

# AQUATOX Training Workshop (Day 2)

Web Training Materials, August 2012

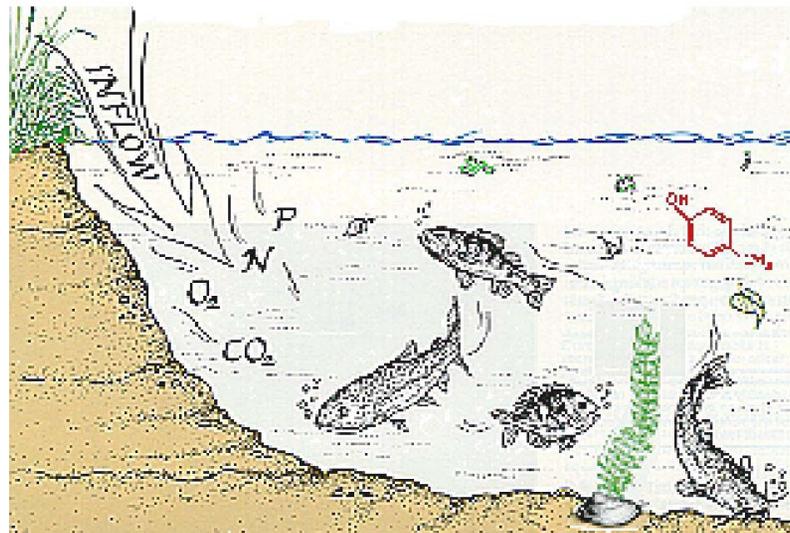
Based on Workshop Given for EPA Region 6, Dallas, Texas, December 2010  
and Columbia River Intertribal Fish Commission, November 2011



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# Lab 4: Application to Minnesota Rivers

Objectives:

- familiarization with using model as forecasting tool
- analyzing impacts of development on pristine and moderately impacted rivers

If bank erosion along the Rum River doubled TSS, what would be the impacts? Use **Lab4\_Rum R MN.aps**.

If summer houses with septic tanks doubled TP in the Crow Wing River, what would be the impacts? Use **Lab4\_Crow Wing R MN.aps**.

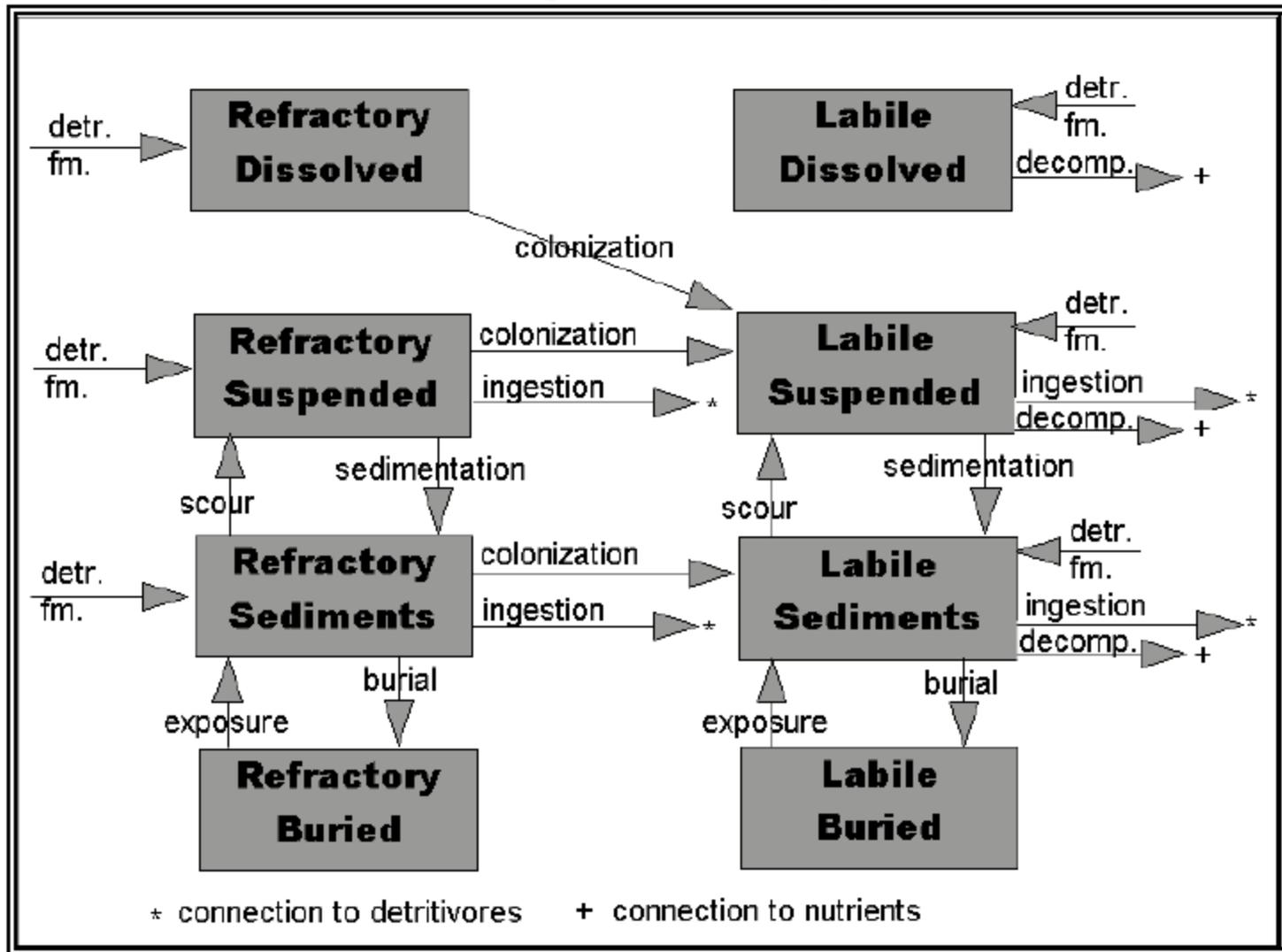
You can set up the simulations and let them run during the next lecture, then we will discuss the results.

# Remineralization

- Detritus
- Variable stoichiometry
- Nutrients
- Variable pH
- Dissolved oxygen and anoxia

# Detritus Compartments in AQUATOX

Figure 54  
Detritus Compartments in AQUATOX



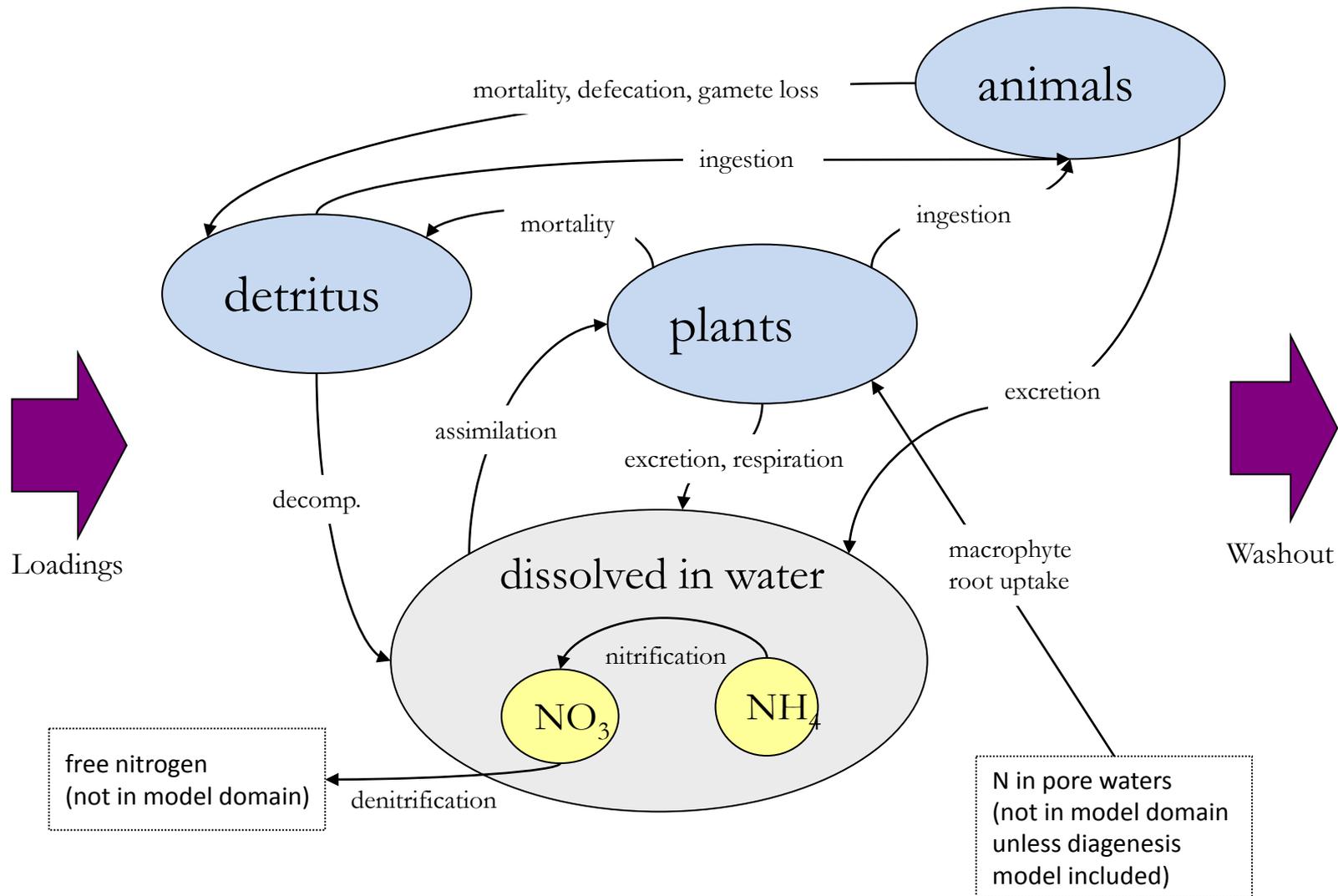
# Variable Stoichiometry

- Ratios of elements in organic matter are editable on an organism by organism basis as well as for detrital state variables.
- Stoichiometry can vary among compartments but is constant within a compartment
- Nutrient mass balance tracked to machine accuracy (nitrogen & phosphorus).
- Nutrient fate can be tracked as well as mass of nutrients dissolved in water, in detritus, in animals, and in plants.

