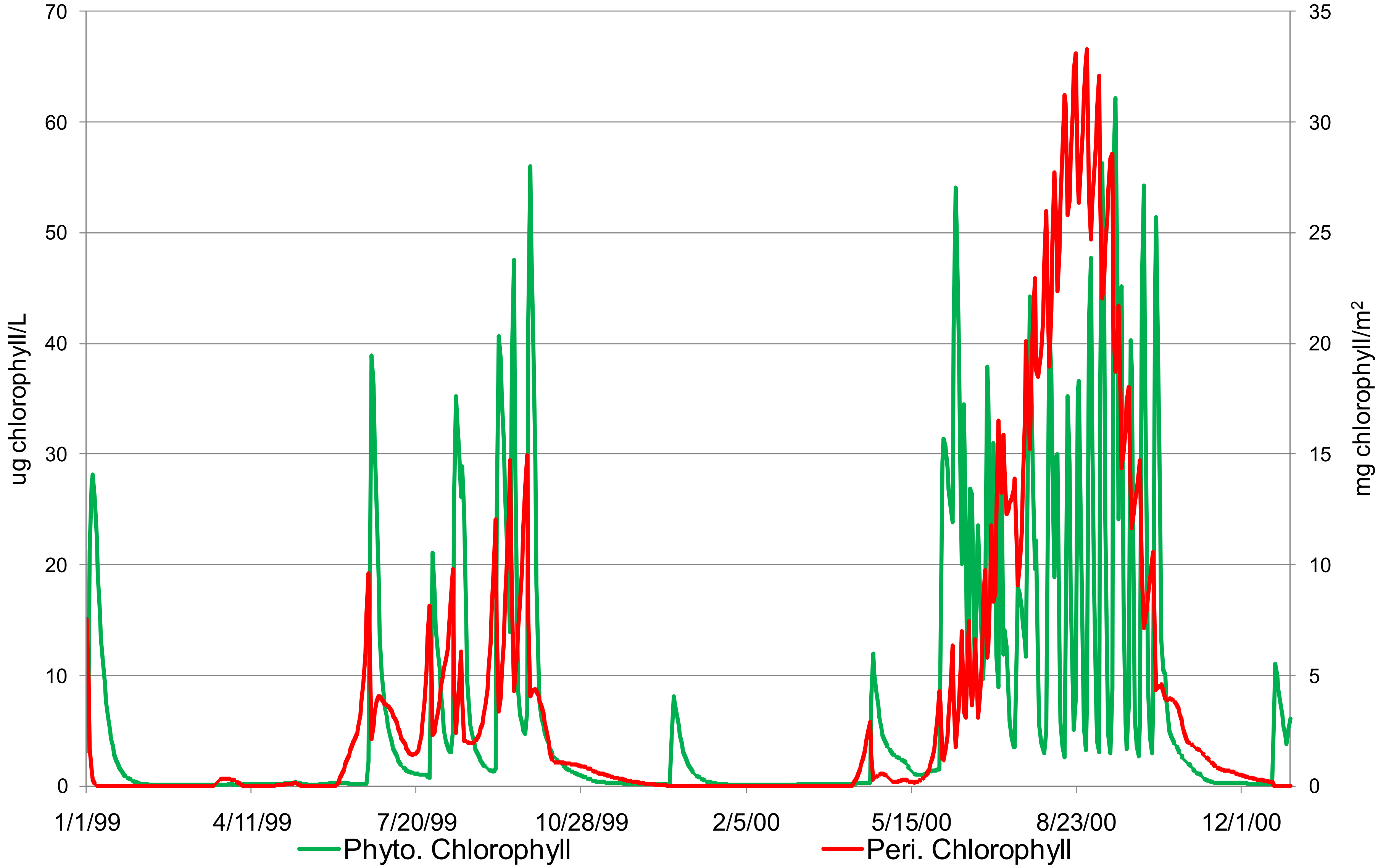
Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Blue Earth River at mile 54



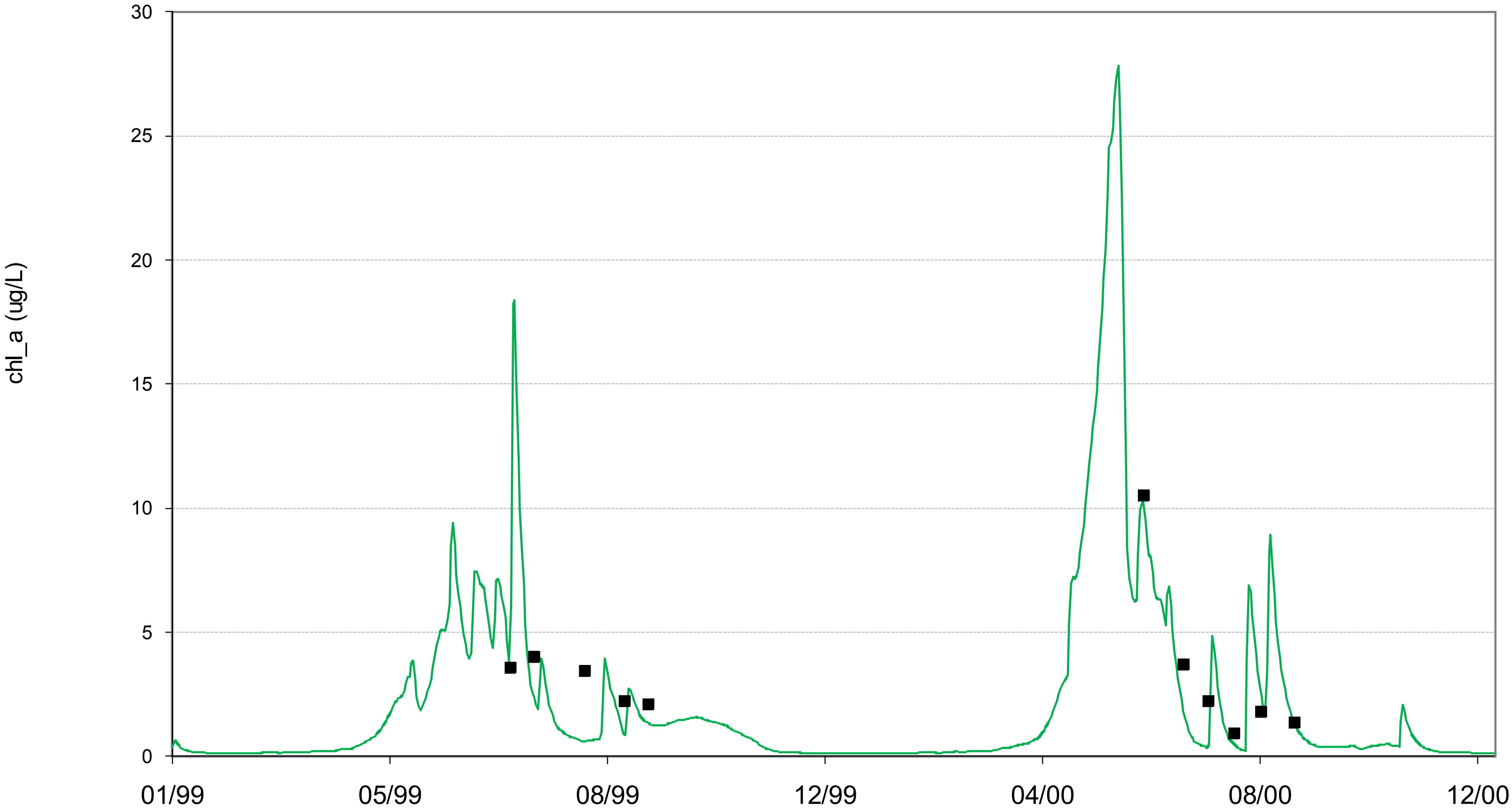
Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Rum River at mile 18



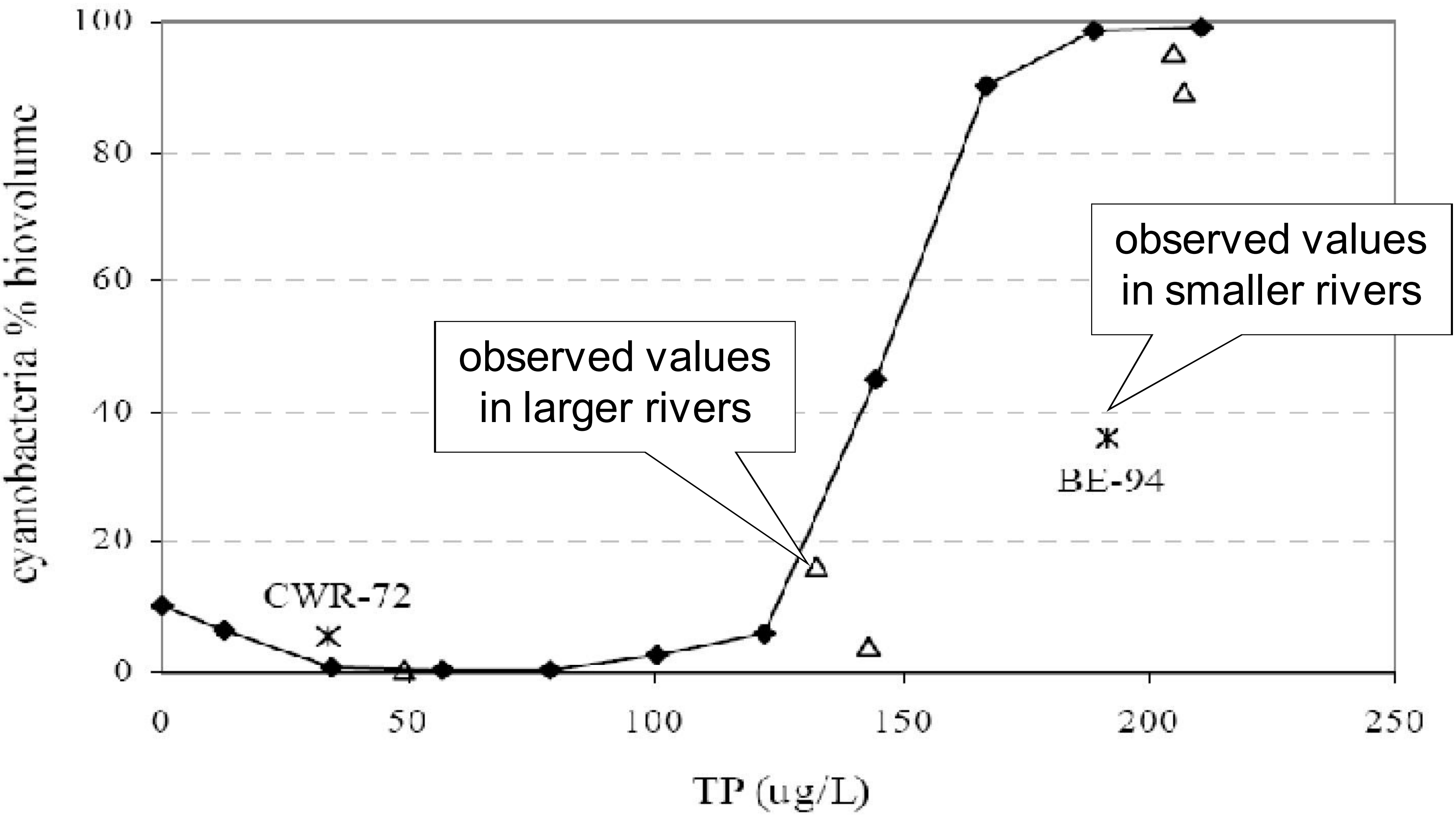
Sestonic algae are largely a result of sloughed periphyton in the Rum, a very shallow river



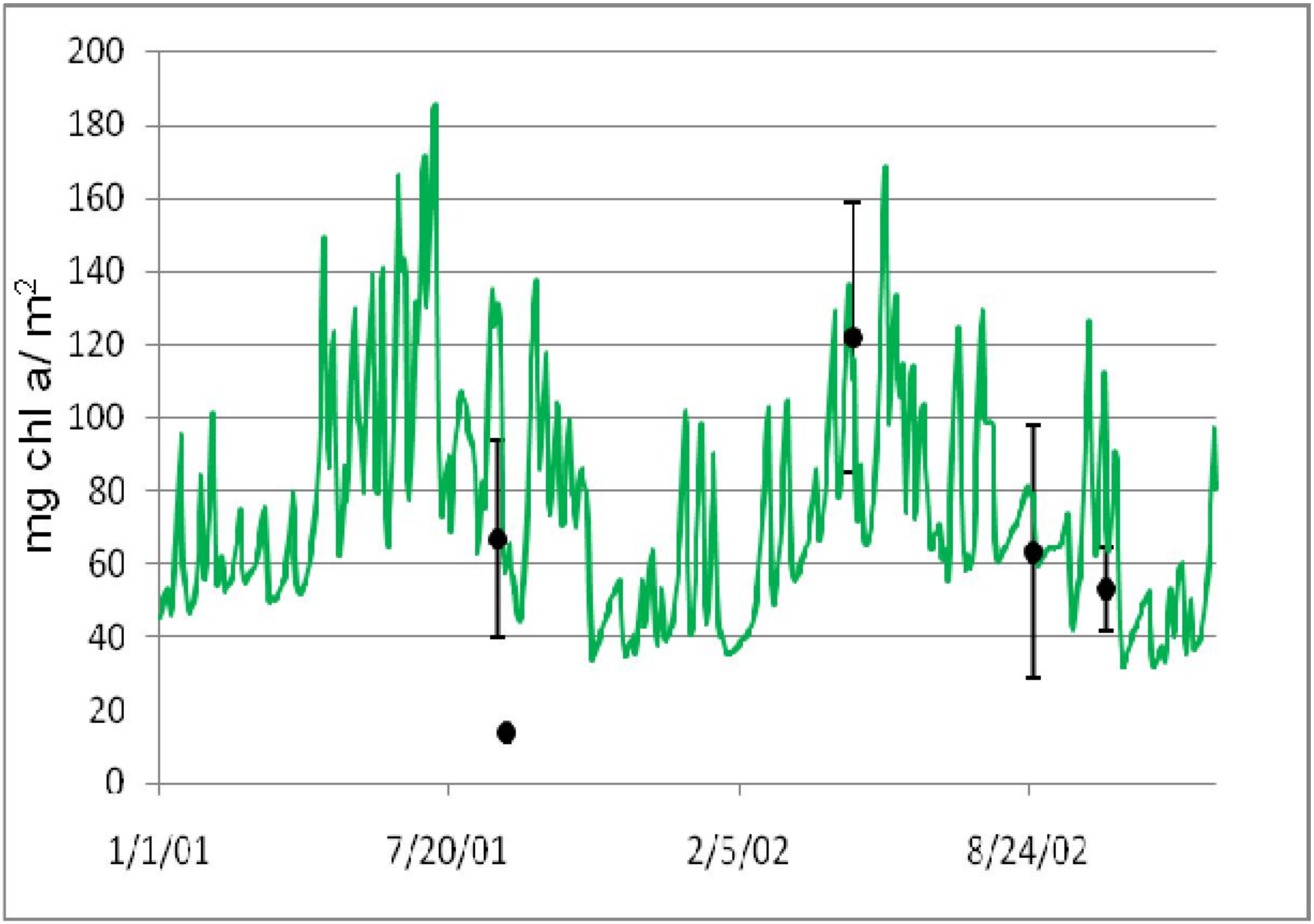
Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Crow Wing at mile 72



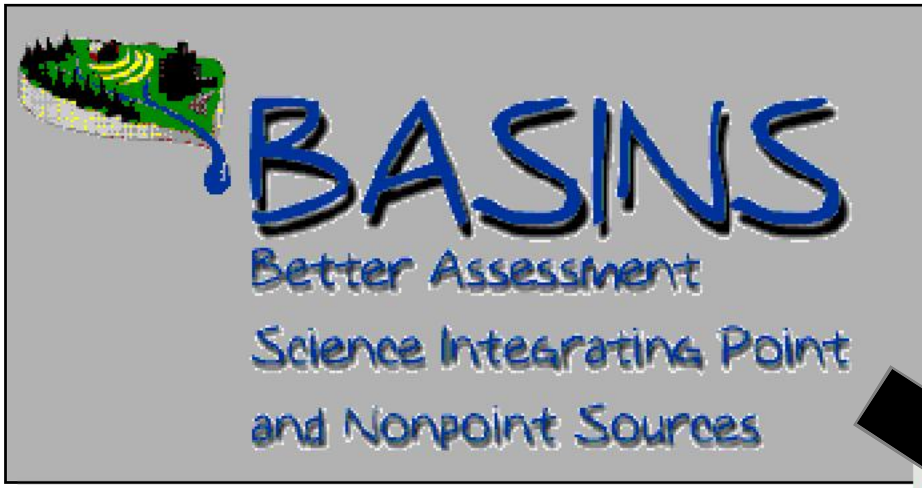
Summer mean percent phytoplankton composed of cyanobacteria-- BE-54 simulations with fractional multipliers on TP, TN, and TSS



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



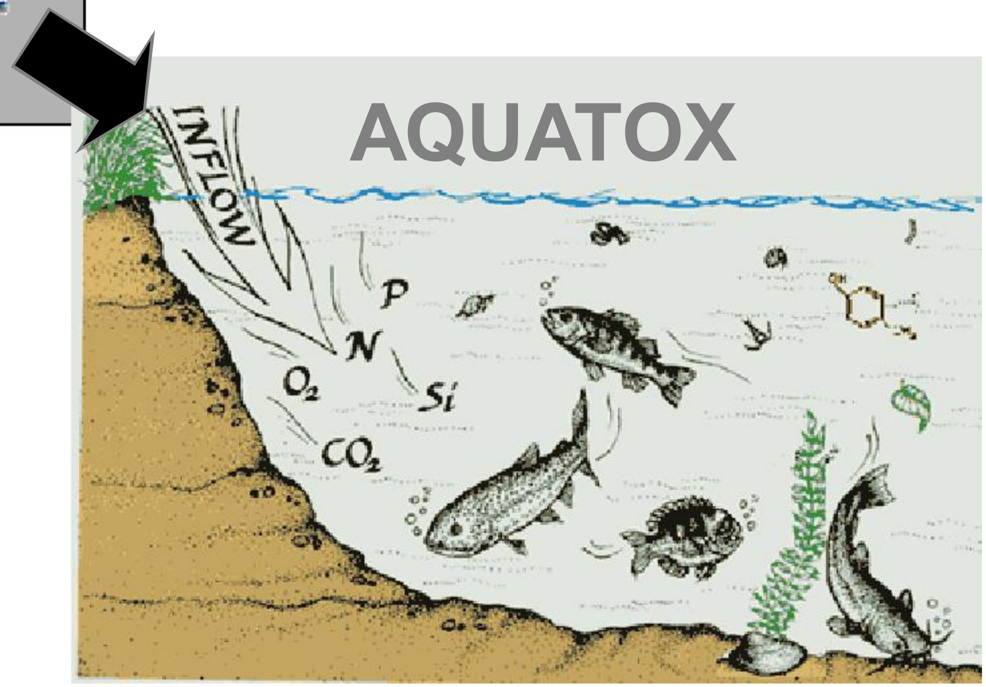
AQUATOX -- BASINS Linkage



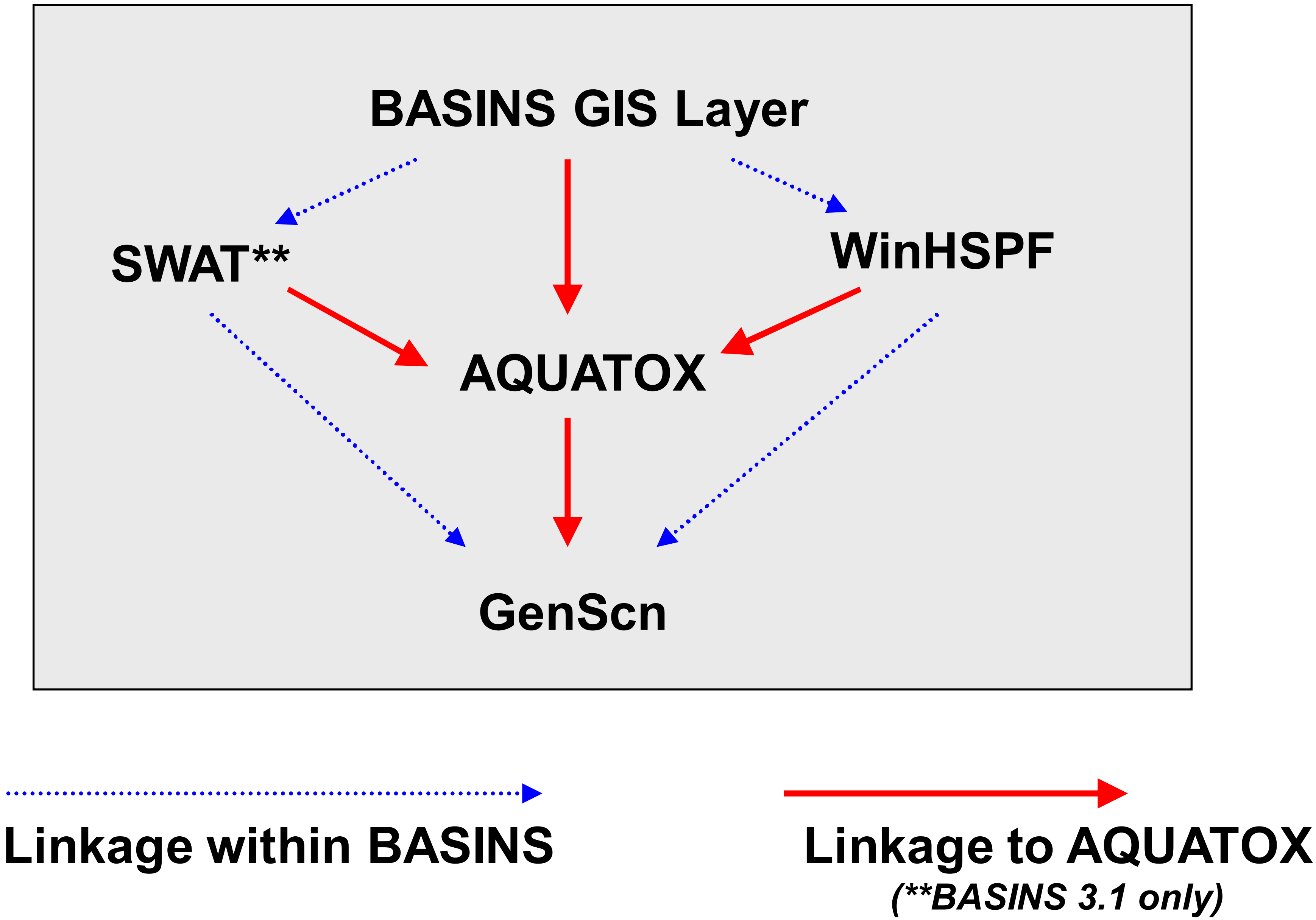
Integrates point/nonpoint source analysis with effects on receiving water and biota

Provides time series loading data and GIS information to AQUATOX

Creates AQUATOX simulations using physical characteristics of BASINS watershed



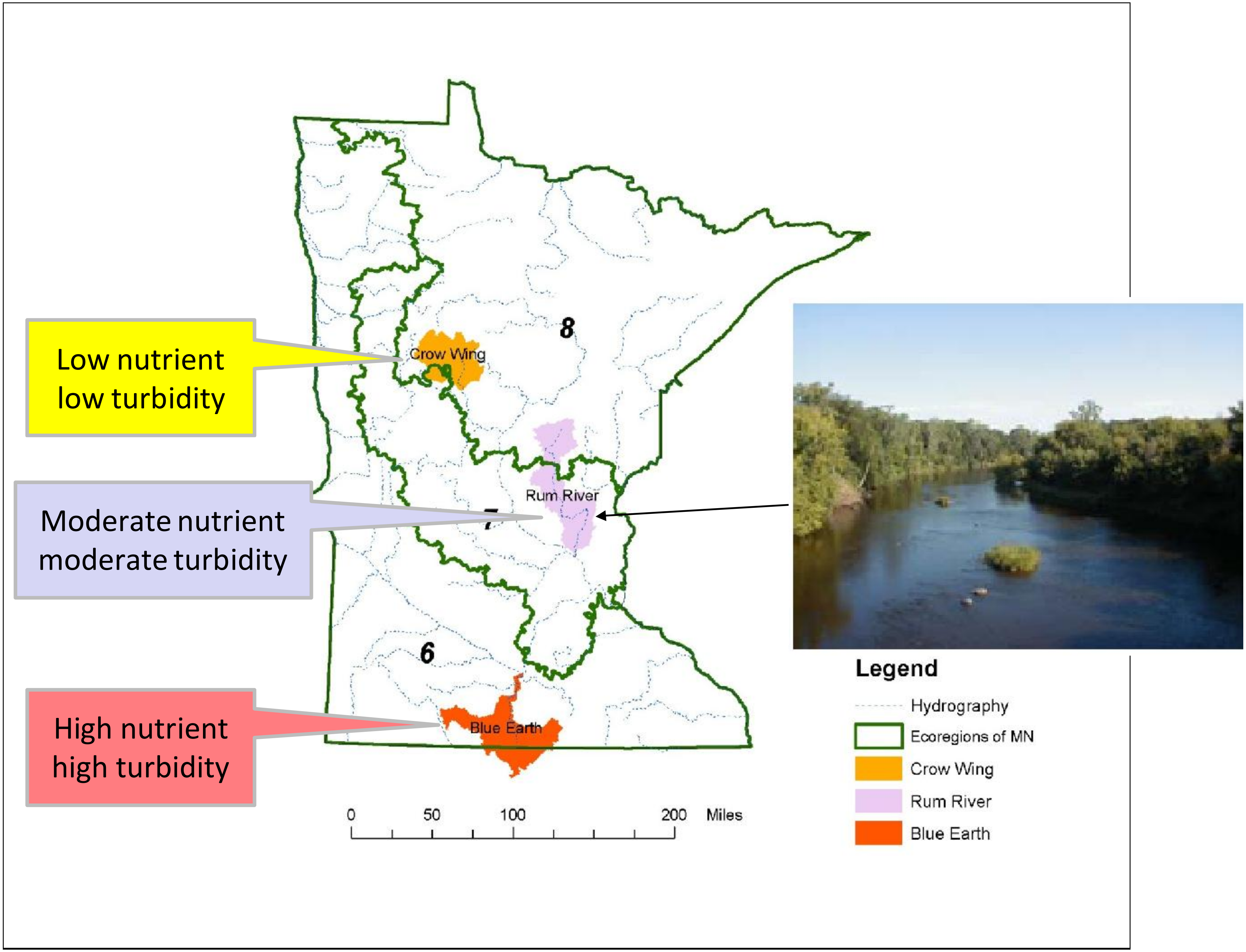
Linkages Between Models



Use of AQUATOX in Water Quality Management Decisions

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

Minnesota Nutrient Sites

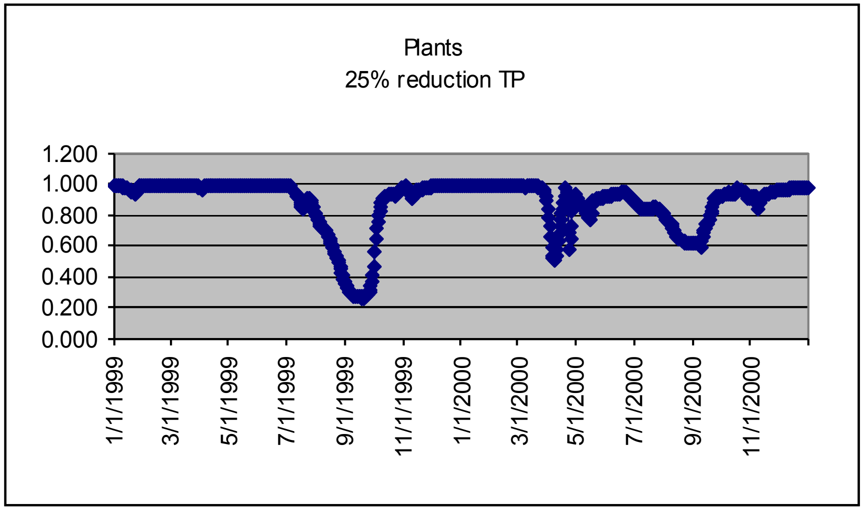


Example Nutrient Analyses from Minnesota

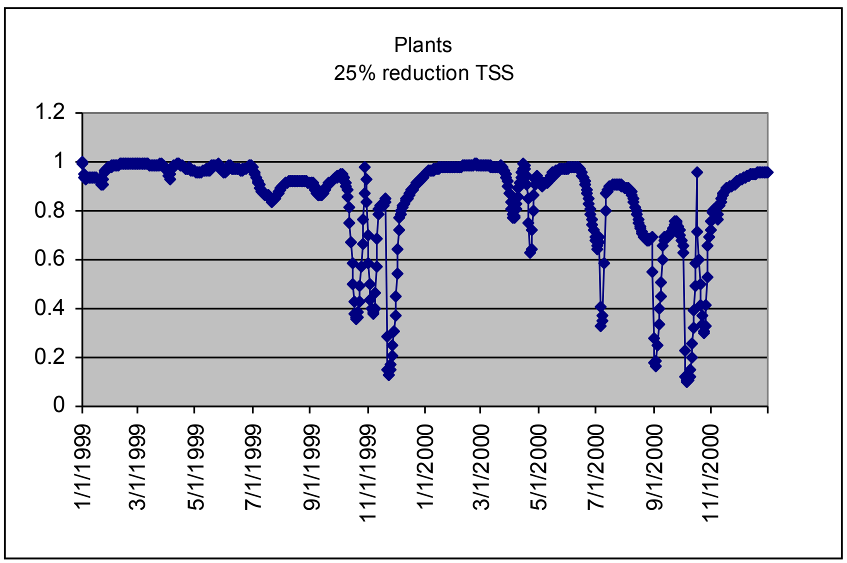
- Calibrated AQUATOX across nutrient gradient
- Set up HSPF, linked loadings to AQUATOX
- Ran iterative simulations with various nutrient reductions
- Applied 2 ways of developing nutrient target
  - Method #1: Accept the ecoregion chl *a* target, use AQUATOX to get corresponding TP level
  - Method #2: Use AQUATOX to develop both chl *a* and TP targets 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?

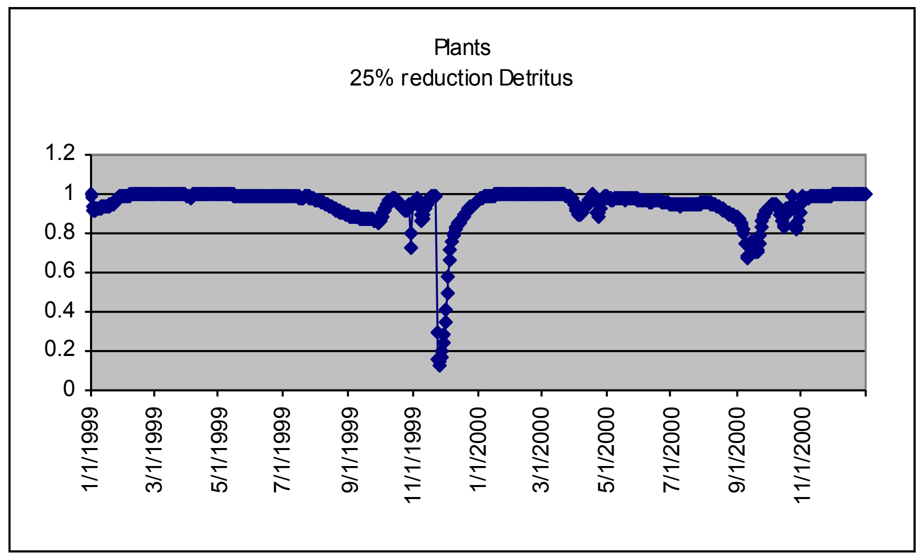
Step 1: Stressor ID using Biotic Index

Algal community response dependent upon stressor



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





Step 2: Run AQUATOX with multiple load reduction scenarios.

Compare Mean TP and Chl a

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

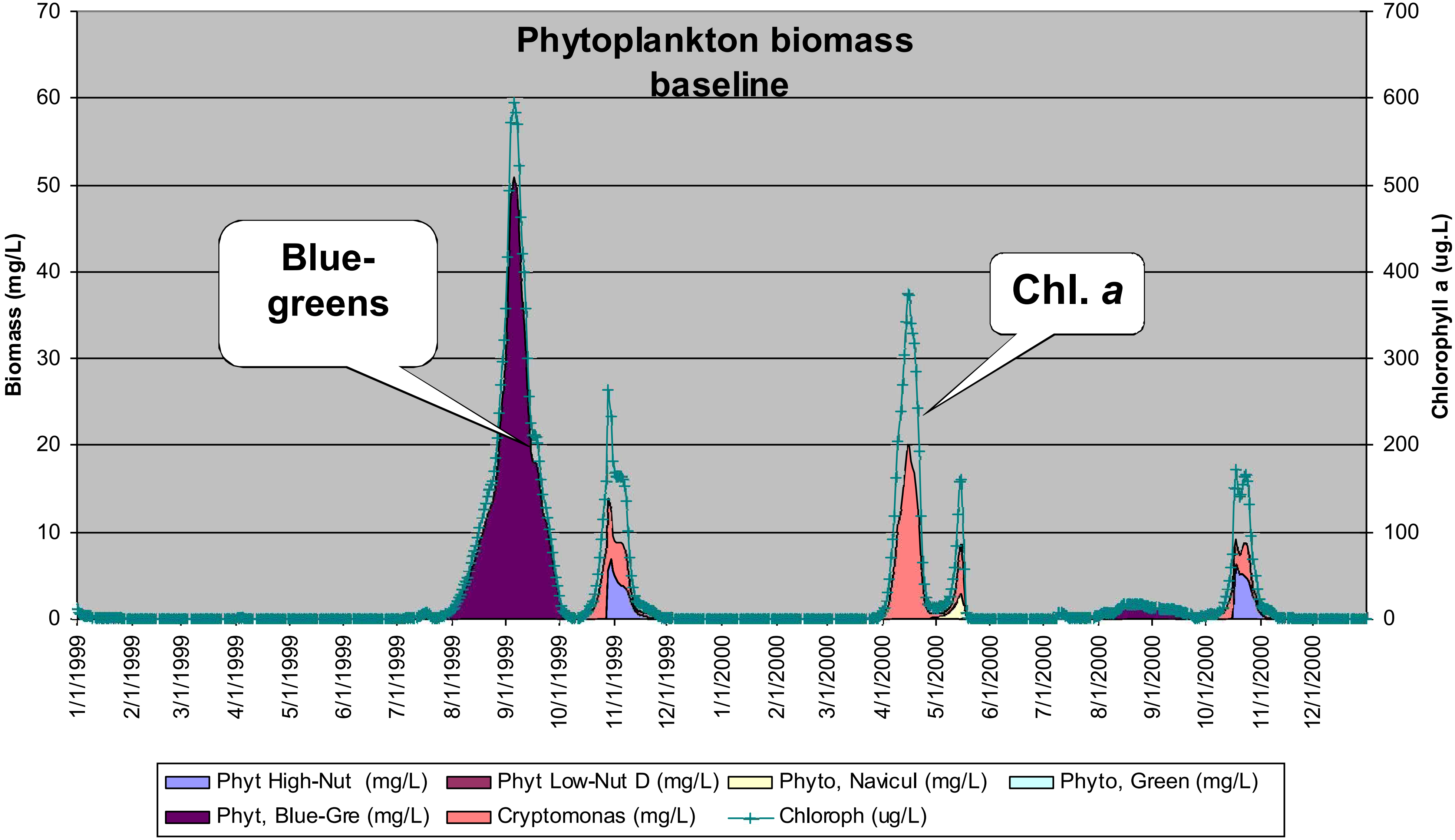
Step 3a: Water Quality Target Development Method #1

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

Step 3b: Water Quality Target Development
Method #2

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

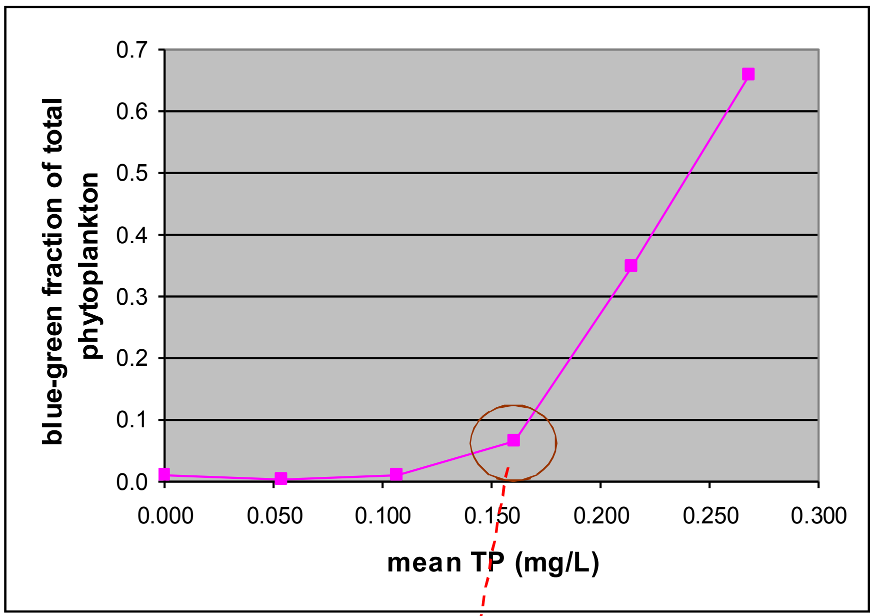
Algal Composition Changes Seasonally and from year to year



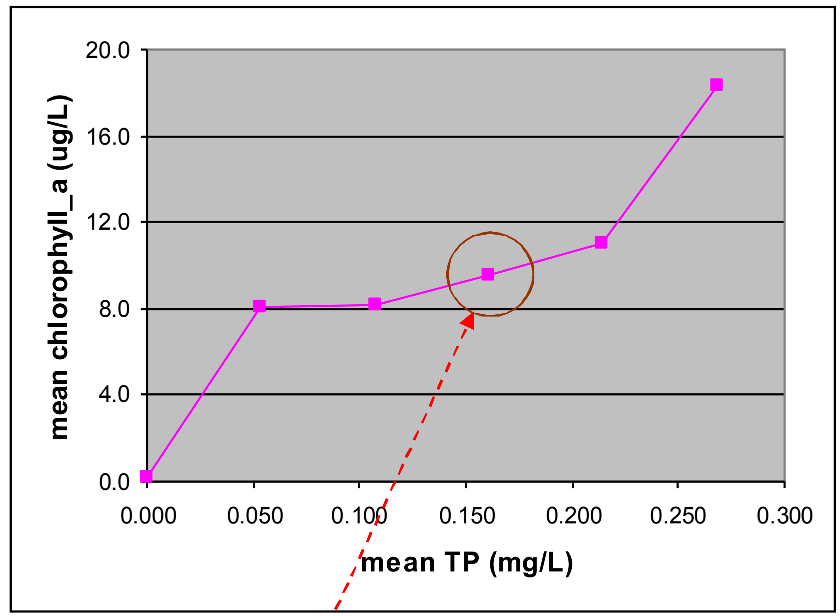
Target Development

- **<u>Method 2</u>: Use AQUATOX to estimate chl *a* level associated with a shift in algal community.**

Mean TP vs %blue-greens



Mean TP vs mean chl a



Inflection point ***– corresponds with <10% blue-greens, 0.161 mg/L mean TP, and. 9.5 ug/L mean chl_a.***

Represents ~40% reduction in TP and TSS.