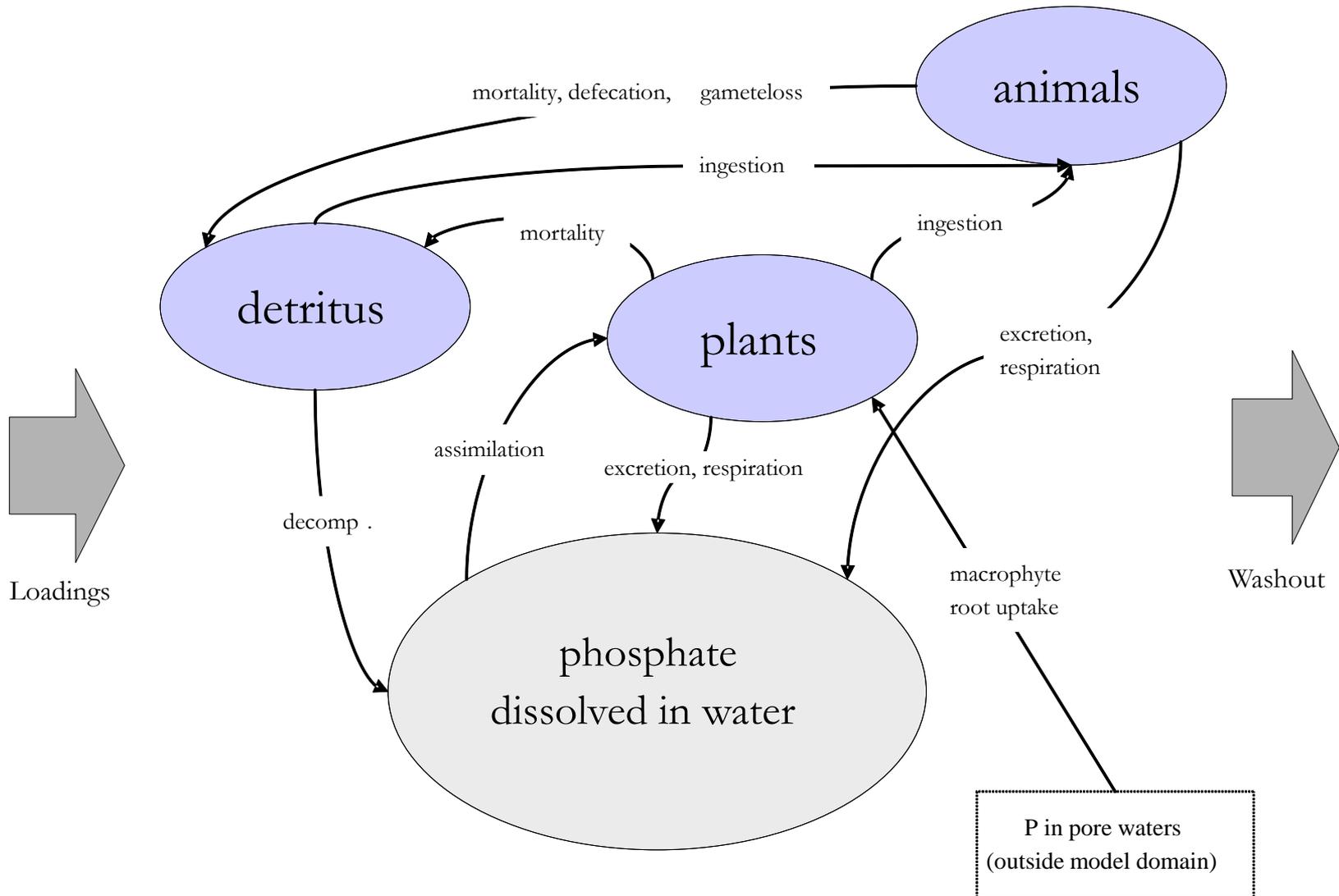
# Default Nutrient to Organic Matter Ratios

<b>Compartment</b>	<b>Frac. N (dry)</b>	<b>Frac. P (dry)</b>	<b>Reference</b>
Refrac. detritus	0.002	0.0002	Sterner & Elser 2002
Labile detritus	0.059	0.007	same as phytoplankton
Phytoplankton	0.059	0.007	Sterner & Elser 2002
Bl-greens	0.059	0.007	same as phytoplankton for now
Periphyton	0.04	0.0044	Sterner & Elser 2002
Macrophytes	0.018	0.002	Sterner & Elser 2002
Cladocerans	0.09	0.014	Sterner & Elser 2002
Copepods	0.09	0.006	Sterner & Elser 2002
Zoobenthos	0.09	0.014	same as cladocerans for now
Minnows	0.097	0.0149	Sterner & George 2000
Shiner	0.1	0.025	Sterner & George 2000
Perch	0.1	0.031	Sterner & George 2000
Smelt	0.1	0.016	Sterner & George 2000
Bluegill	0.1	0.031	same as perch for now
Trout	0.1	0.031	same as perch for now
Bass	0.1	0.031	same as perch for now

# Nutrient Cycle in AQUATOX (Nitrogen)

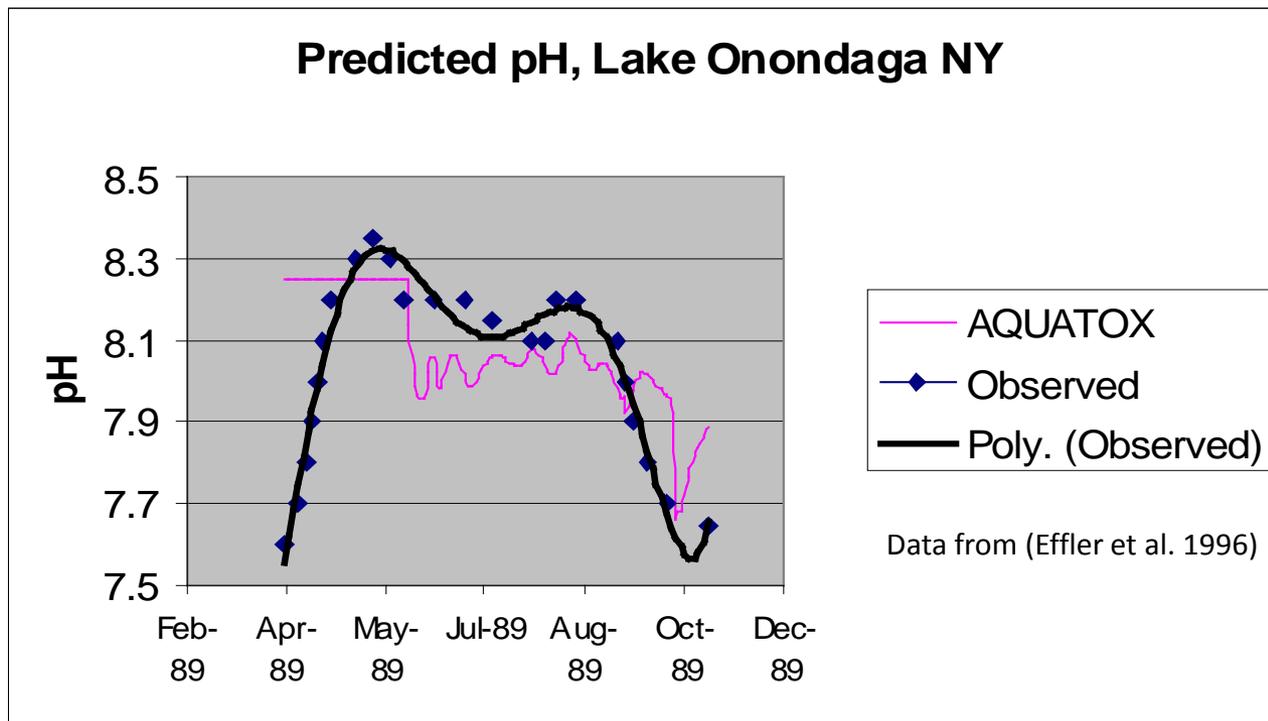


# Nutrient Cycle in AQUATOX (Phosphorus)



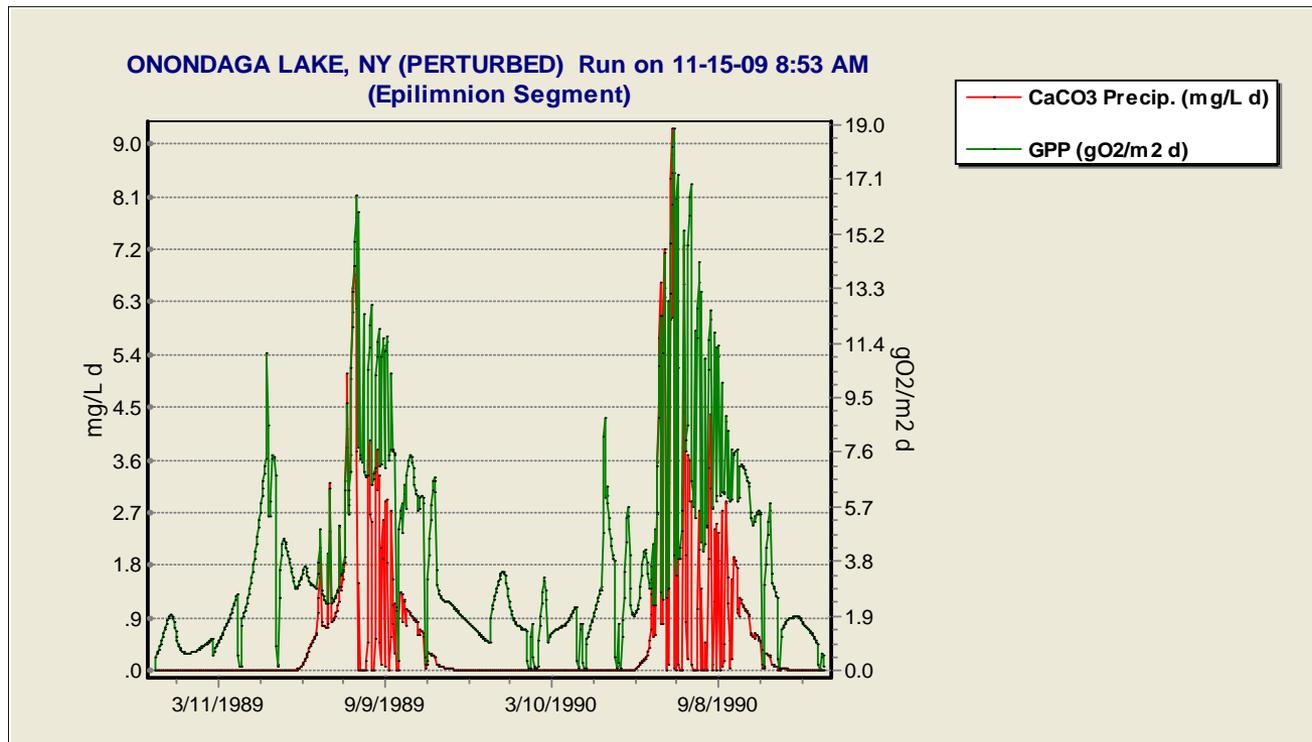
# Dynamic pH also added to variable stoichiometry version:

semi-empirical computation employed for simplicity as in (Small and Sutton 1986; Marmorek et al. 1996) :



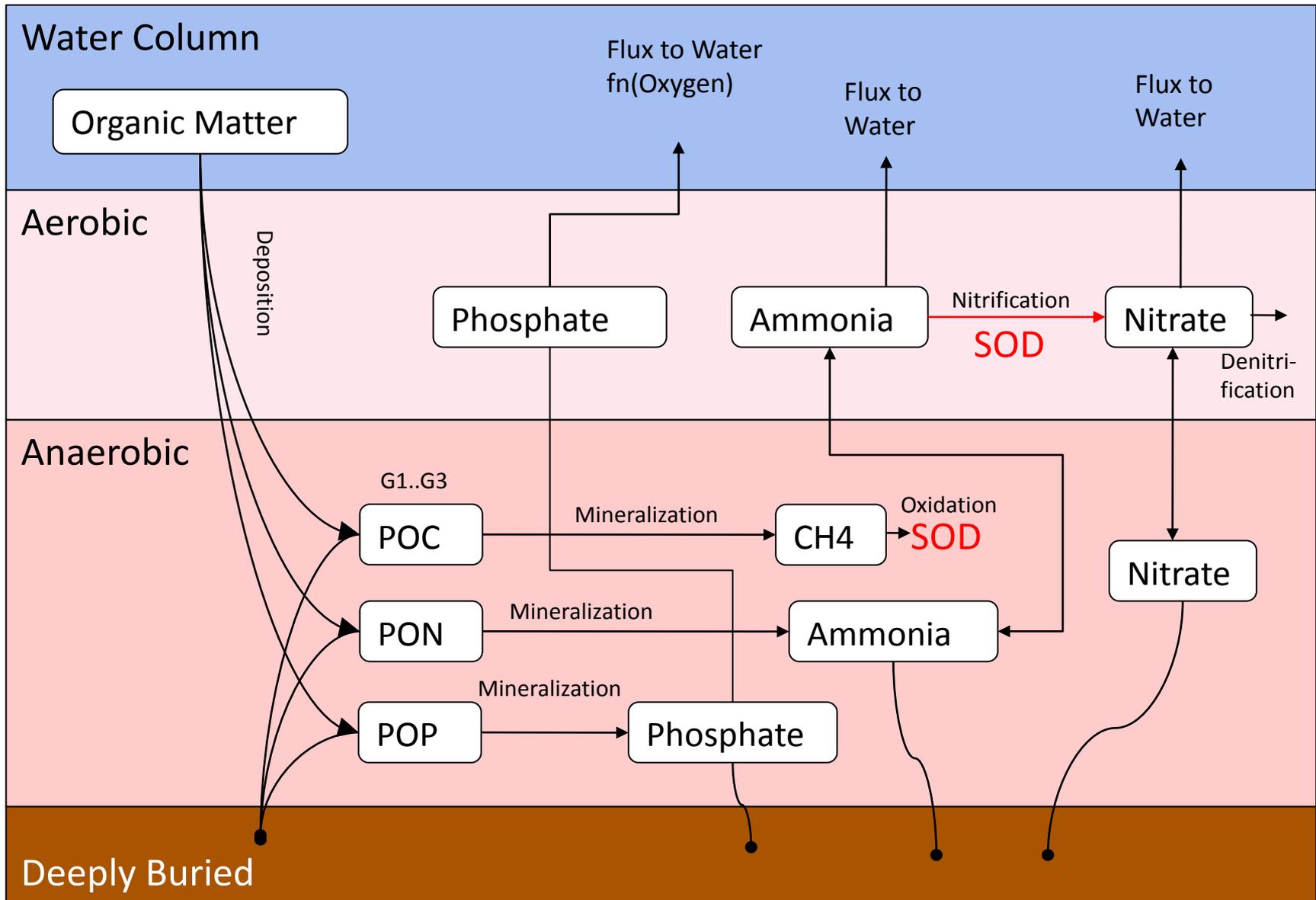
# Calcium Carbonate Precipitation

- Predicted as a function of pH and algal type
  - When pH  $\geq 7.5$ , precipitation is predicted
  - Precipitation rate is dependent on photosynthesis rate (gross primary production) in some, but not all, plants
- $\text{CaCO}_3$  sorbs phosphate from the water column



# 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 (Di Toro, 2001)

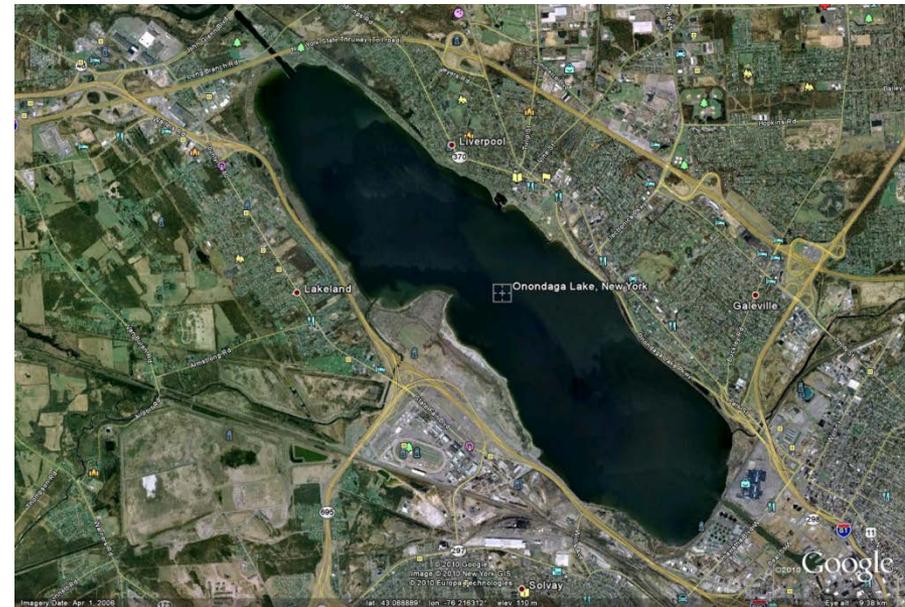


# Key Points: Diagenesis Model

- 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 oxidized 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
- Steady-state mode dramatically reduces execution time

# Sediment Diagenesis Demo

- Lake Onondaga, NY
  - Significant nutrient inputs from wastewater treatment plant; combined sewers
  - successive algal blooms
  - hypoxia in hypolimnion
  - build-up of organic sediments in bottom
  - More details to follow!