Summary of Minnesota Analysis

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

Other Possible Analyses to Support Development of Water Quality Targets

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

Modeling Animals with AQUATOX

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

Animal Modeling Overview

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

Animal Parameters

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

Animal Type: Fish

Toxicity Record: Trout | Edit All

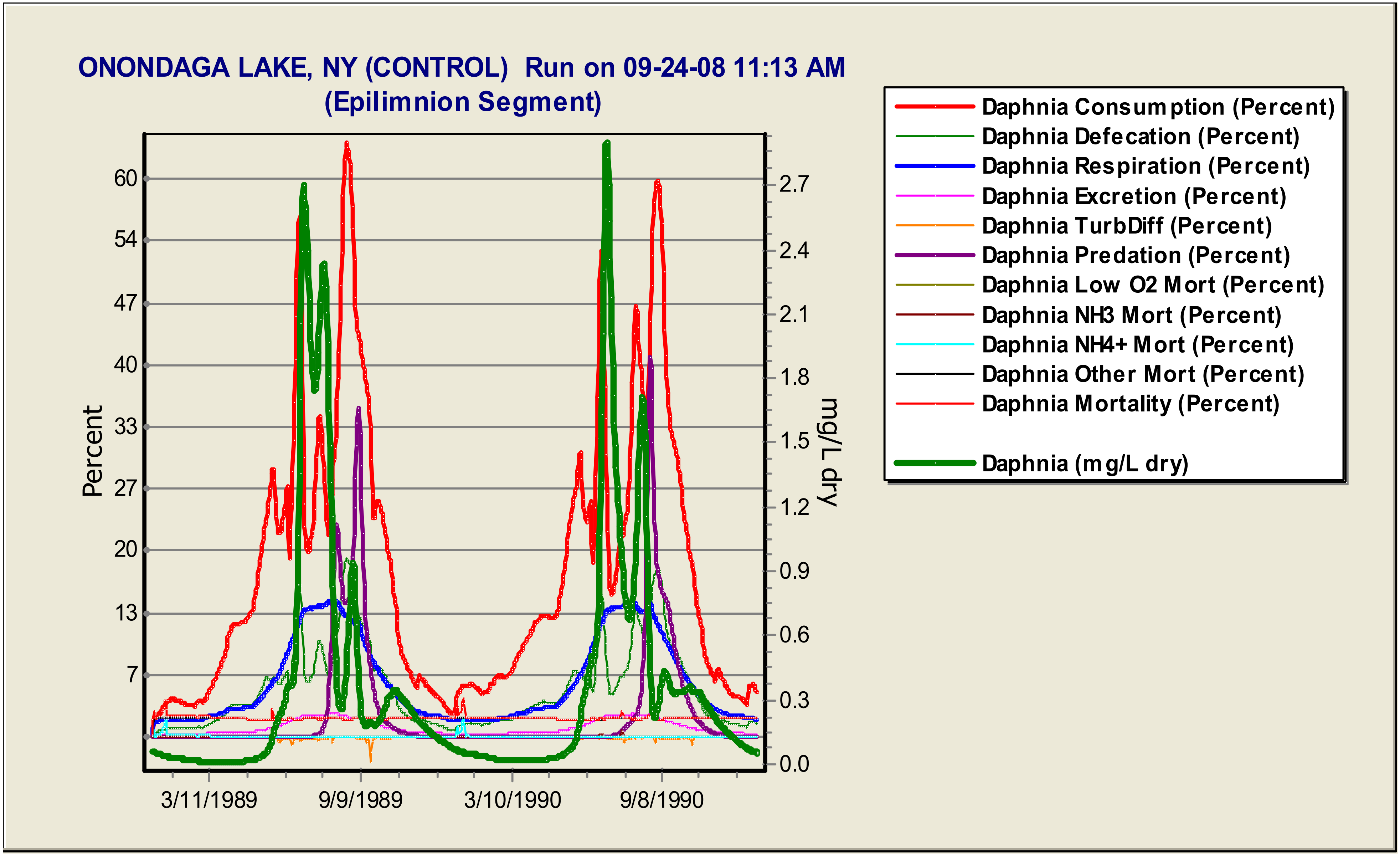
Taxonomic Type or Guild: Game Fish

Trophic Interactions

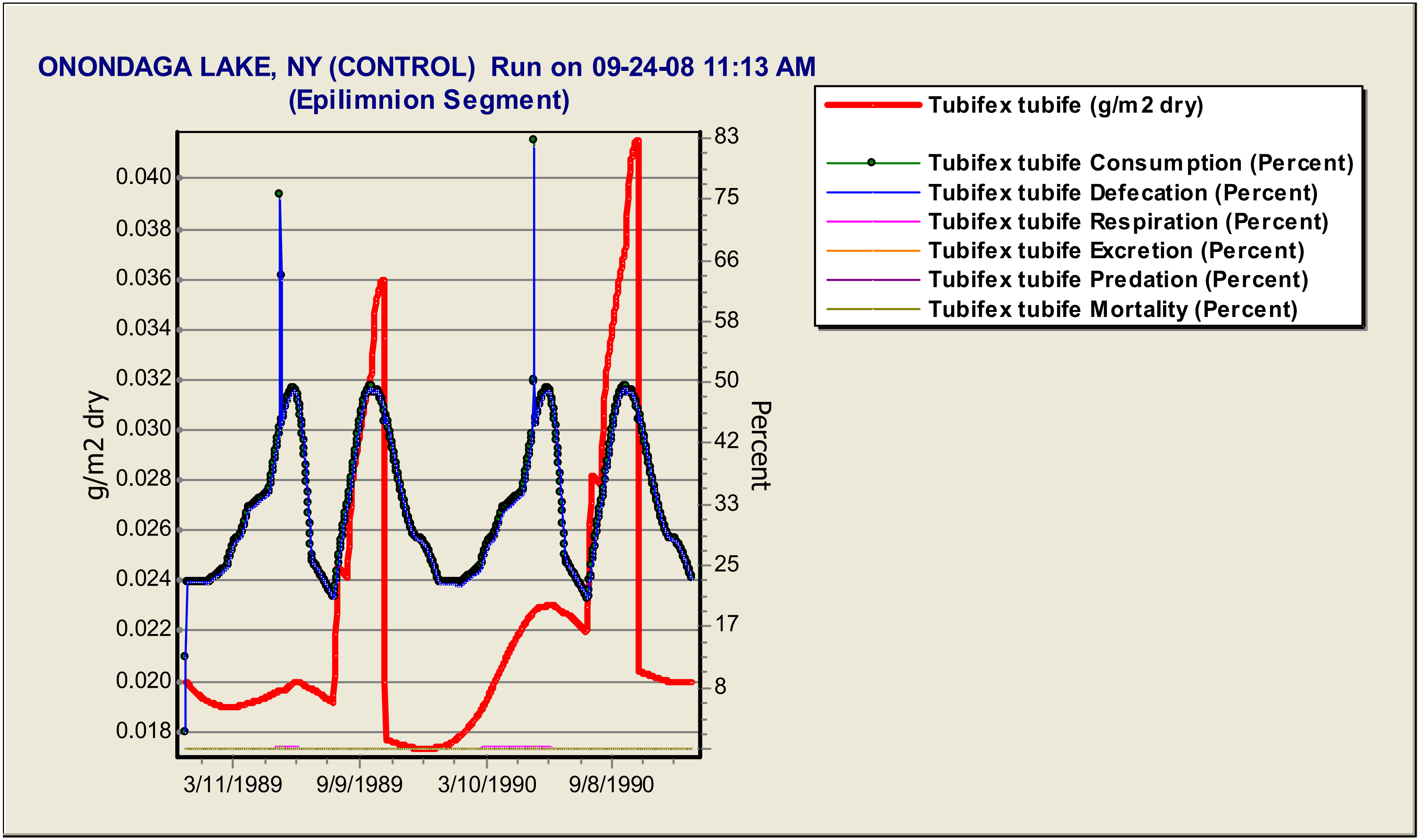
Animal Data:

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

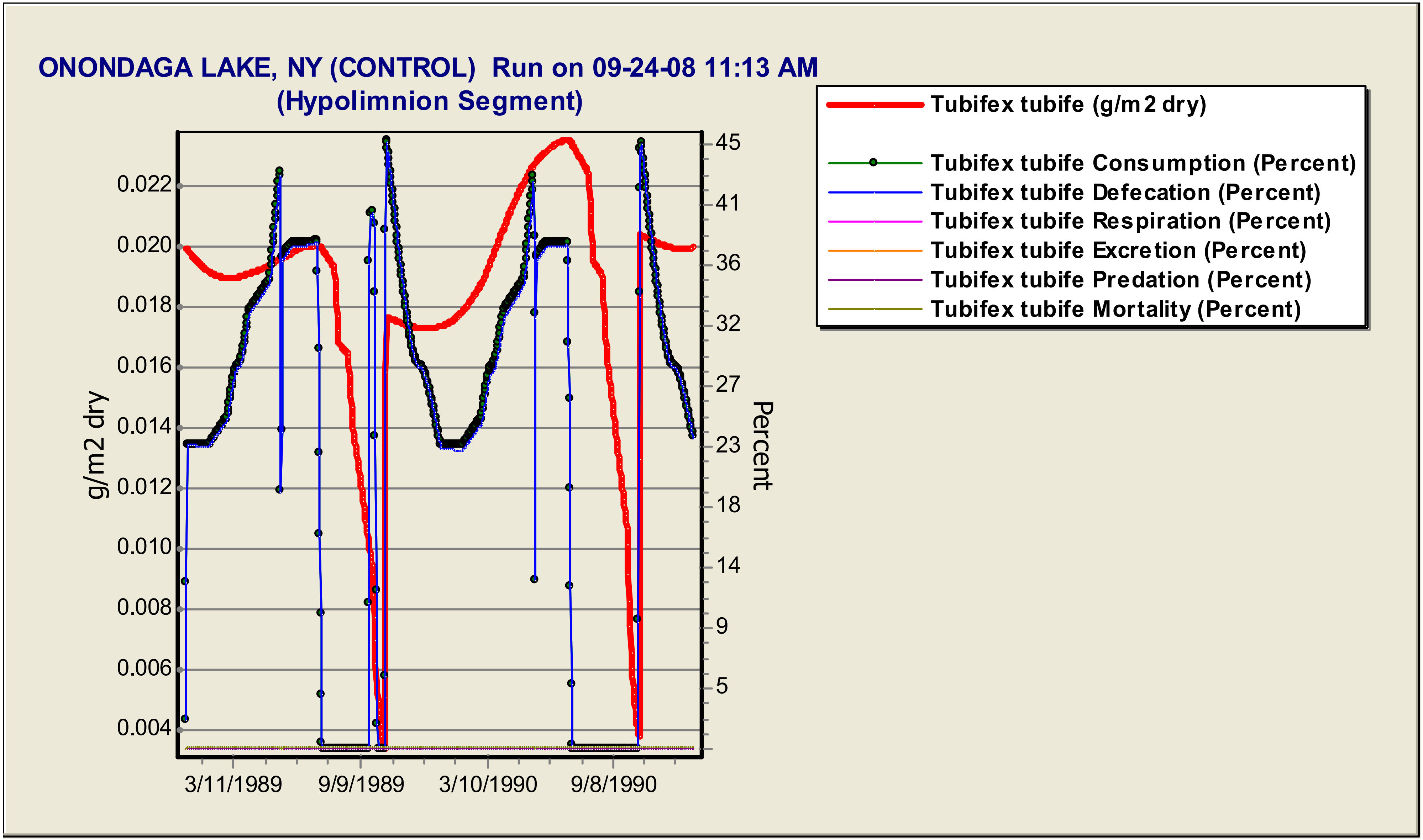
Zooplankton consumption is often tied to phytoplankton productivity



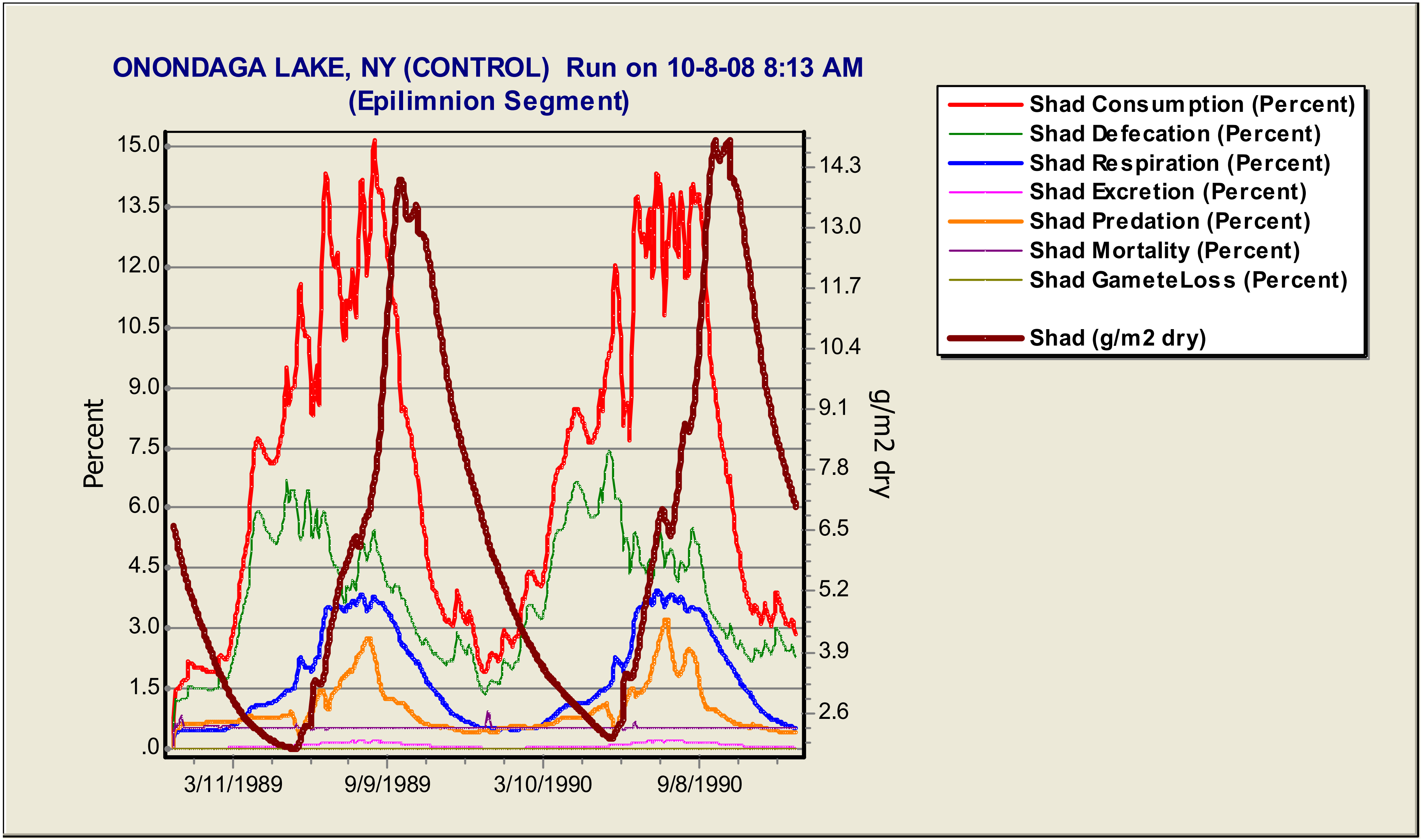
Benthic invertebrates are also tied to phytoplankton productivity through detritus



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



Fish exhibit seasonal patterns based on food availability and temperature



Foodweb Model specified as Trophic Matrix

Interactions are normalized to 100%

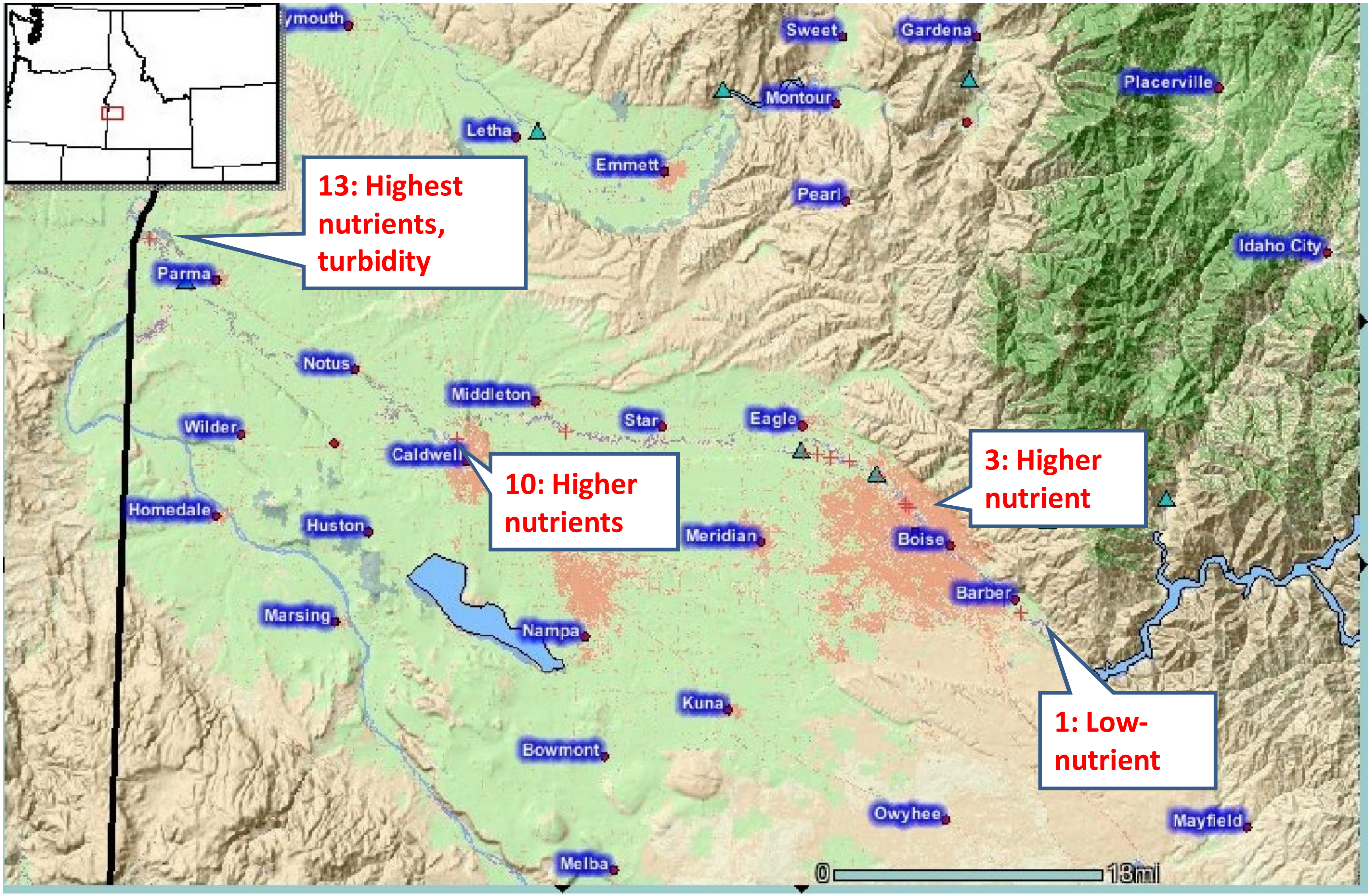
AQUATOX-- Trophic Interaction Matrix

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

Show Preferences Show Egestion Coefficients Show Comments

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

Lower Boise River, Idaho
with WWTPs and agricultural drains

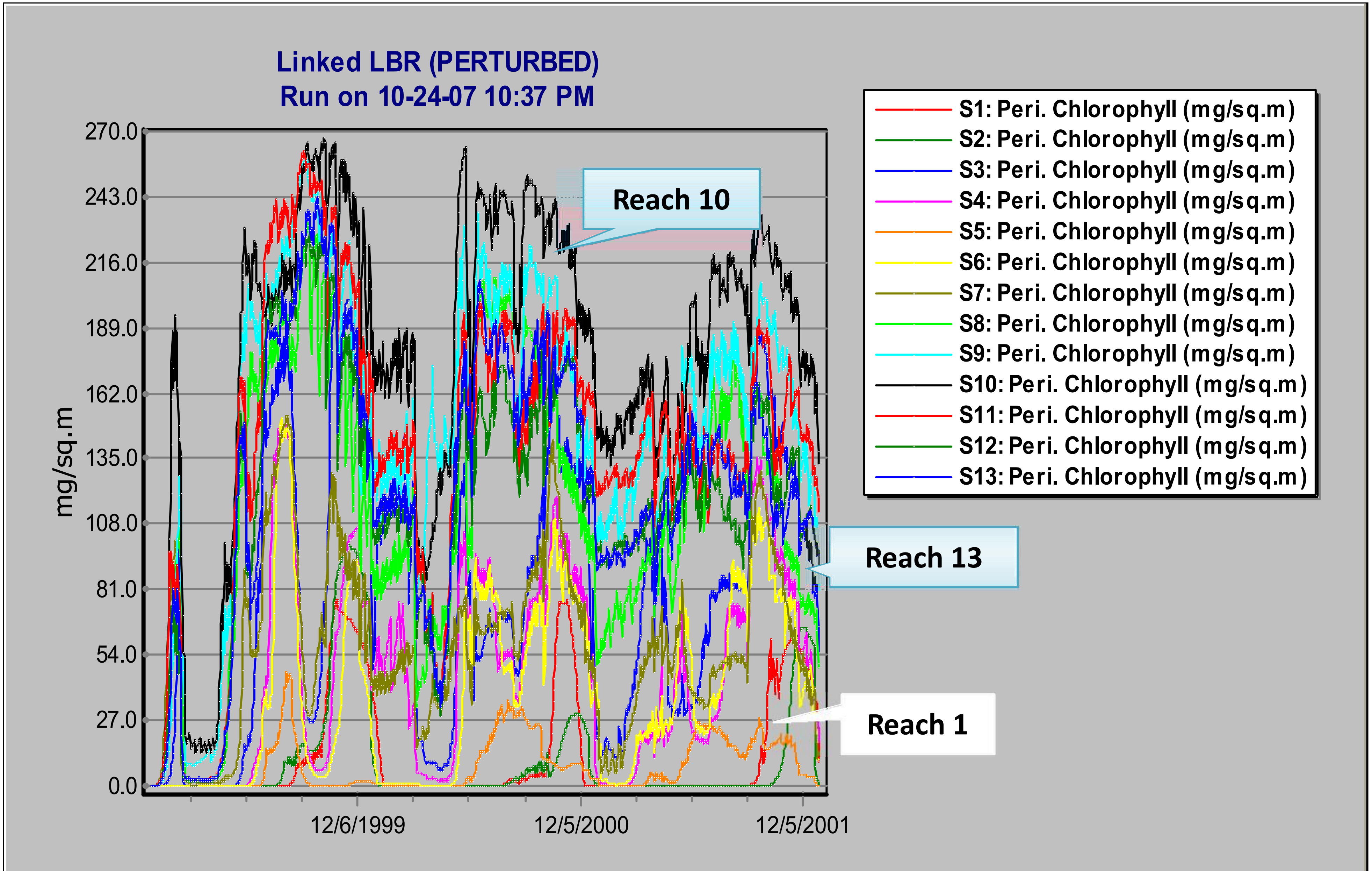


Lower Boise River in Boise, Idaho

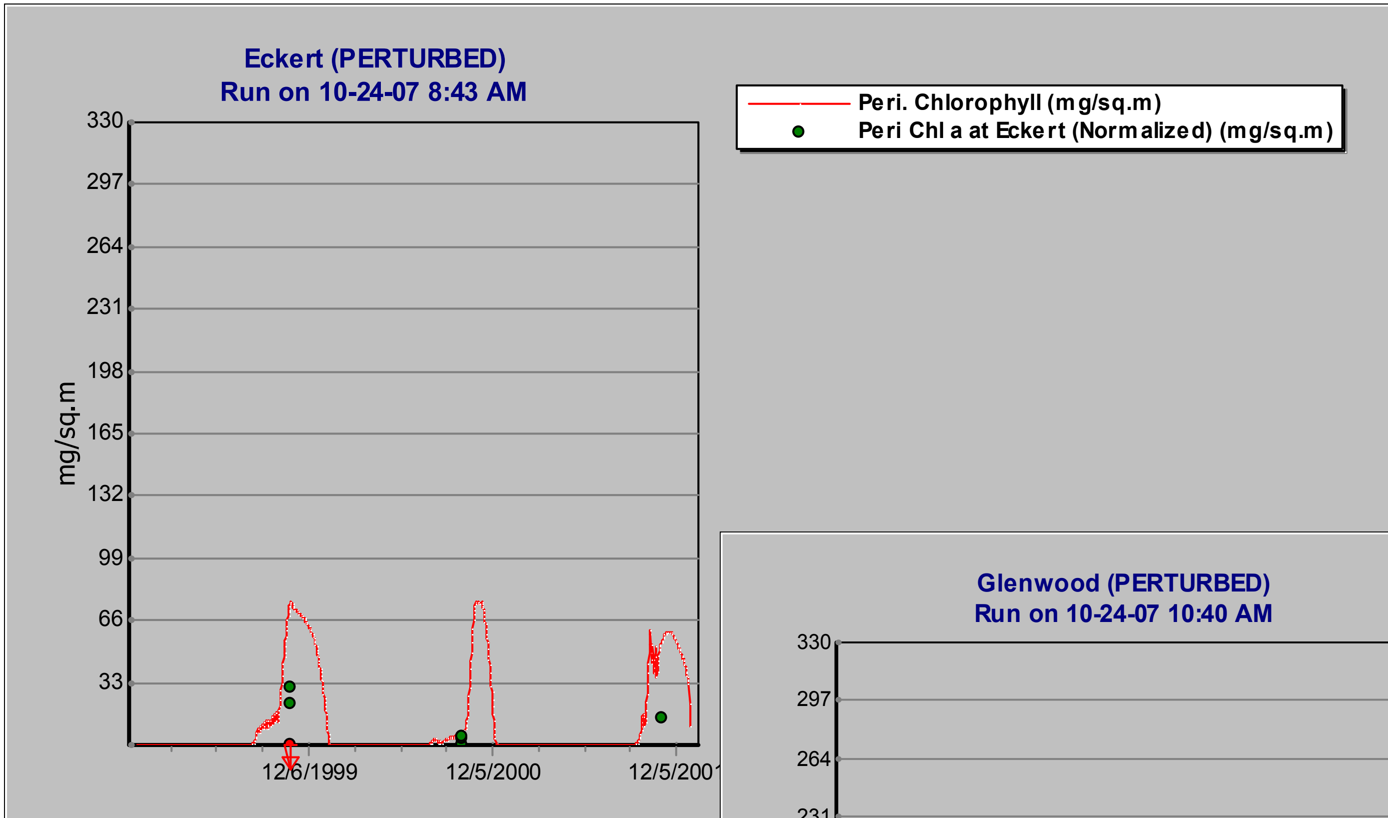
Complex Linked Model

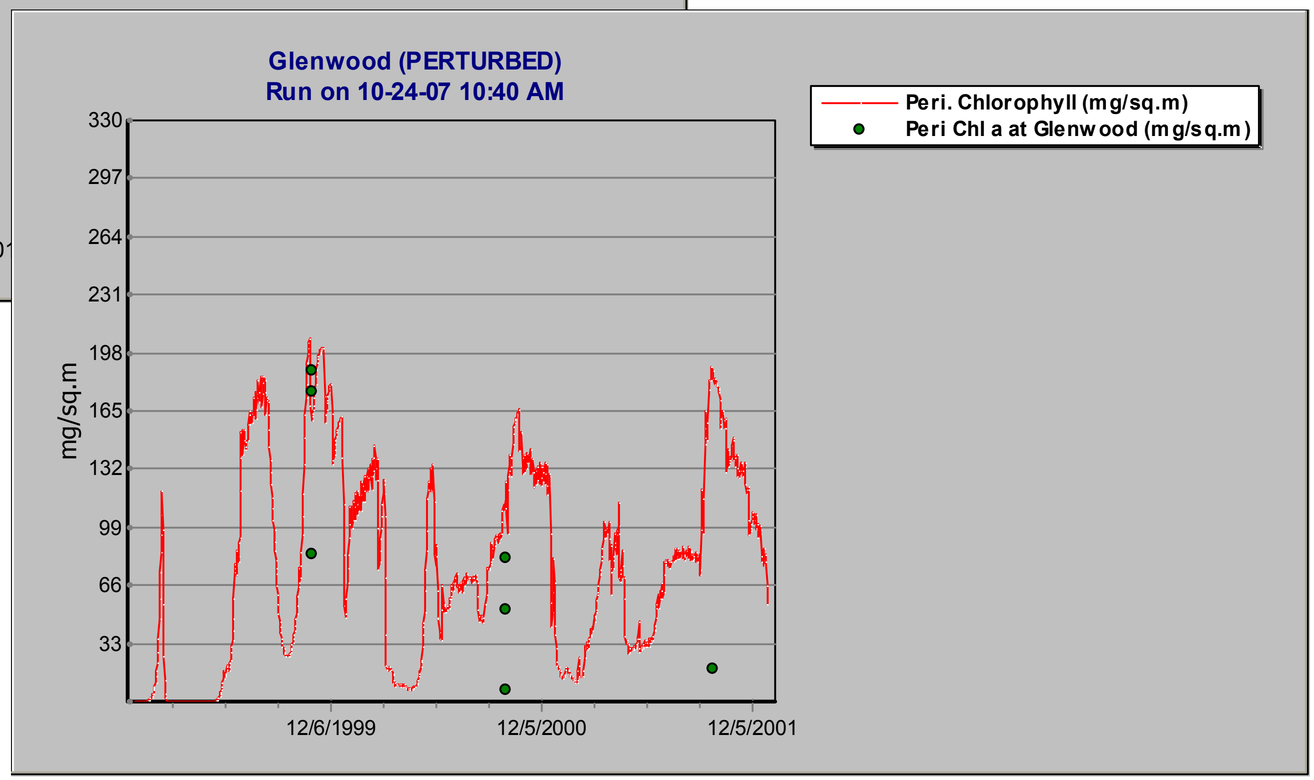
- 13 main-stem segments modeled
- 26 “tributary inputs”
  - Groundwater inputs
  - Waste Water Treatment Facilities
  - Input drains and tributaries
- Extensive water withdrawals
- Complex water-balance model
- Nutrients are integrated within main-stem

LBR Downstream Periphyton Trend

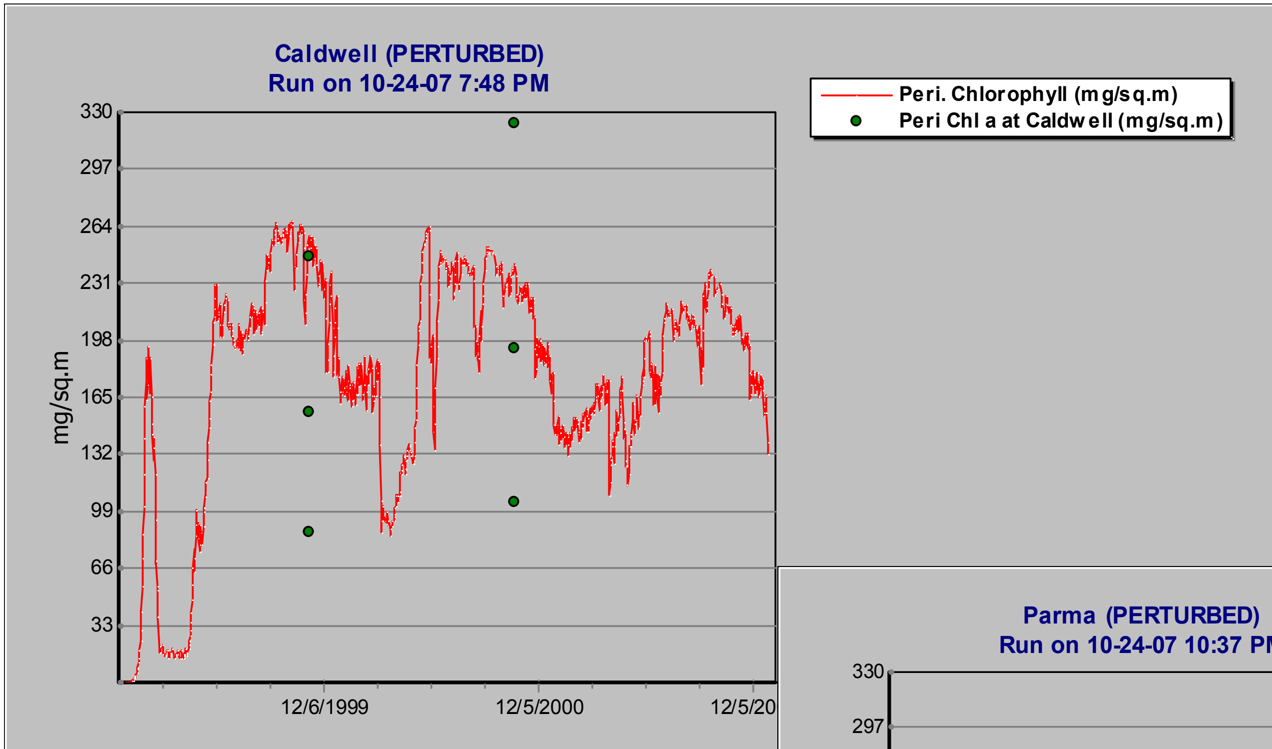


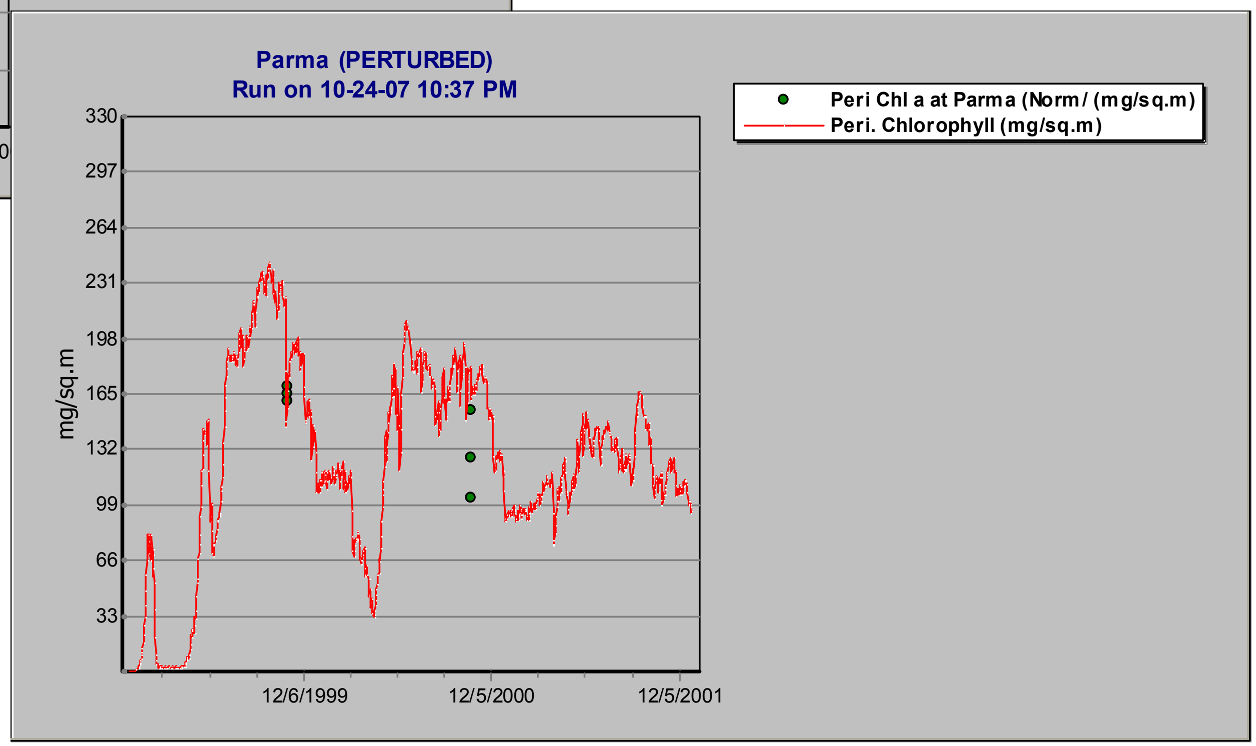
Periphyton in Reaches 1 and 3, LBR



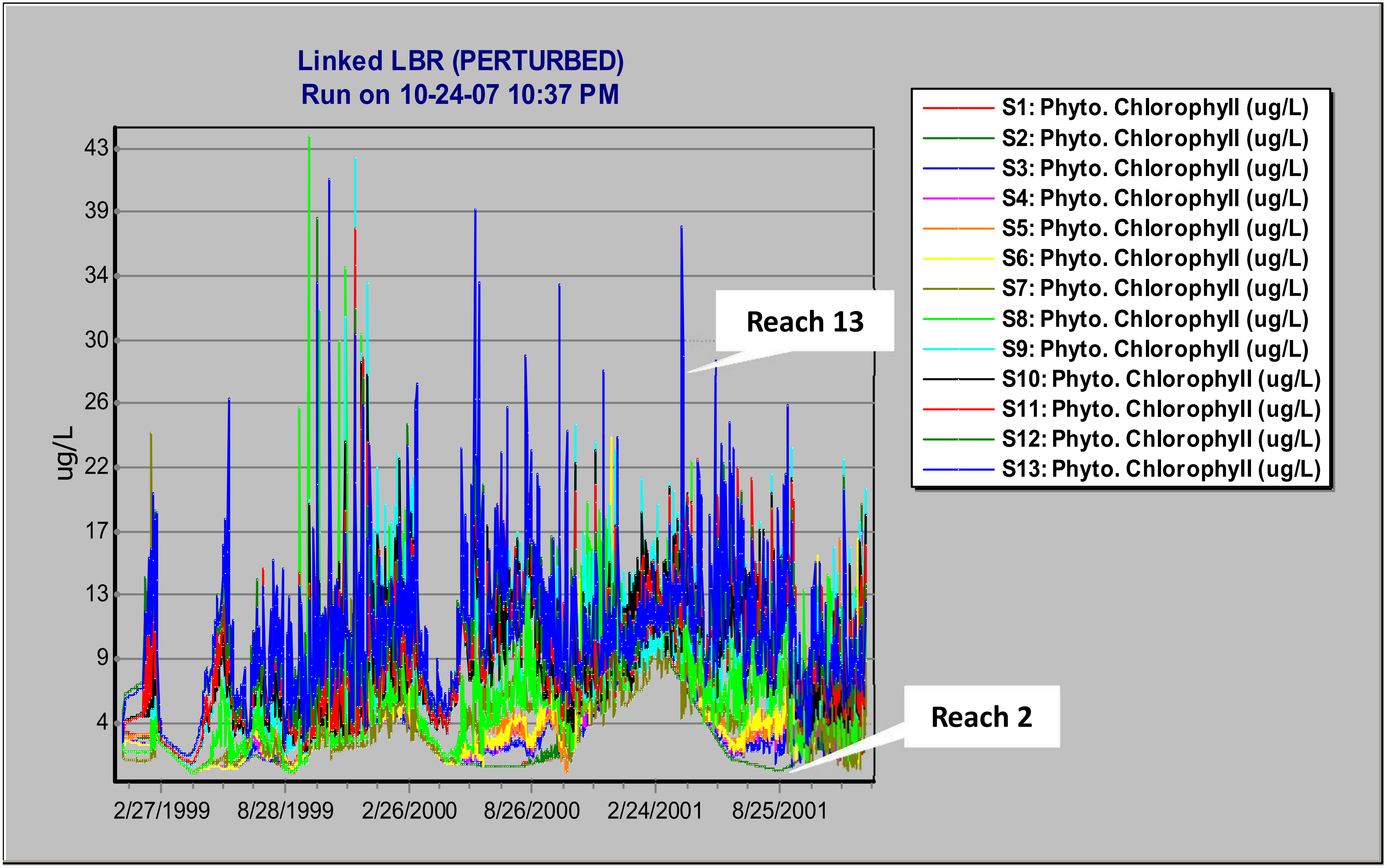


Periphyton in Reaches 10 and 13, LBR

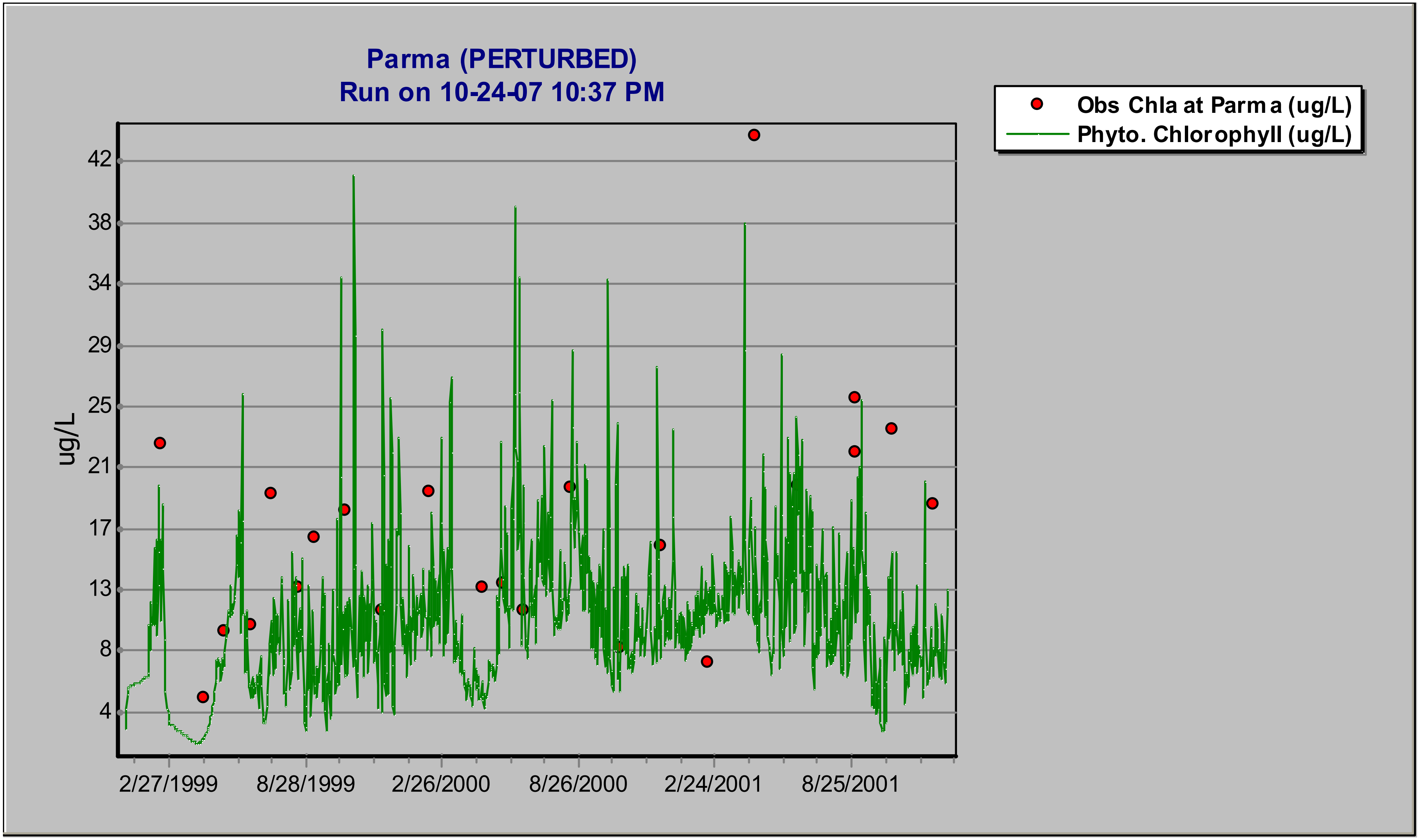




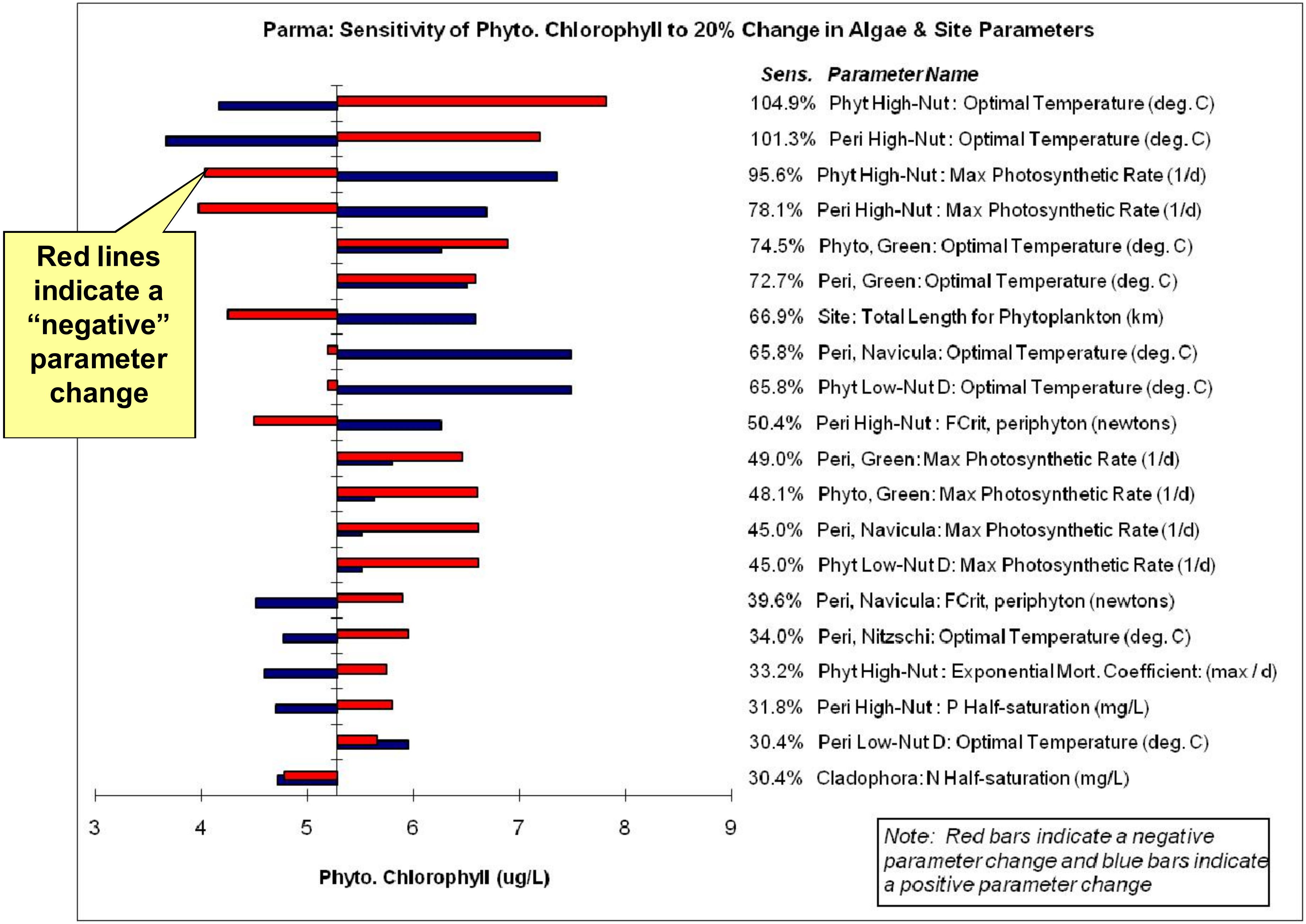
LBR Downstream Phytoplankton Trend



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



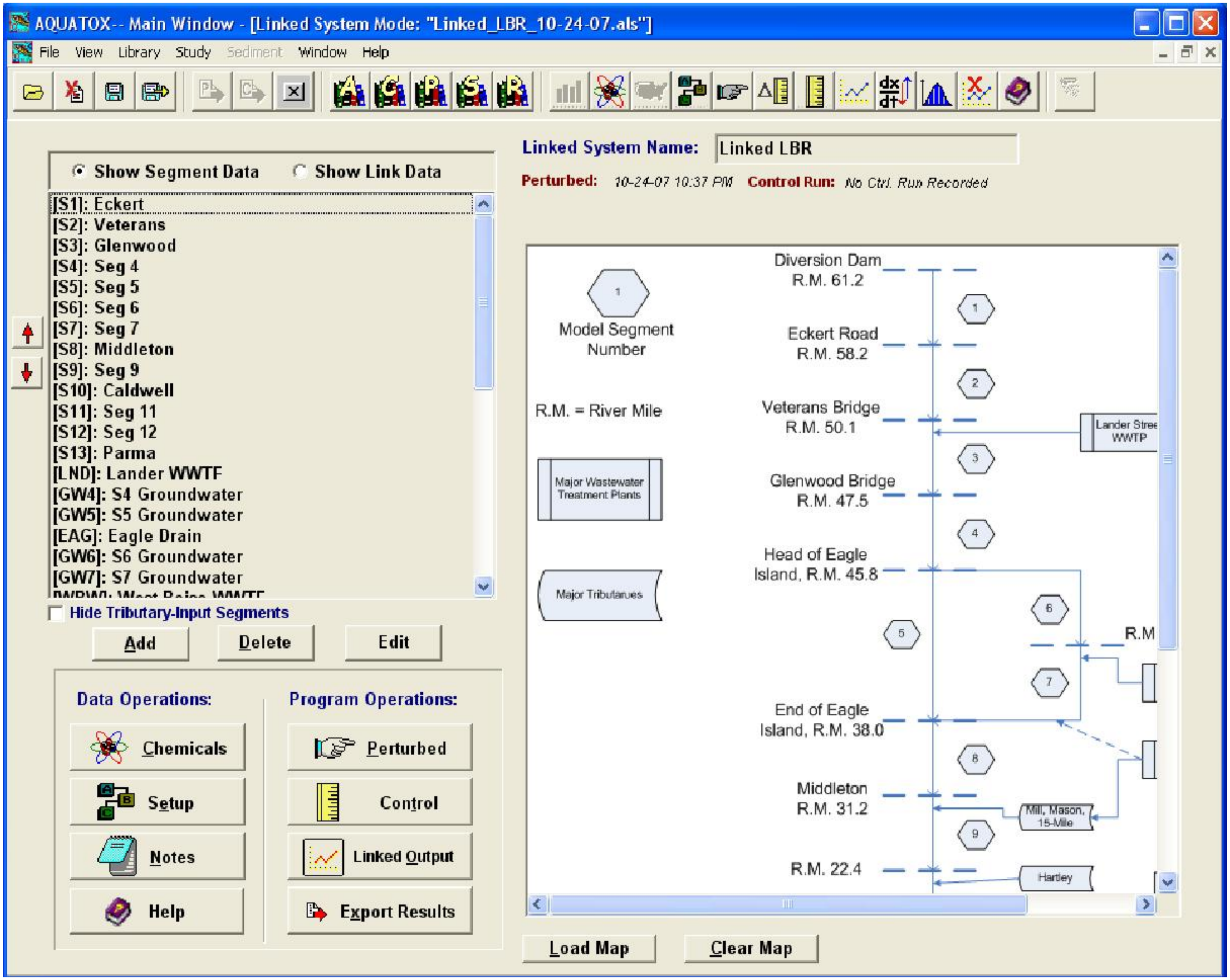
Phytoplankton Sensitivity, Parma LBR could choose parameters for better fit