# Sediment Bed Initialization

AQUATOX\_Sed\_Bed\_Inputs.xls

INPUTS			AQUATOX "CLASSIC" PARAMS			SED-DIAGENESIS PARAMS		
Name	Value	Units	Name	Value	Units	Name	Value	Units
foc	0.01	frac OC	L Detr Sed	37.2	g/m2	POC G1	196	g C/m3
depth	0.1	meters	R Detr Sed	3683	g/m2	POC G2	38766	g C/m3
sed dens.	3720	kg/m3				POC G3	196	g C/m3
frac. Labile	0.01					PON G1	29	g N/m3
<b>Diagenesis Only:</b>						PON G2	147	g N/m3
frac G3 (nonreactive)	0.01					PON G3	0.7	g N/m3
<b>Diagenesis Assumptions:</b>						POP G1	6.7	g P/m3
P to Org, Refr	0.0002	frac dry				POP G2	14.7	g P/m3
N to Org, Refr	0.002	frac dry				POP G3	0.07	g P/m3
P to Org, Labile	0.018	frac dry						
N to Org, Labile	0.079	frac dry						
C to Org, All	0.526	frac dry						

# Sediment Diagenesis Parameters

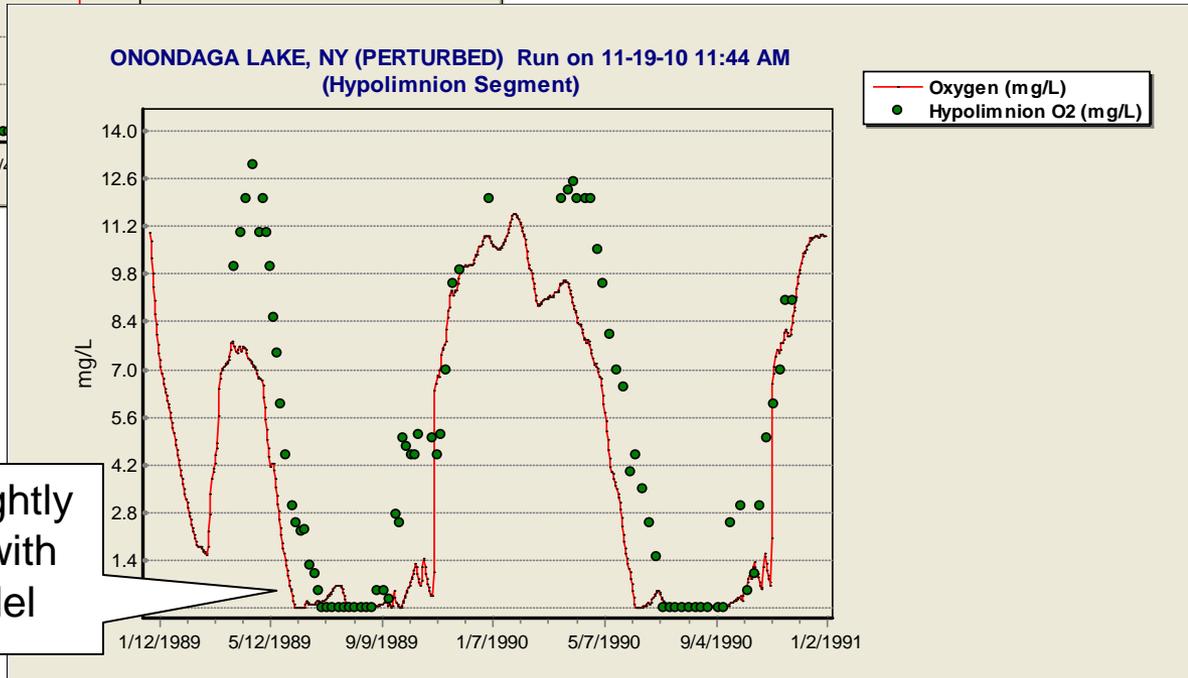
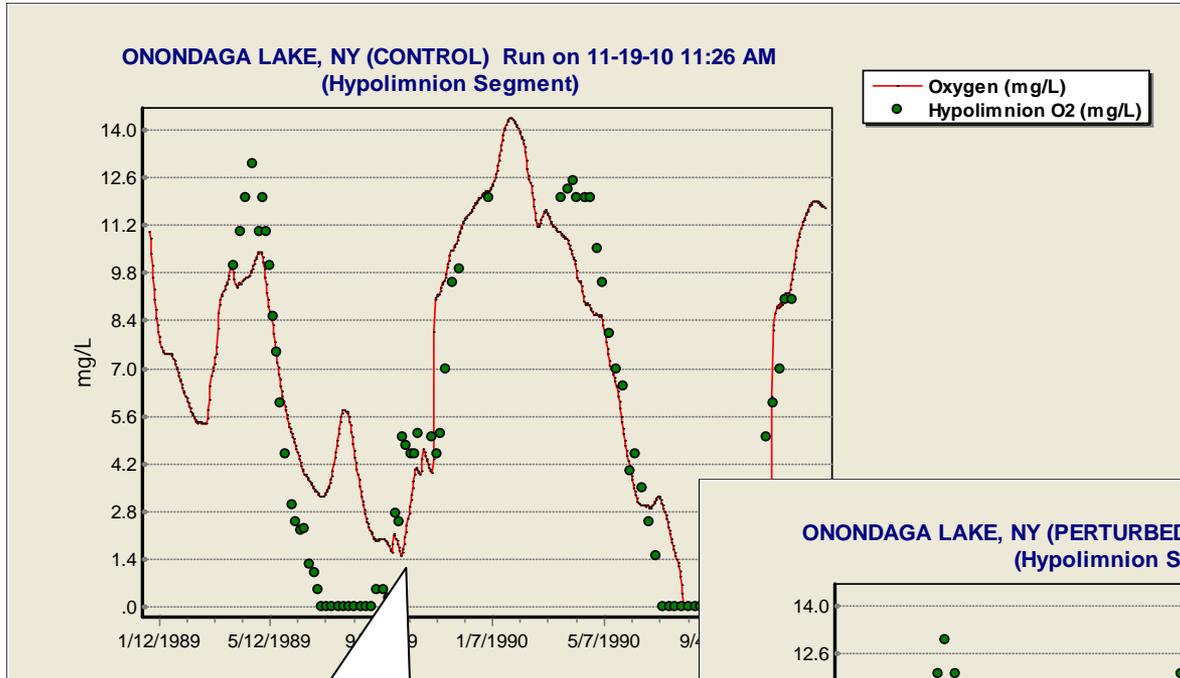
Edit Sediment Diagenesis Parameters

Symbol	Value	Units	Description	Comment
m1	0.5	kg/L	Solids concentration in layer 1	
m2	0.5	kg/L	Solids concentration in layer 2	
H1	0.01	m	Thickness of sediment aerobic layer 1	1 mm default, r
Dd	0.001	m <sup>2</sup> /d	pore water diffusion coefficient	
w2	0.0003	m/d	Deep burial velocity	(Q2K uses 0.0)
H2	0.1	m	Thickness of sediment anaerobic layer 2	
KappaNH3f	0.131	m/d	Freshwater nitrification velocity	(Cerco and Co
KappaNH3s	0.131	m/d	Saltwater nitrification velocity	
KappaNO3_1f	0.1	m/d	Freshwater denitrification velocity	(Cerco and Co
KappaNO3_1s	0.1	m/d	Saltwater denitrification velocity	
KappaNO3_2	0.25	m/d	Denitrification in the anaerobic layer 2	

Copy to All Segments      Save Table to Excel      Help      Cancel      OK

Copy Diagenesis Parameters

# Results are Improved



Hypoxia not predicted before addition of diagenesis

Perhaps even slightly "overpredicted" with diagenesis model

# **AQUATOX also simulates:**

- Diel oxygen
- Effects of low dissolved oxygen
- Ammonia toxicity

# **AQUATOX as a Part of BASINS**

Integration of tools

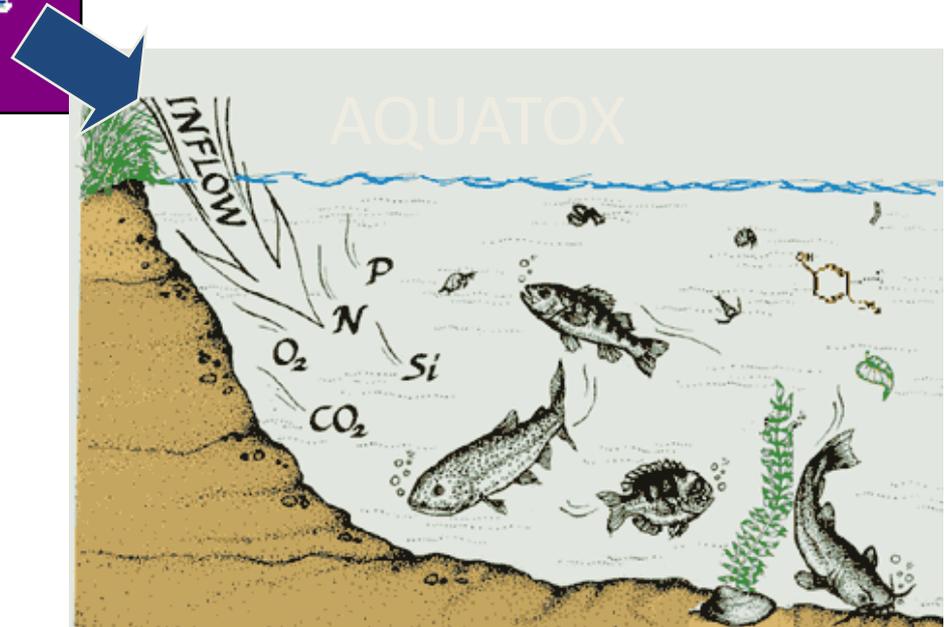
# AQUATOX BASINS Linkage



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



# BASIN GIS System Overview

Web Data Download Tool



**Political Boundaries**  
**TIGER Line and Census Data**  
**Monitoring Data**  
**Hydrography**  
**Land Use**  
**Digital Elevation Data**  
**State Soils Data**  
**Meteorological Data (Weather Stations)**

**Additional User Supplied Data**

## Tools and Utilities

**Watershed Reports**  
  
**WDMUtil**  
  
**Watershed Delineation**  
  
**Parameter Estimation**  
**PEST**  
  
**HSPFParm**  
  
**DFLOW**

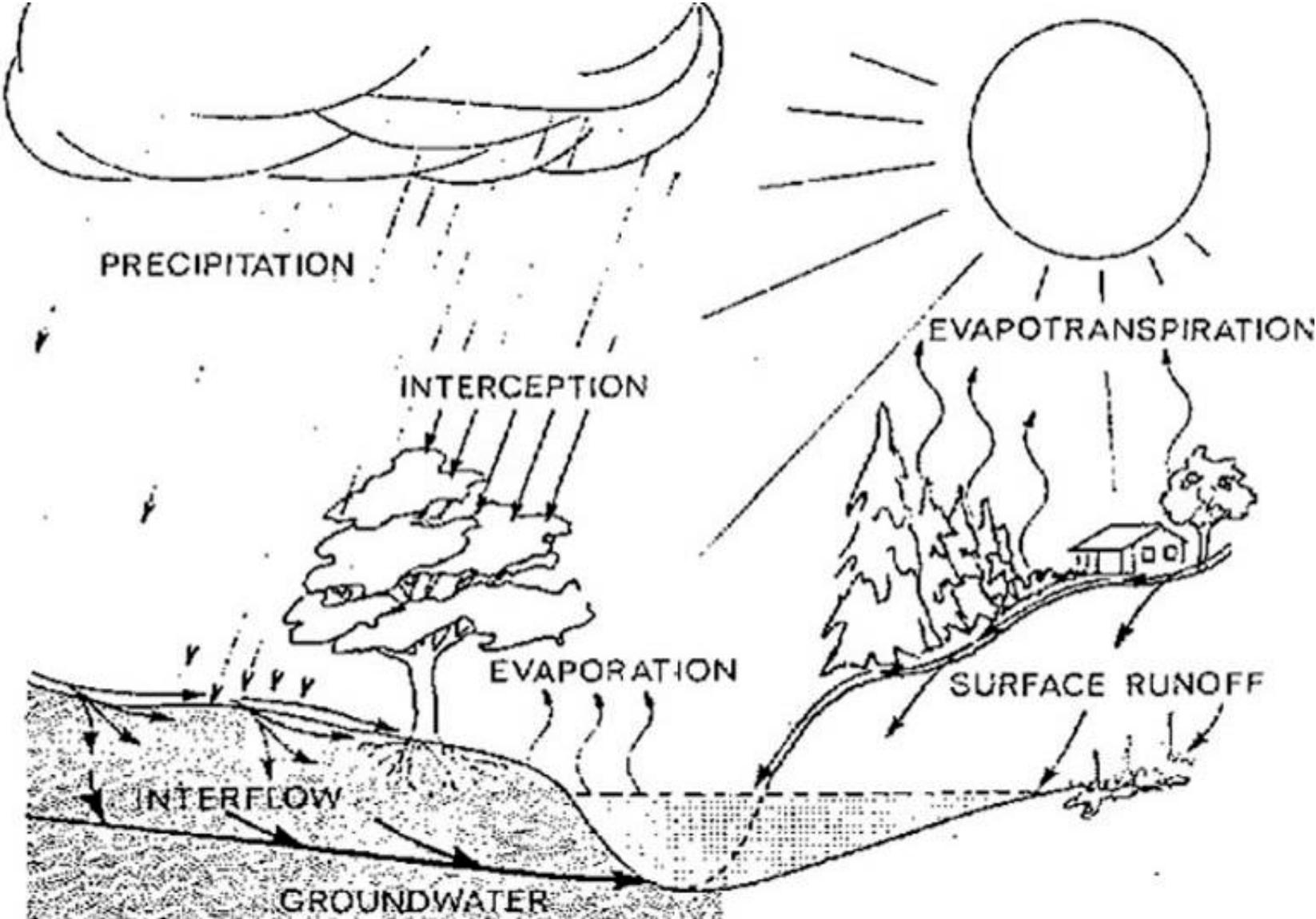
## Models

**HSPF/WinHSPF**  
  
**AQUATOX**  
  
**Pollutant Loading Estimator**  
  
**SWAT**  
  
**SWMM**  
  
**WASP**  
  
**GWLF (Coming Soon)**

## Decision Making and Analysis

**PostProcessing**  
**GenScn**  
  
**Reporting/Scripts**  
**Watershed Management**  
**Sensitivity Analysis**  
**Climate Analysis**  
  
**Nutrient Management**  
  
**Source Water Protection**  
**TMDLs**  
**UAAs**  
**Project Archive**

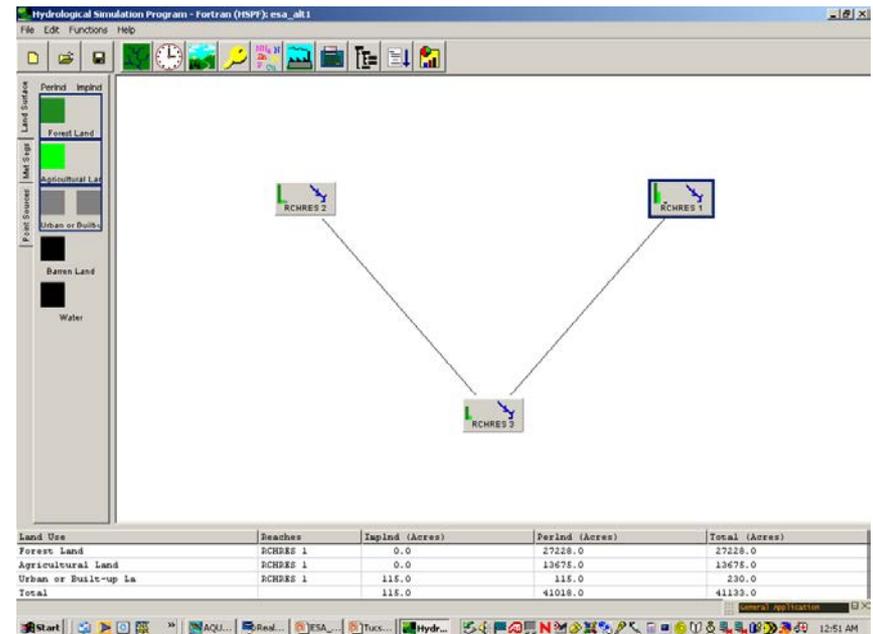
# Simplified Hydrologic Model



# WinHSPF

## Hydrologic Simulation Program–FORTRAN

- Predicts loadings in mixed land use settings for bacteria, metals, *sediments, nutrients, algae as Chlorophyll a*
- Considers point source and nonpoint source loadings
- Natural and developed watersheds and water systems
- Continuous simulation, hourly meteorology
- Lumped parameters by landuse/watershed
- **AQUATOX 3.1 will include a link to HSPF (external to BASINS)**