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



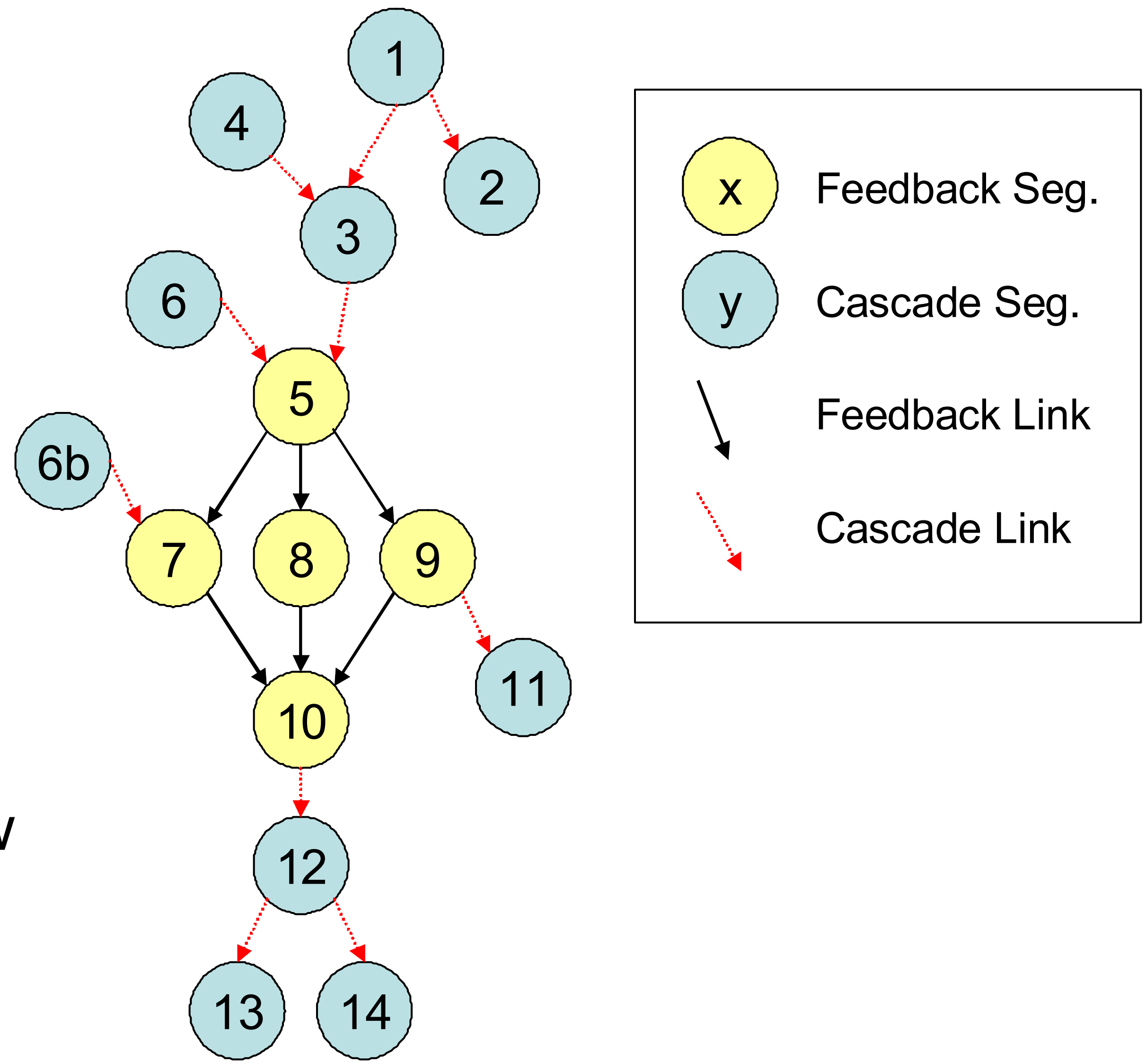
Cascade & Feedback Linkages

<u>Cascade Linkages:</u>

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

<u>Feedback Linkages:</u>

Two-way linkages that allow for backwards flow and diffusion

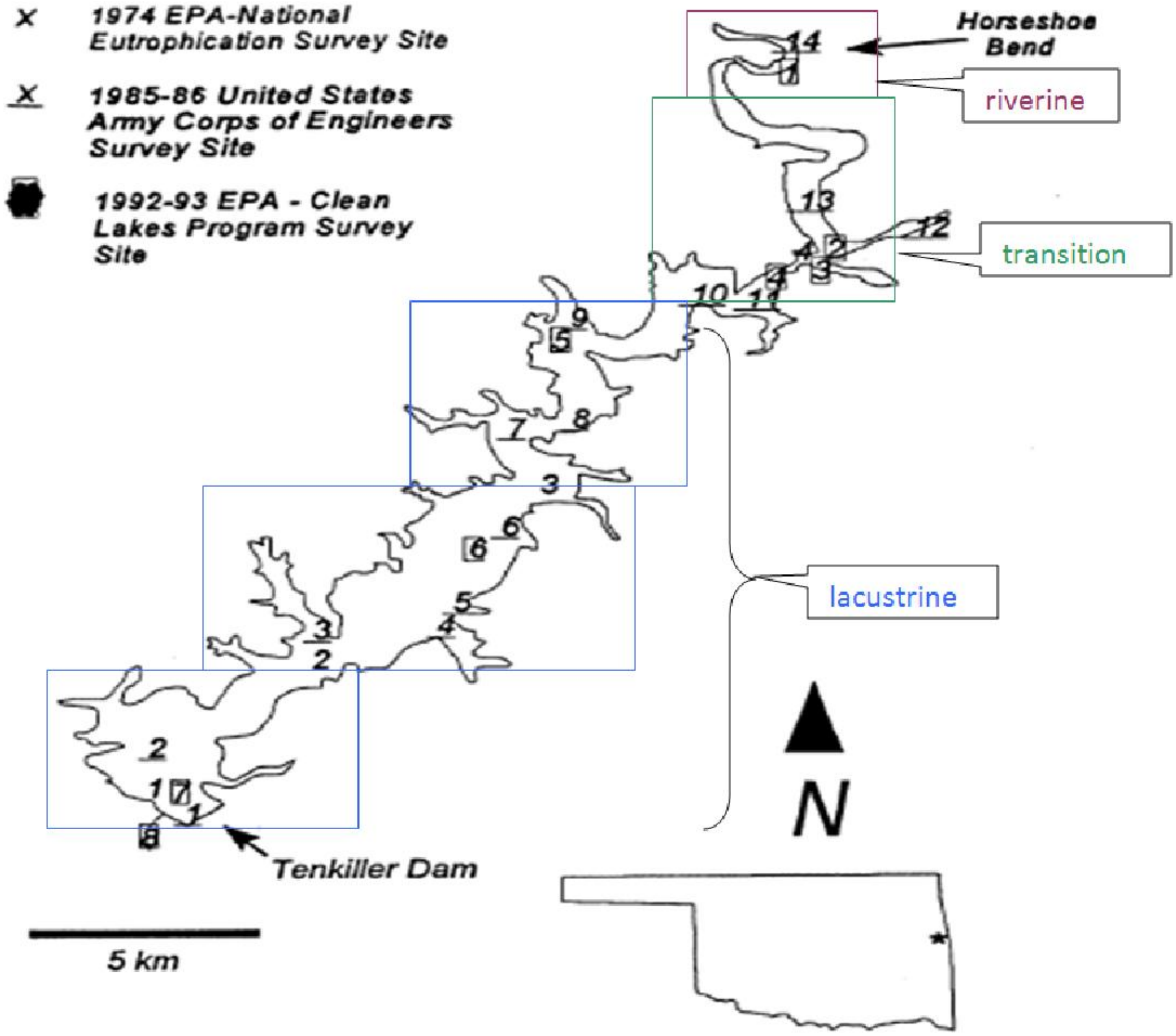


Linked Segment Model Data Requirements

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

Interface Demonstration to follow

Tenkiller Lake, OK



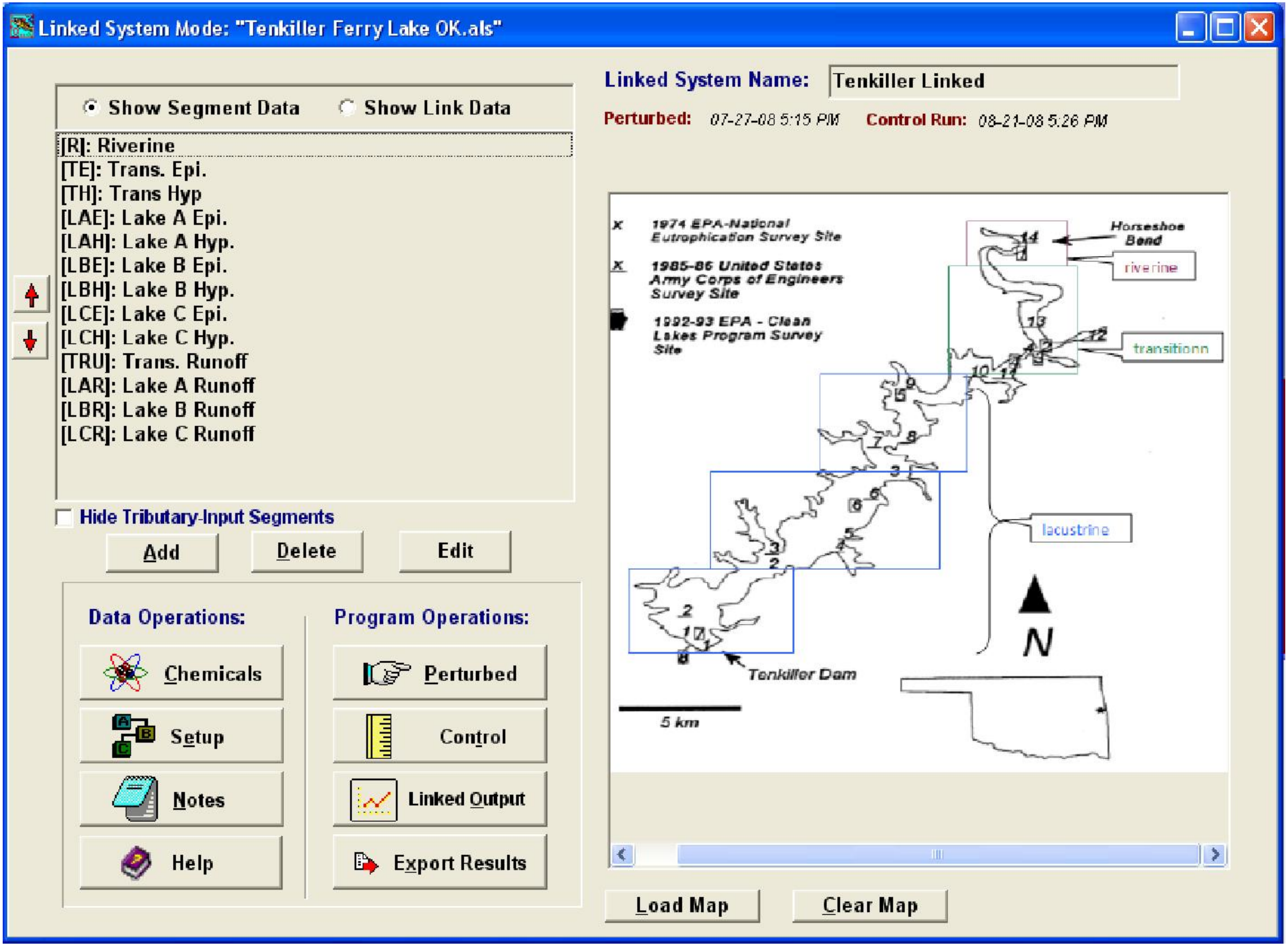
Tenkiller Lake Background

- 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)

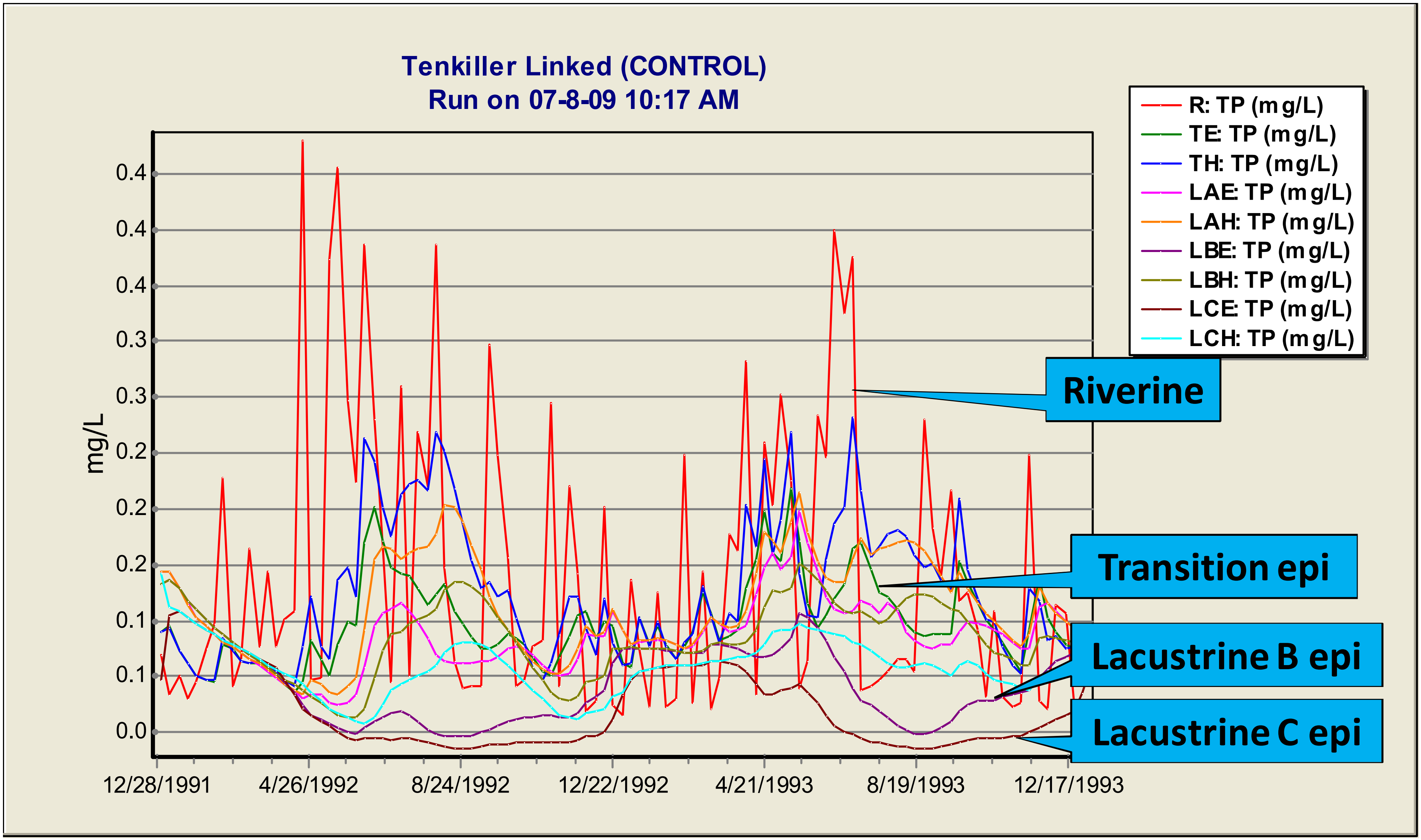
Tenkiller Lake OK



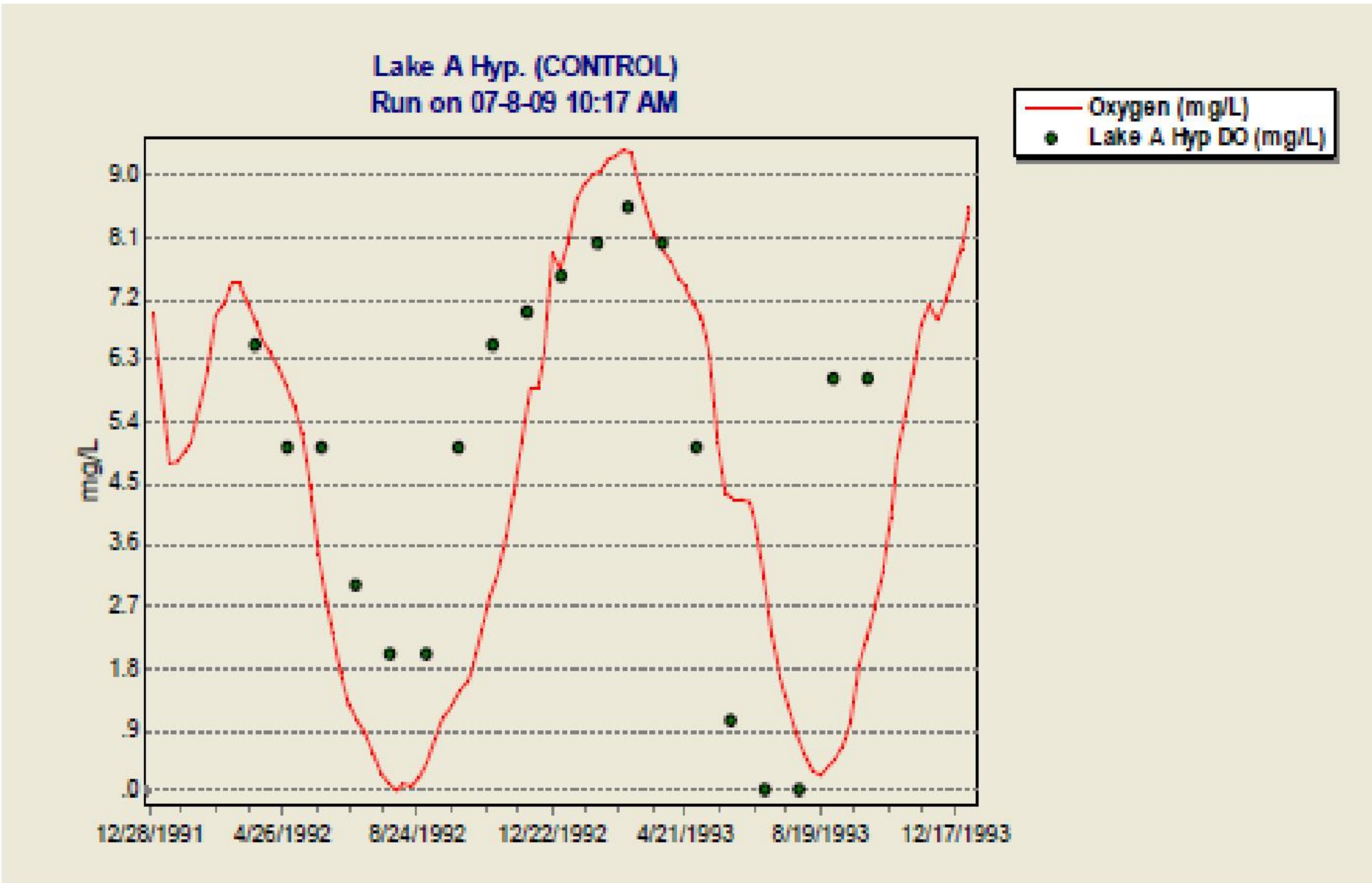
Storm-water plume, algae-rich riverine segment

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

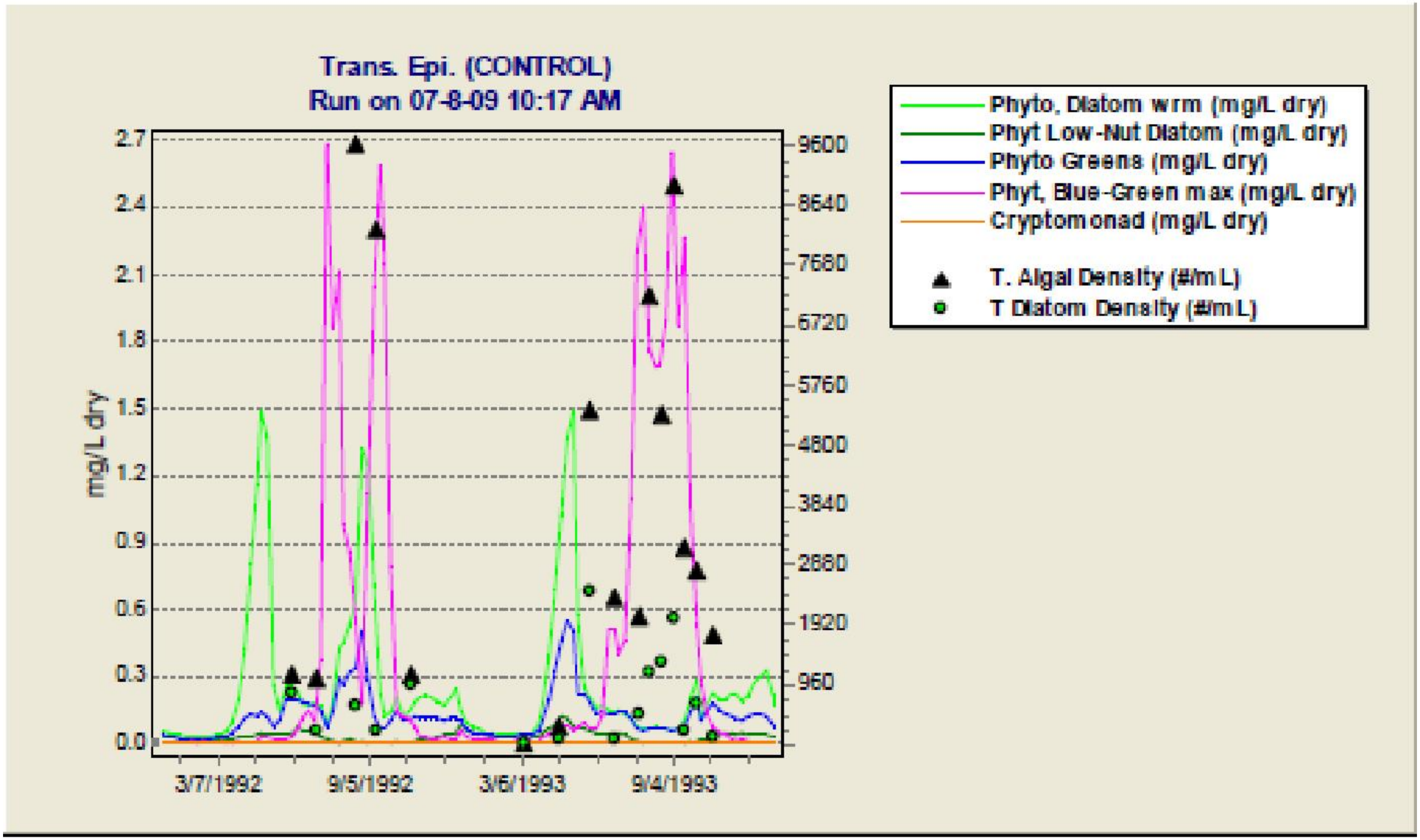
Total phosphorus in water column decreases toward dam; loss to sediments is simulated



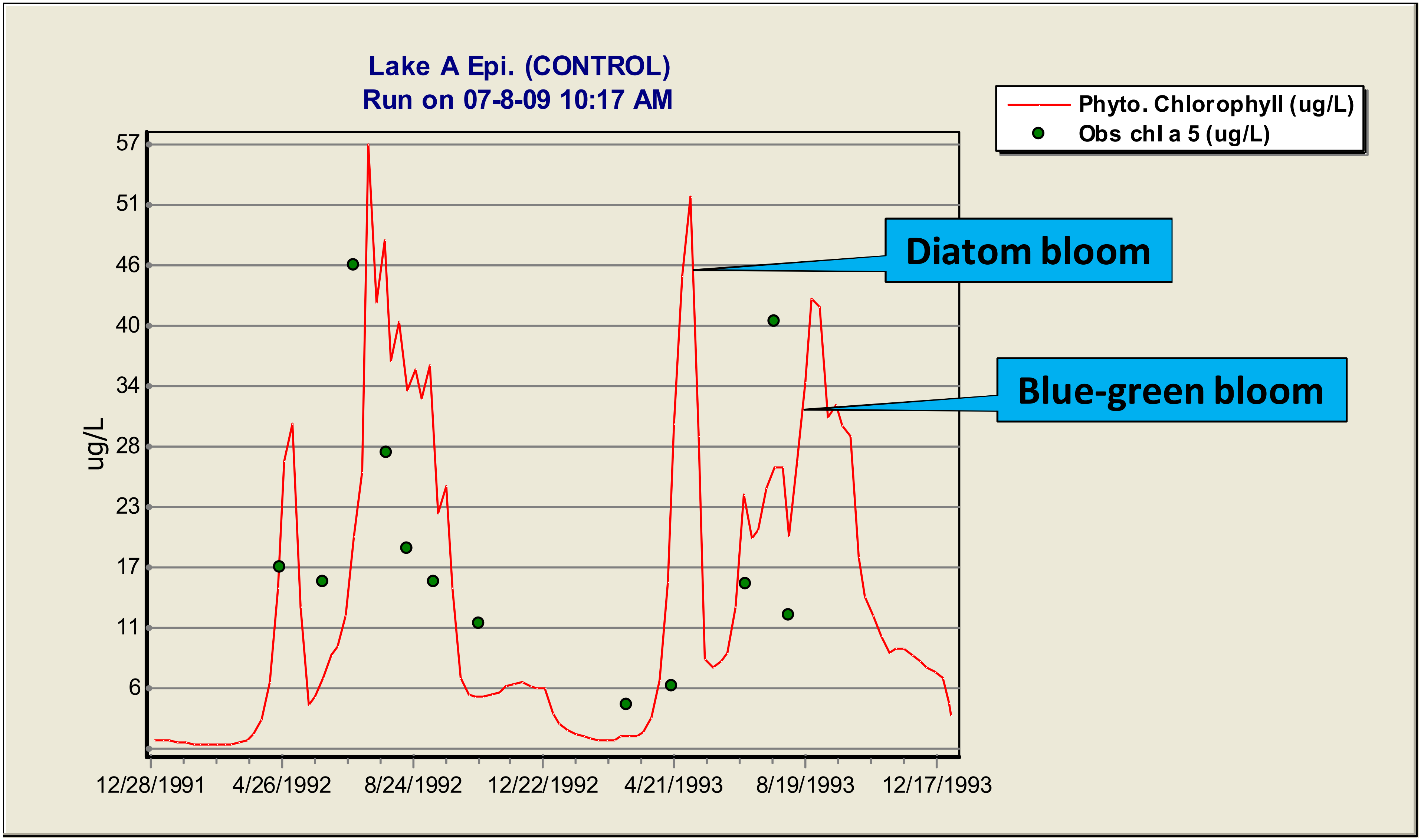
Simulated hypoxia in hypolimnion of Lacustrine A



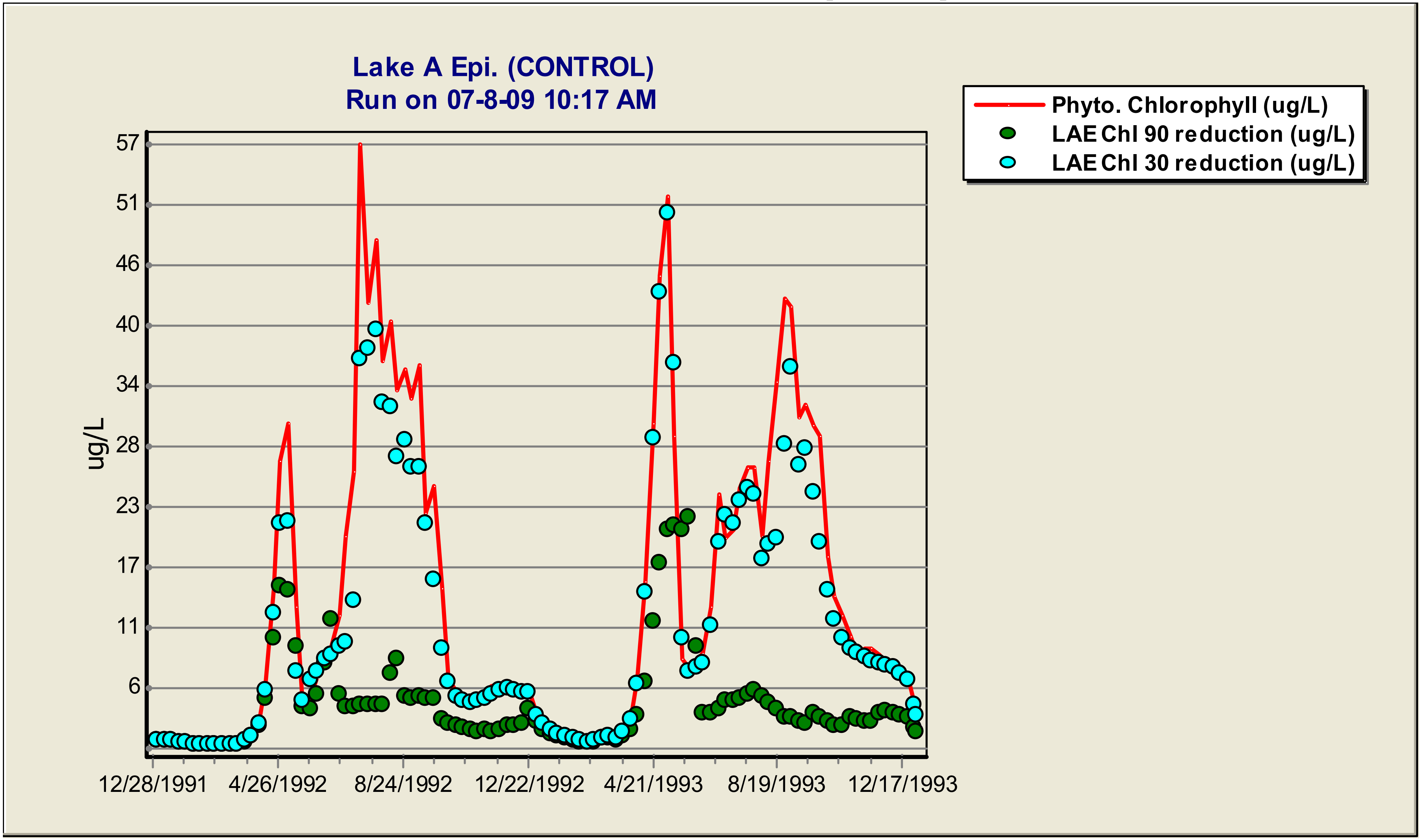
Simulated & observed algal composition in epilimnetic Transition



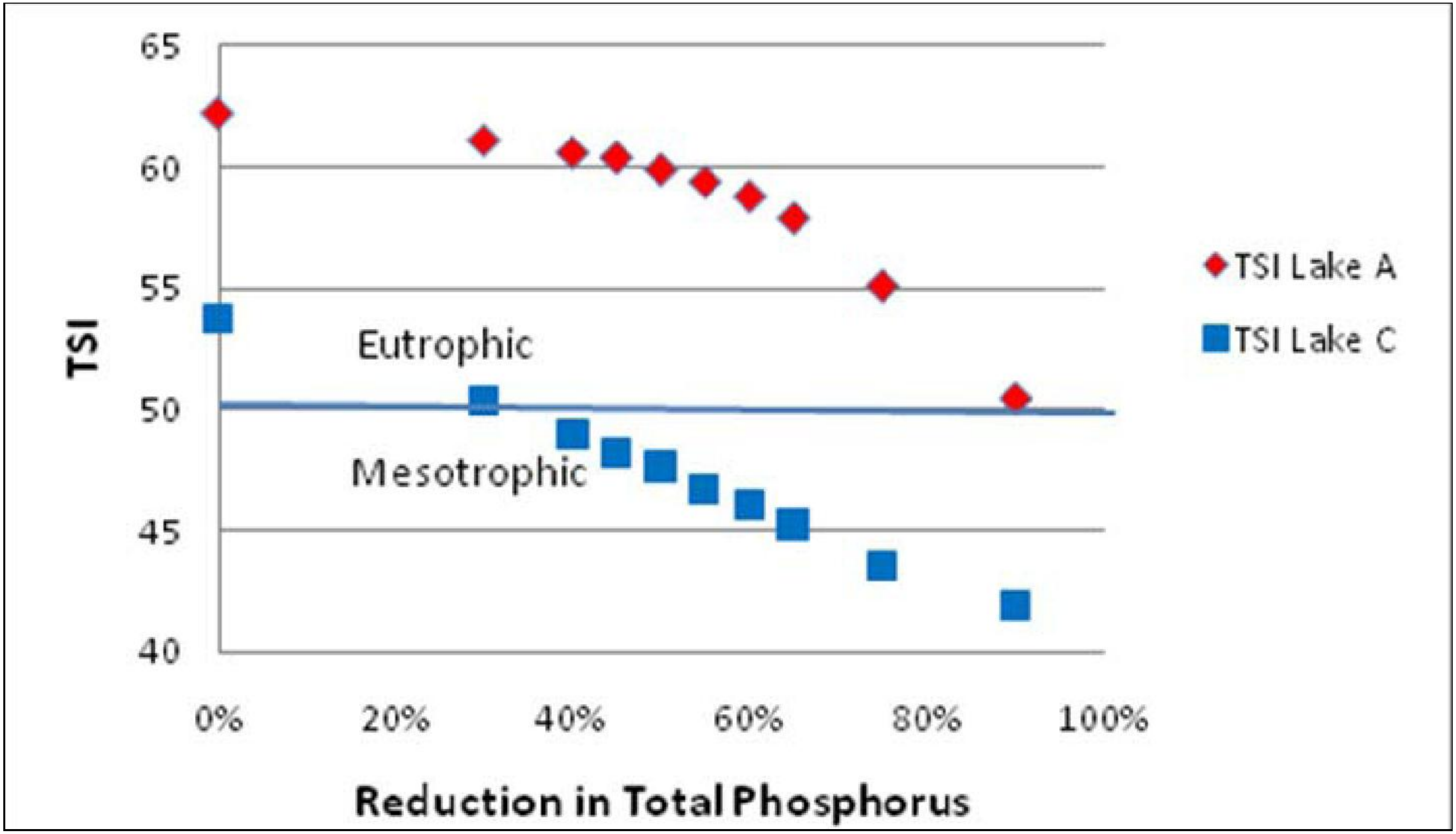
Simulated & observed chlorophyll *a* in Lacustrine A



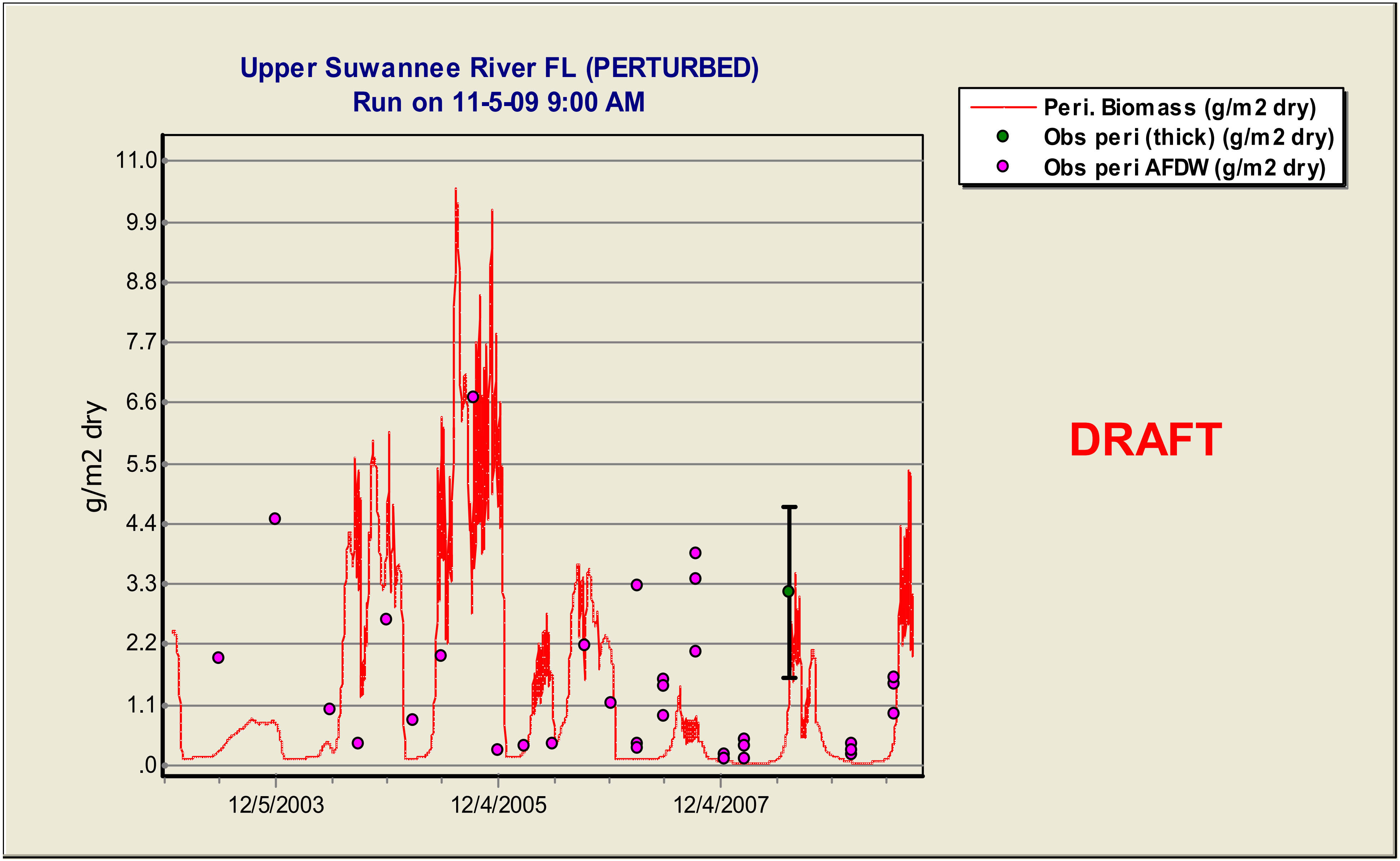
Predicted chlorophyll *a* in Lacustrine A with 30% and 90% load reduction of TP compared to baseline (red)



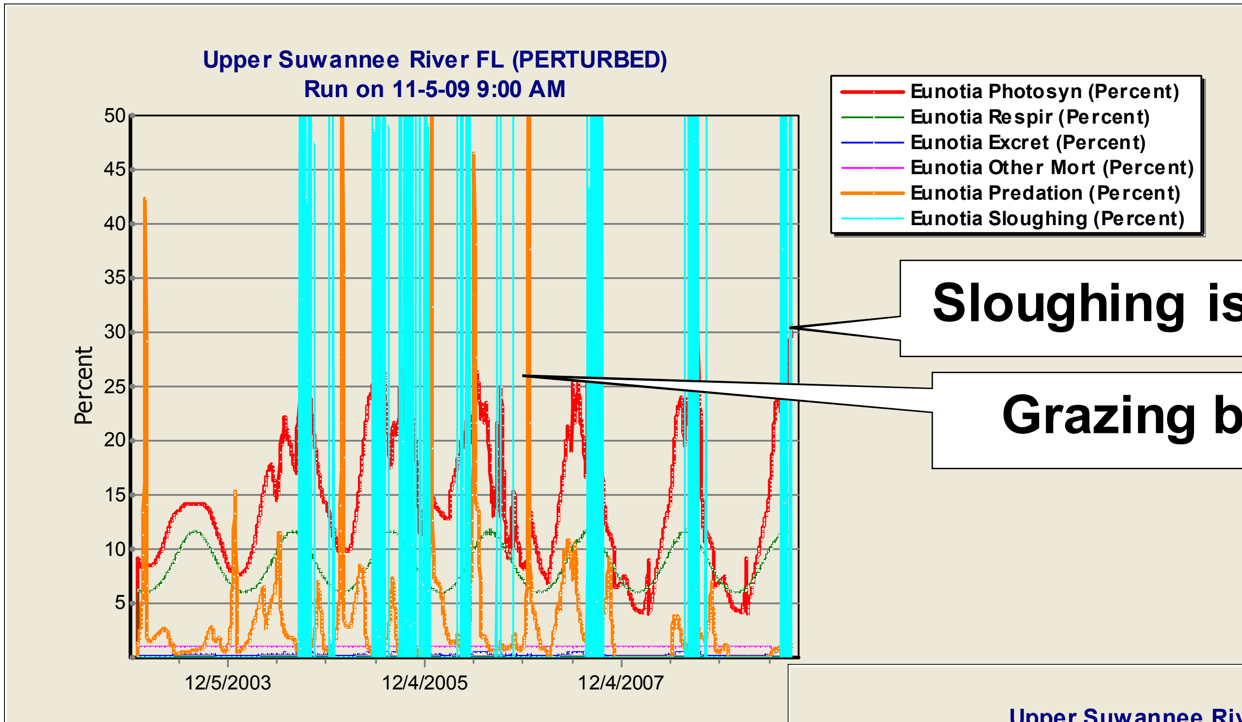
Predicted Trophic State Indices (Apr-Sep) in Lacustrine A & C as a function of load reductions



Model is being applied to numerous FL streams, including the Suwannee River



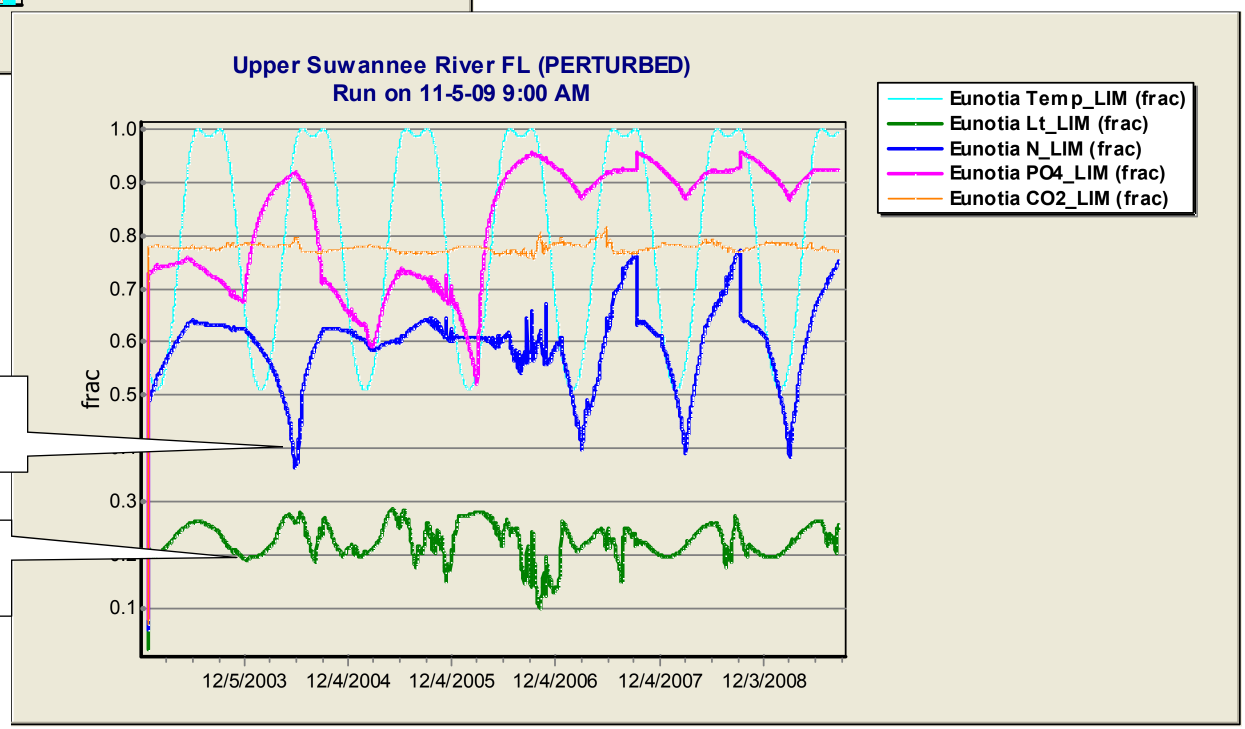
Can diagnose algal response



Sloughing is important

Grazing by mayflies

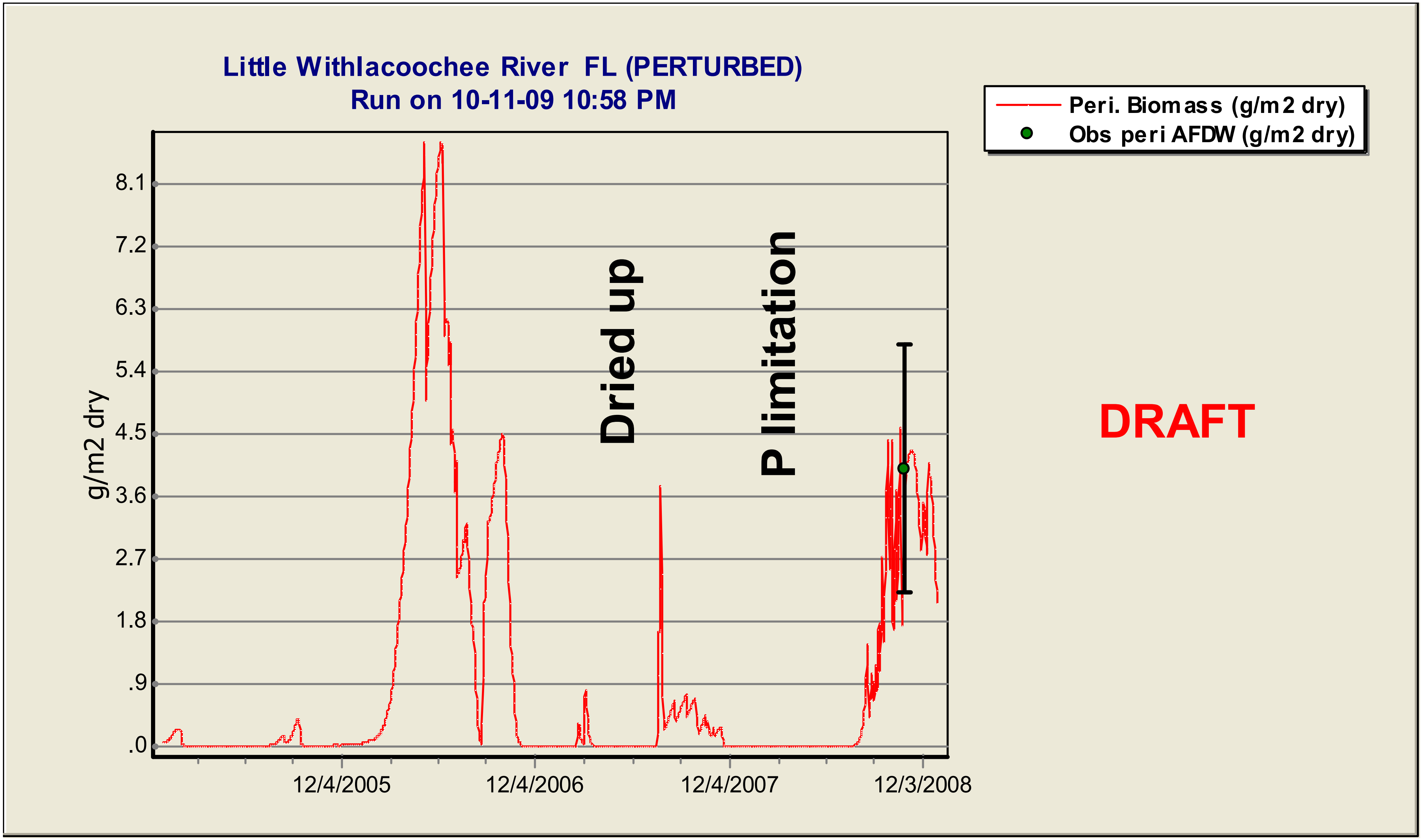
DRAFT



Nitrogen is limiting

Light is more limiting

The Little Withlacoochee River has mean TP of 0.044 mg/L



AQUATOX– Chemical Fate Overview

- Can model up to twenty chemicals simultaneously
- Fate processes:
  - microbial degradation
  - photolysis
  - ionization
  - hydrolysis
  - volatilization
  - sorption
- 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