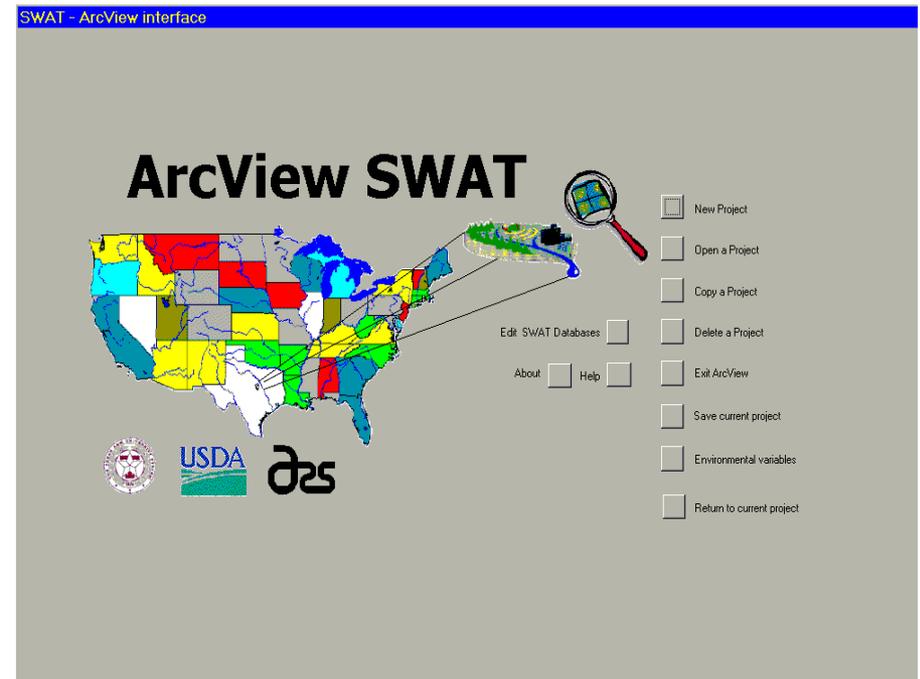


*Note: red indicates parameter that may be loaded into AQUATOX*

# SWAT

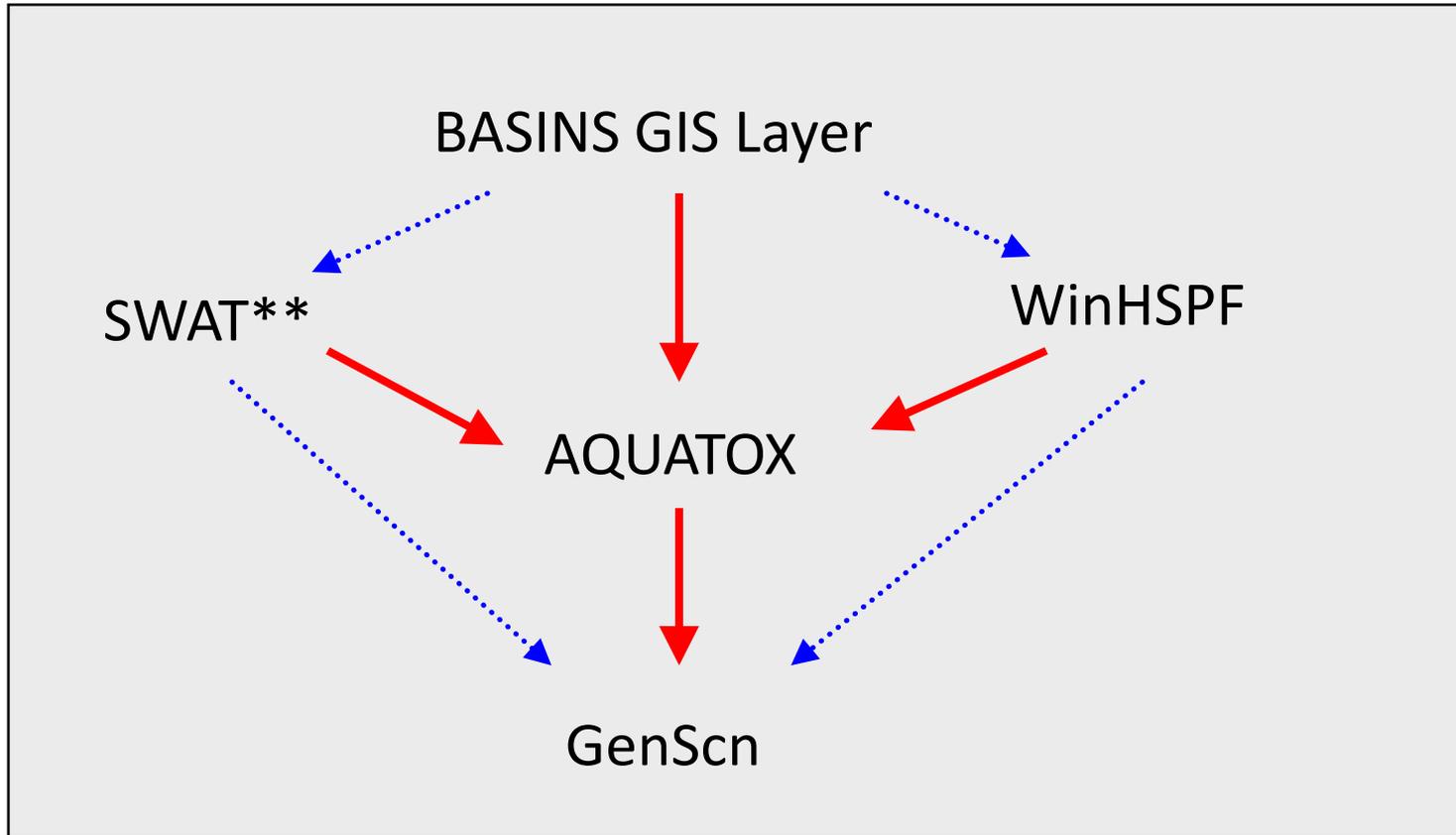
## Soil and Water Assessment Tool

- Physically-based, watershed scale model
- Predicts impacts of land management practices on water, sediment, and agricultural chemical yields in large complex watersheds
- Models *water and sediment movement, nutrient cycling*, crop growth, metals, *pesticides*, etc.
- *Current AQUATOX linkage only to SWAT in BASINS 3.1, due to different SWAT version in BASINS 4*



**Note: red indicates parameter that can be loaded into AQUATOX**

# Linkages Between Models



Linkage within BASINS



Linkage to AQUATOX  
(\*BASINS 3.1 only)

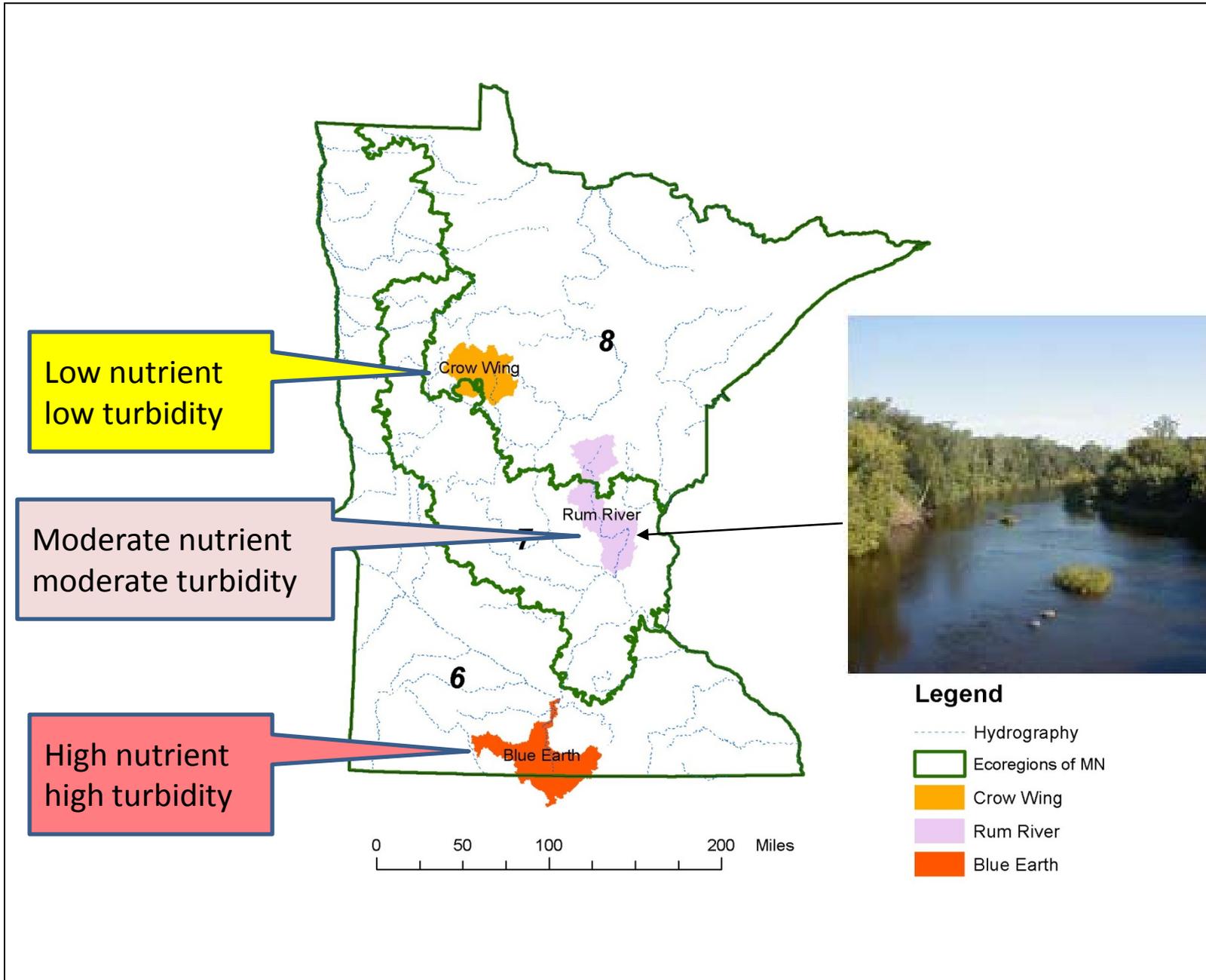
# Potential Applications

- Evaluate potential effects of land use changes on aquatic biota
- Evaluate whether BMPs will lead to attainment of water quality standards
- Using new Climate Assessment Tool (CAT) linked to HSPF, evaluate effects of climate change on aquatic ecosystems
- Etc....

# 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

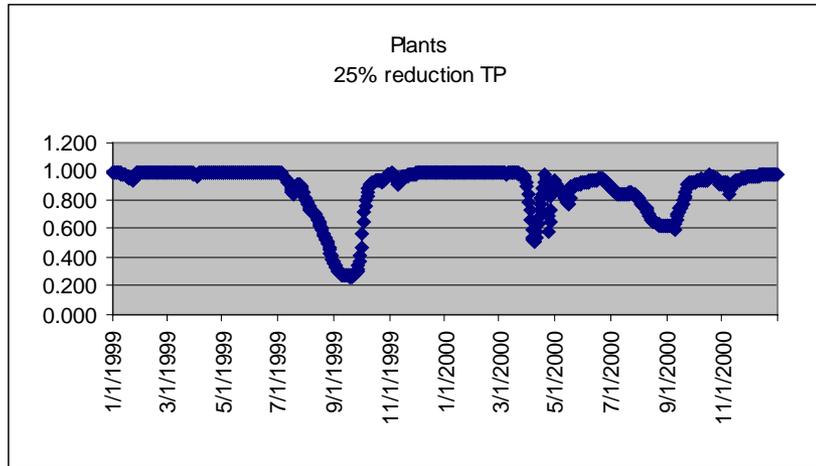


# Example Nutrient Analyses from Minnesota

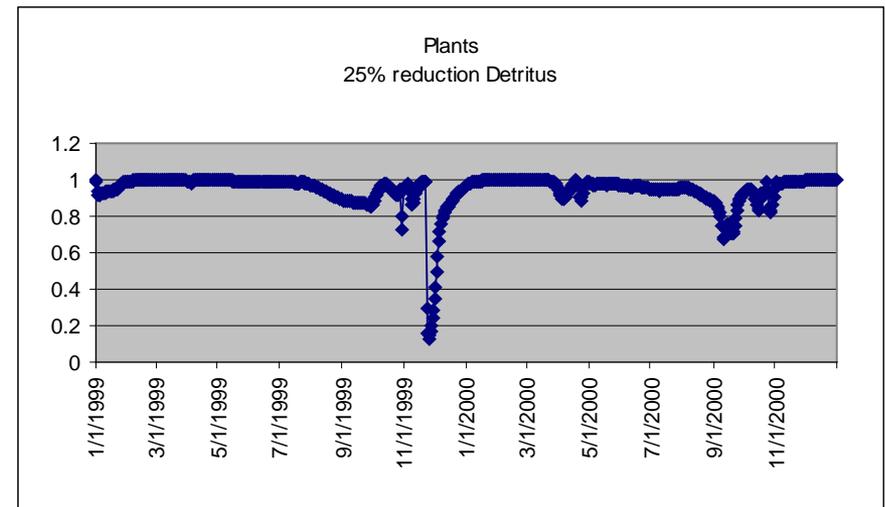
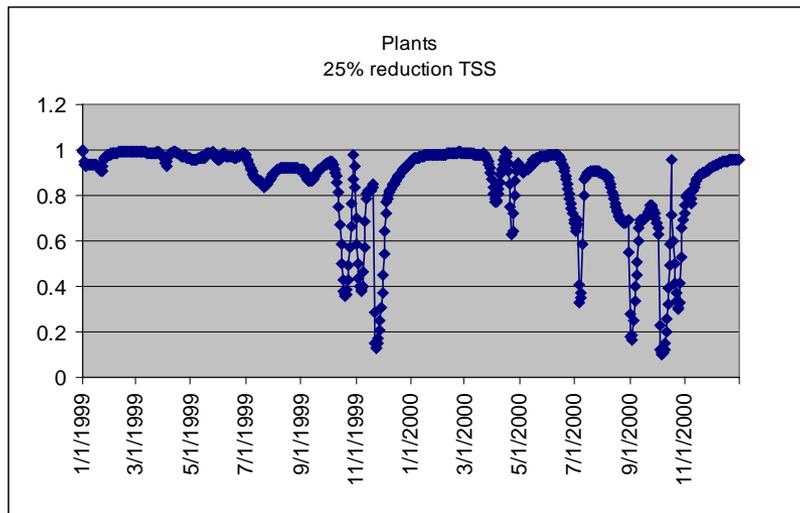
- Calibrated AQUATOX across nutrient gradient
- Set up HSPF, linked loadings to AQUATOX
- Ran iterative simulations with various nutrient reductions
- Applied 2 ways of developing nutrient target
  - Method #1: Accept existing chl *a* target, use AQUATOX to get corresponding TP level
  - Method #2: Use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



- Reductions in TSS and TP loadings had significant effects on algal community
- BOD reductions had only short-lived effects
- NO<sub>3</sub> and NH<sub>3</sub> reductions had little effect



## Step 2: Run AQUATOX with multiple load reduction scenarios.

Calculate and compare Mean TP and Chl a

	TP/TSS multiplier	Mean TP (ug/L)	Mean chl_a (ug/L)
Baseline condition	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
	<b><i>Ecoregional criteria</i></b>	<b><i>118.13</i></b>	<b><i>7.85</i></b>

# Step 3a: Water Quality Target Development

## Method #1

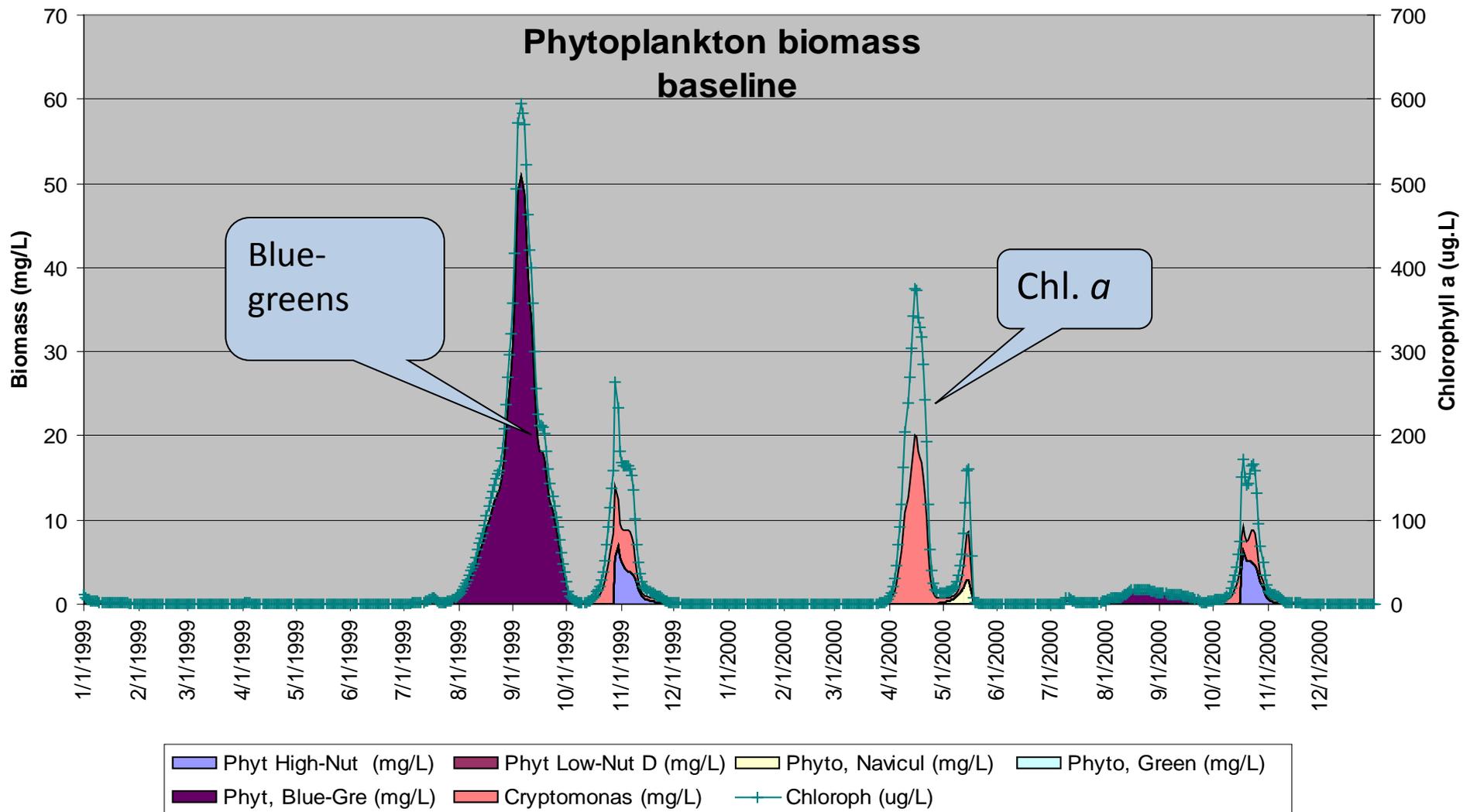
- Focus on TP and chl *a* only
- Model results: 80% TP reduction required to meet 7.85 ug/L chl *a*
- Ecoregional WQC: 56% TP reduction required to meet same chl *a* level

# Step 3b: Water Quality Target Development

## Method #2

- Focus on algal community, not total chl *a*
  - Blue Earth had periodic blooms of blue-green algae (cyanobacteria)
    - Noxious, 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?

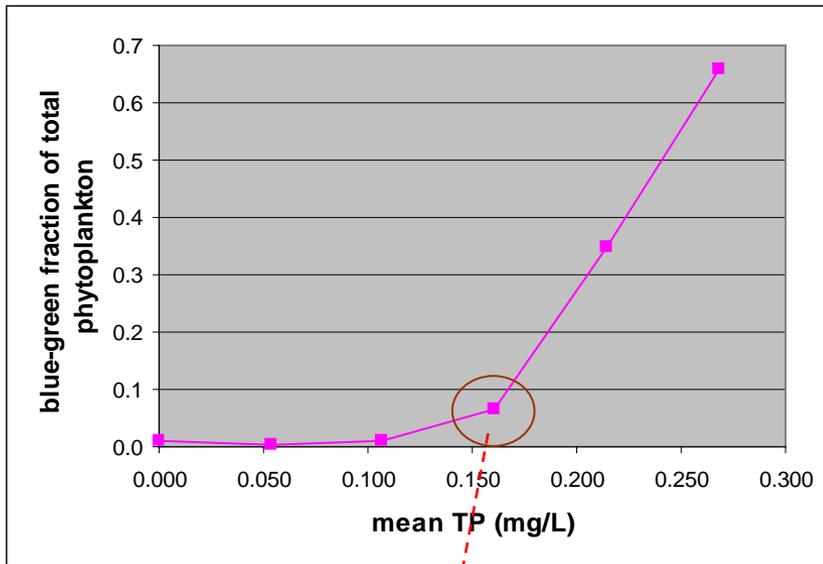
# Algal Composition Changes Seasonally and from year to year



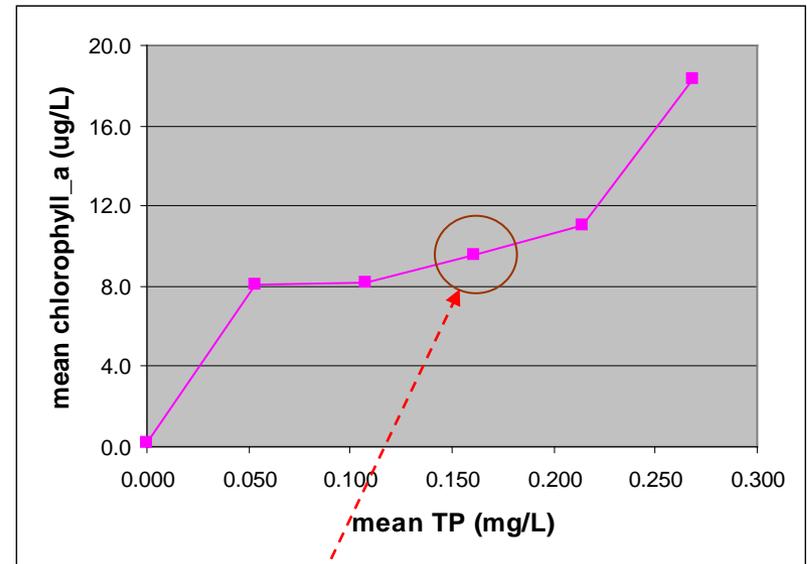
# Target Development

- Method 2: 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<sub>a</sub>.