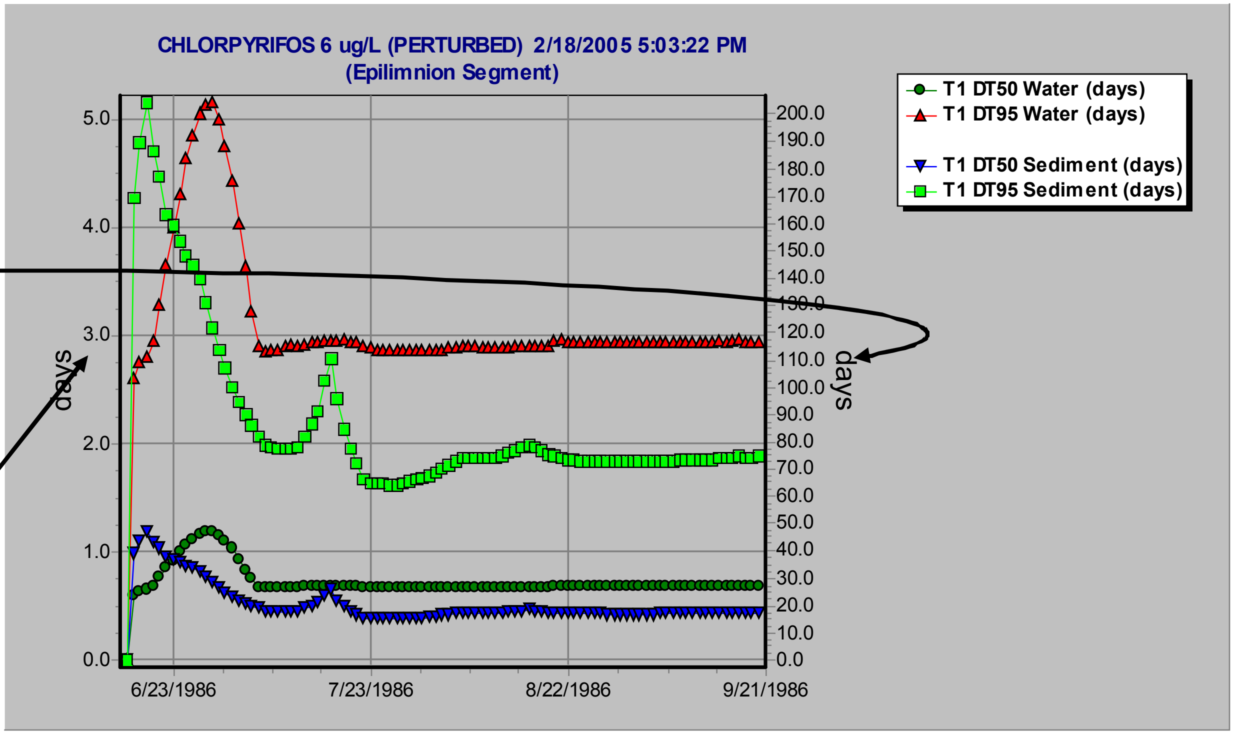
$$Loss_{Water} = \frac{Hydrolysis_{Water} + Photolysis + Microbial_{Water} + Washout + Volat. + Sorption}{Mass_{Water}}$$

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

For this Chlorpyrifos Study:

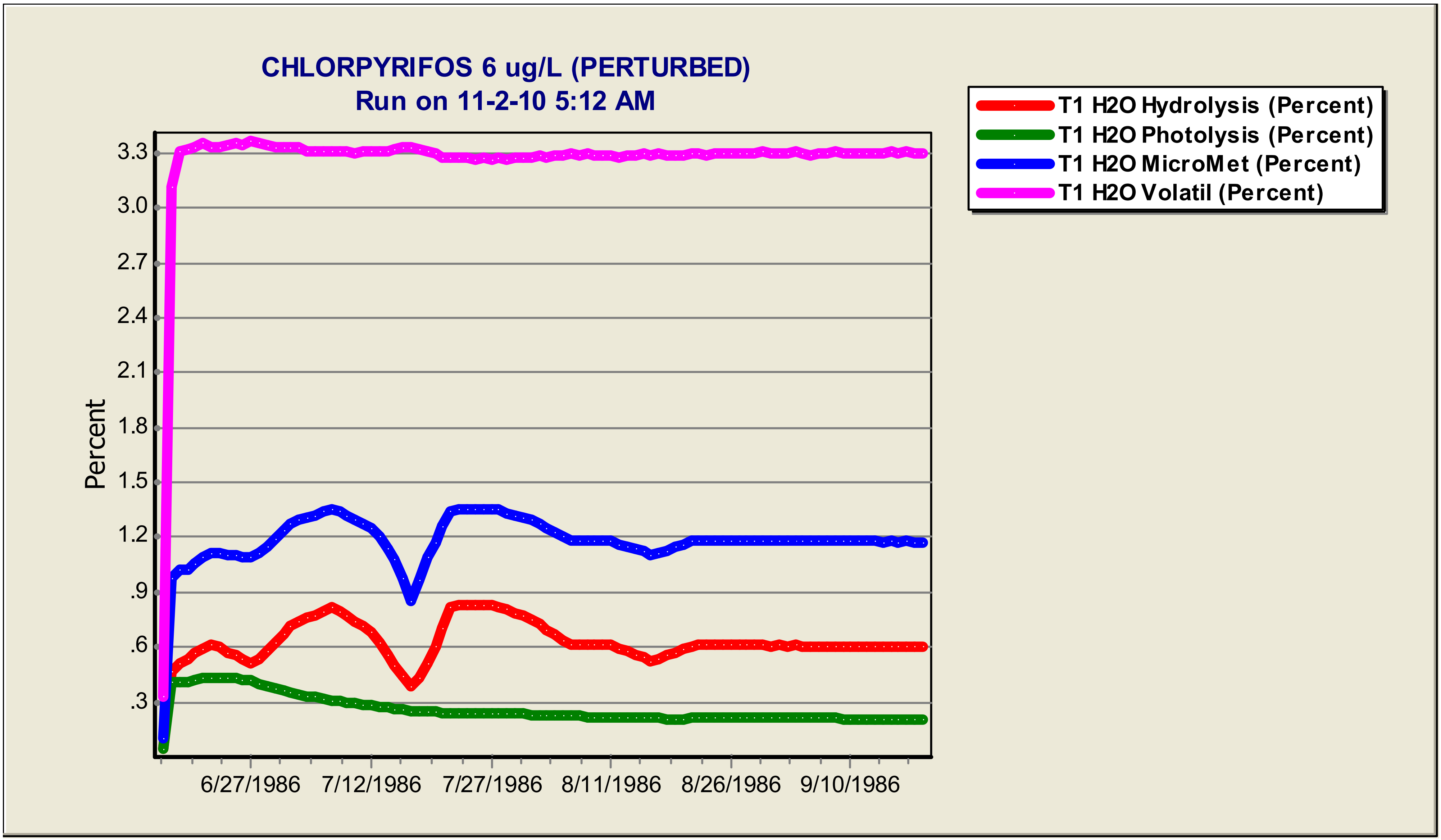
Half-life in Sediment of roughly 20 days
DT95 of roughly 75 days

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



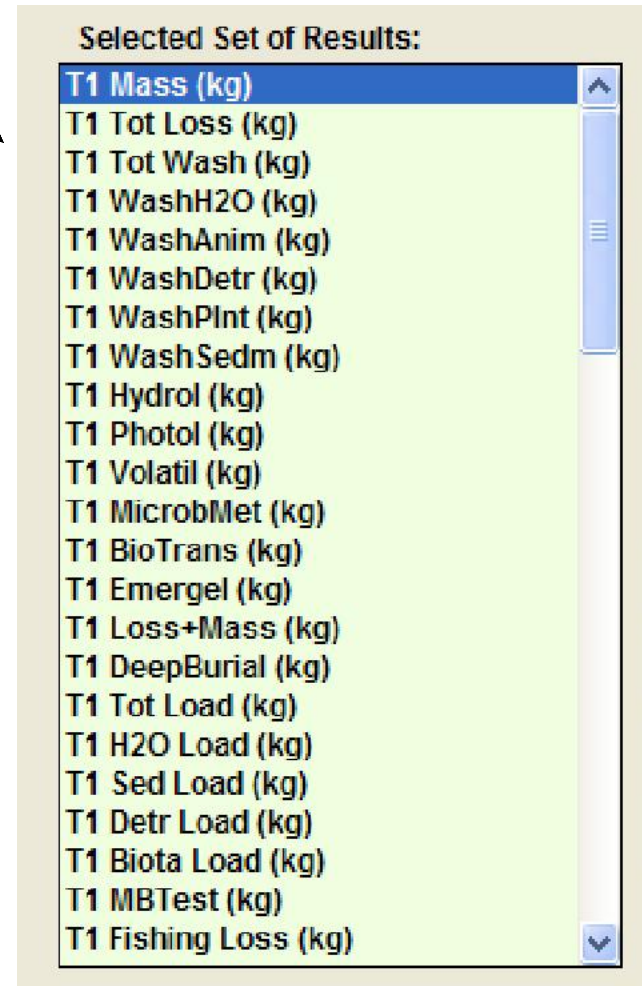
Chemical rates may be tracked

Predicted In-situ Degradation Rates for Chlorpyrifos in Pond



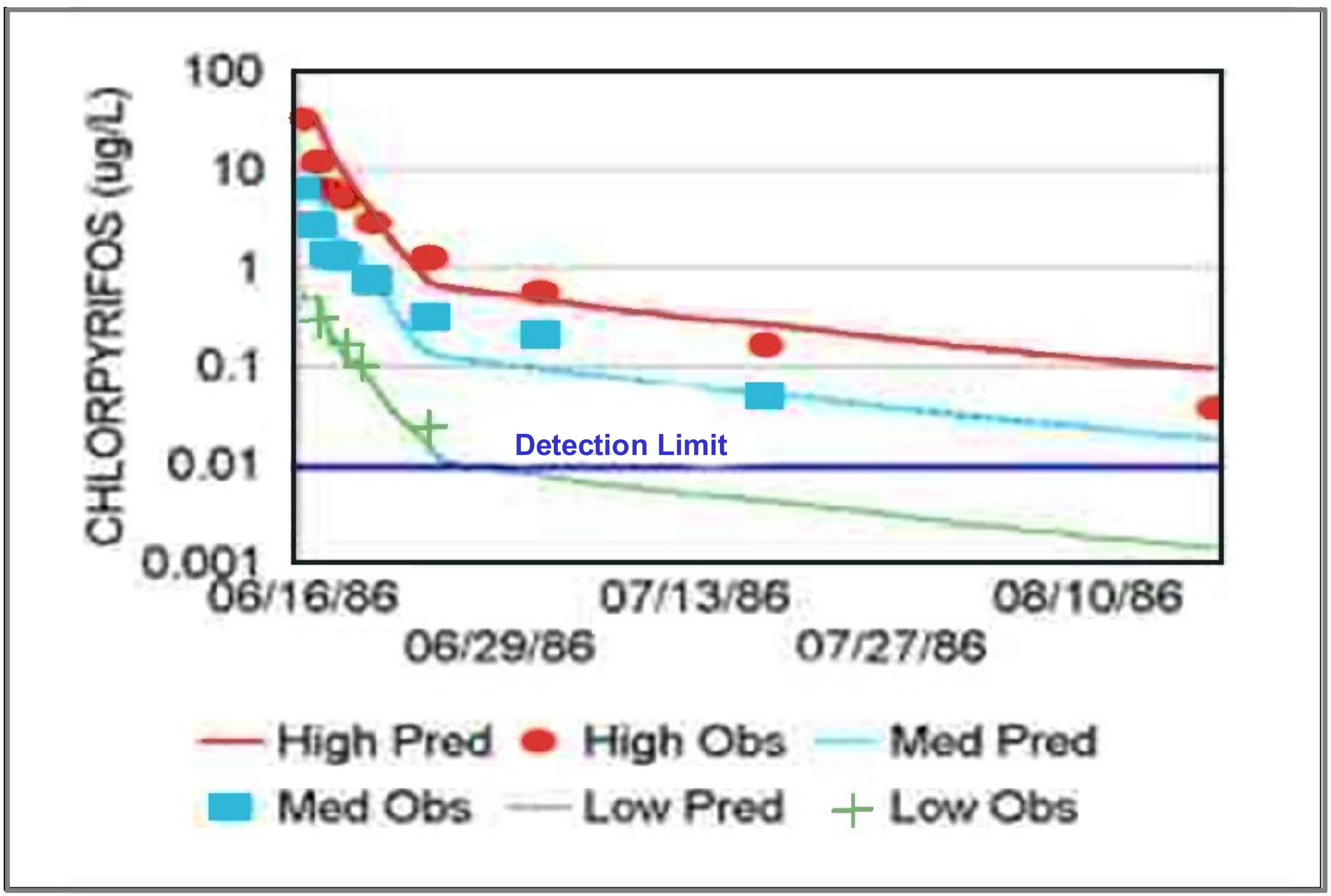
Toxicant mass balance tracking

- 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



Fate of Chlorpyrifos in the Duluth MN Pond was Predicted Successfully

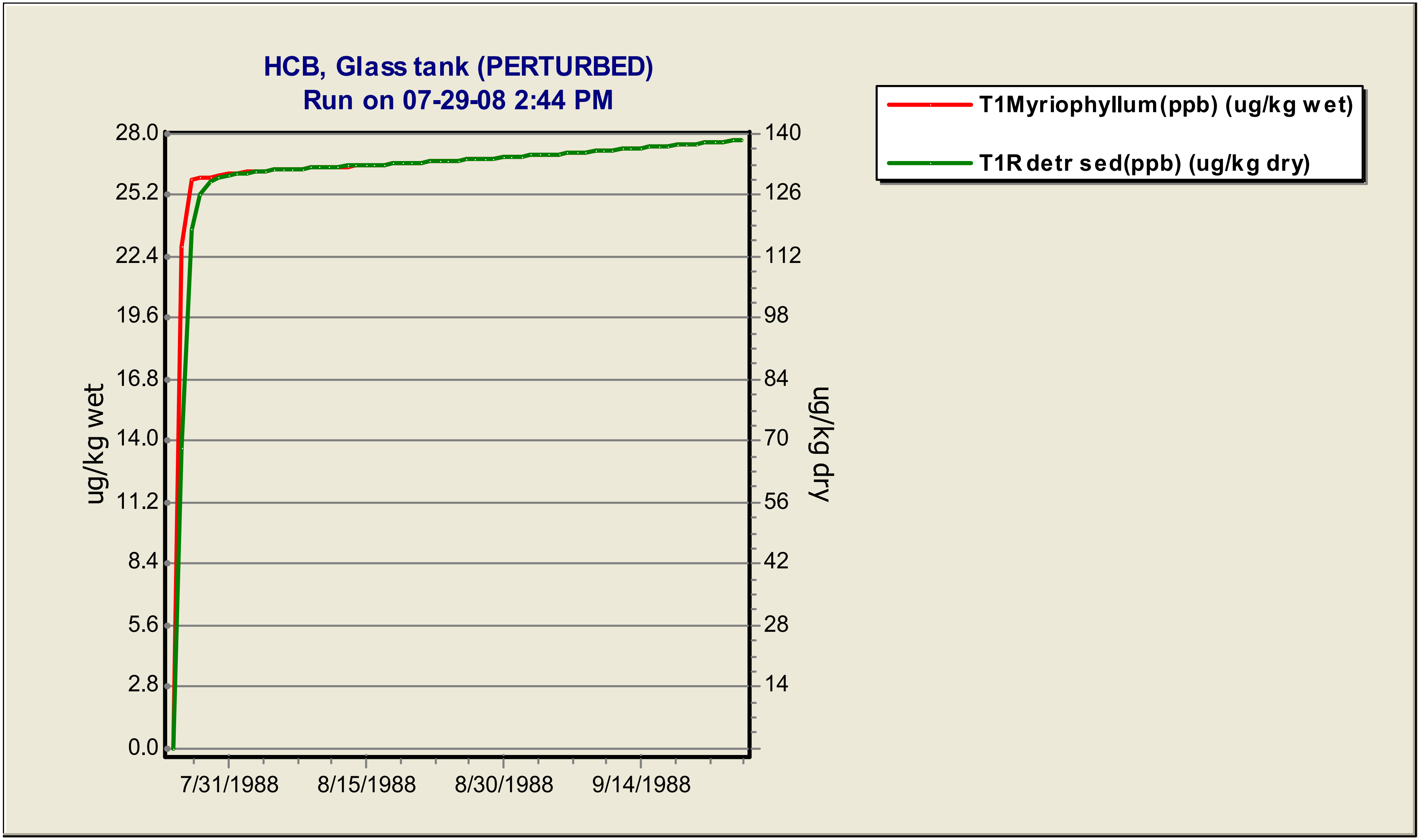
Multiple Dosing Levels



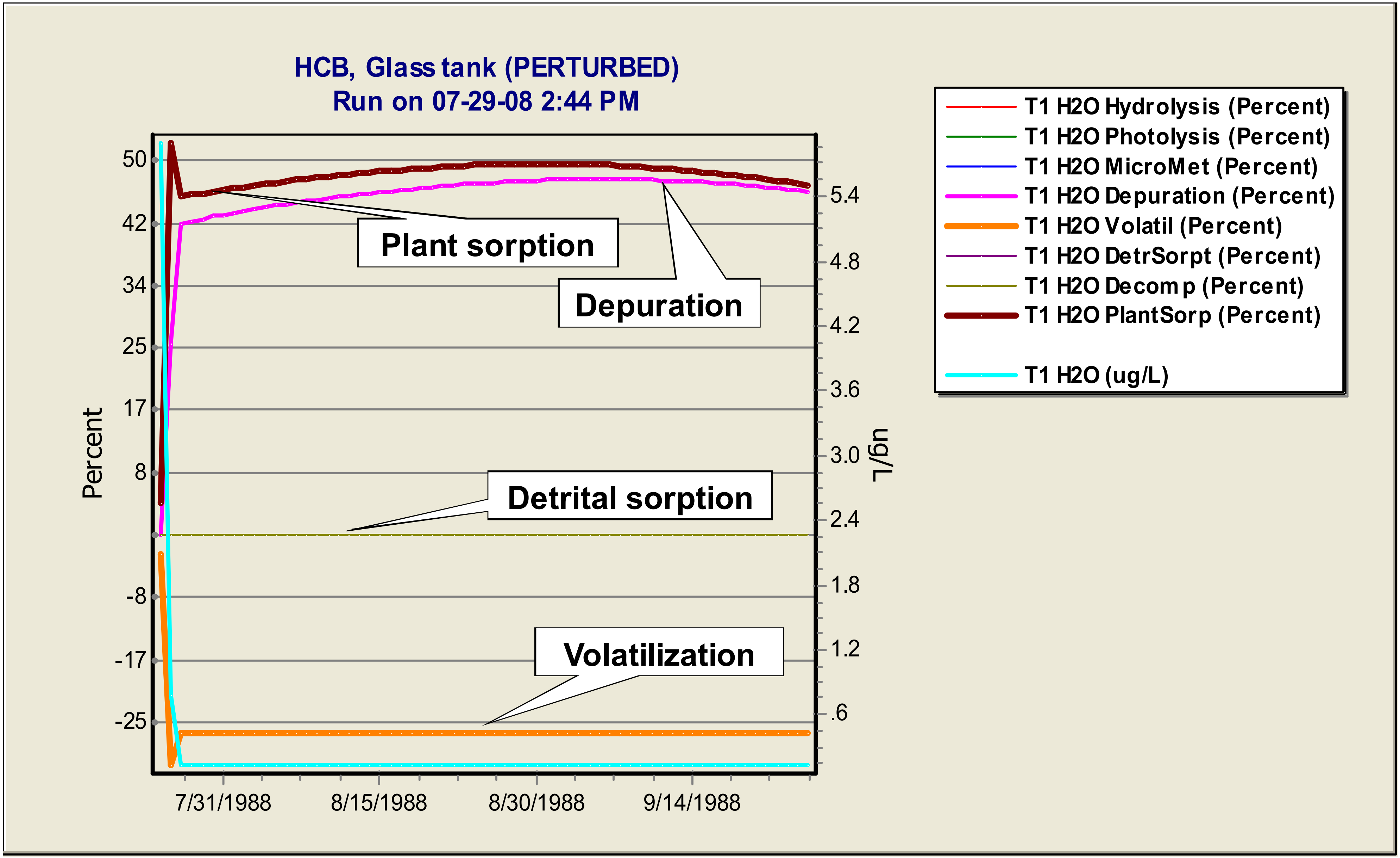
HCB in tank

- 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



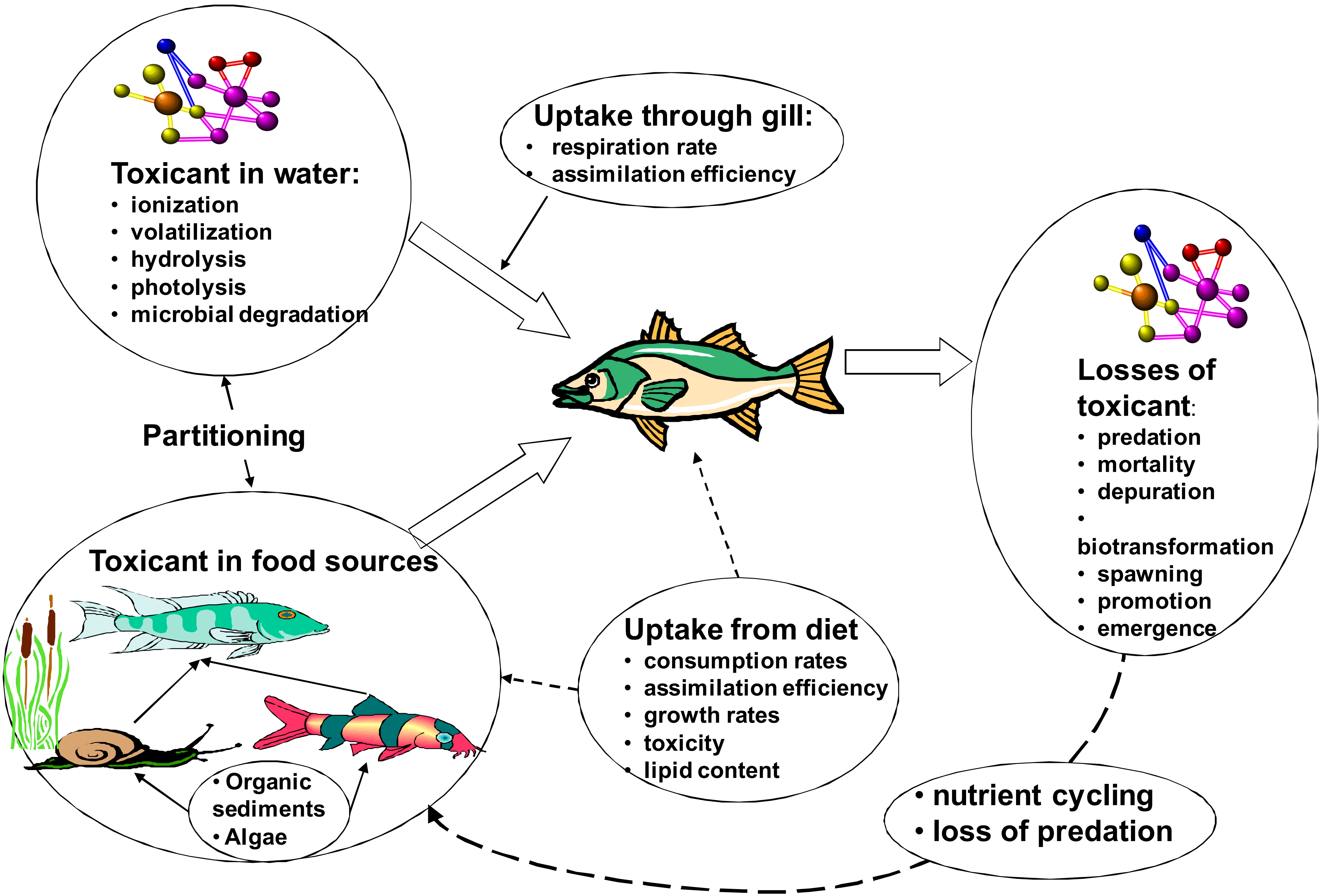
HCB loss rates can be plotted, showing that sorption to detritus is negligible (due to mass)



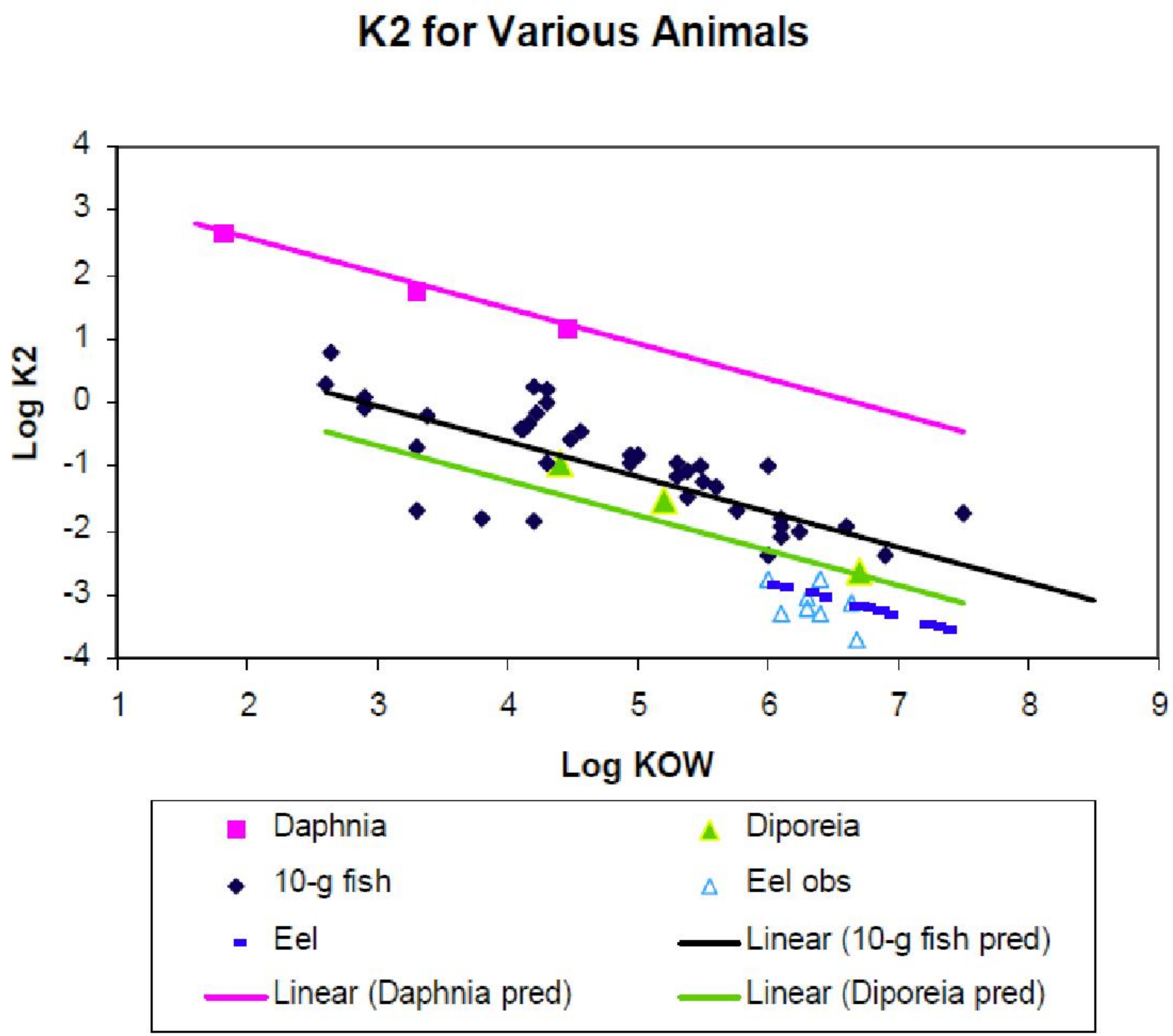
Chemical Bioaccumulation Overview

- 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



Alternative Chemical Uptake Model

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

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

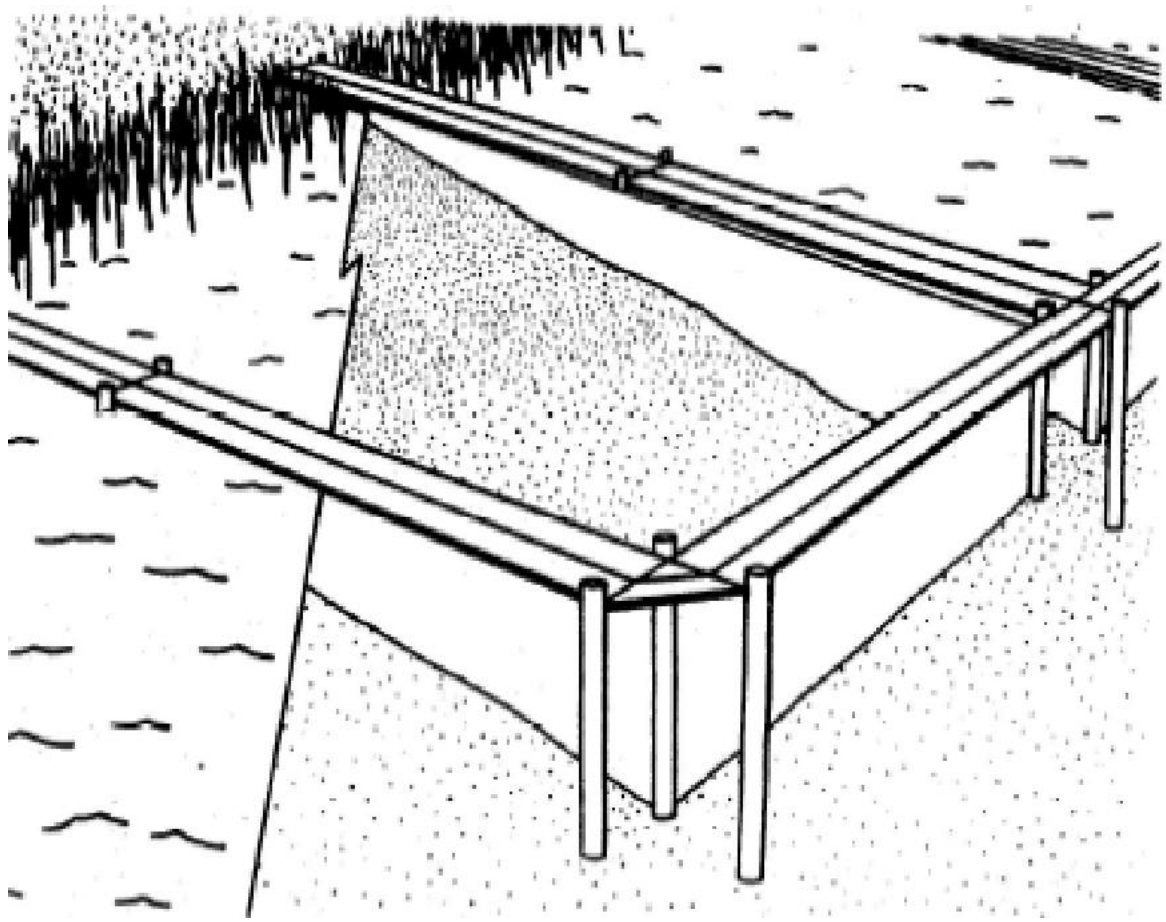
Given these parameters, AQUATOX calculates uptake and depuration in plants and animals as kinetic processes.

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

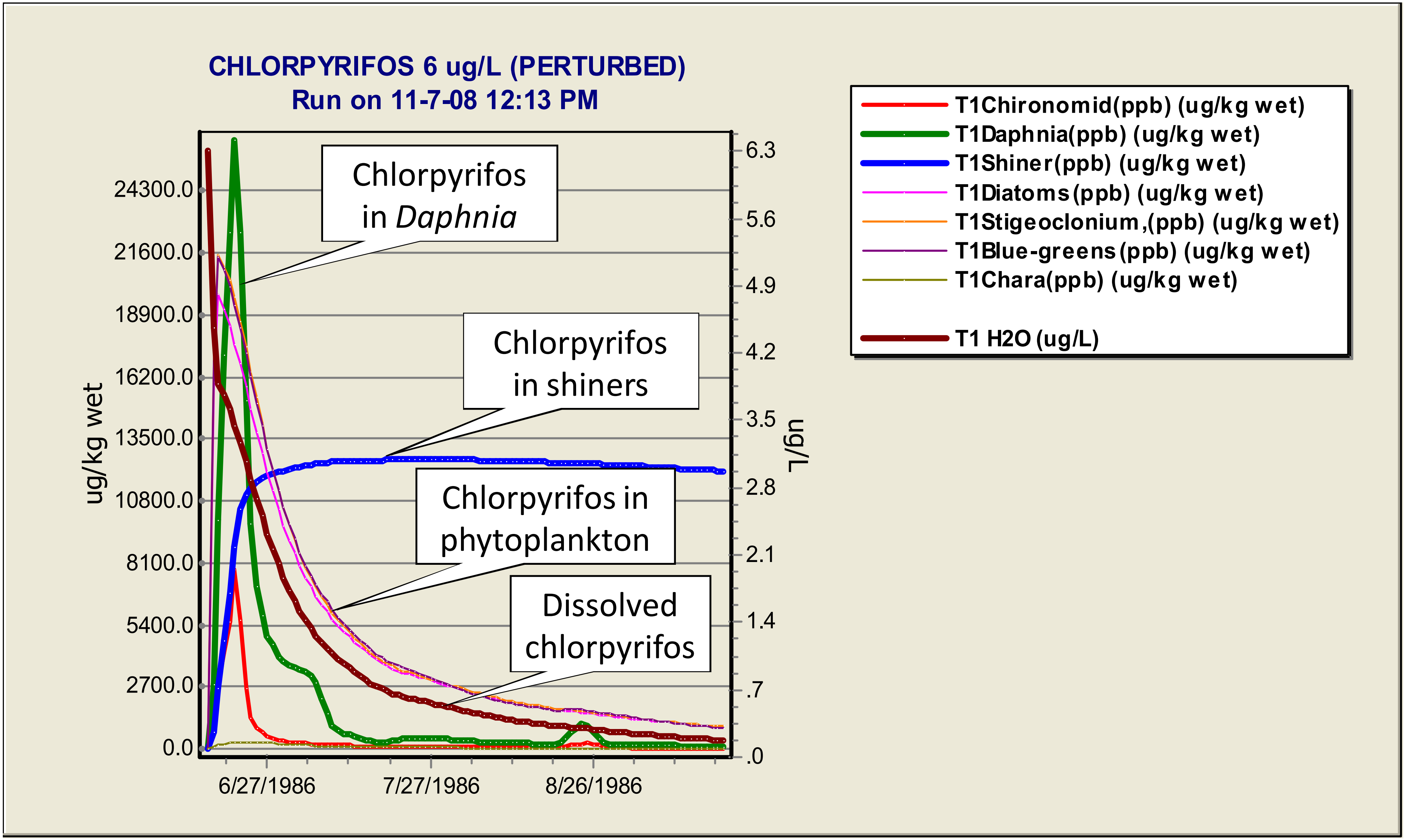
Chlorpyrifos in Pond

- 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

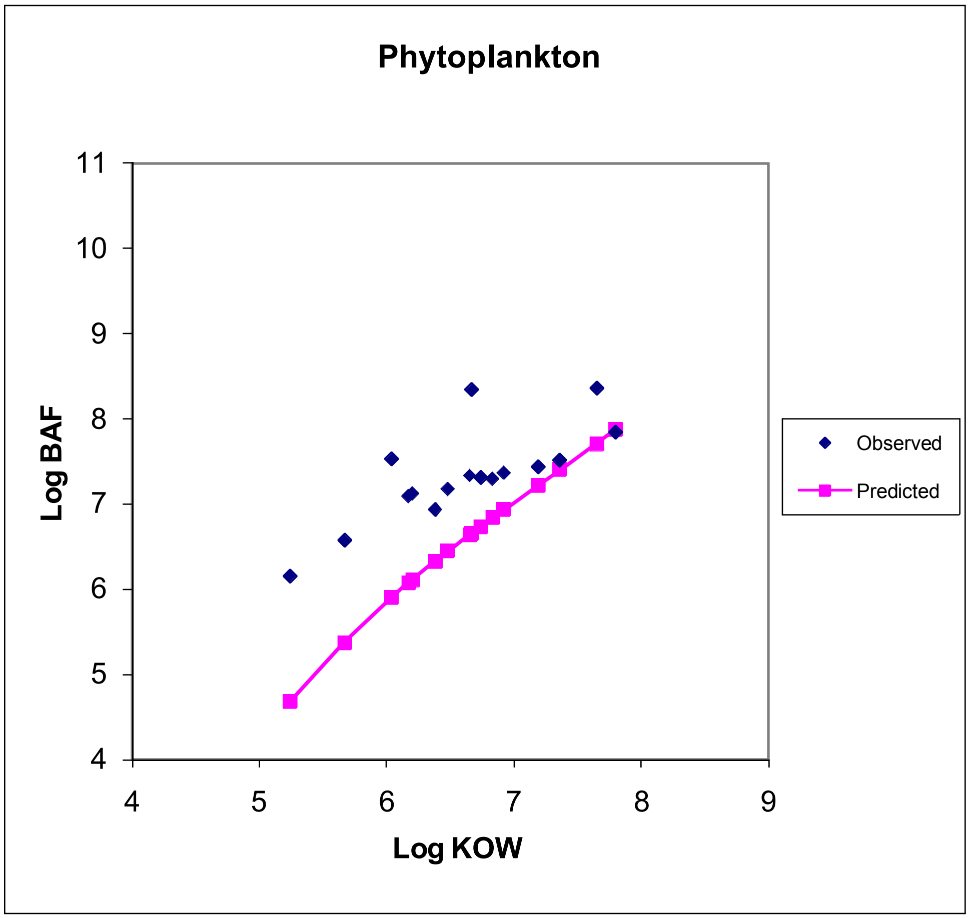


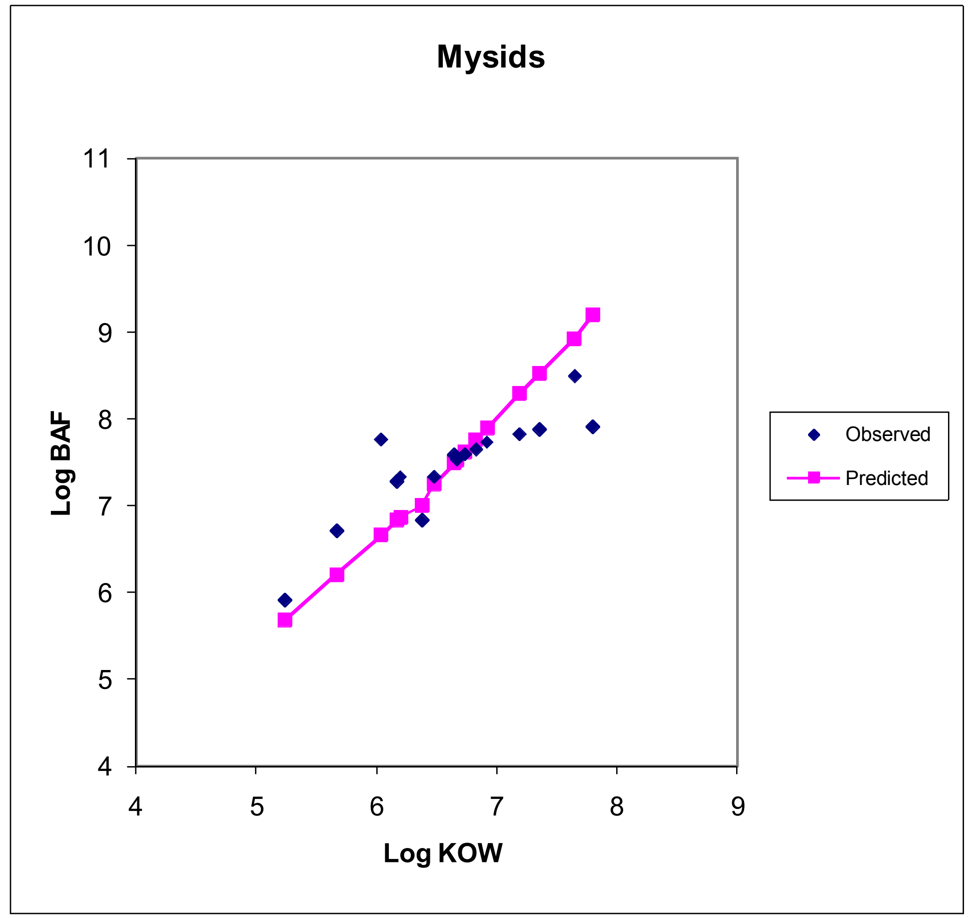
Model can trace how the toxicant is partitioned in the biota



Lake Ontario Bioaccumulation

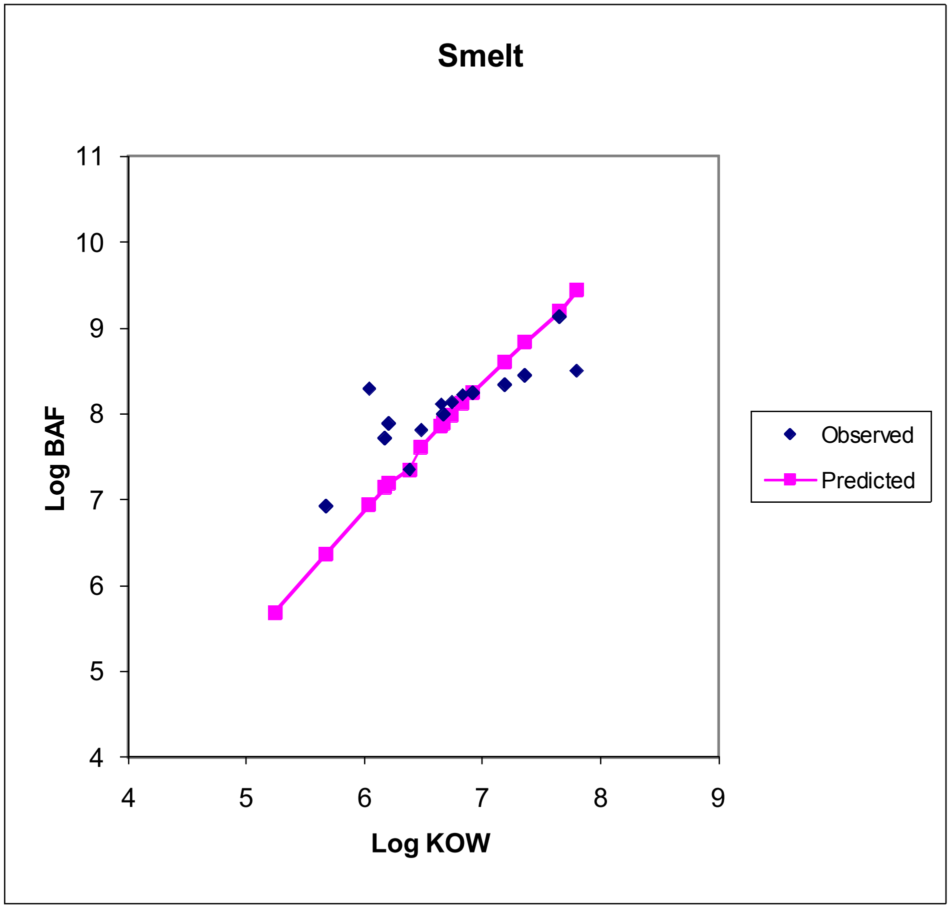
Observed and predicted lipid-normalized and freely dissolved BAFs for PCBs in Lake Ontario ecosystem components.

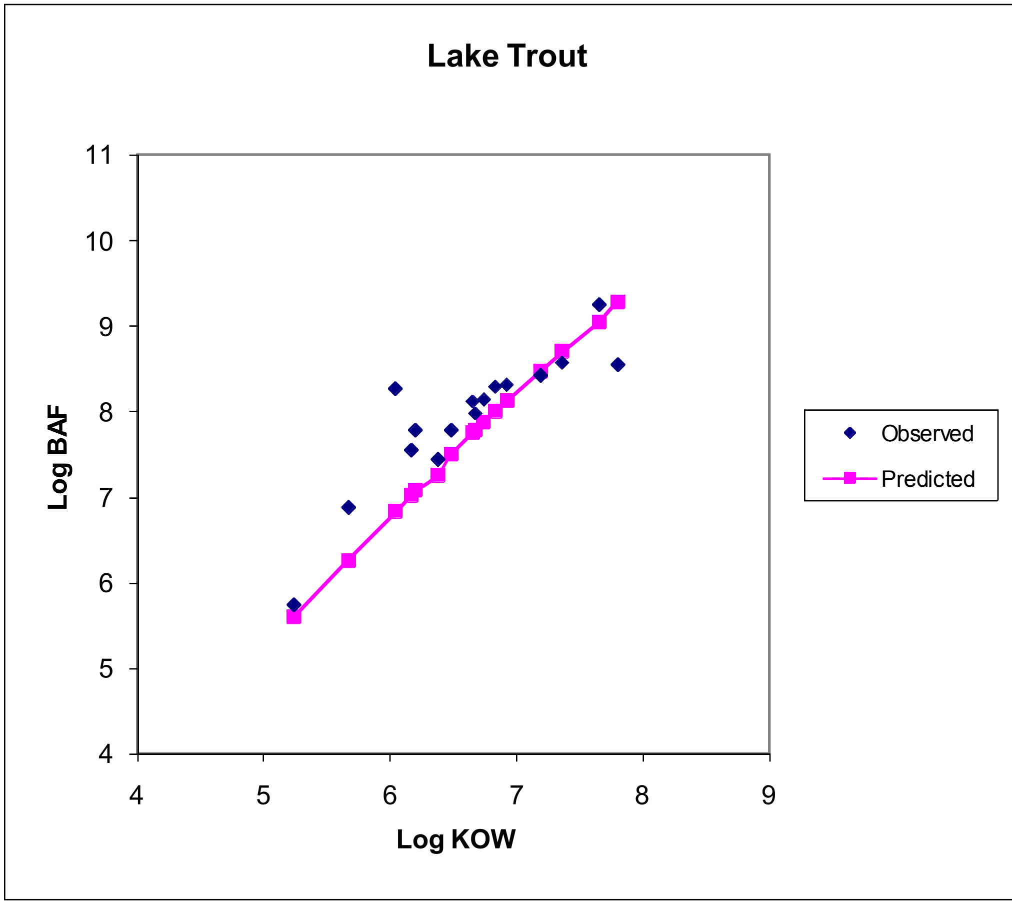




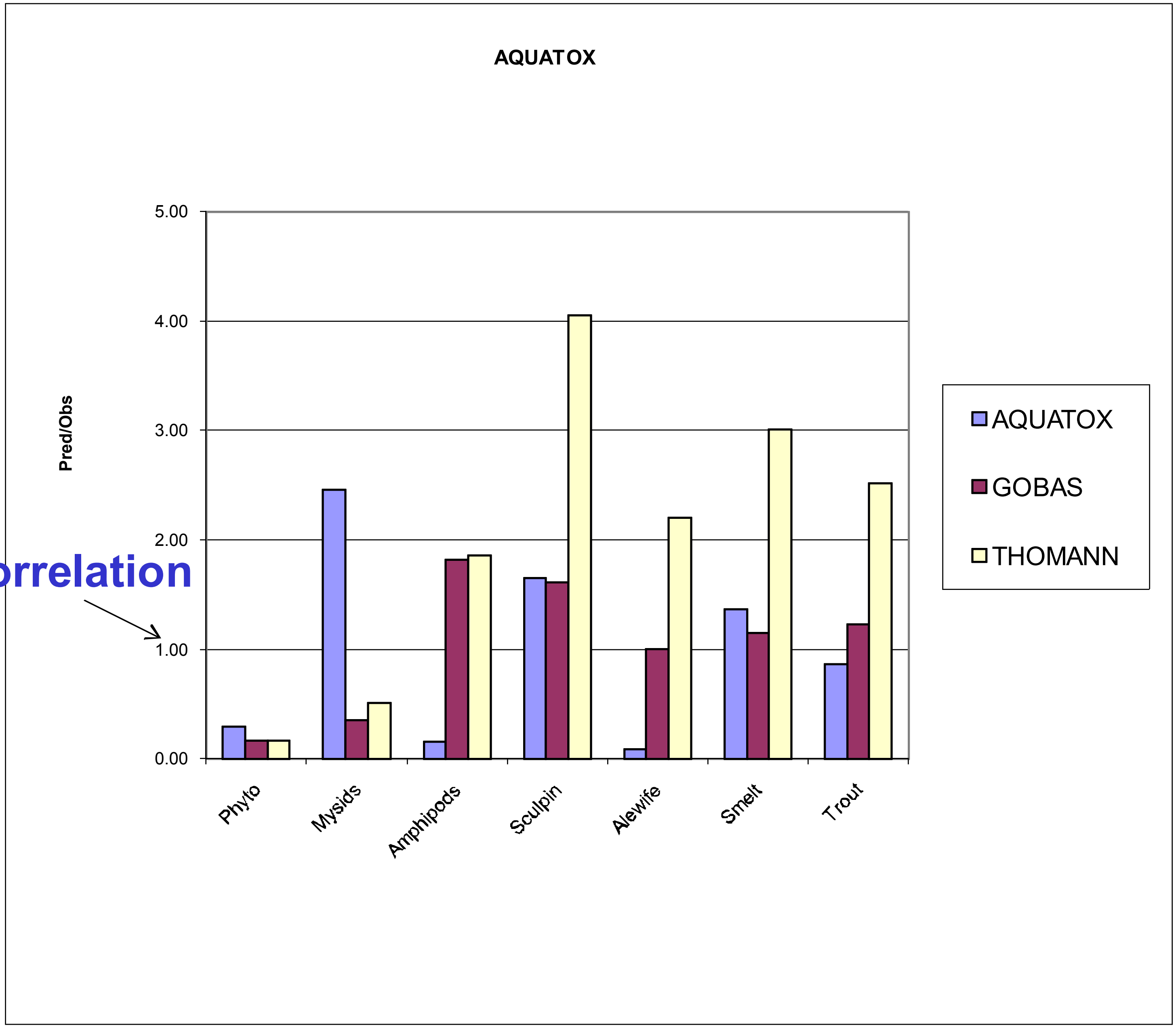
Lake Ontario Bioaccumulation

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





Lake Ontario BAF model comparison



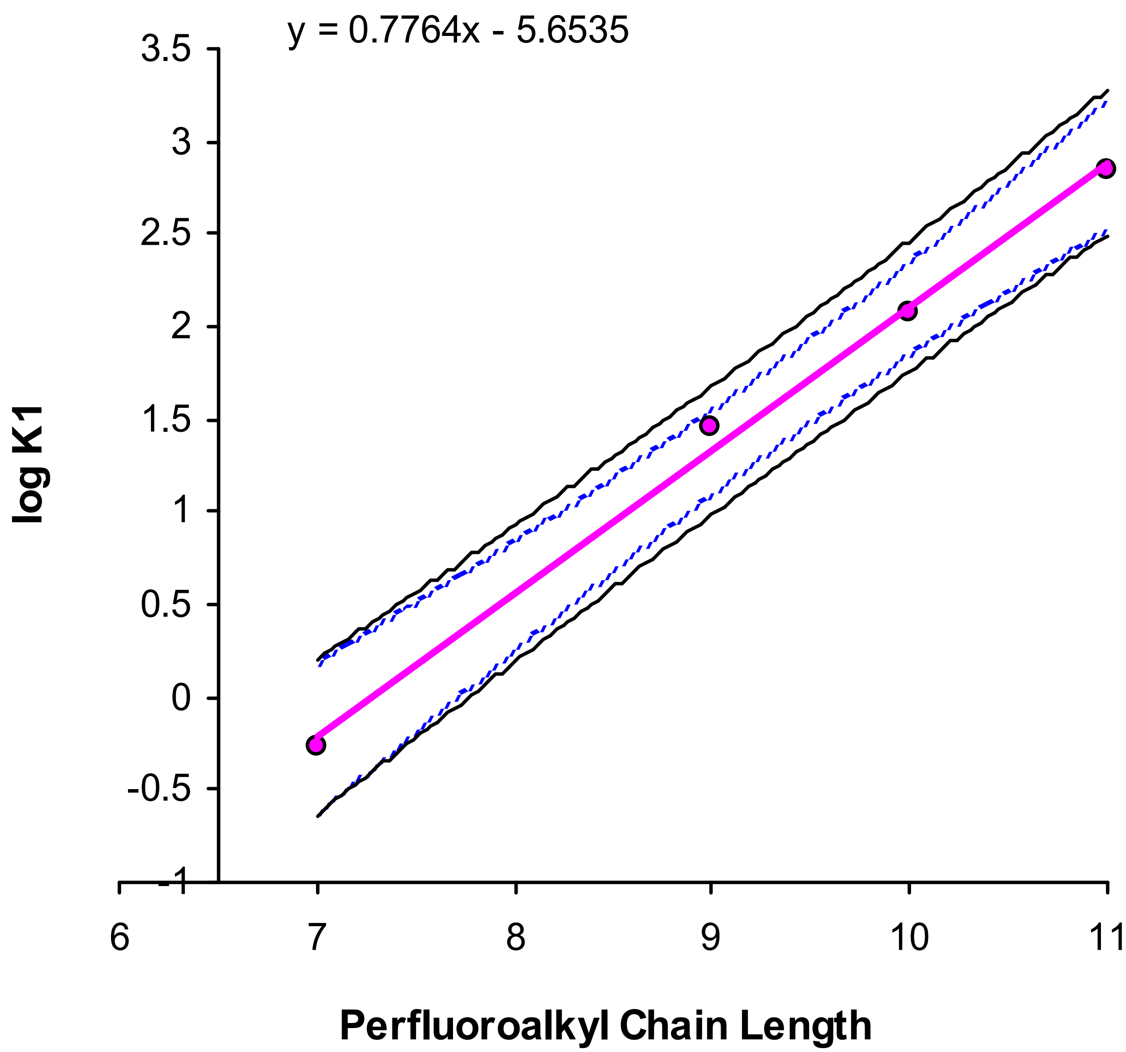
Perfect correlation

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

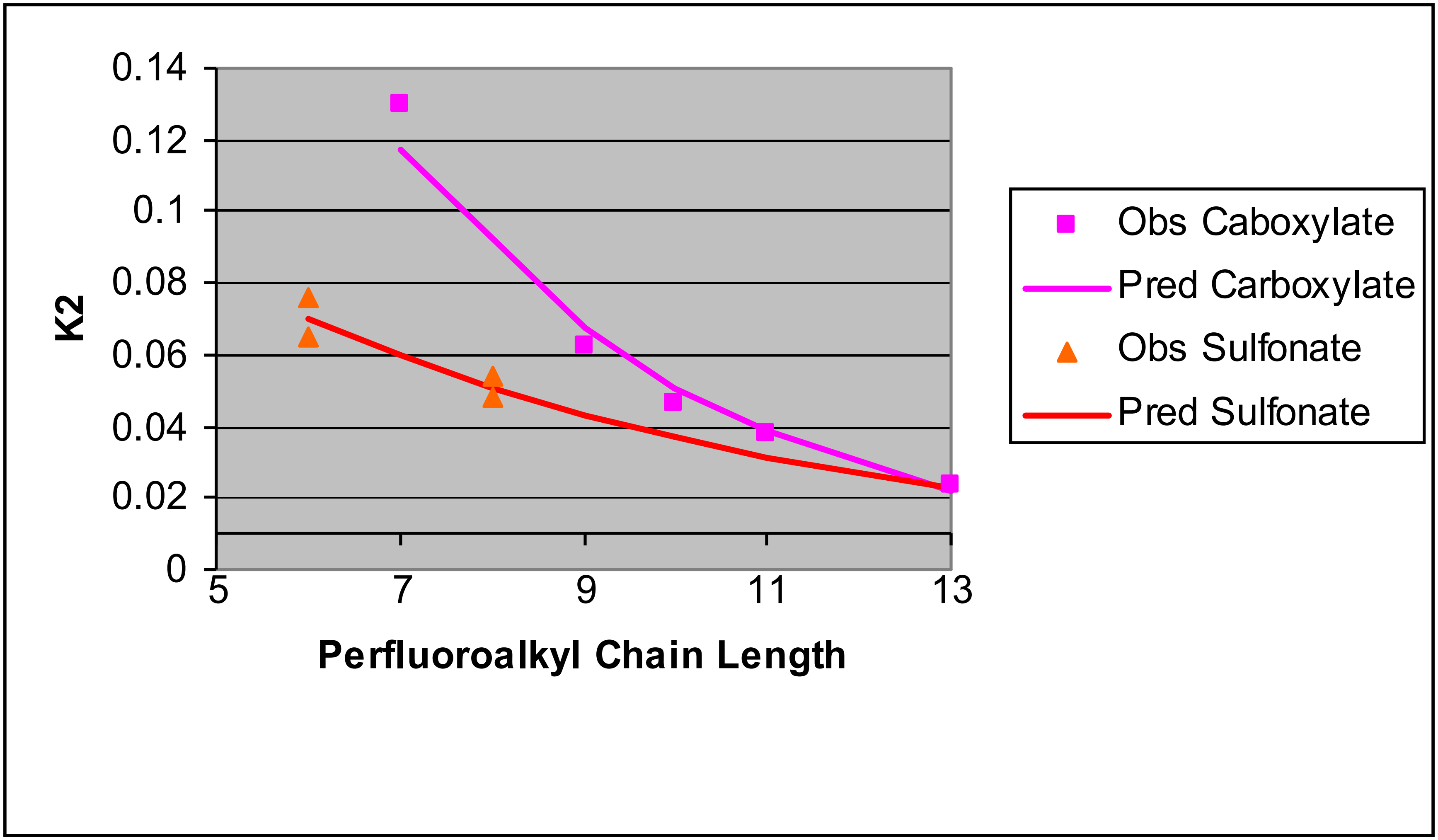
Uptake of carboxylates can be predicted by chain length

data from Martin et al., 2003



Depuration rate is also a function of chain length

data from Martin et al., 2003

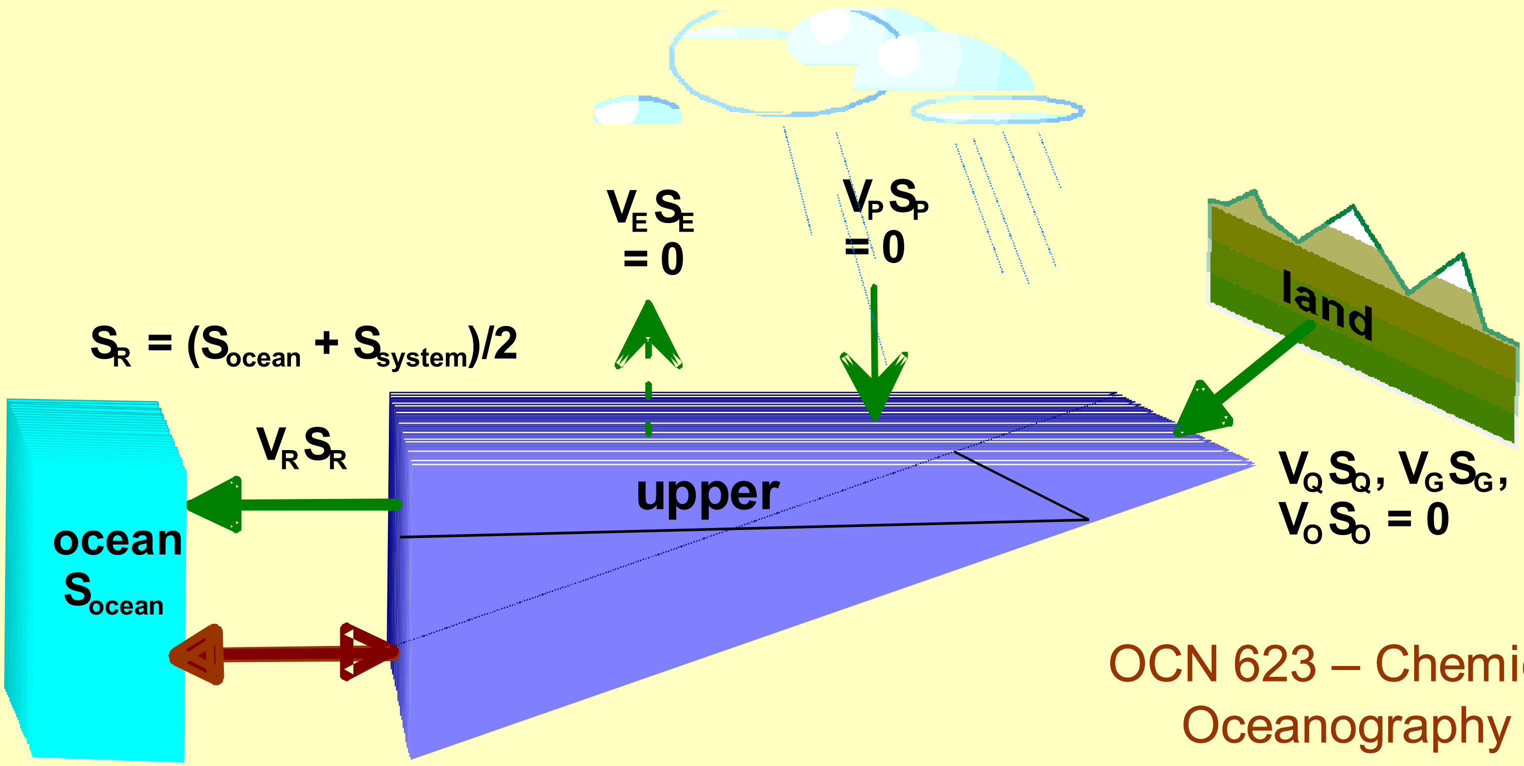


Estuarine version applied to Galveston Bay, Texas, to evaluate toxicants

Photo Courtesy NASA Johnson Space Center

Estuarine Features

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

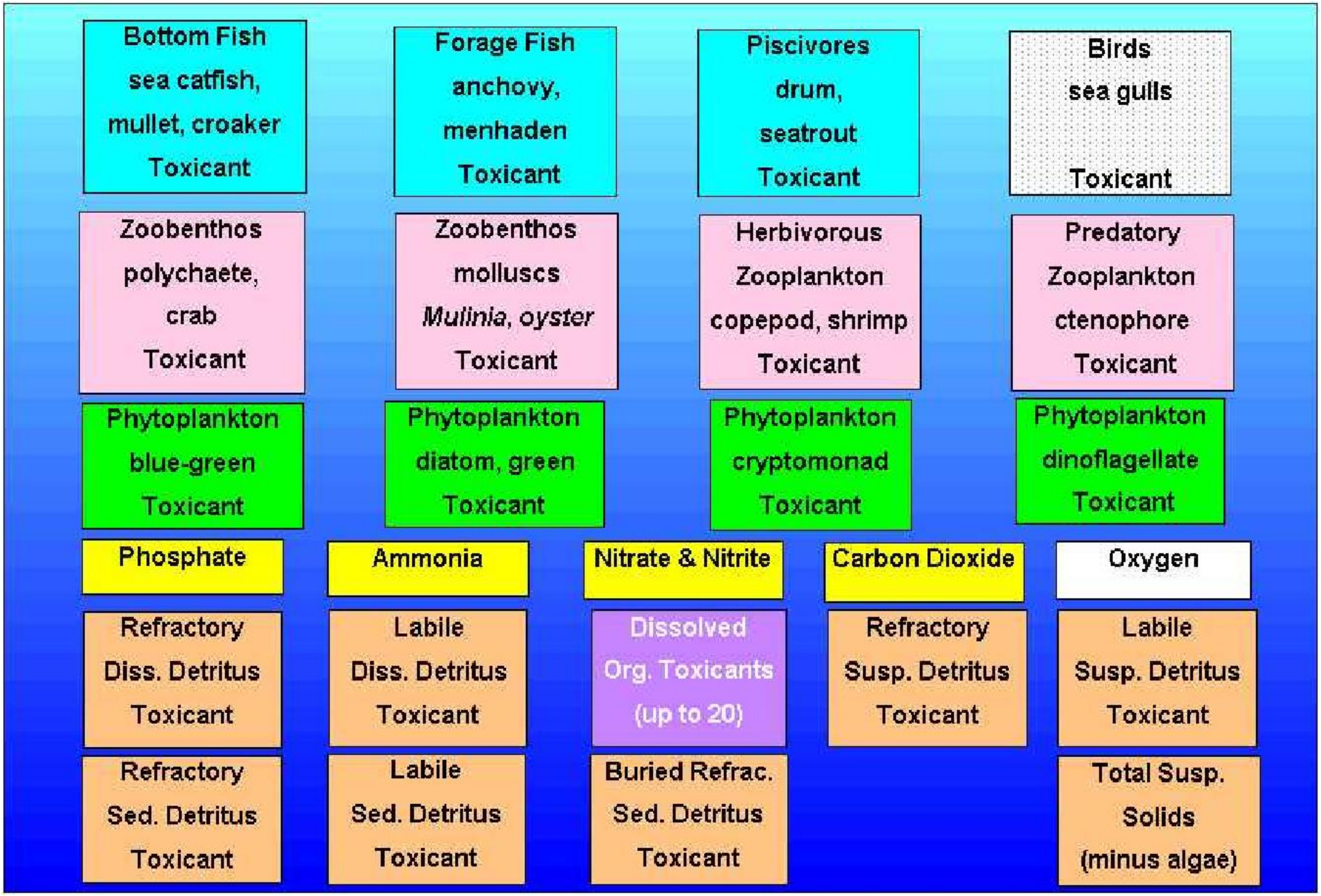


OCN 623 – Chemical Oceanography University Hawaii

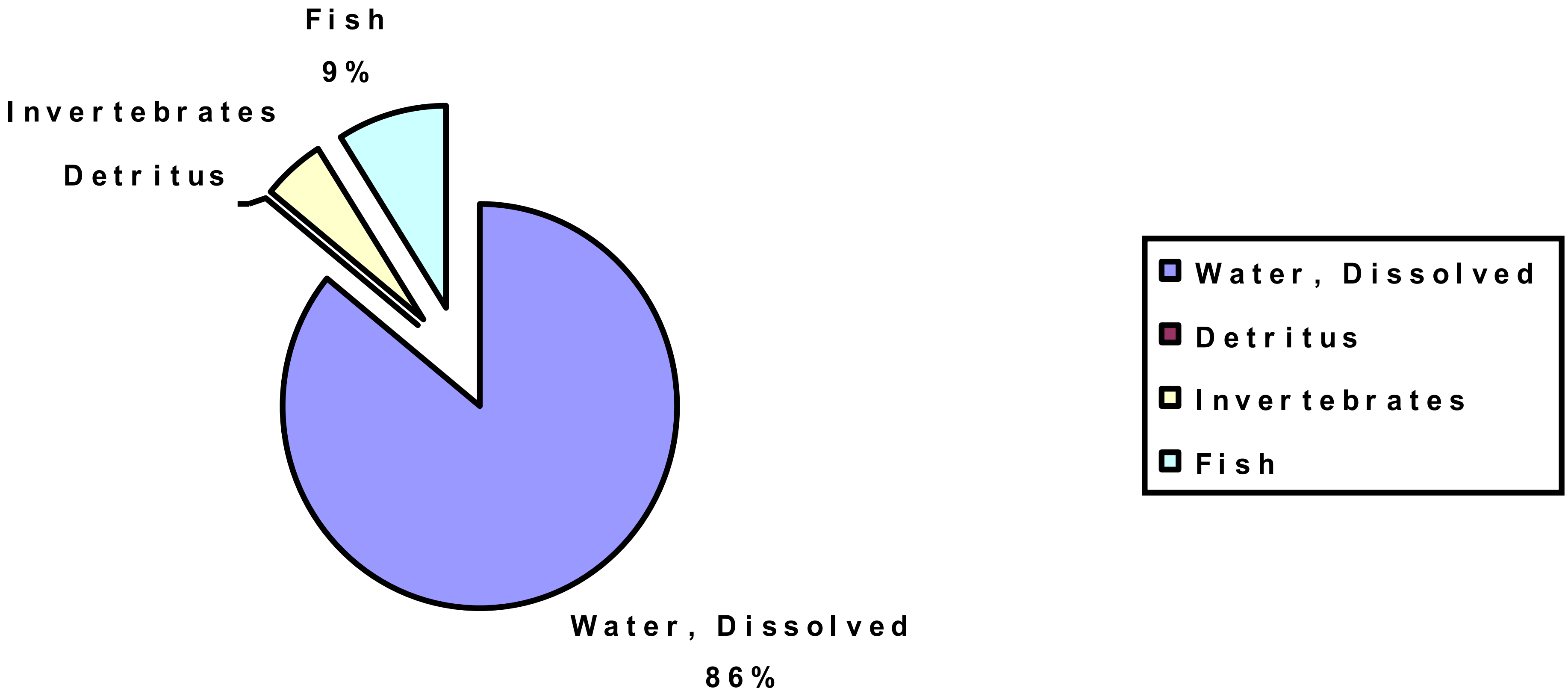
Estuary Model Data Requirements

- 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

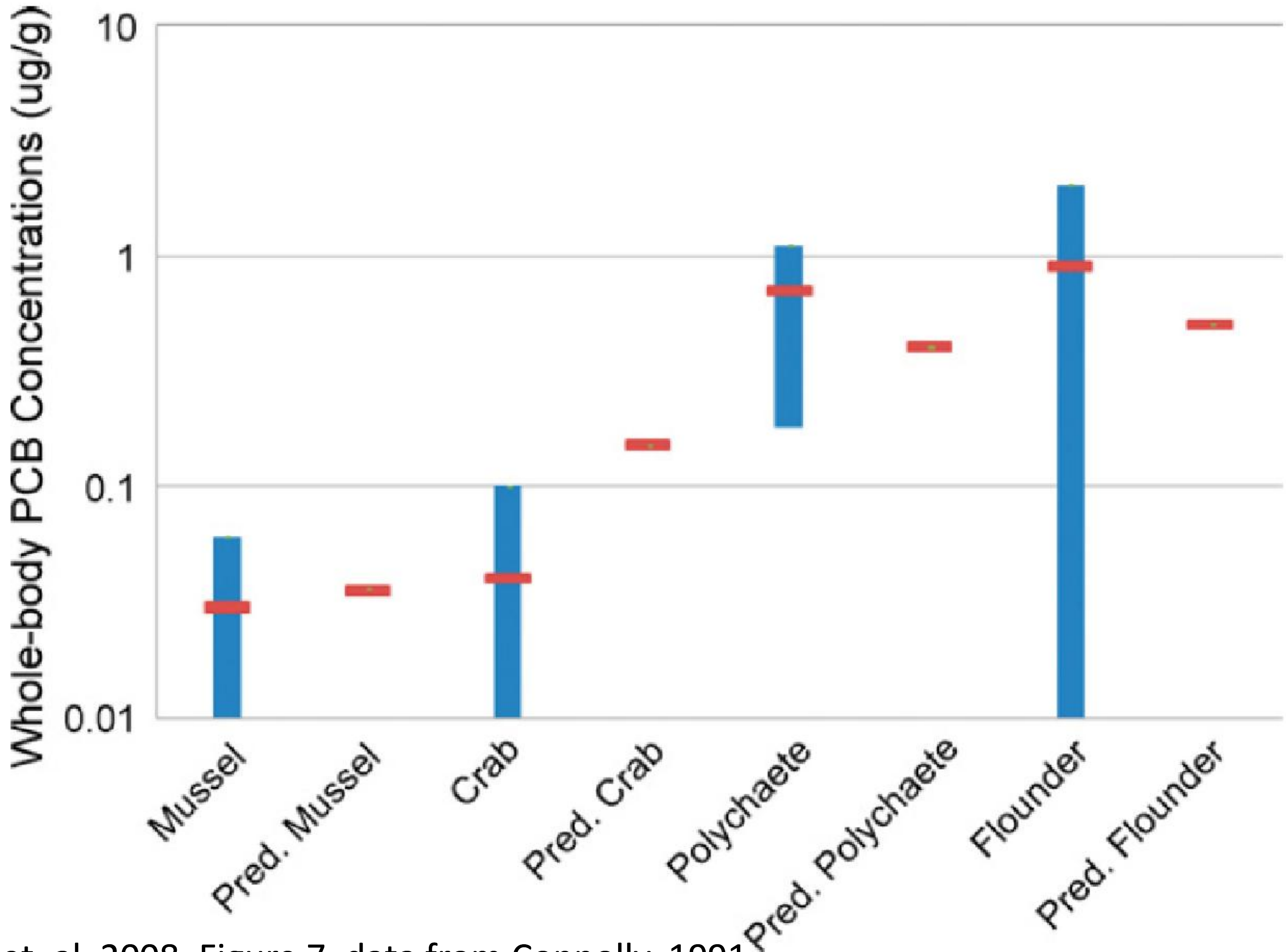
Galveston Bay, Texas, compartments



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



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



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

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

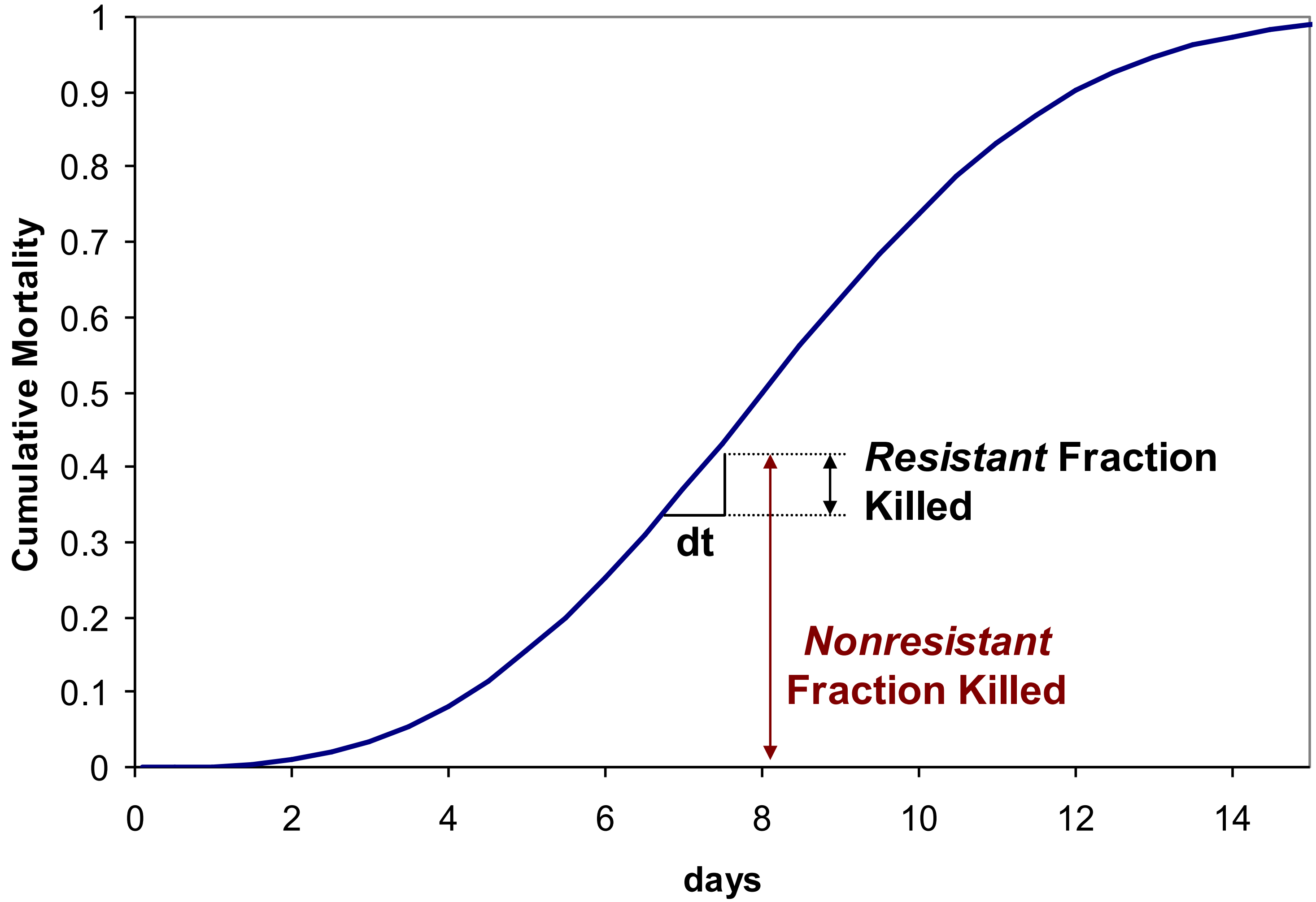
Table 3.5. Toxicity Models	AQUATOX Release 2	BASS v 2.1	Biotic Ligand 1.0.0	RAMAS Ecosystem
Domain of Toxicity Models				
Acute Toxicity	★	★	★	★
Chronic Toxicity	★	★		★
Sub-Lethal Effects	★			
Toxicity Effects Feed Back to Bioconcentration Model	★	★		★
Toxicity Mechanisms				
Based on Total Internal Concentrations	★	★		★
Based on Concentrations in Organs			★	
User Input Required				
LC50 values	★	★		
EC50 values	★			★
Weibull Shape Parameter	★			★

Imhoff et al. 2004

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



Option to Model with External Concentrations

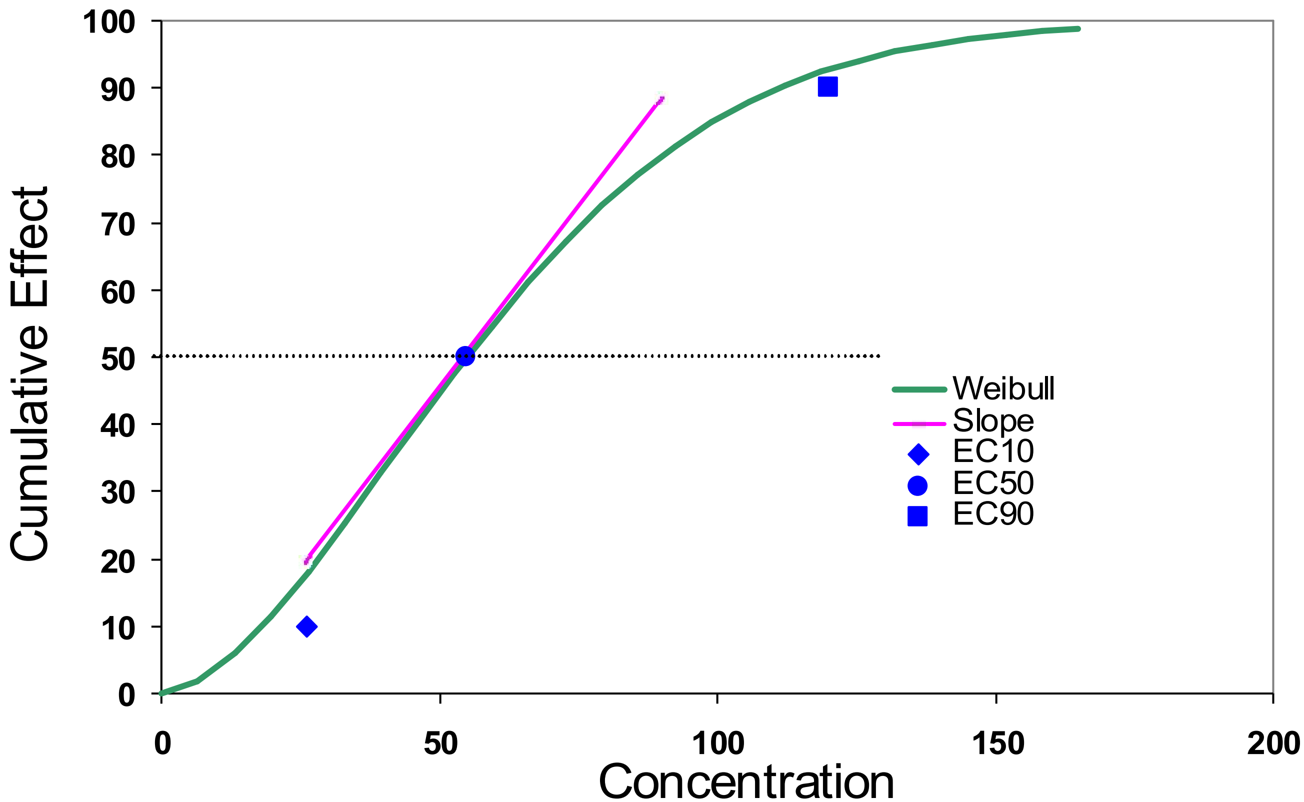
Two-parameter Weibull distribution as in Christiensen and Nyholm (1984)

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

Two Required Parameters:

LC50 (or EC50)

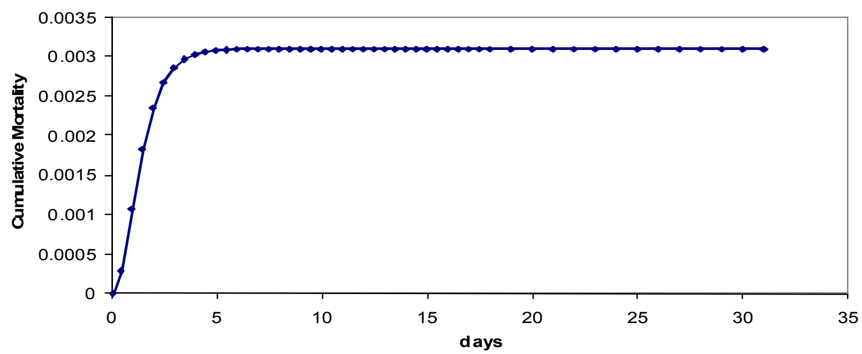
"Slope Factor" = Slope at LC50 multiplied by LC50

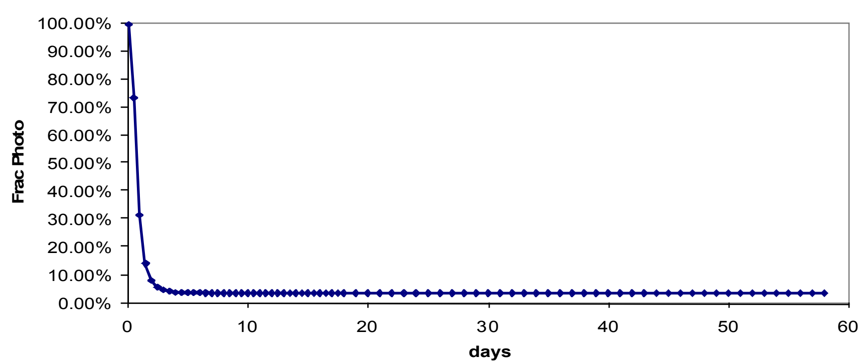


Spreadsheet Demo

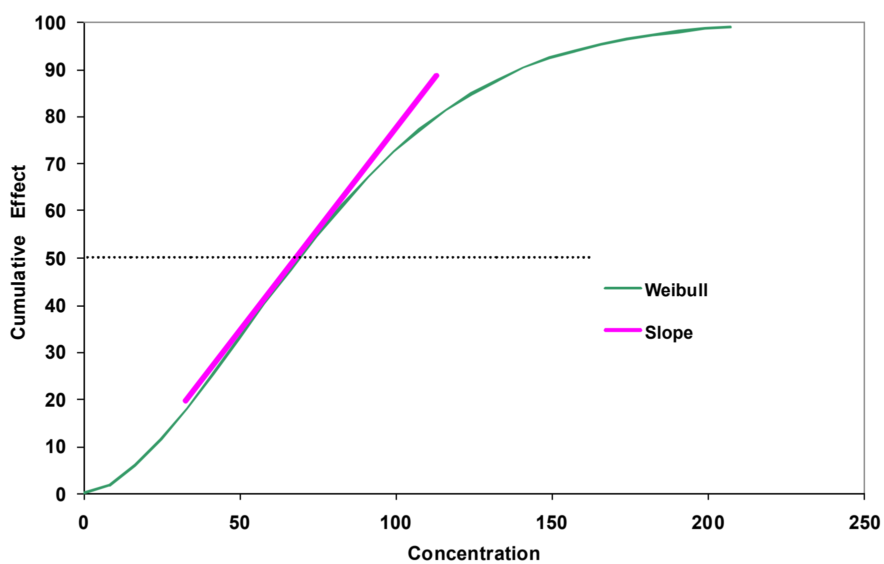
AQUATOX is distributed with two spreadsheets useful in understanding the model's toxicity components

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)	Biotrnsfm. 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)	Biotrnsfm. rate (1
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.

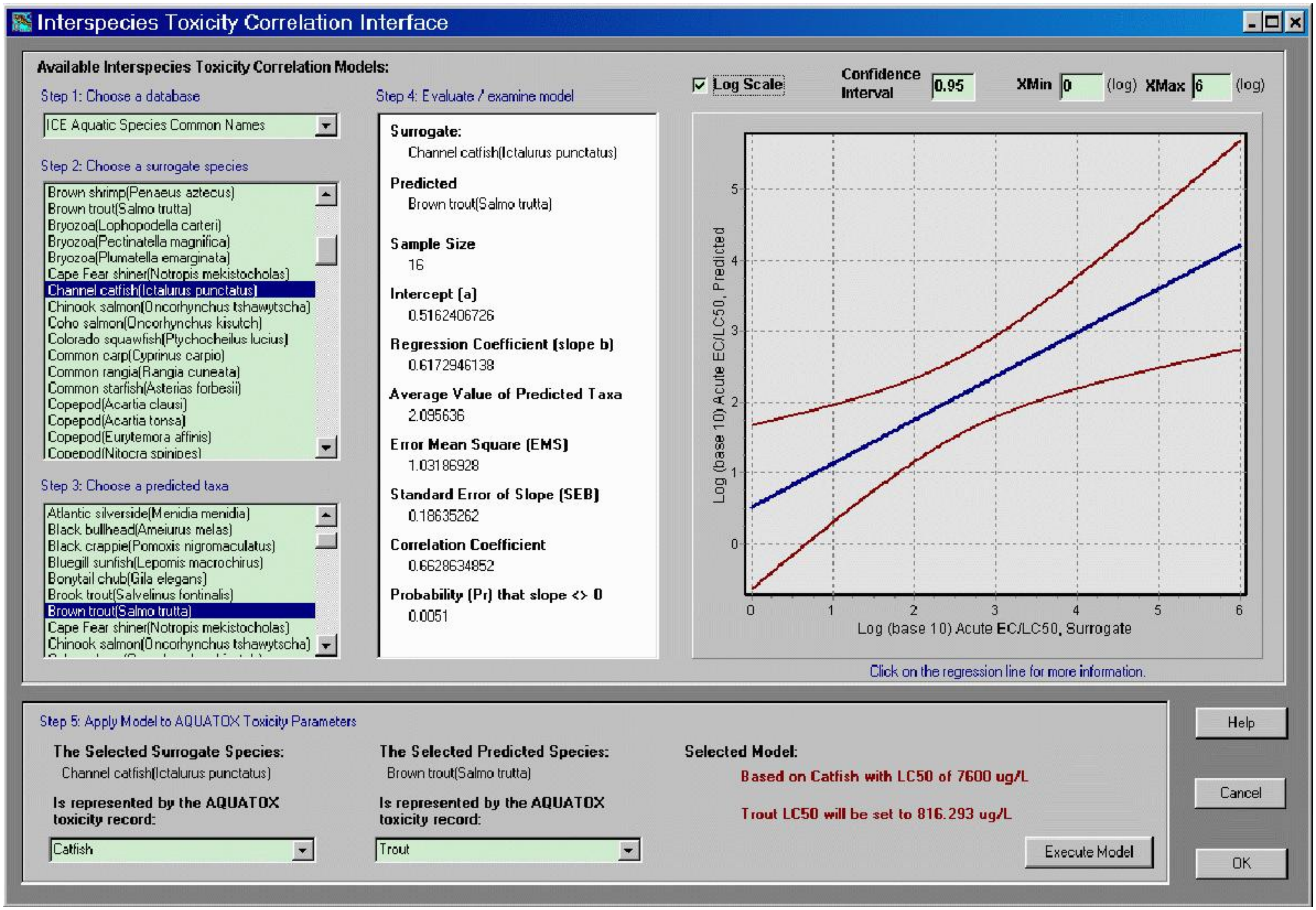
Estimate Animal K2s using Kow | Estimate Plant K2s using Kow | Interspecies Toxicity Correlation Models

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**

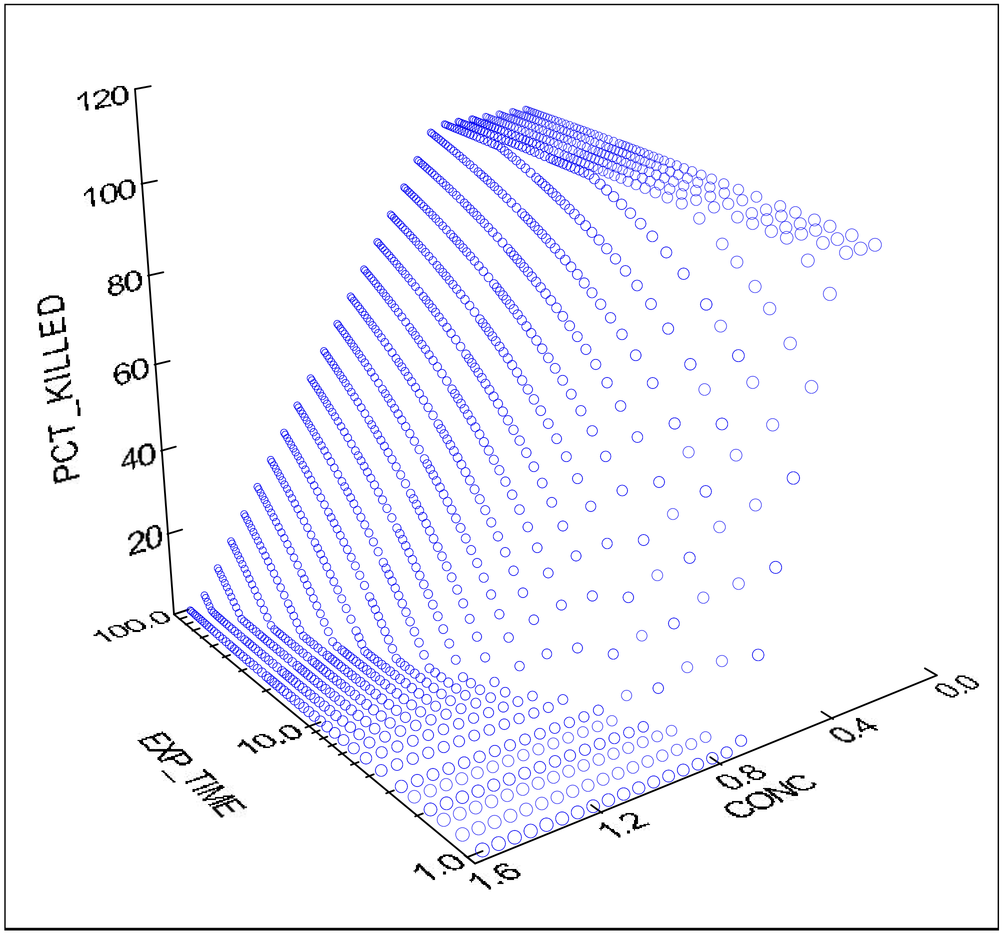


Release 3: Additional Toxicity Features

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

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

Includes non-lethal effects on consumption and reproduction

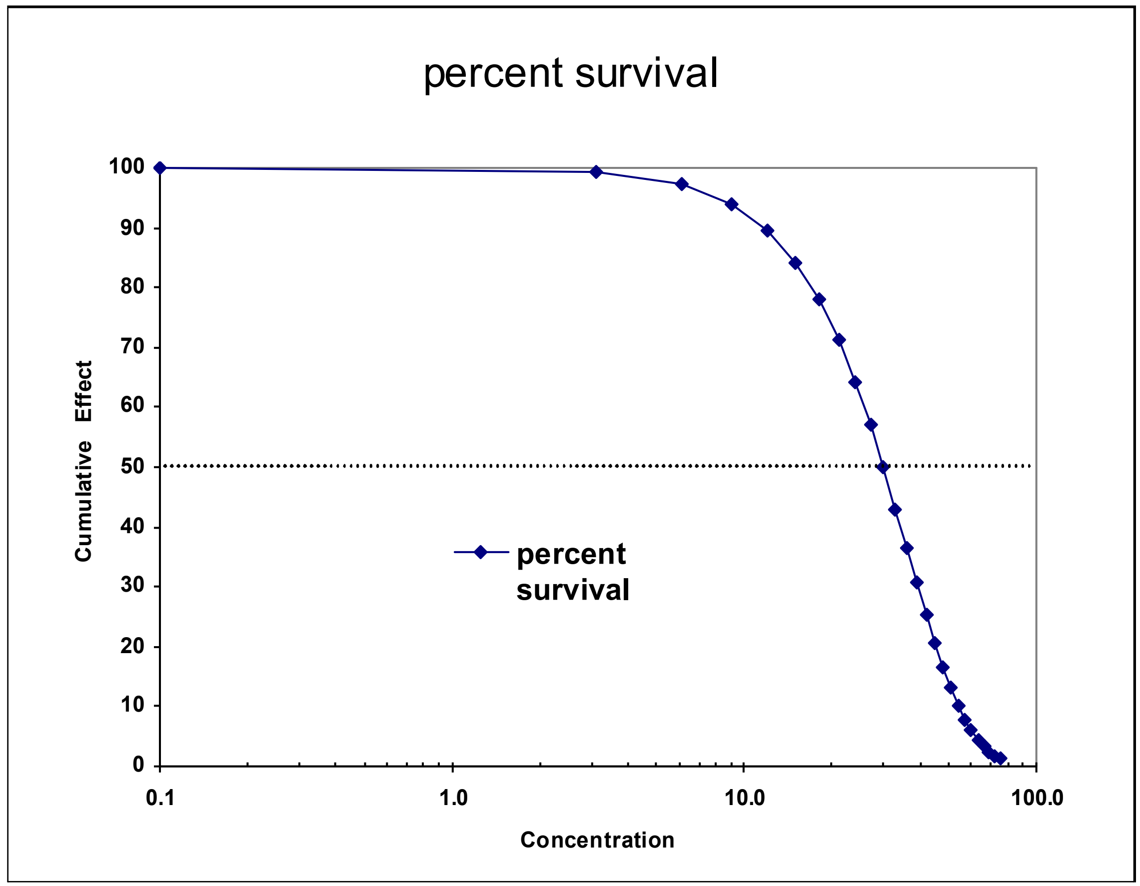


Release 3: Additional Toxicity Features

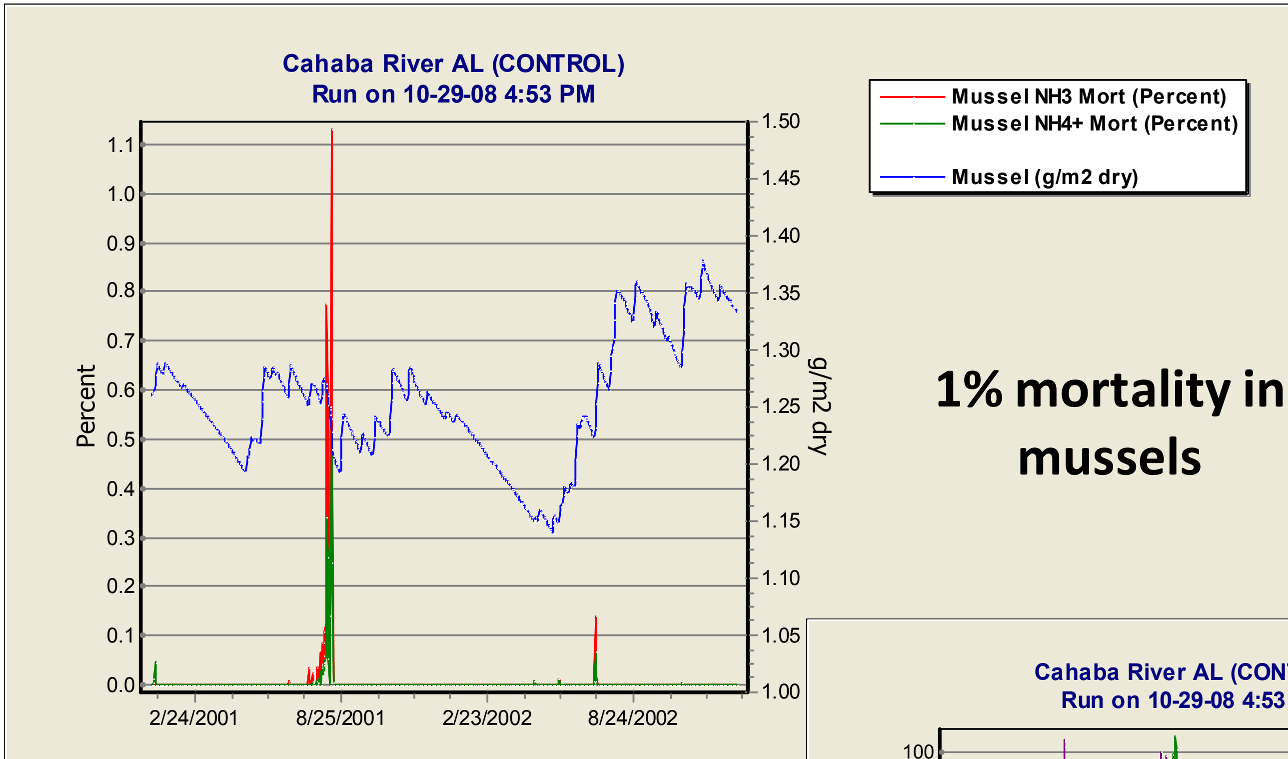
- Integration with ICE: a large EPA database of toxicity regressions
- Dissolved Oxygen effects
- Ammonia effects

External Toxicity Model Utilized

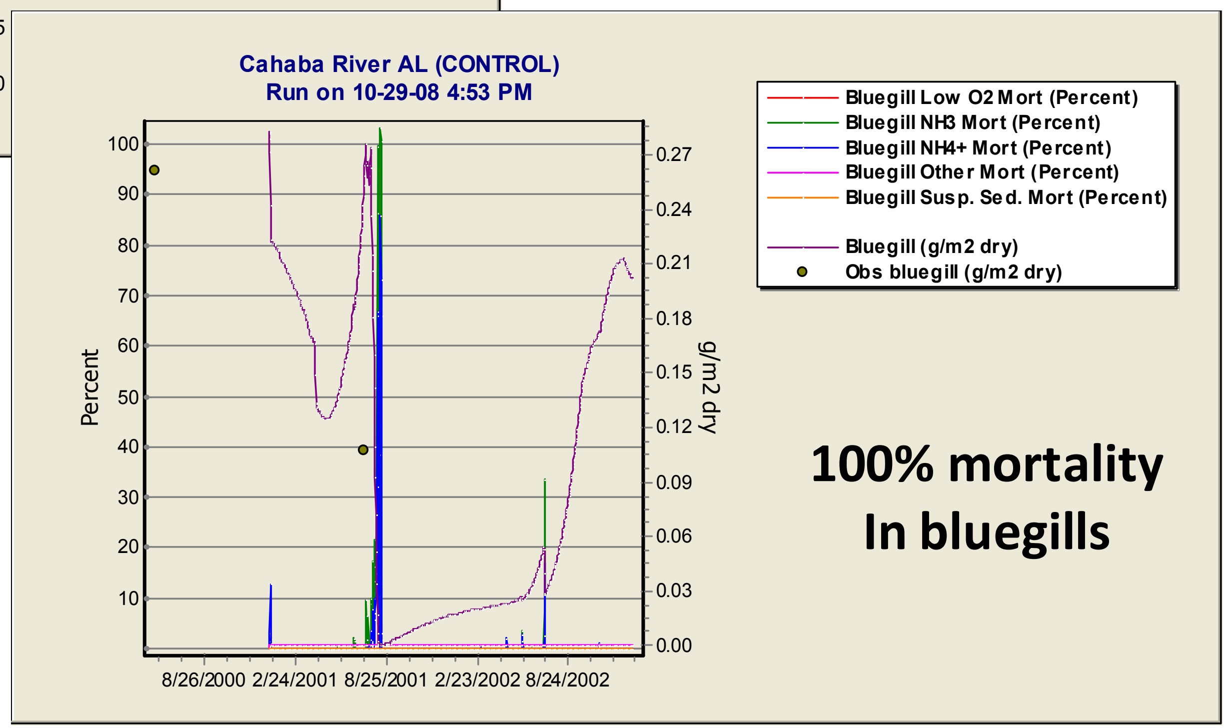
Effects from un-ionized and ionized ammonia are additive



Predicted ammonia toxicity in Cahaba River AL

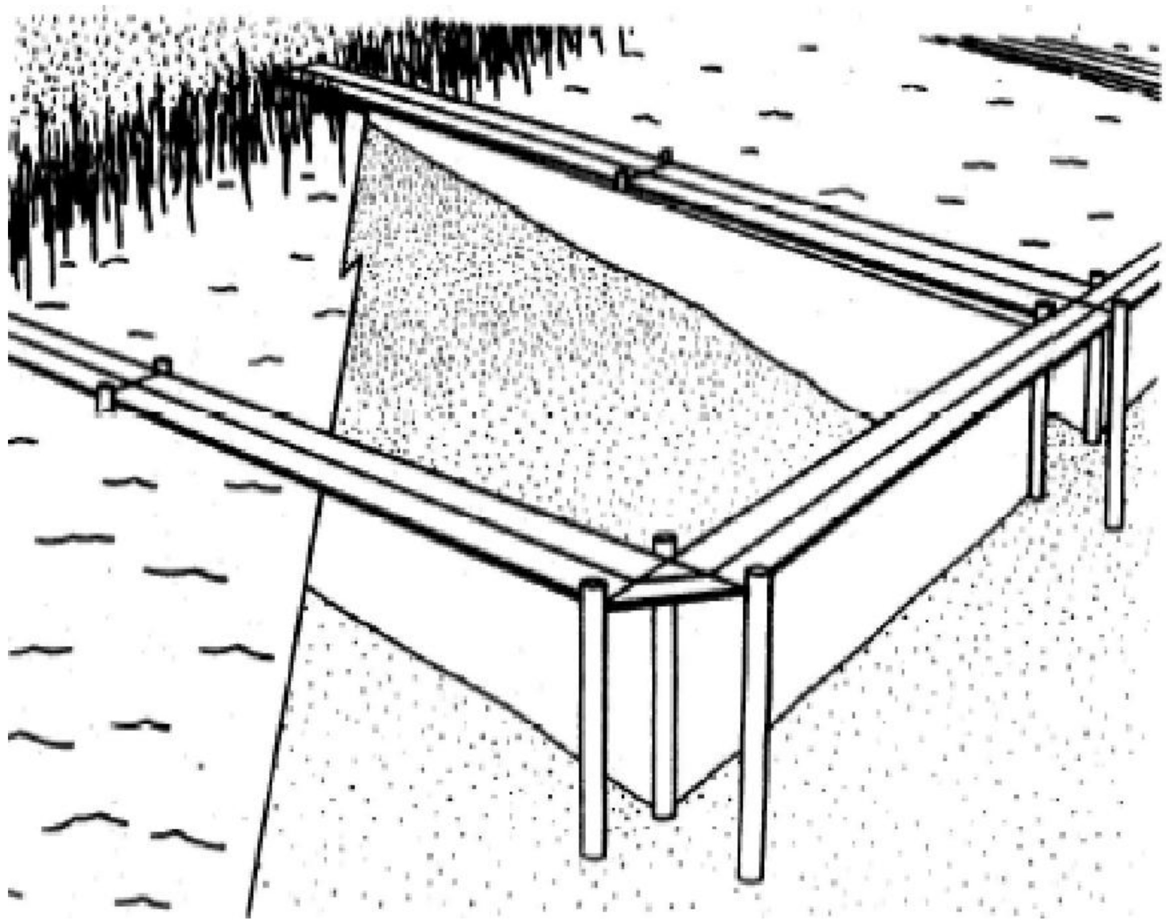


1% mortality in mussels

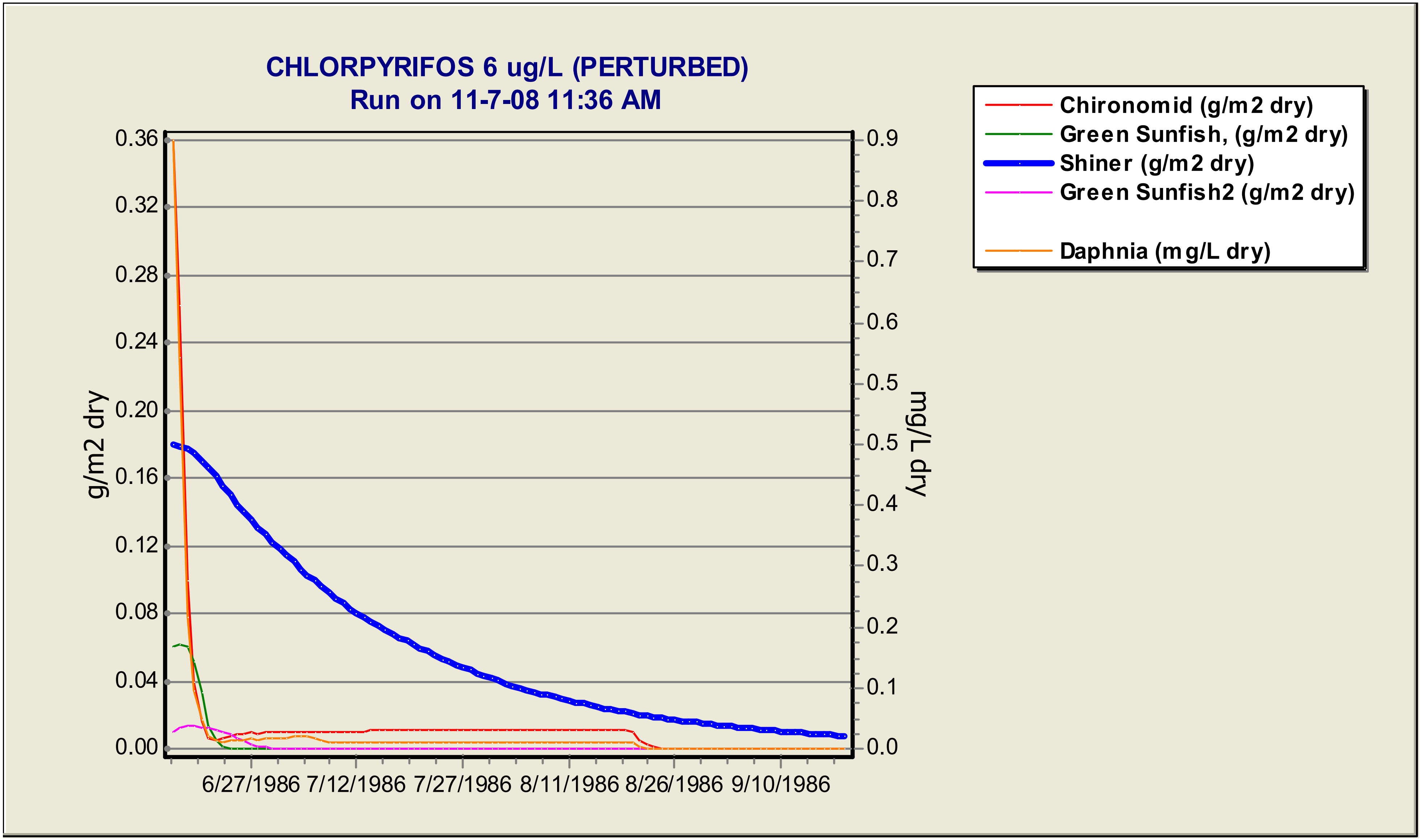


100% mortality In bluegills

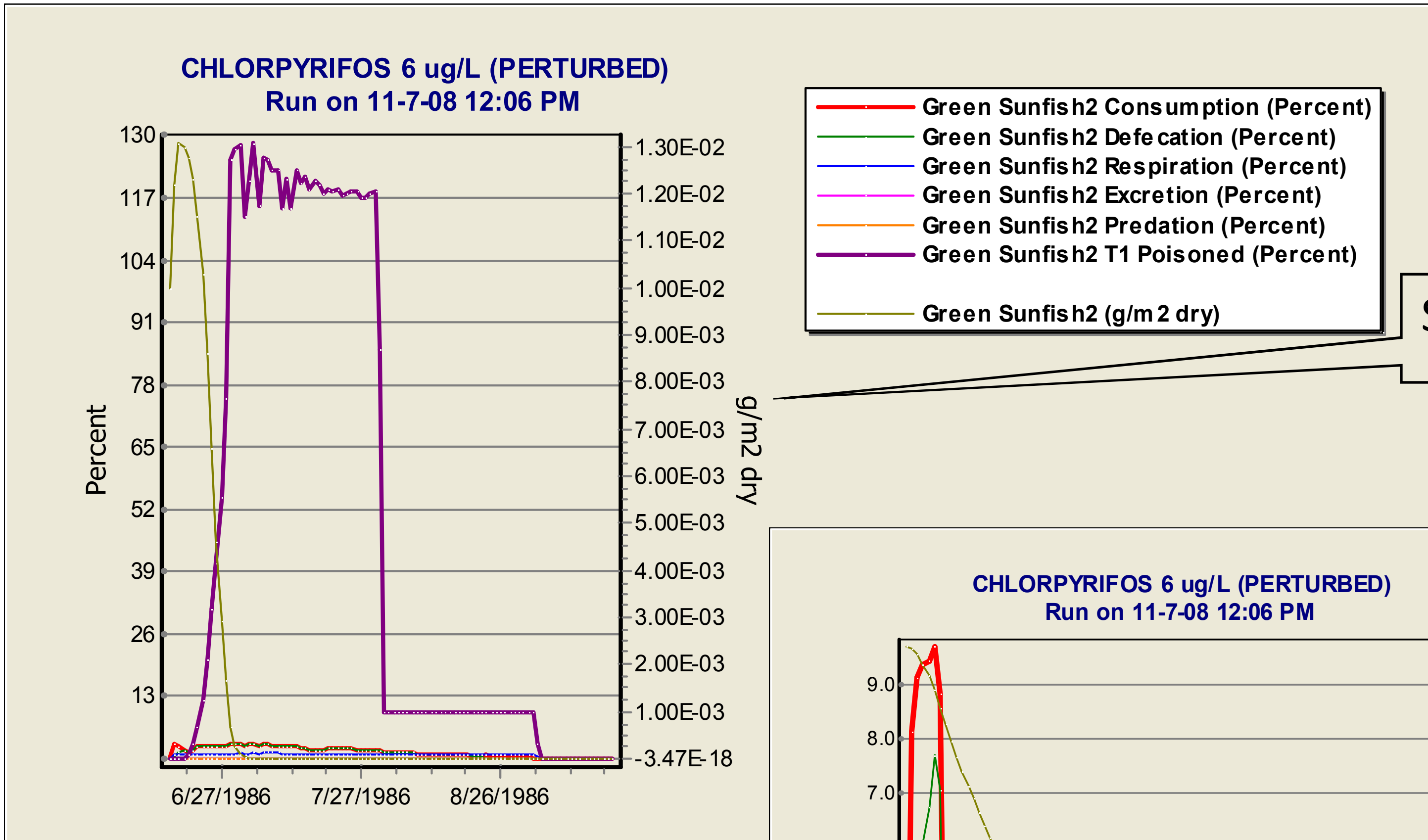
Returning to the Enclosure in Duluth MN . . .



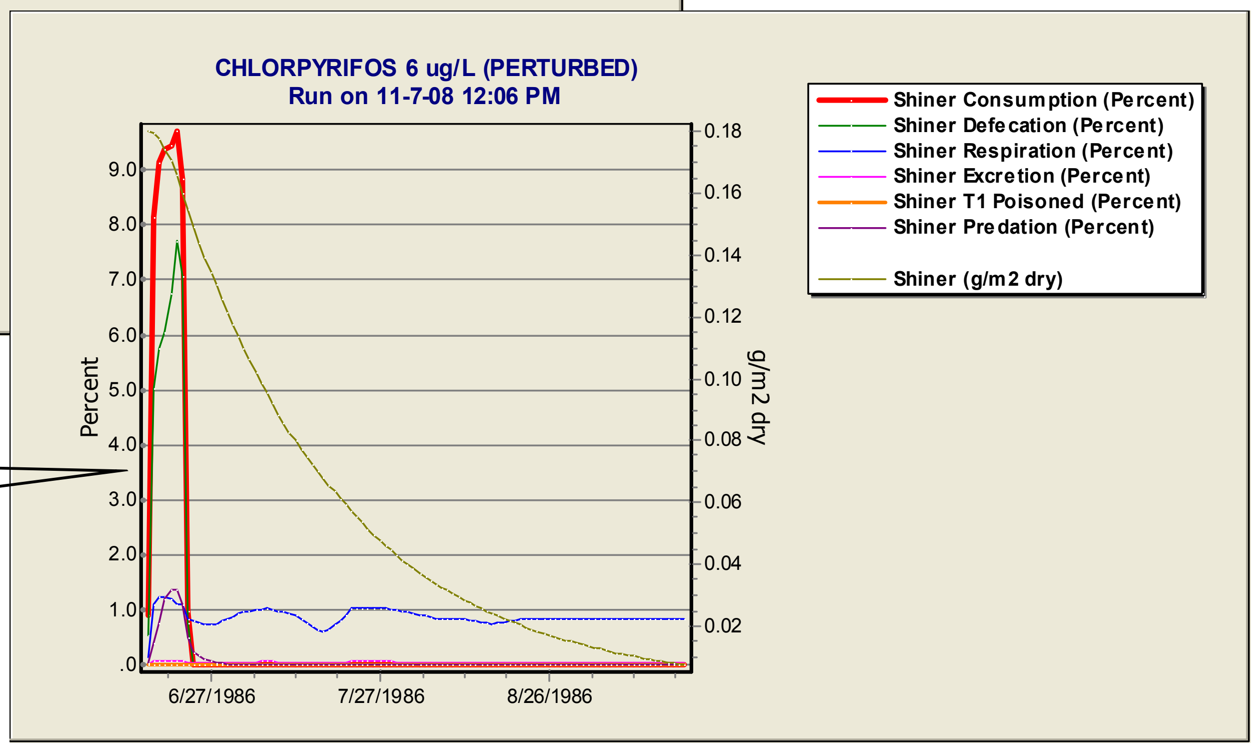
Animals all decline at varying rates following a single initial dose of chlorpyrifos



Sunfish have lethal effects, shiners have sublethal effects from chlorpyrifos

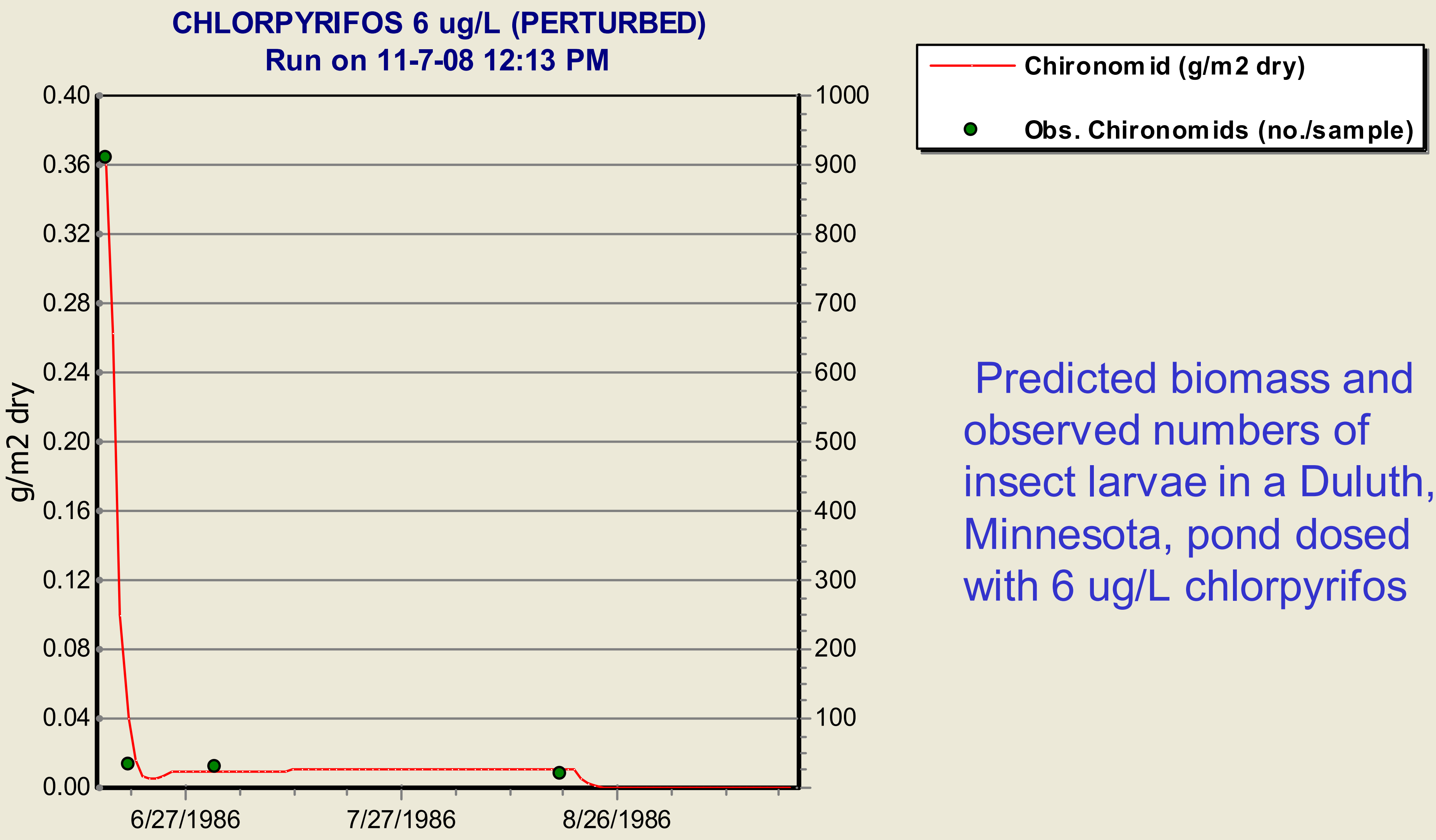


Sunfish with lethal effects



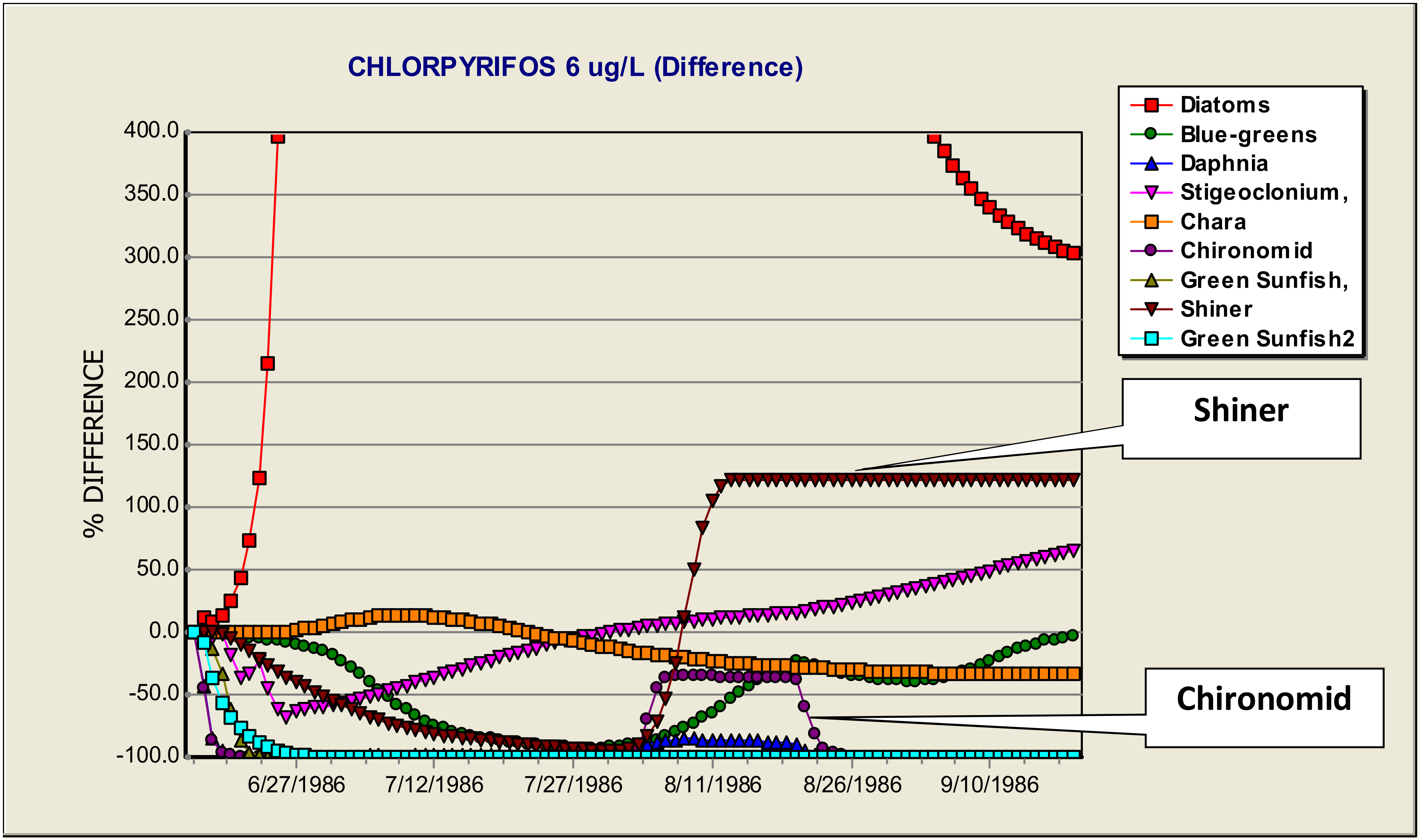
Shiner with sublethal effects only

Toxic effects of Chlorpyrifos in Duluth pond

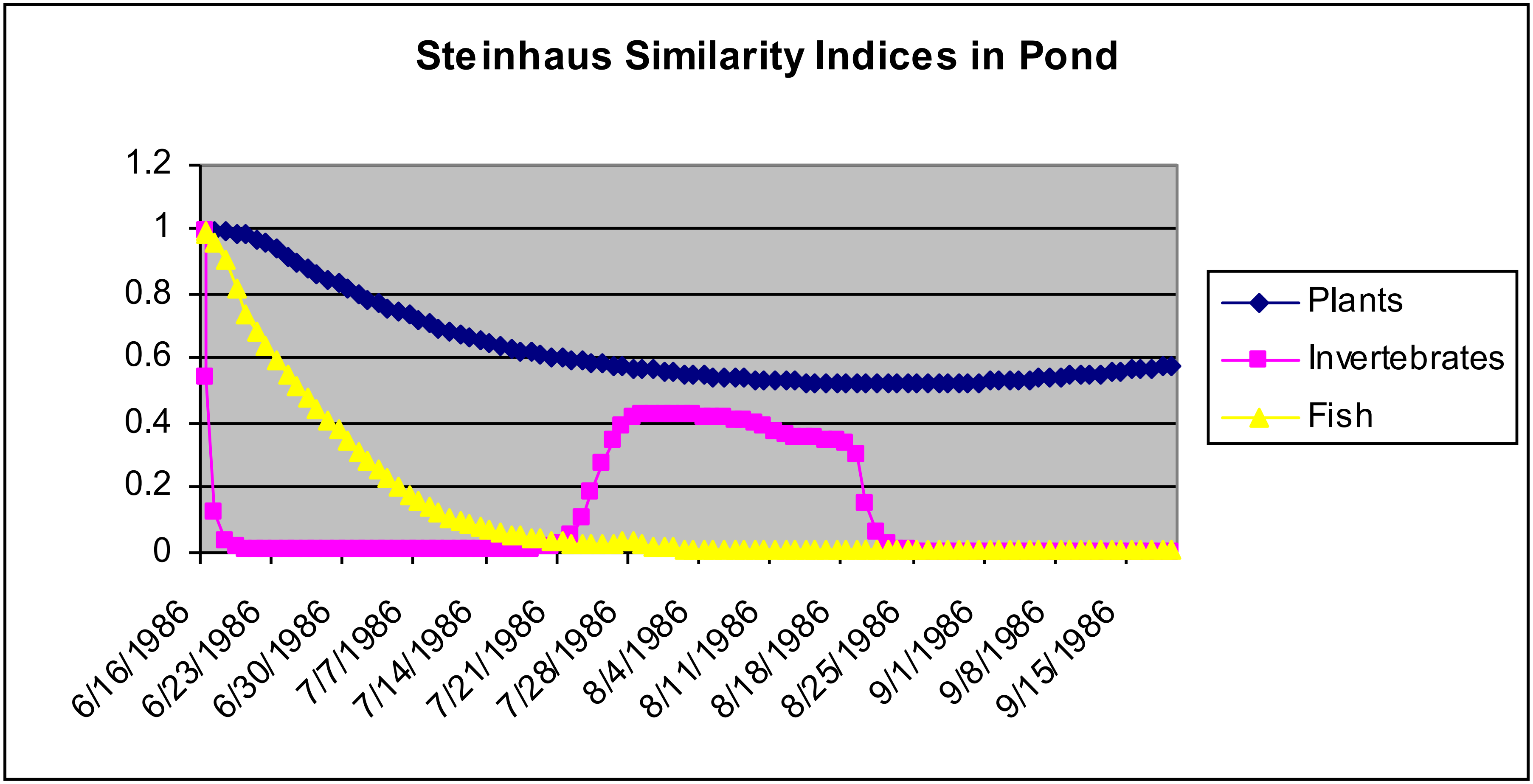


Predicted biomass and observed numbers of insect larvae in a Duluth, Minnesota, pond dosed with 6 ug/L chlorpyrifos

% Difference Graph shows differences in species response to toxicant



Steinhaus Indices show ecosystem impacts predicted by the model



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

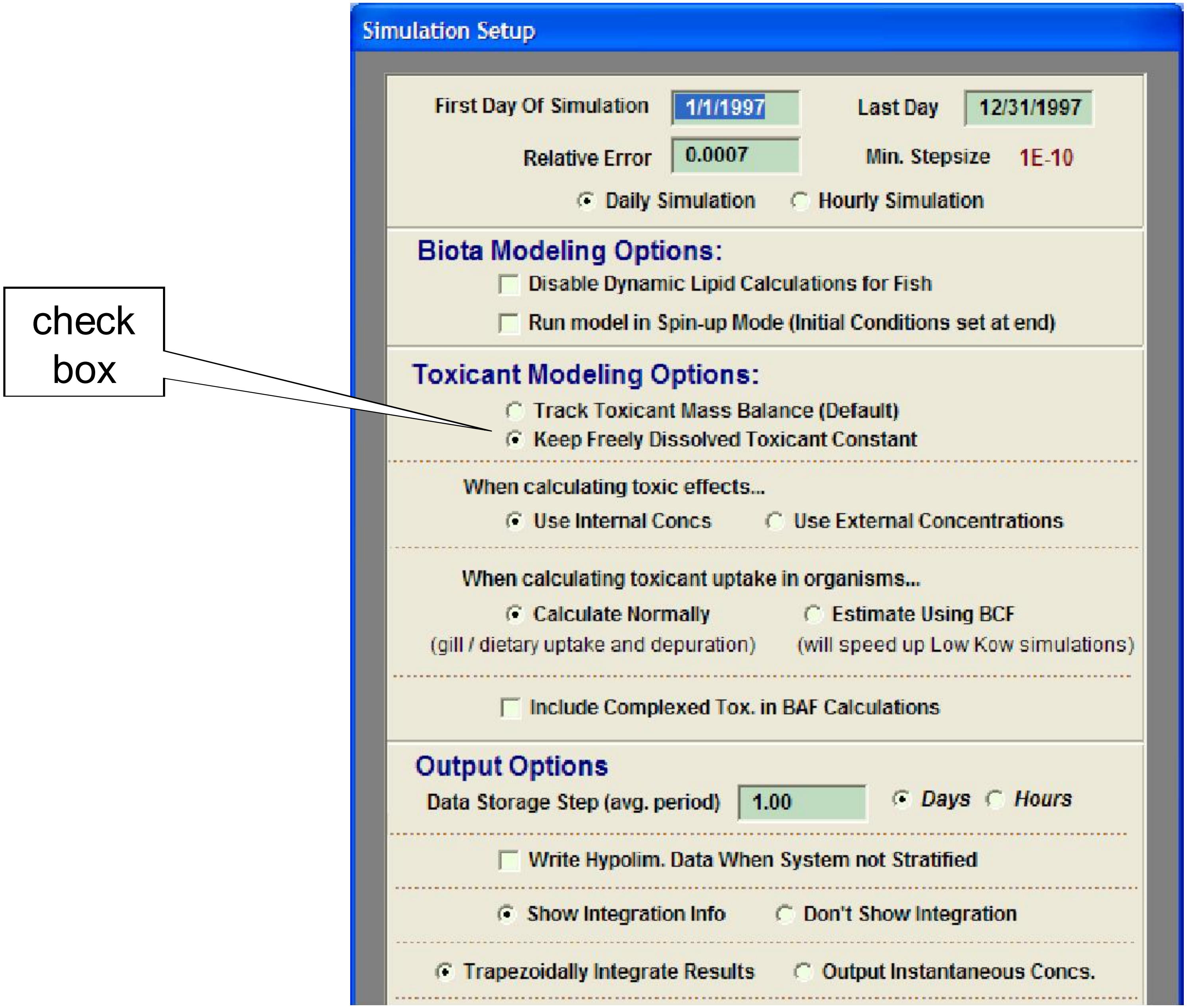
Chlorpyrifos in Stream

Objective: analyze direct and indirect ecotoxicological effects with model

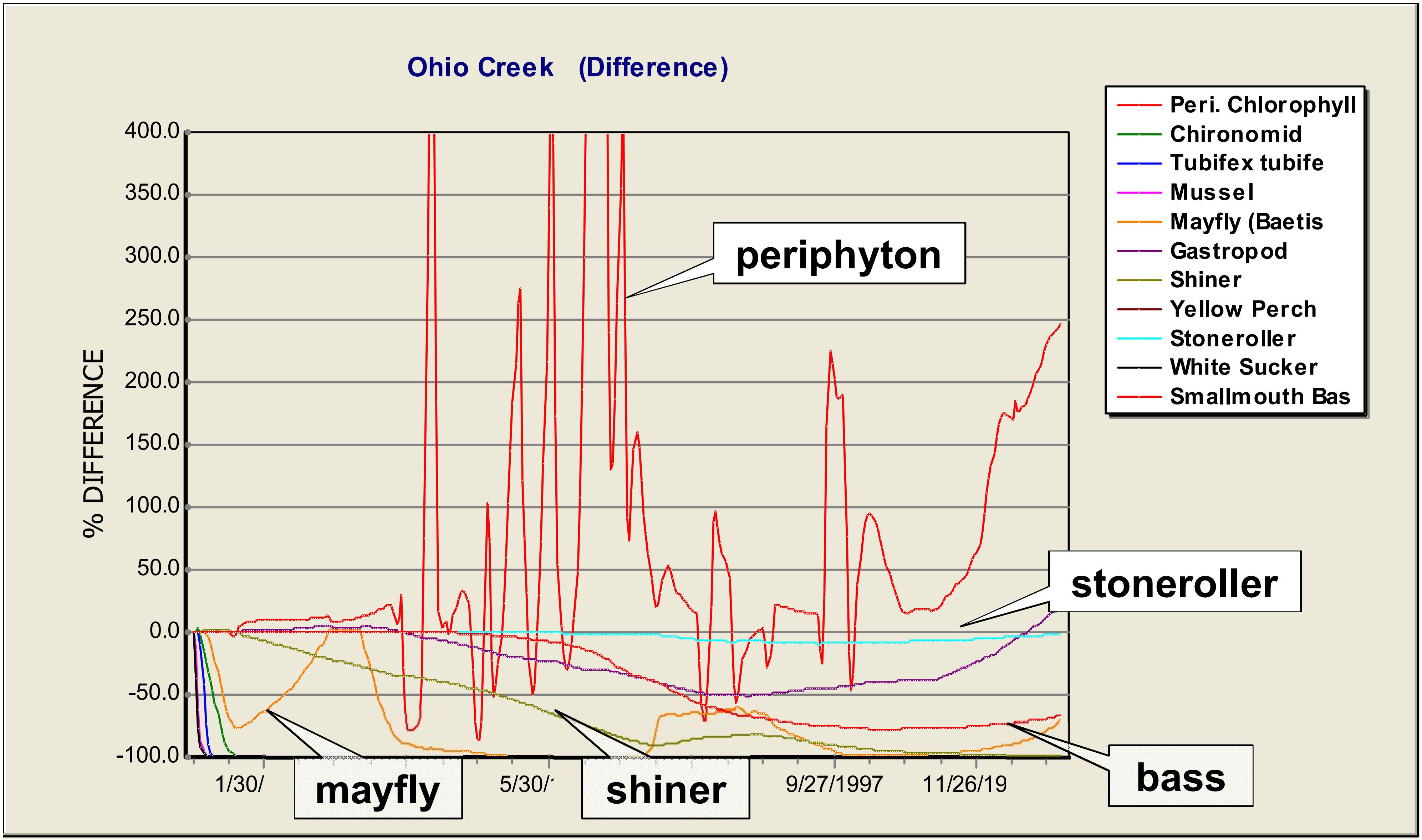
- Assessment of chlorpyrifos in a generic stream
  - small stream in corn belt
  - exposure to constant level of Chlorpyrifos assessed (0.4 ug/L)
  - optionally simulate with the initial condition of 0.4 ug/L as a one-time dose

Set exposure to a constant in Study Setup

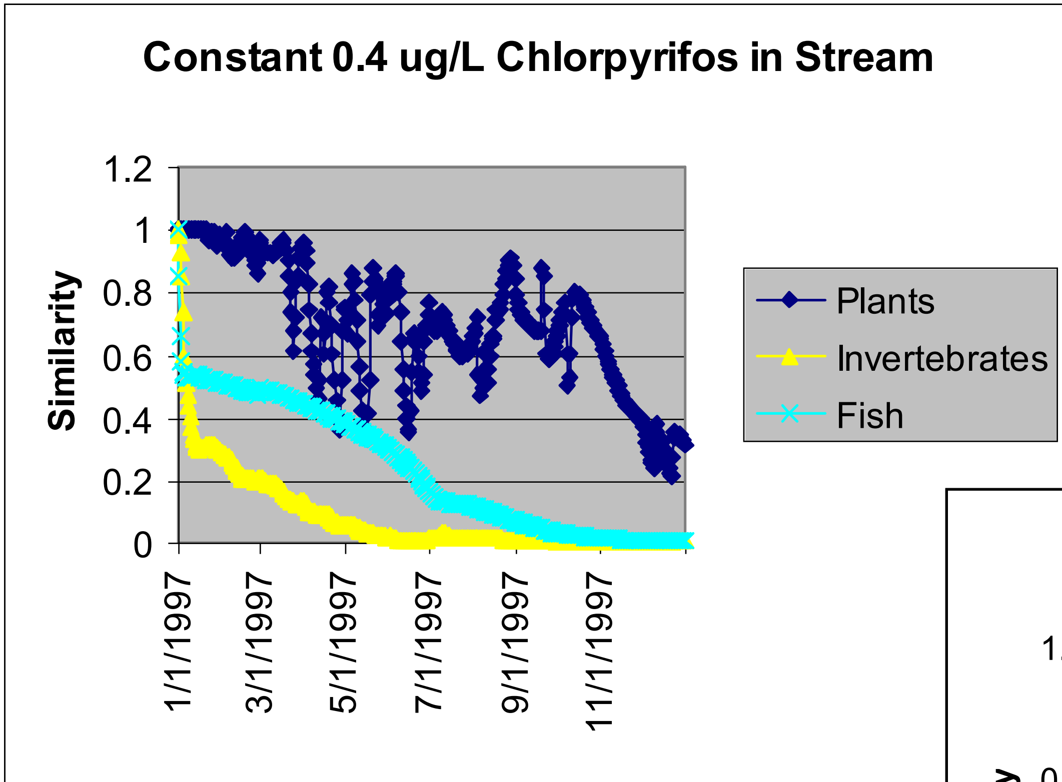
Set "Control Setup" to omit toxicants from "control" results

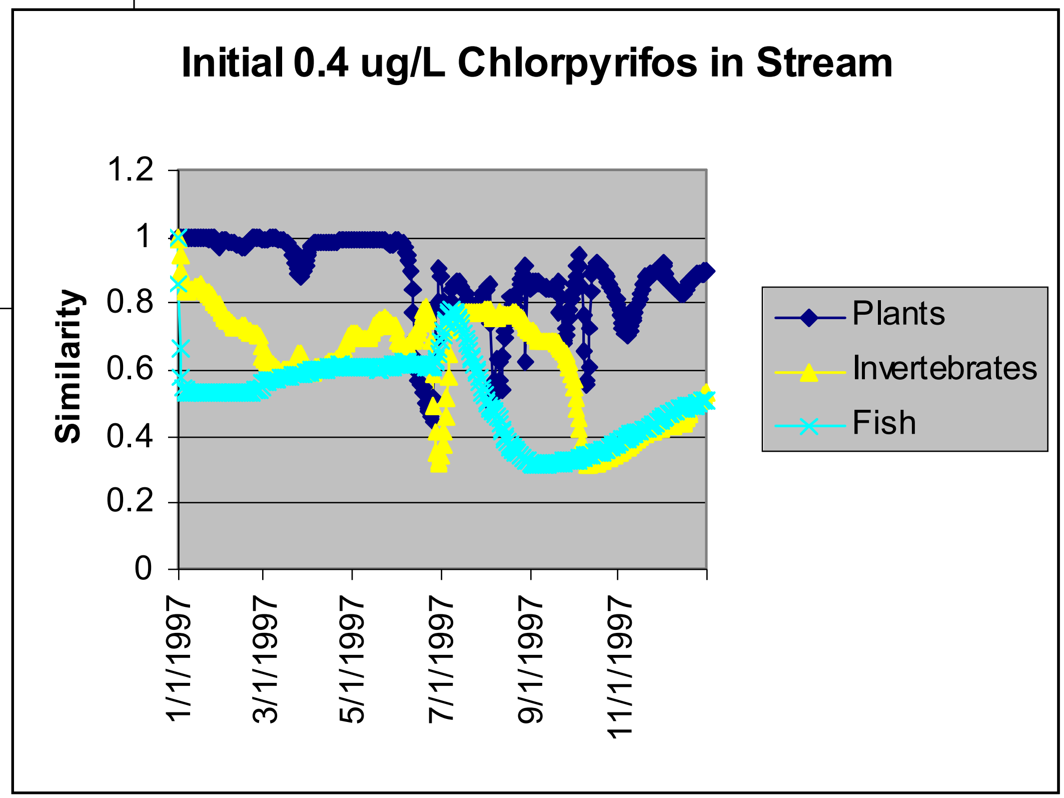


Impacts of constant chlorpyrifos are dramatic: animals decline, algae increase (less herbivory)



Plot of Steinhaus indices shows lasting impacts predicted by the model

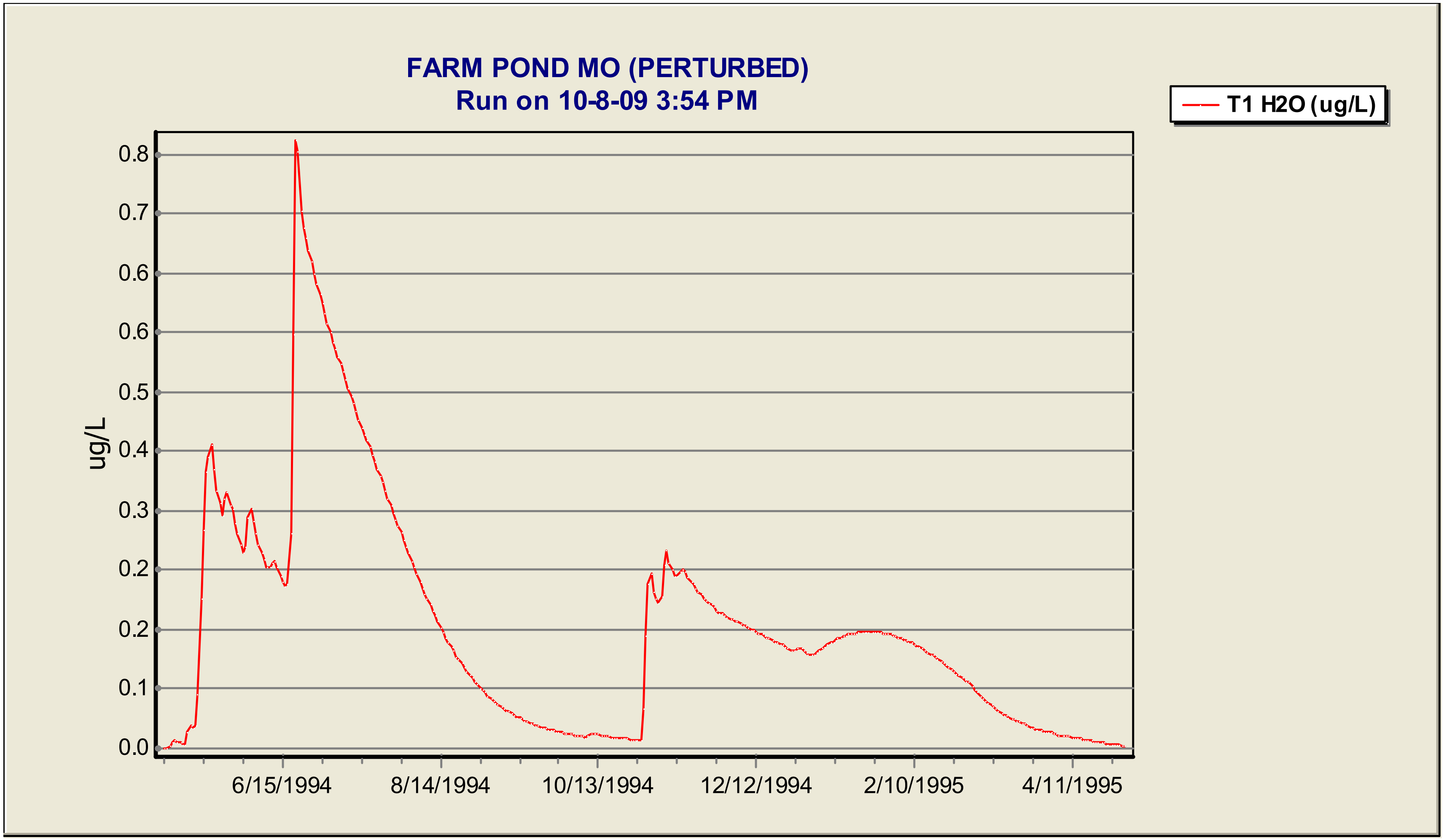




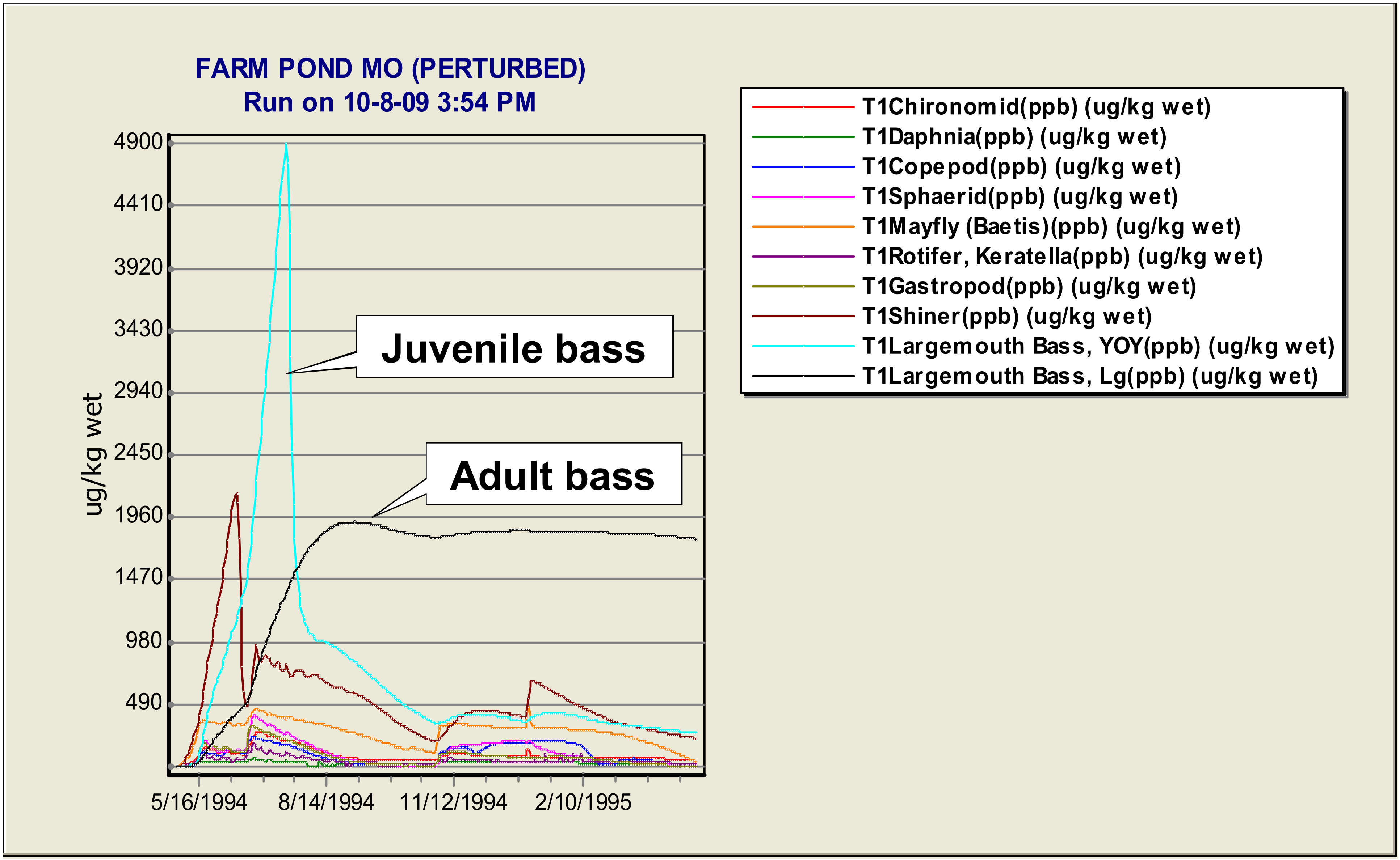
You can also uncheck the "keep constant" choice to see how the model responds to an initial dose of 0.4 ug/L

Farm Pond MO, Esfenvalerate

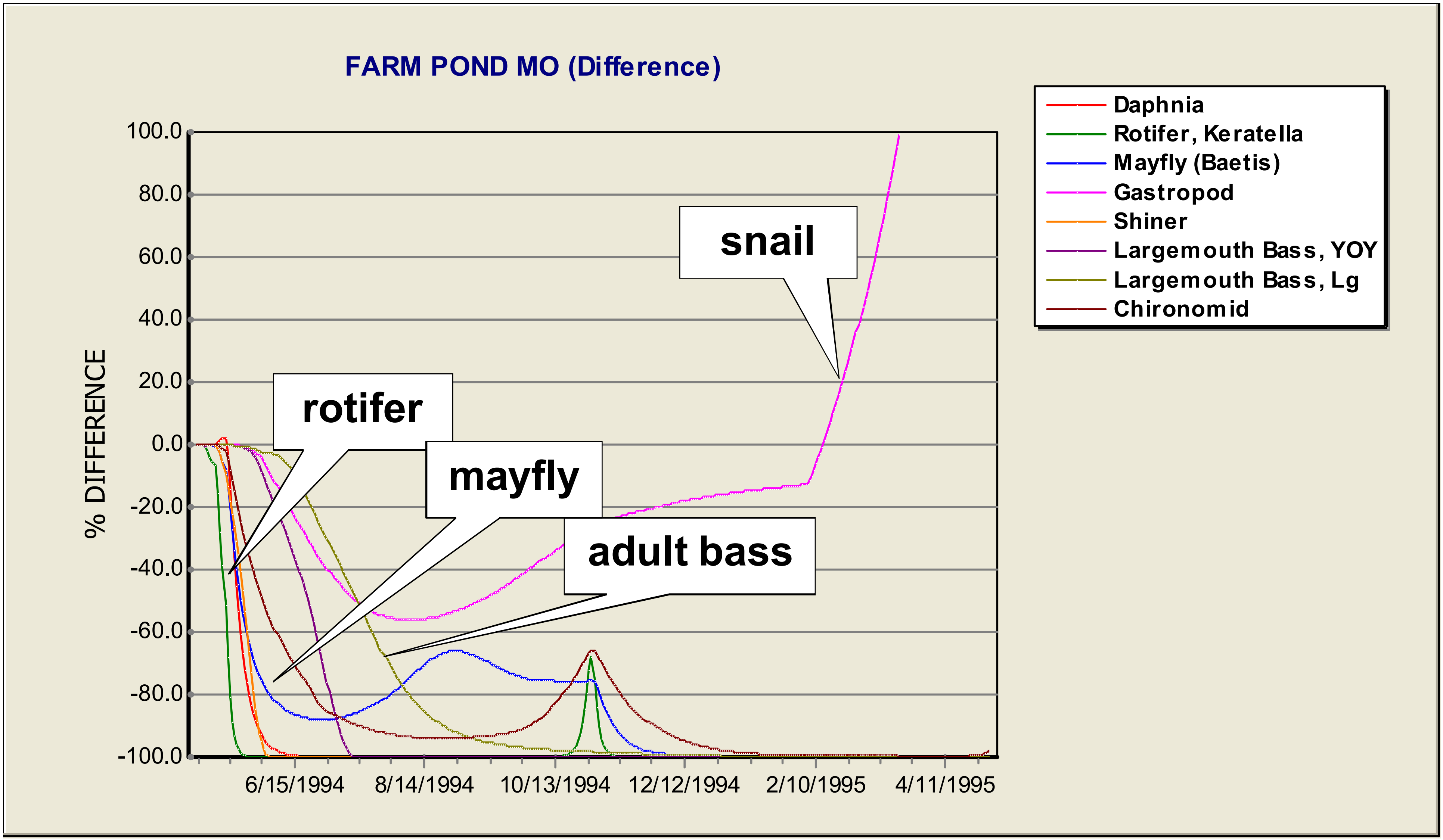
- Loadings from PRZM for adjacent cornfield
- Worst case scenario for runoff of pesticide predicted by PRZM



Farm Pond, Esfenvalerate Chemical Uptake in animals

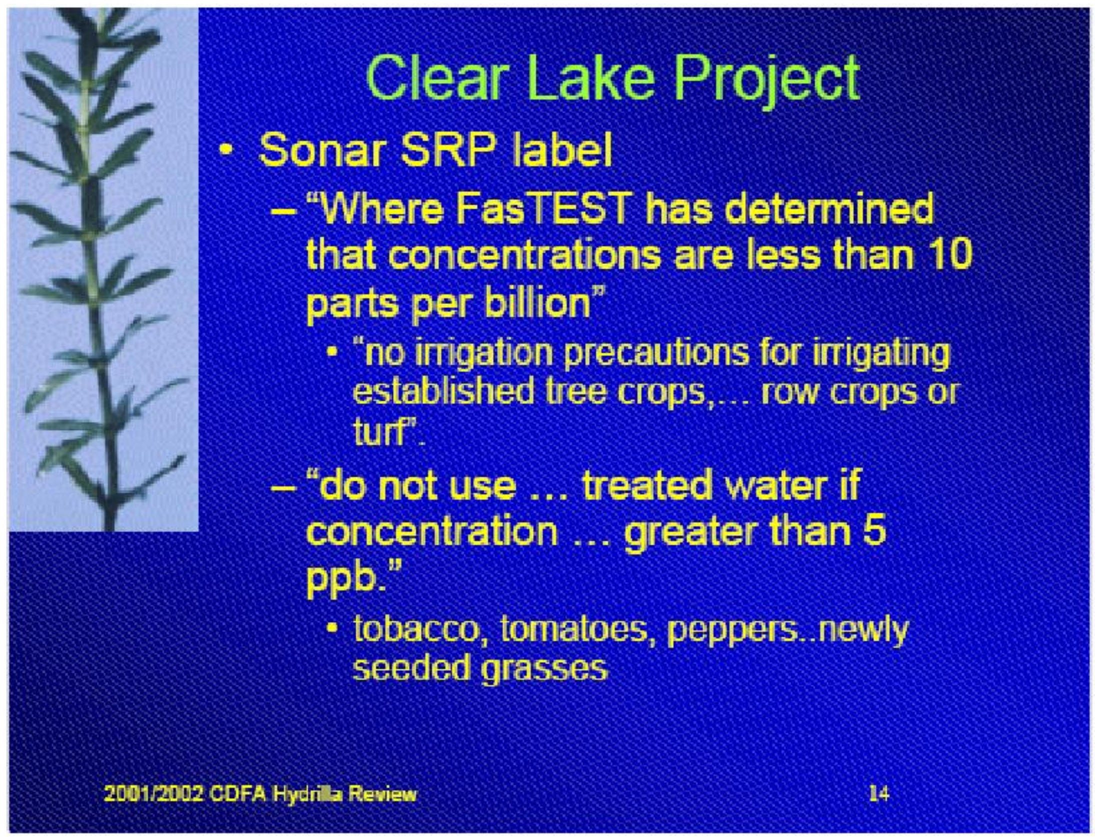


Farm Pond, Esfenvalerate Difference Graph

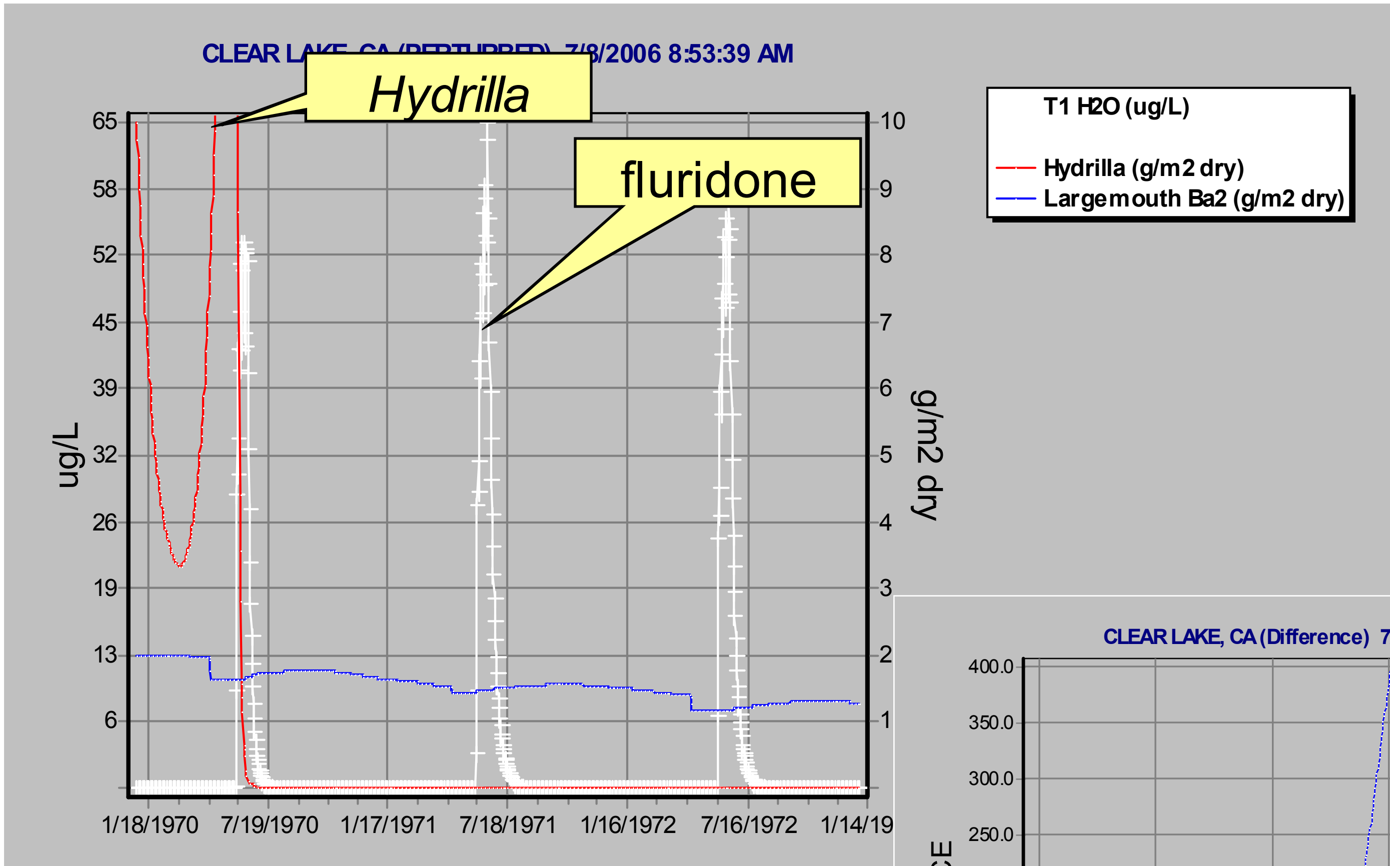


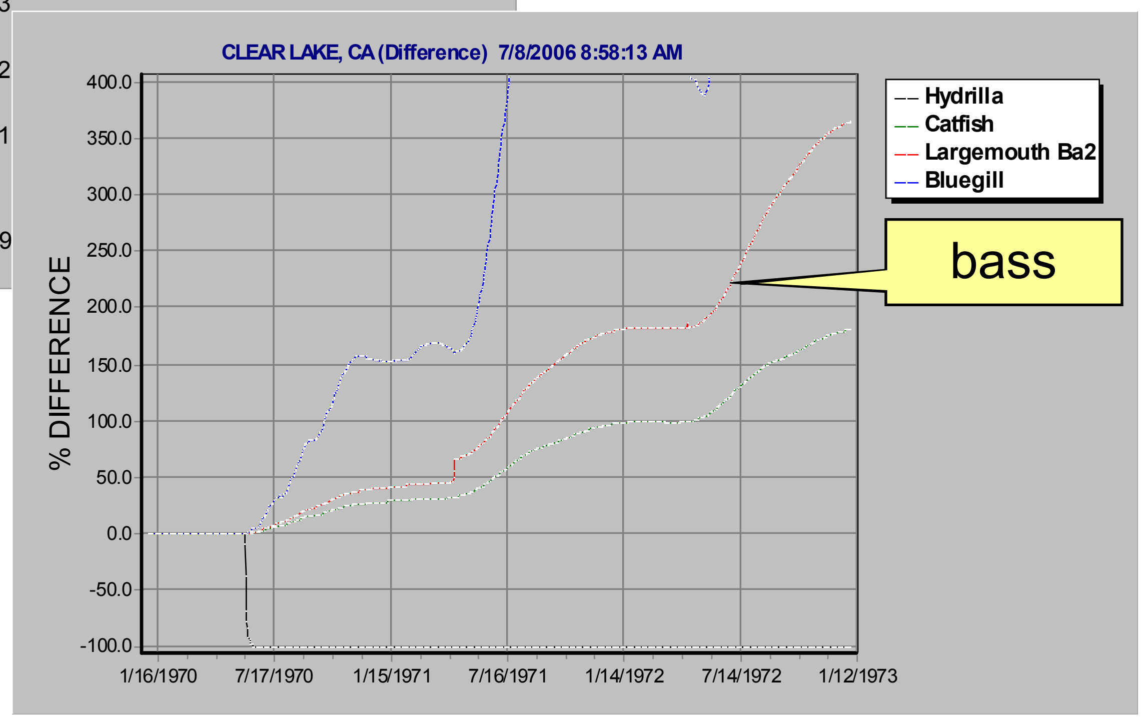
Fluridone (Sonar) used to eradicate *Hydrilla* in Clear Lake CA

- 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?



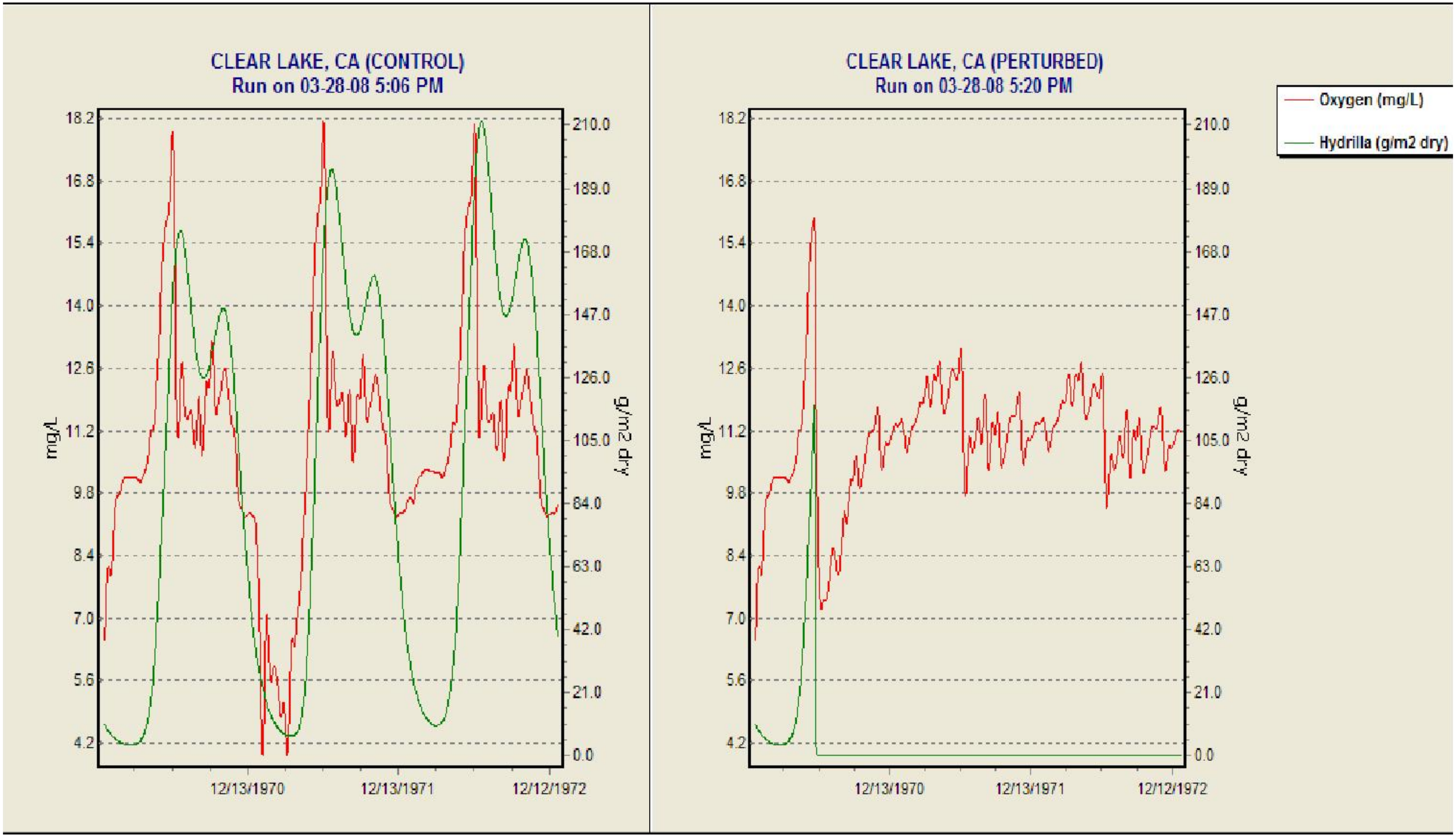
Addition of Fluridone causes dramatic response of Clear Lake ecosystem





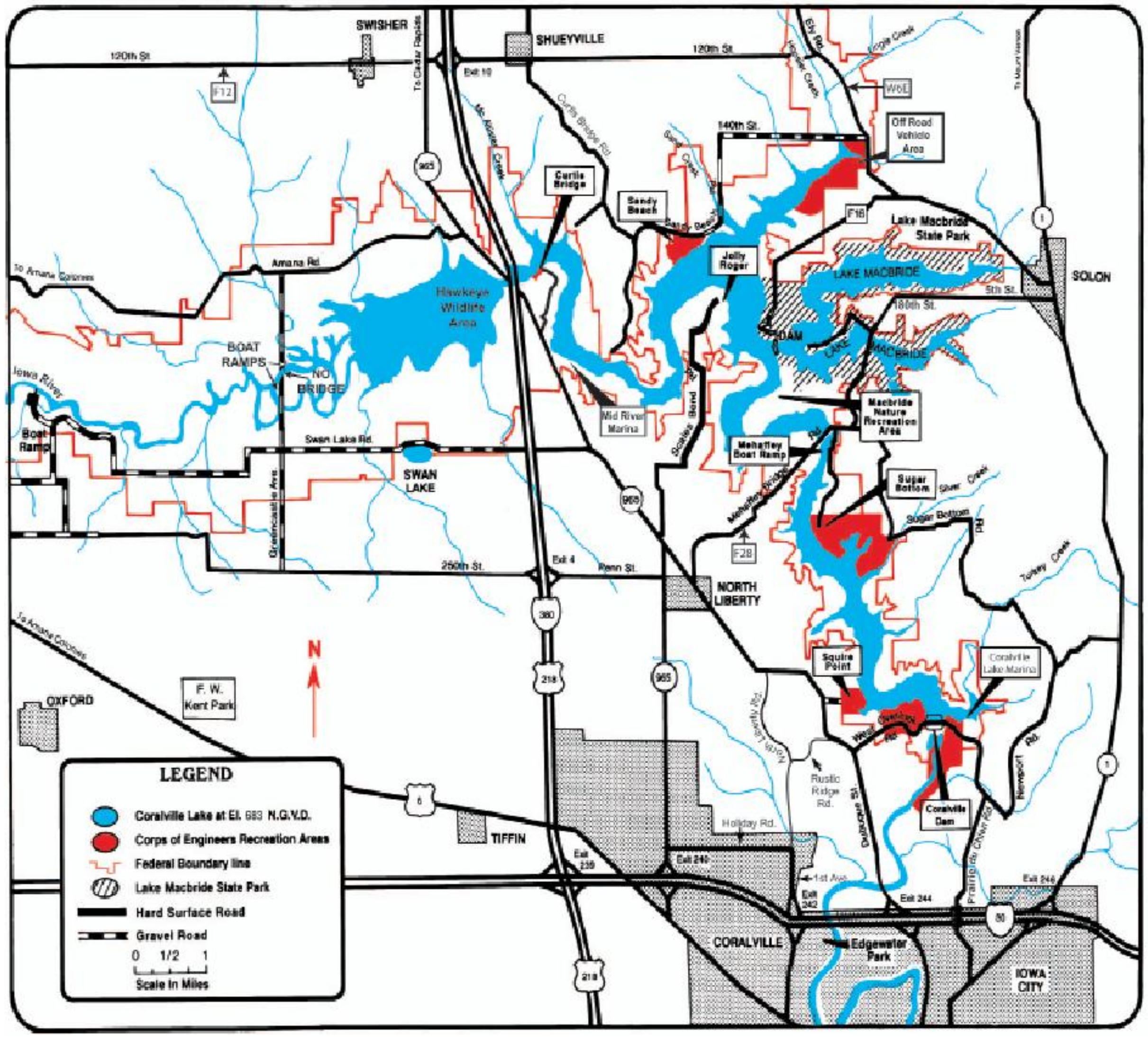
Indirect Effects Captured

e.g. Impact on DO levels is negligible

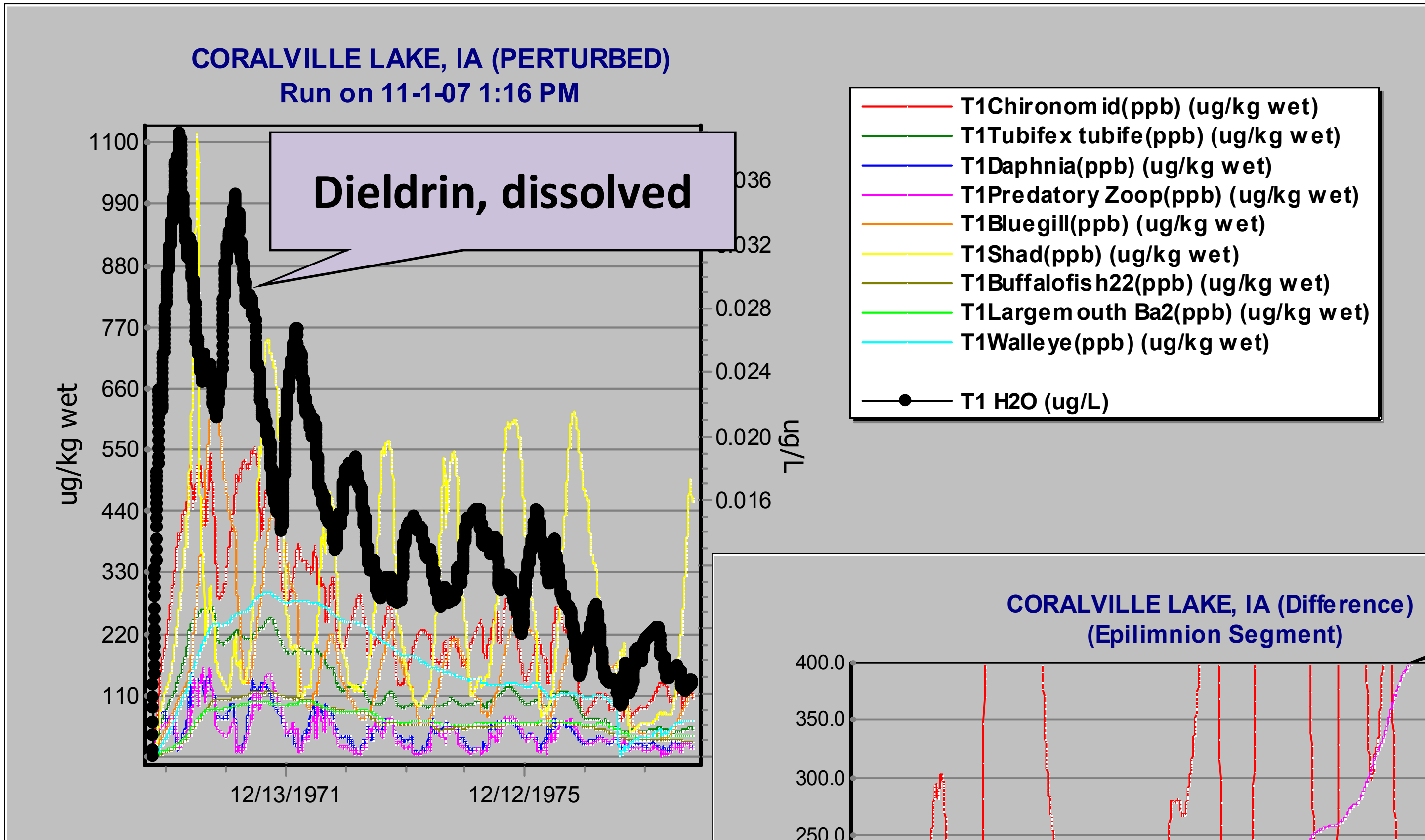


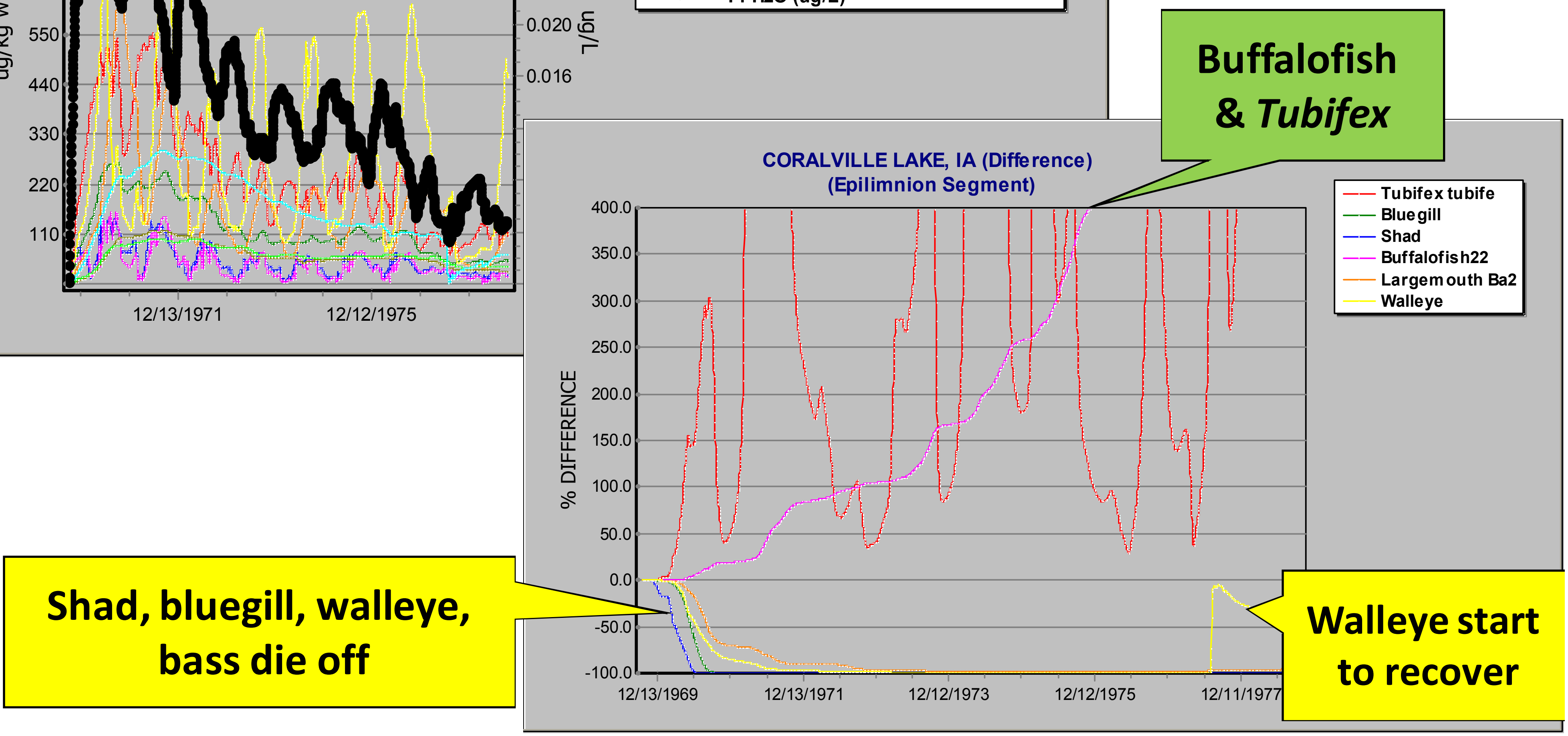
Coralville Reservoir Iowa
long-term contamination with dieldrin

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

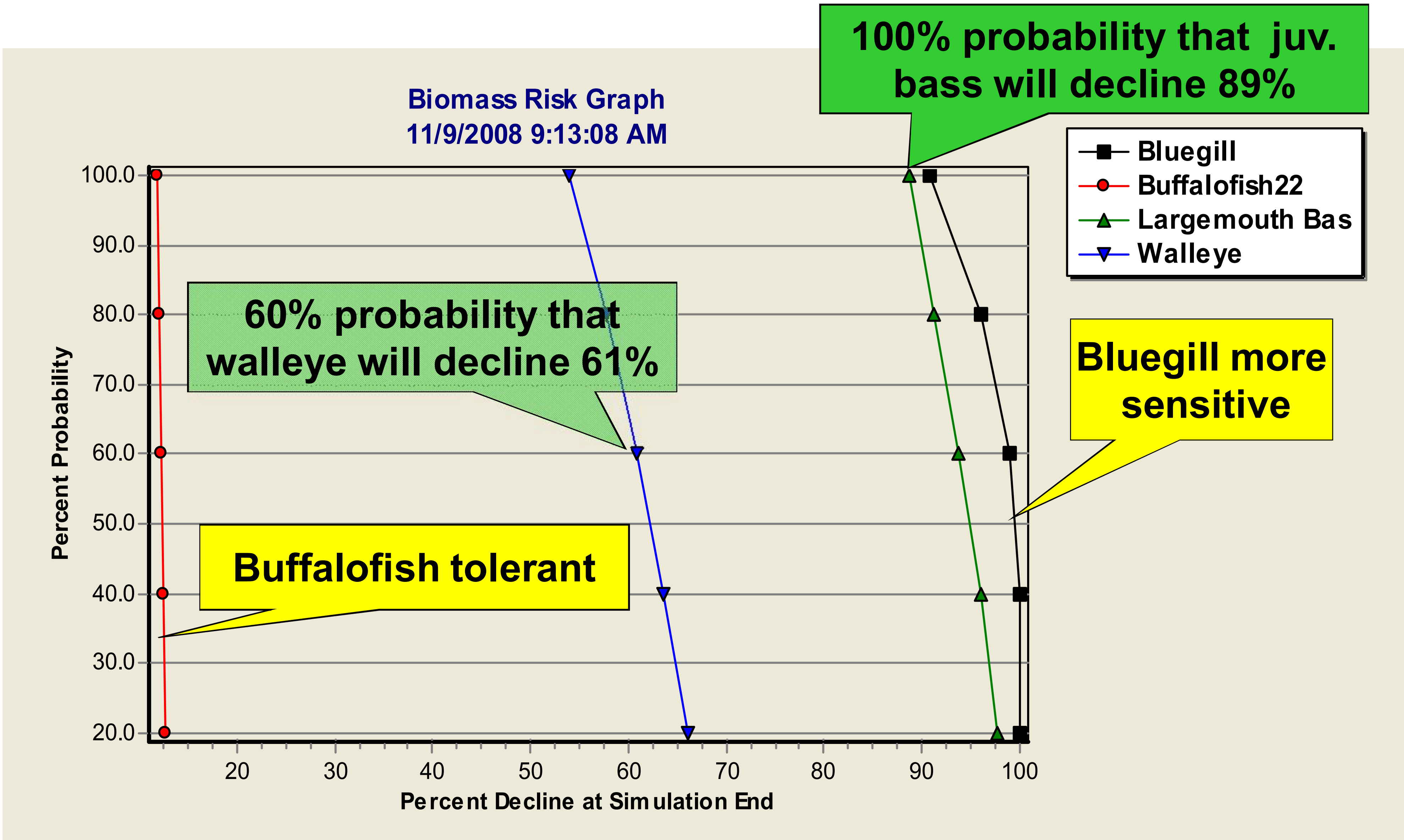


Dieldrin bioaccumulates & declines over 20 years with fish mortality, but tolerant buffalofish, *Tubifex* prosper





Probability of decline in biomass (end of 1st year) can be estimated based on uncertainty

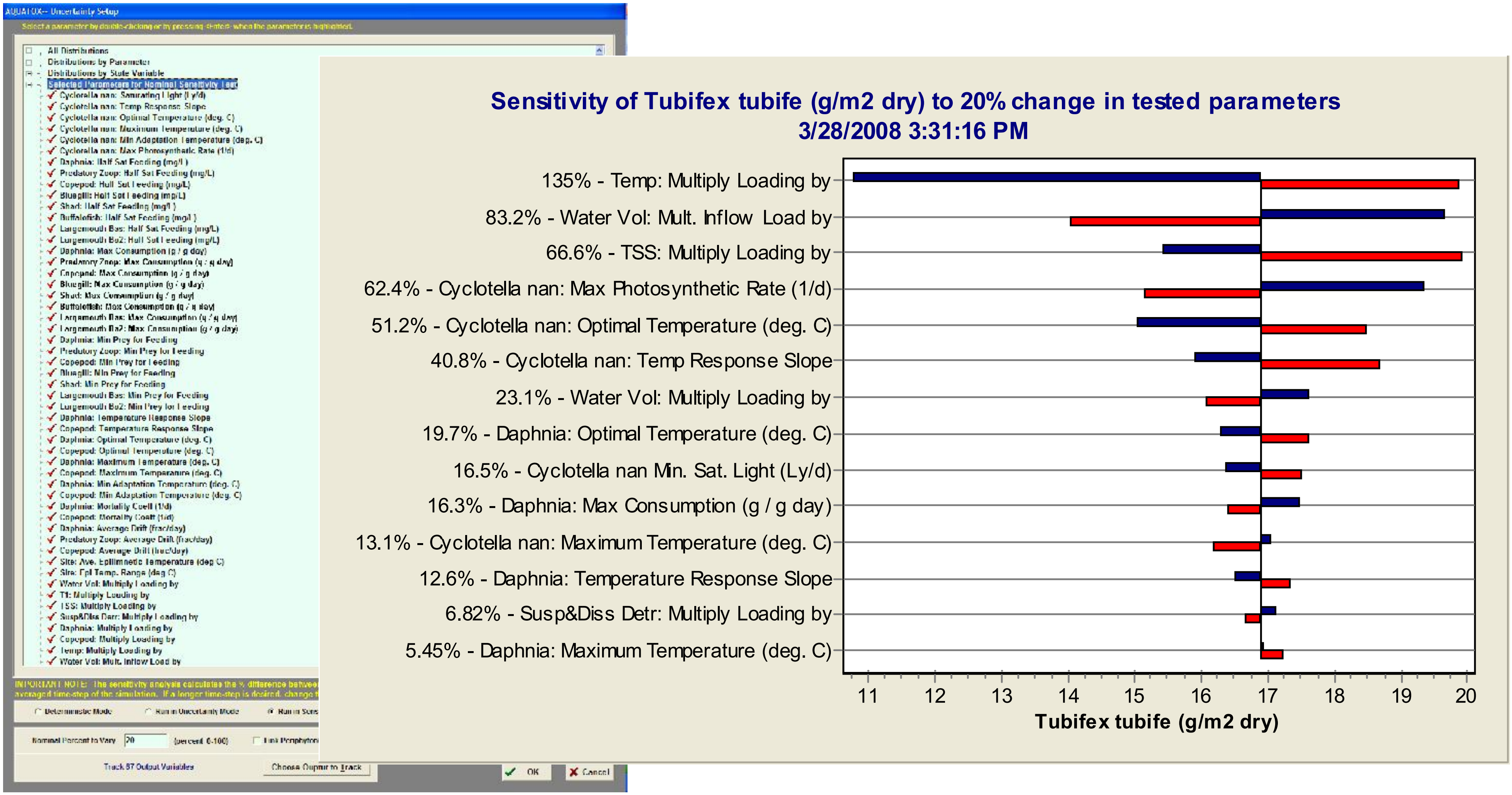


Uncertainty and Sensitivity Analysis

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

Coralville Sensitivity Analysis Demo

Demonstration of inputs and outputs from Coralville analysis

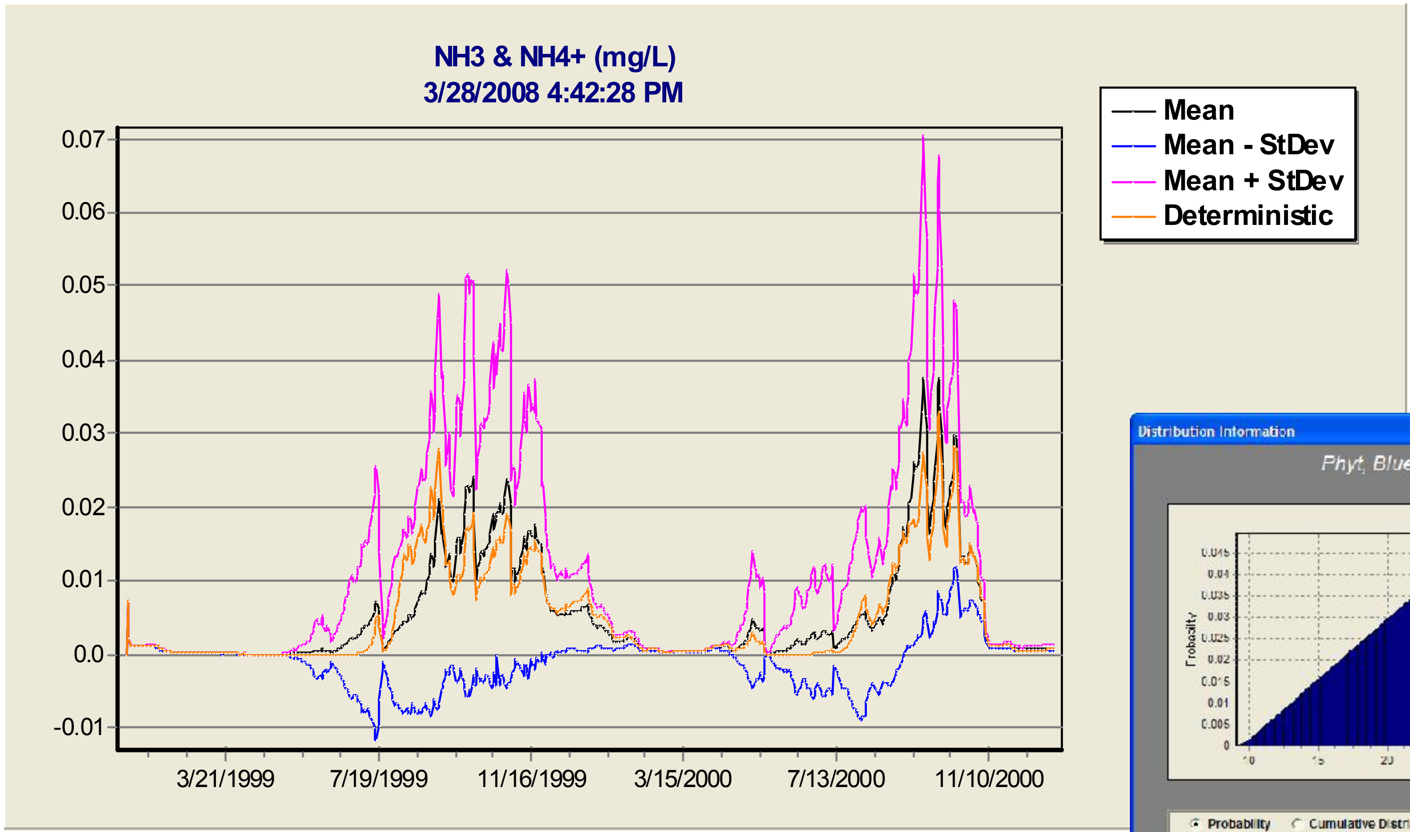


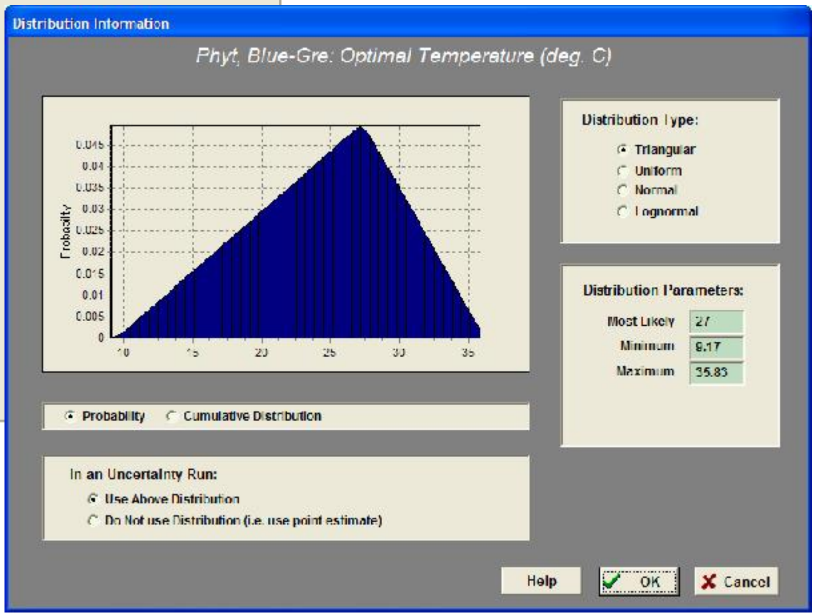
Uncertainty Analysis

- Uncertainty analyses describe sources of incertitude 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” (greatly reduces required iterations)

Blue Earth Uncertainty Analysis Demo

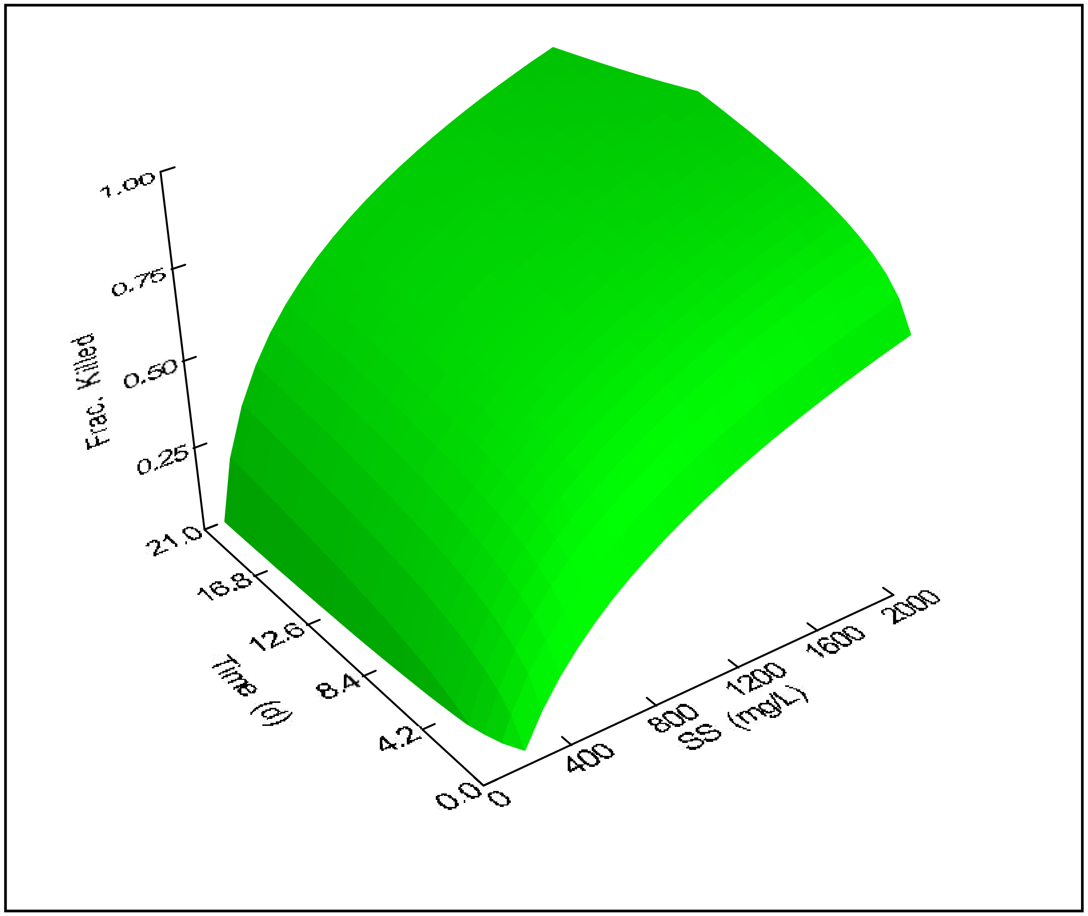
Demonstration of inputs and outputs from Blue Earth River, MN





Sediment Effects Overview

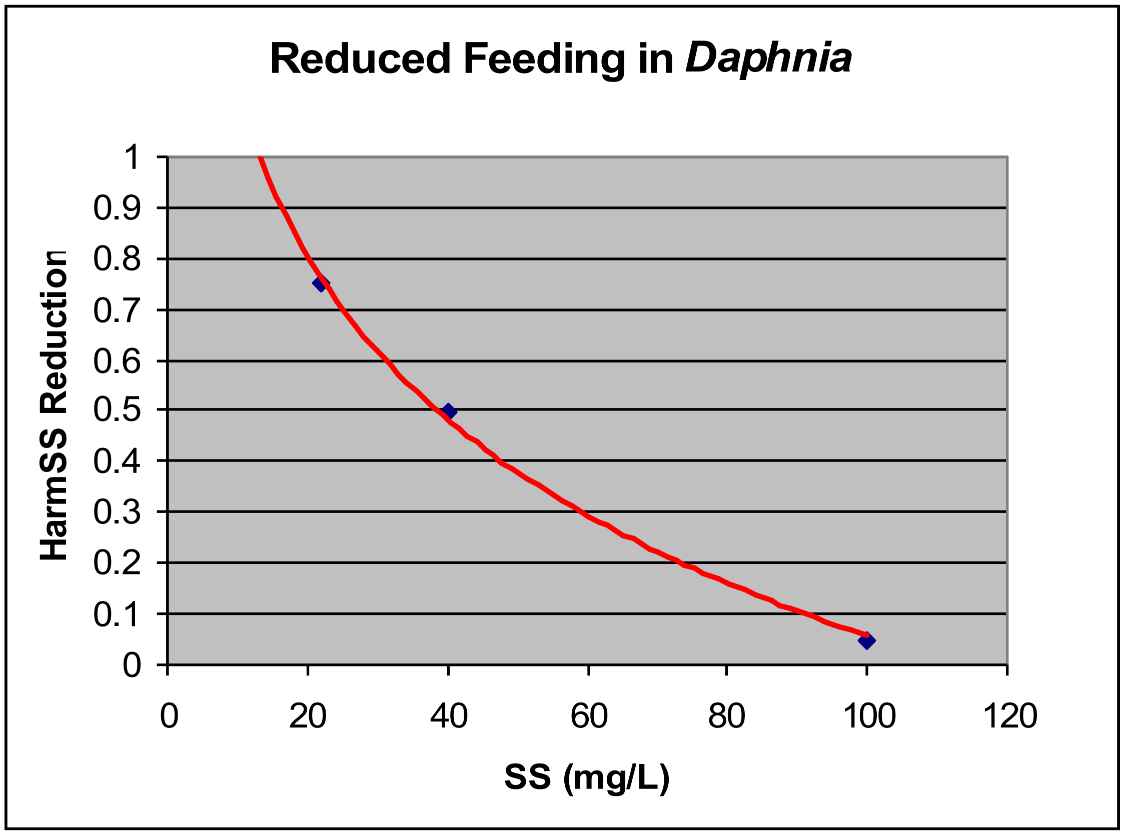
- Suspended and bedded sediment effects
  - **Mortality**
    - Highly Sensitive
    - Sensitive
    - Intolerant
    - Tolerant



Sediment Effects Overview

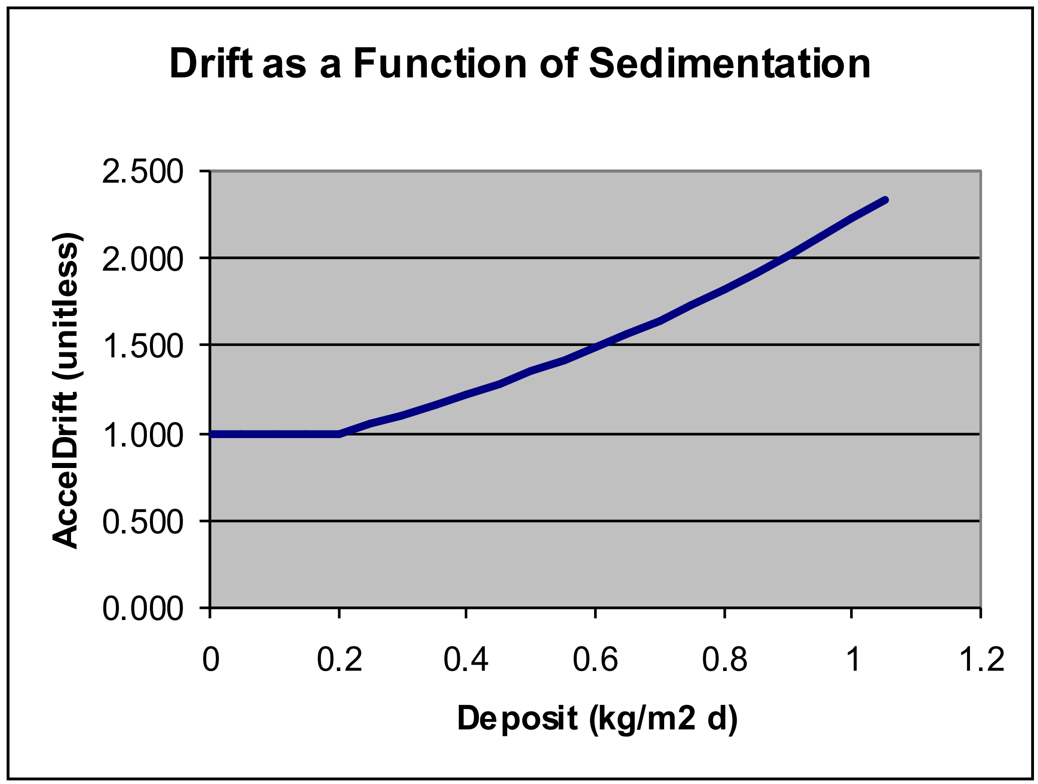
- Suspended and bedded sediment effects
  - Mortality
  - **Reduced Feeding**

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



Sediment Effects Overview

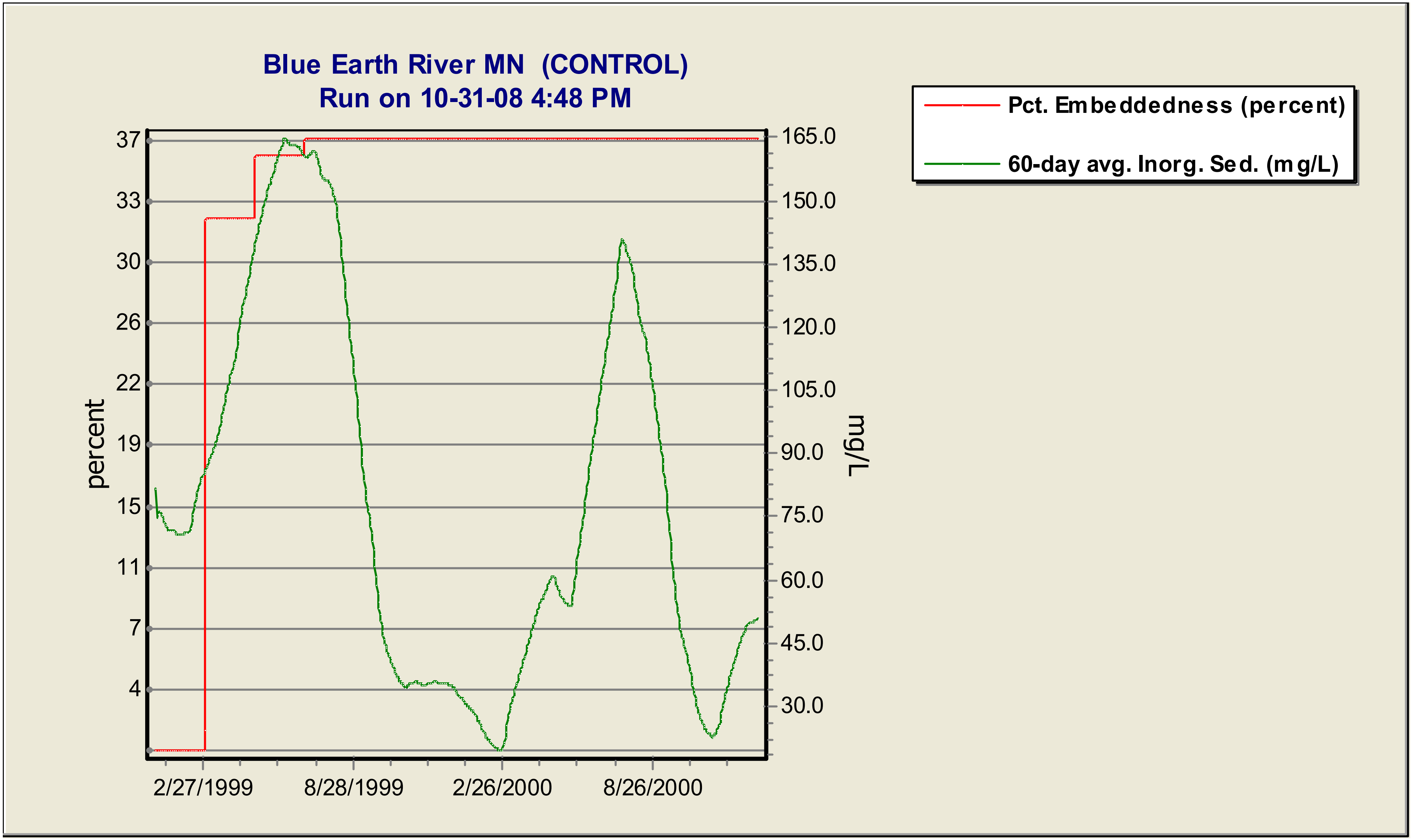
- Suspended and bedded sediment effects
  - Mortality
  - Reduced Feeding
  - **Increased drift of benthos due to sedimentation**



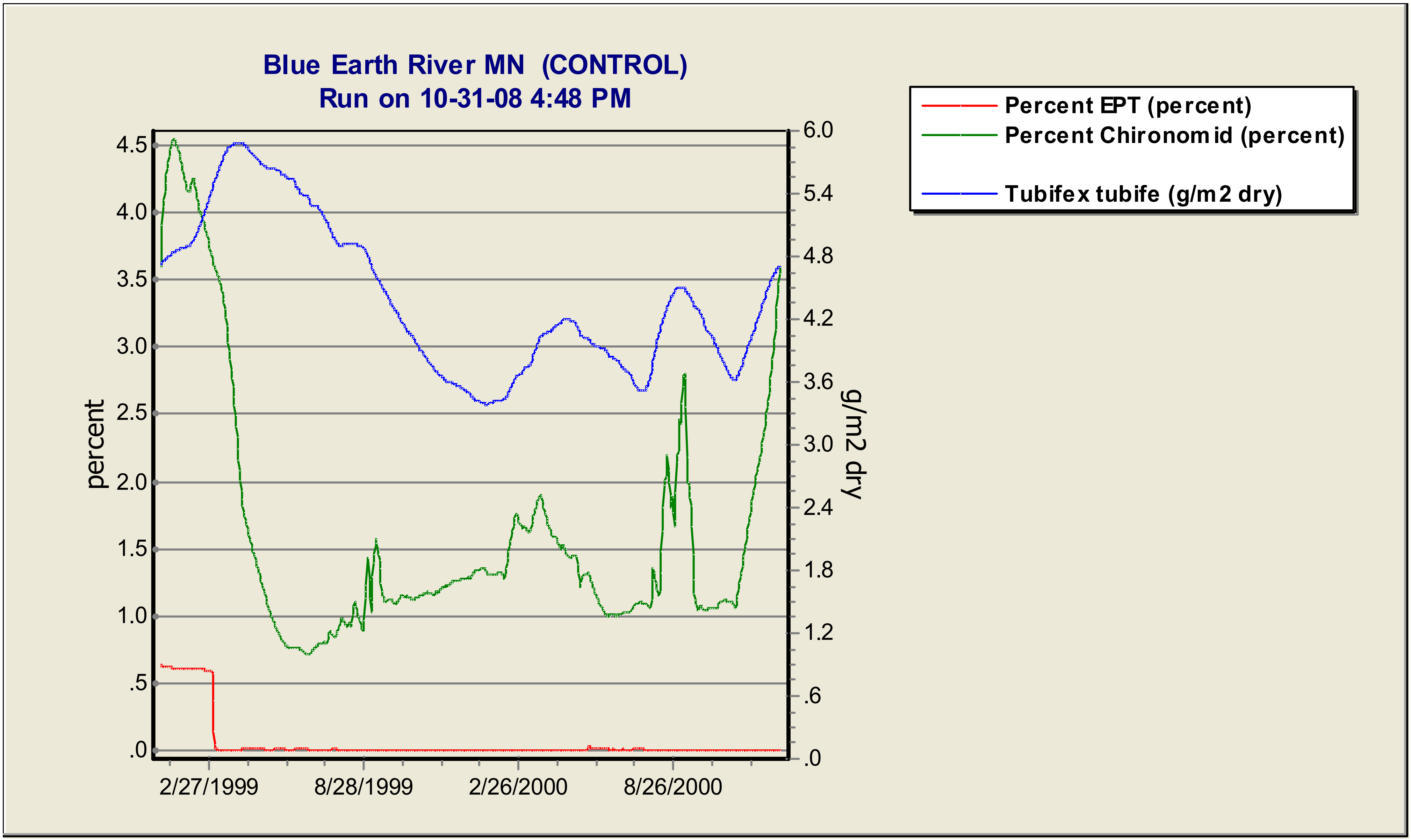
Sediment Effects Overview

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

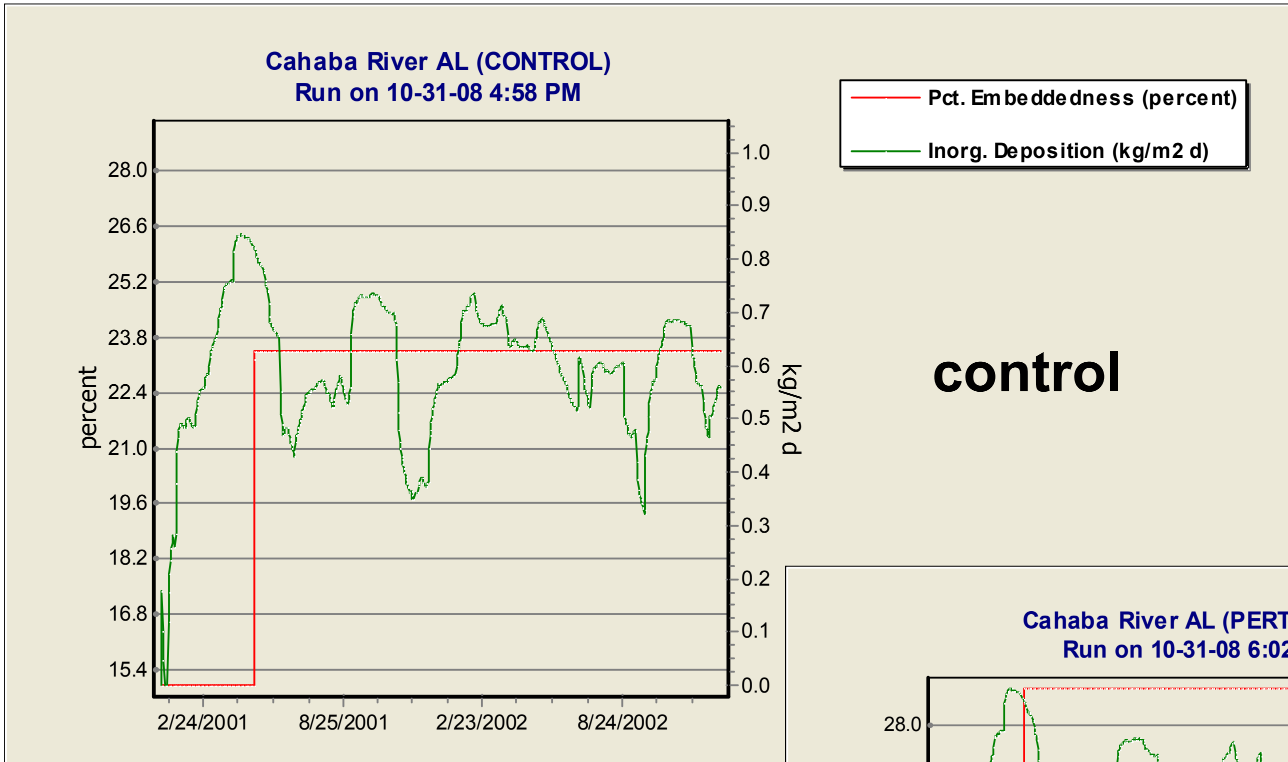
Percent embeddedness is computed from 60-day deposition rate (a function of TSS)

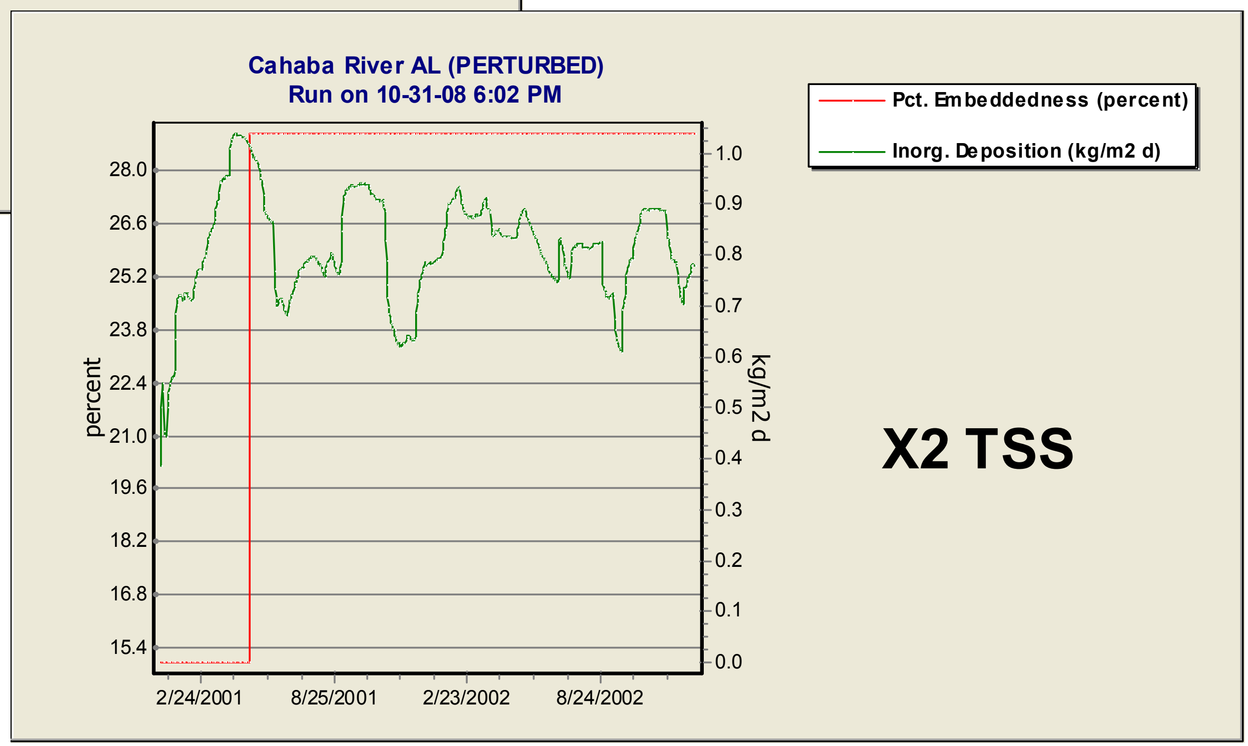


Mayflies, stoneflies, & caddisflies (EPT) are sensitive to embeddedness; chironomids & oligochaetes are not

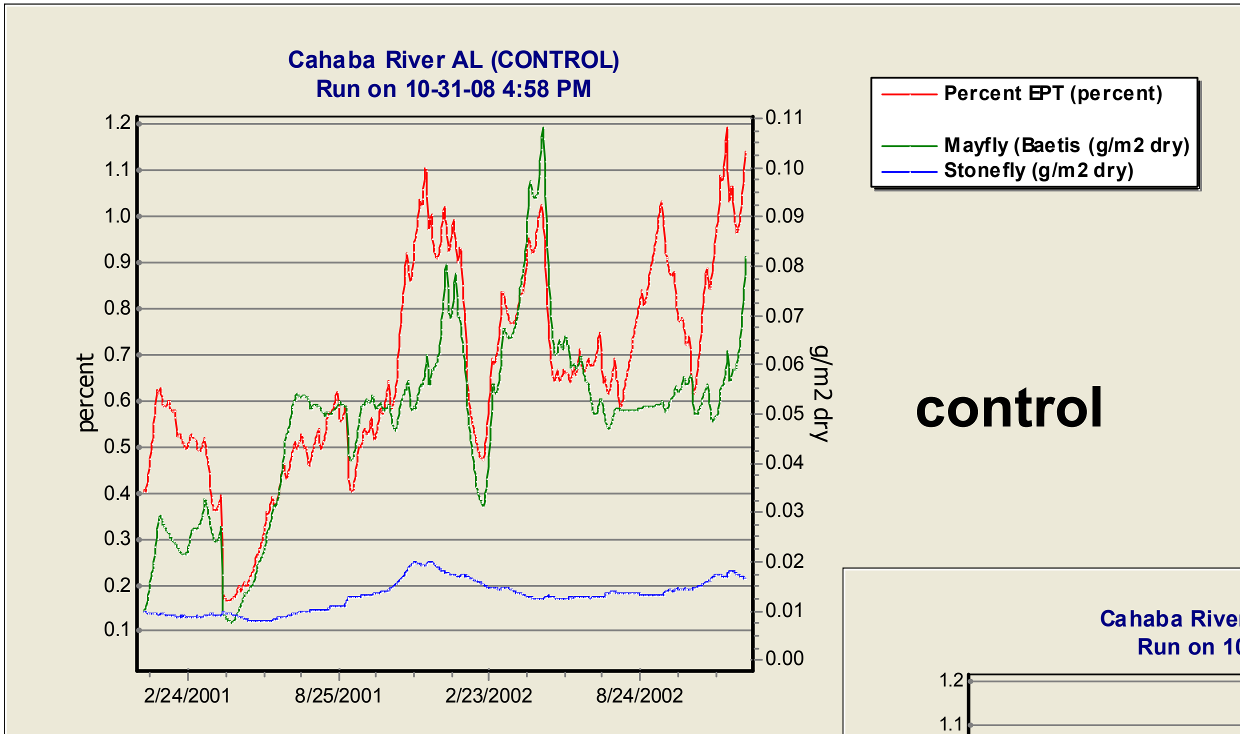


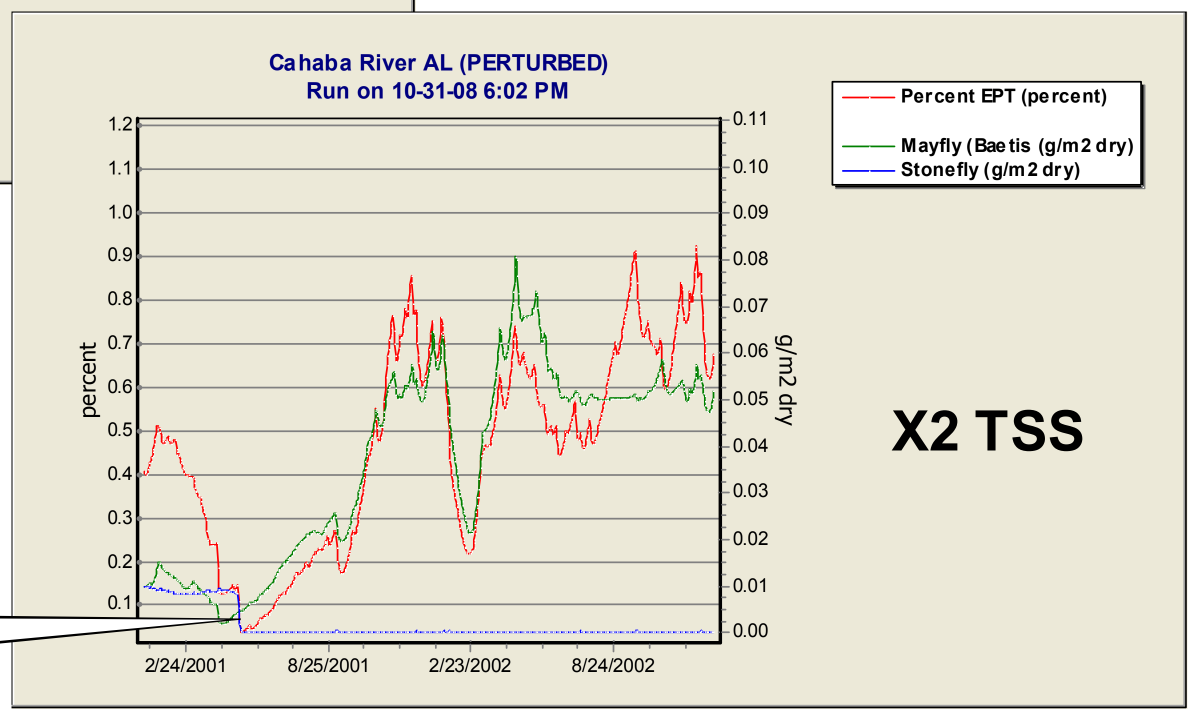
Doubling TSS increases embeddedness in Cahaba River, AL





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





stoneflies crash

Closure

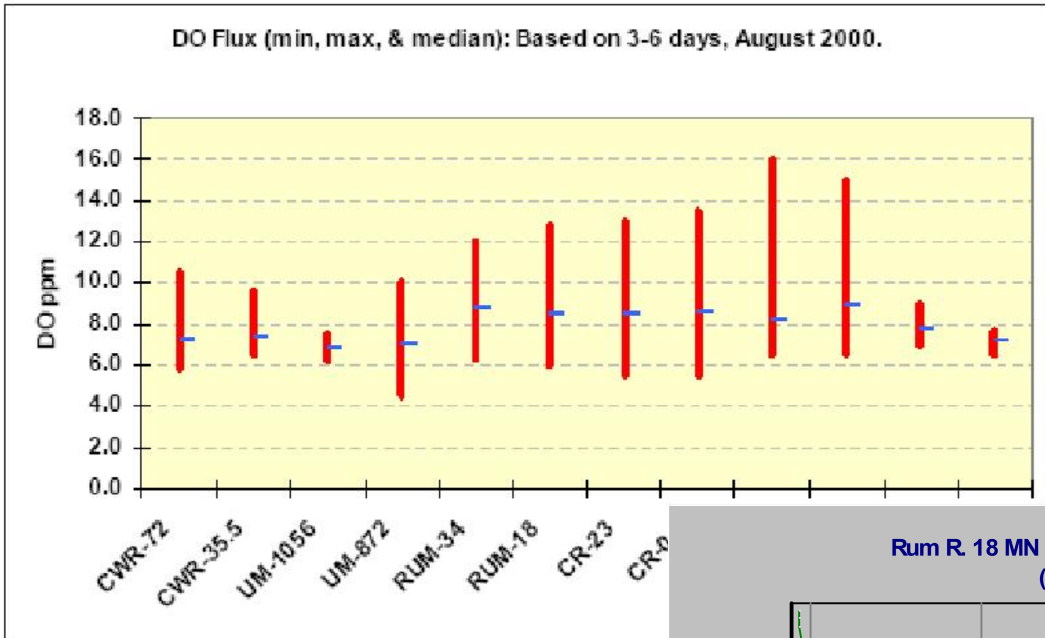
- Topics not yet covered (time-permitting)
  - Diel Oxygen
  - Sand-Silt-Clay model
  - Multi-layer sediment model
- Final Q&A

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://water.epa.gov/scitech/datait/models/aquatox/index.cfm
  - Citations of articles using or reviewing AQUATOX
  - Data sources

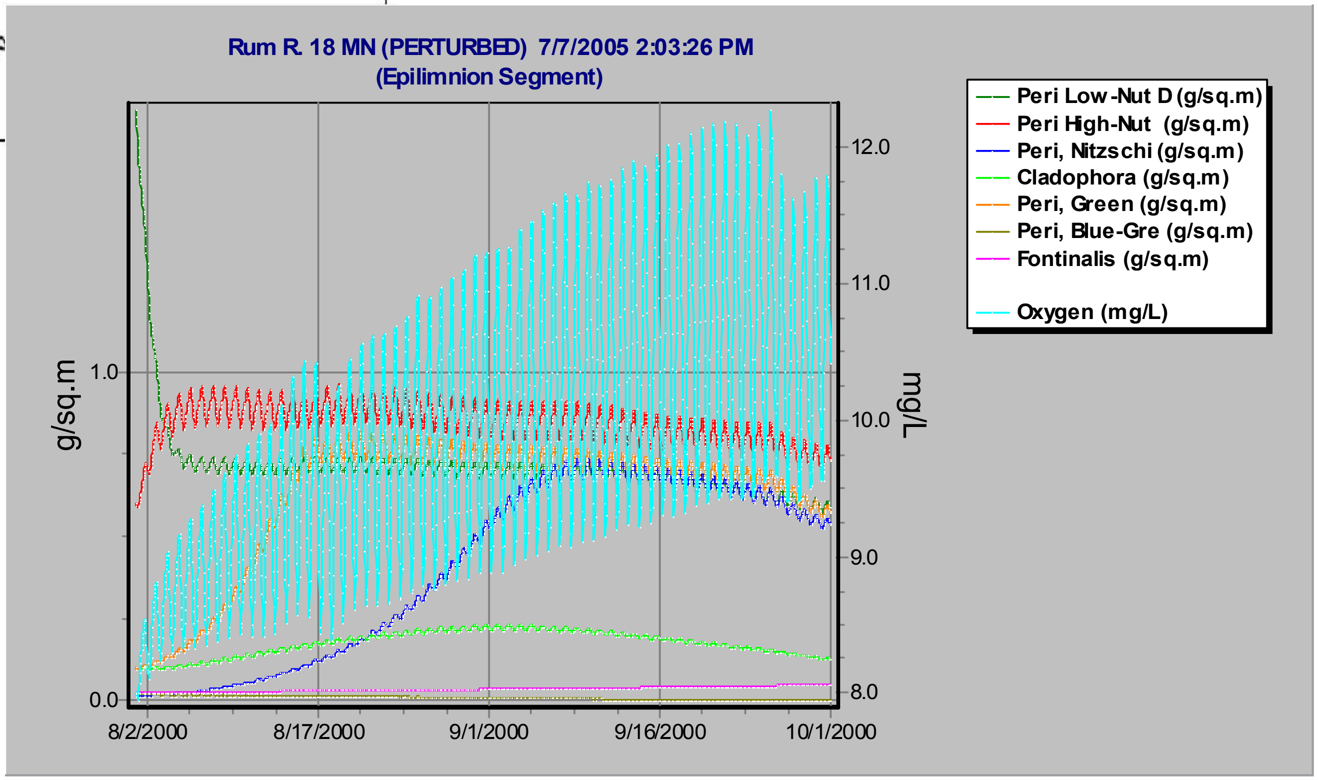
Diel Oxygen, Light; Hourly time-step

Figure 4. Dissolved oxygen flux based on continuous measurement.

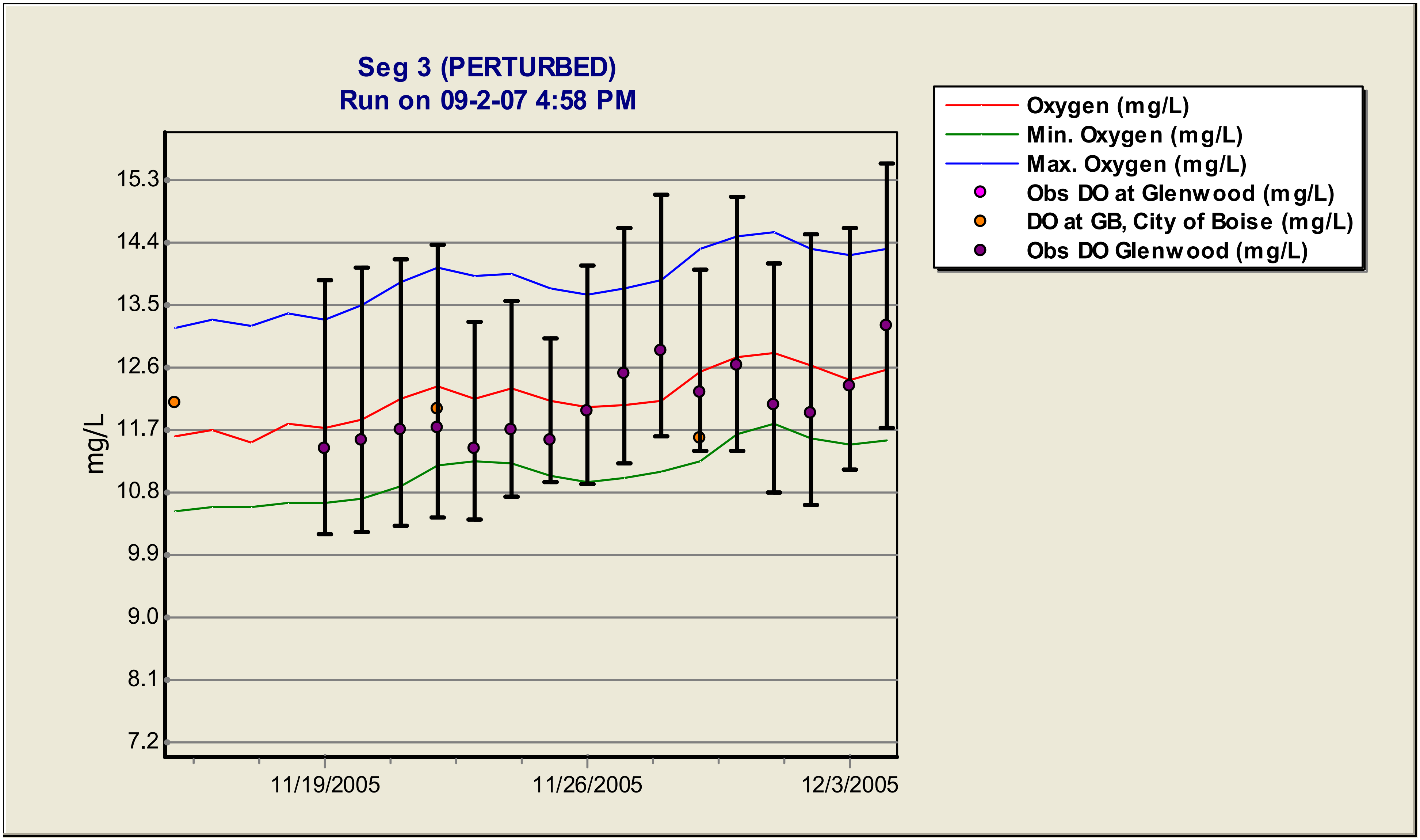


AQUATOX can now run with an hourly time-step including hourly light inputs. This results in a simulation of oxygen concentrations on an hourly basis

Monitoring data indicate that oxygen levels fluctuate daily



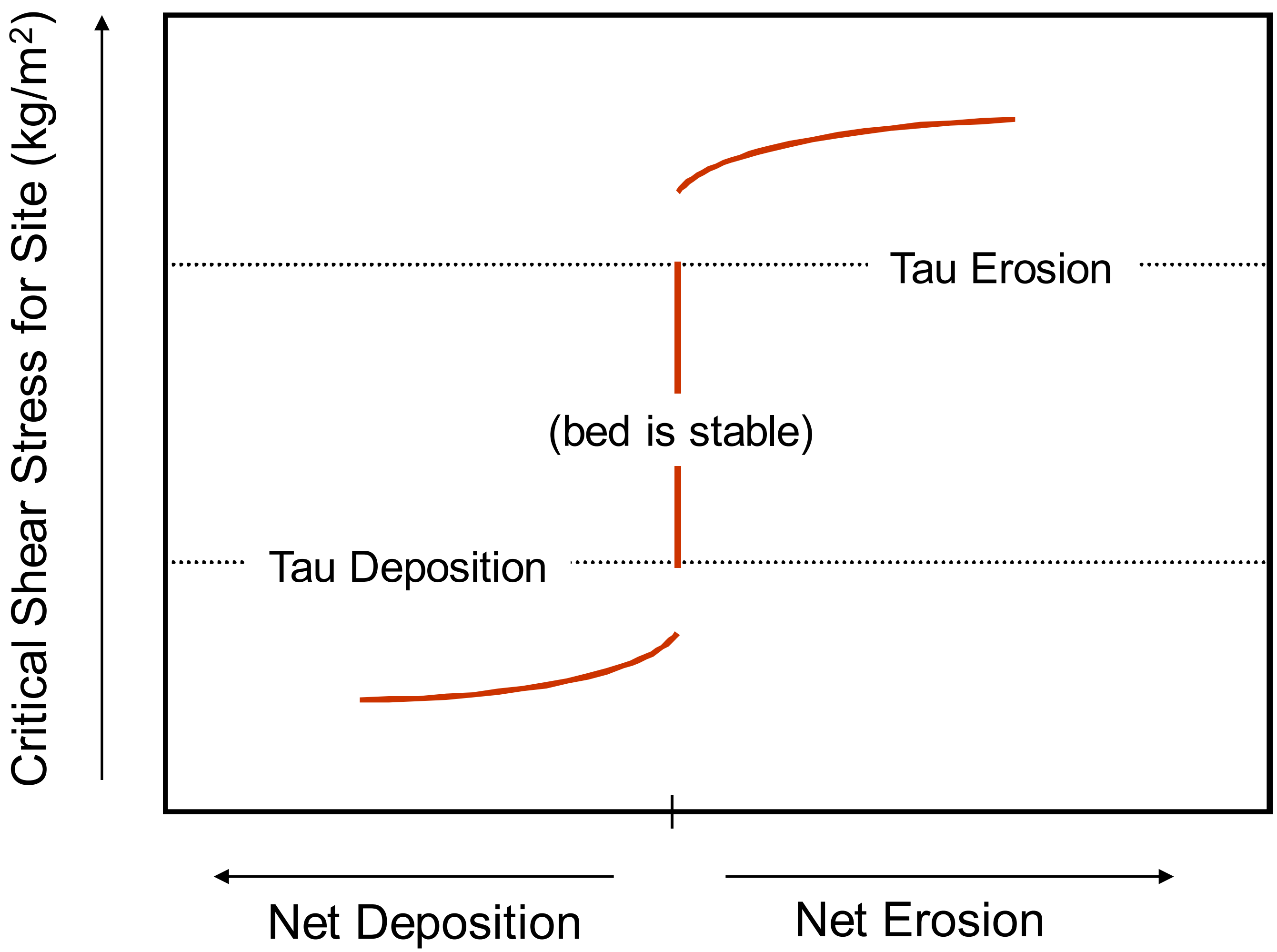
Diel Oxygen, Hourly Time-step



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, and now direct sediment effects

Critical Shear Stress for Erosion and Deposition Key Parameters



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