*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).
  - Decision of “acceptable” target is policy question
- 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

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

# Demonstration: 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

AQUATOX-- Main Window - [Linked System Mode: "Linked\_LBR\_10-24-07.als"]

File View Library Study Sediment Window Help

Linked System Name: **Linked LBR**

**Perturbed:** 10-24-07 10:37 PM **Control Run:** No Ctrl. Run Recorded

Show Segment Data  Show Link Data

- [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
- [MID]: West Point WWTF

Hide Tributary-Input Segments

Add Delete Edit

**Data Operations:**

- Chemicals
- Setup
- Notes
- Help

**Program Operations:**

- Perturbed
- Control
- Linked Output
- Export Results

R.M. = River Mile

Major Wastewater Treatment Plants

Major Tributaries

Load Map Clear Map

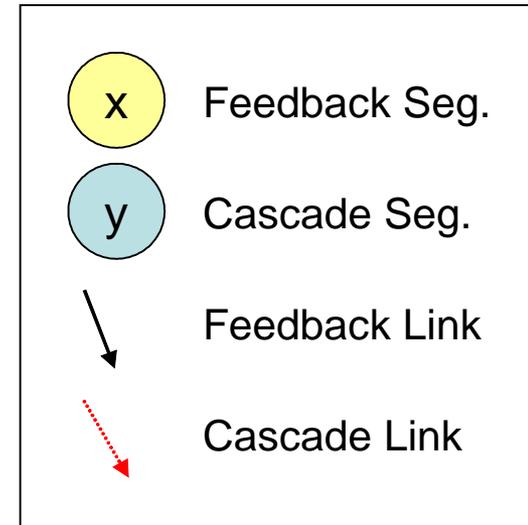
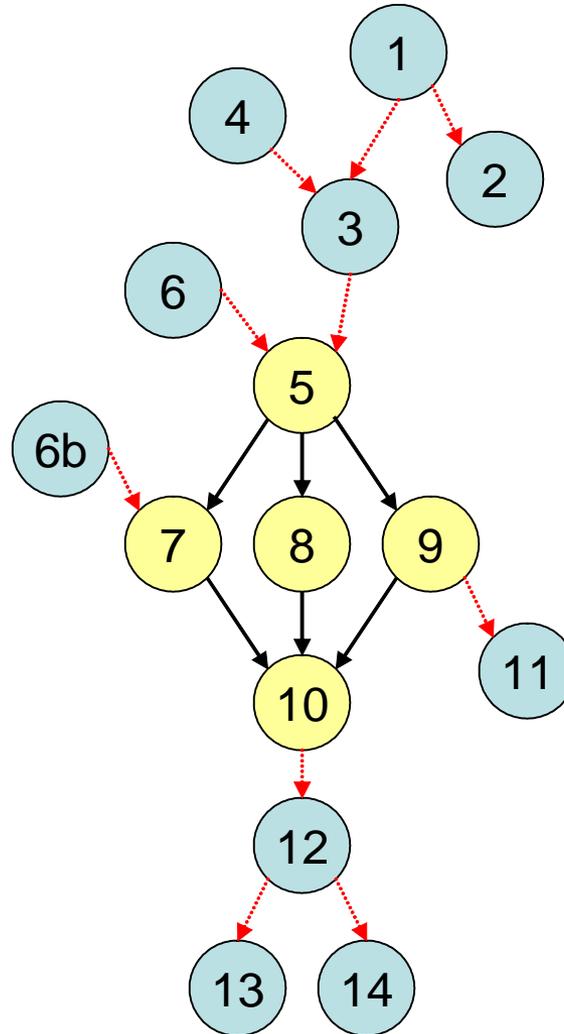
# Cascade & Feedback Linkages

## 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
  - 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

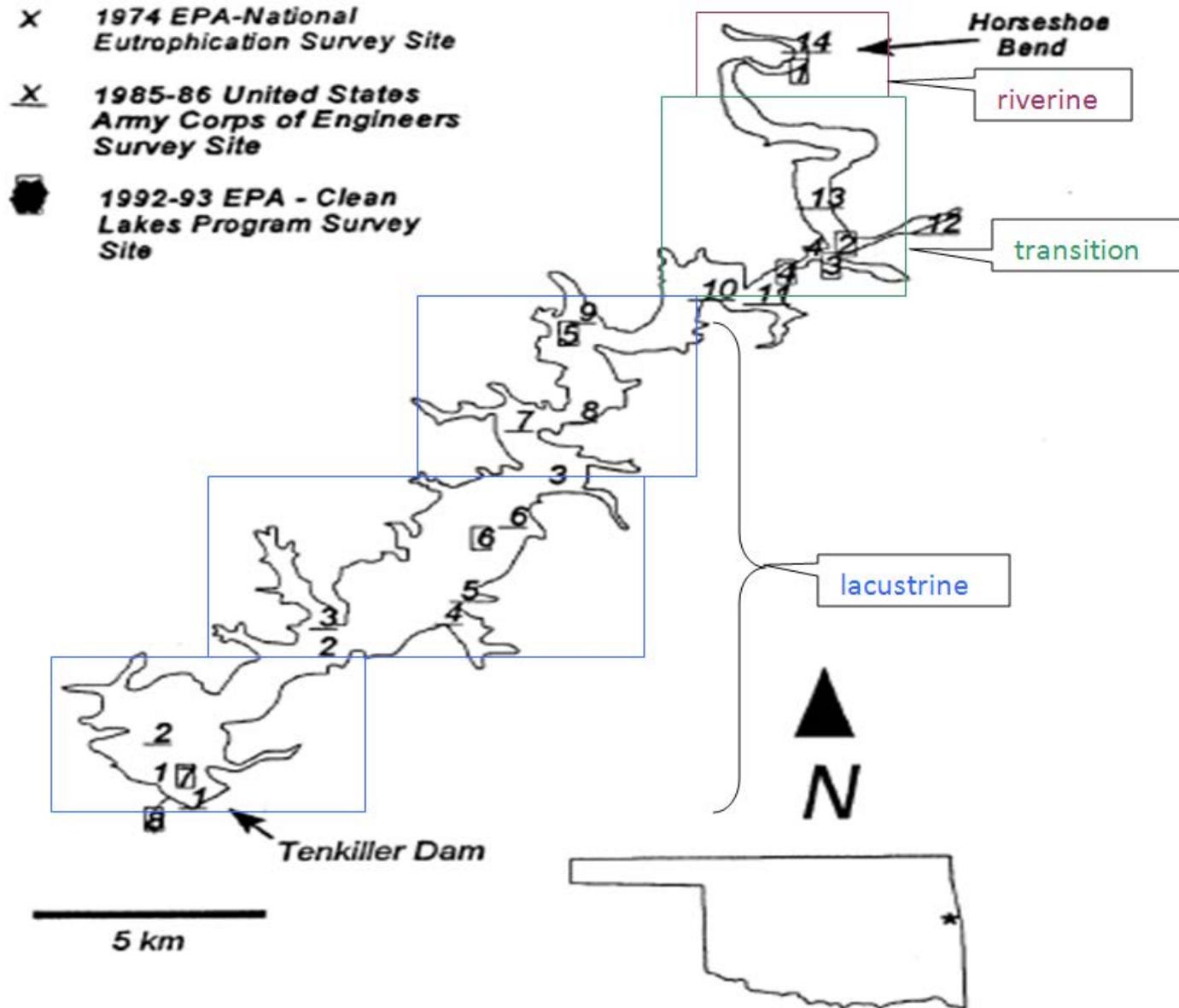
Interface Demonstration to follow

# Modeling Nutrients for Criteria Support in Tenkiller Lake, OK

## 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, OK



# 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

Add Delete Edit

**Data Operations:**

- Chemicals
- Setup
- Notes
- Help

**Program Operations:**

- Perturbed
- Control
- Linked Output
- Export Results

The map displays the Tenkiller Lake system with several key features:

- Survey Sites:** 1974 EPA-National Eutrophication Survey Site (marked with an 'X'), 1985-86 United States Army Corps of Engineers Survey Site (marked with an 'X'), and 1992-93 EPA - Clean Lakes Program Survey Site (marked with a house icon).
- Geographic Features:** Horseshoe Bend, Tenkiller Dam, and a 5 km scale bar.
- System Zones:** riverine (top), transitionn (middle), and lacustrine (bottom).
- Segment Markers:** Numbered markers 1 through 14 along the river and lake system.

Load Map Clear Map

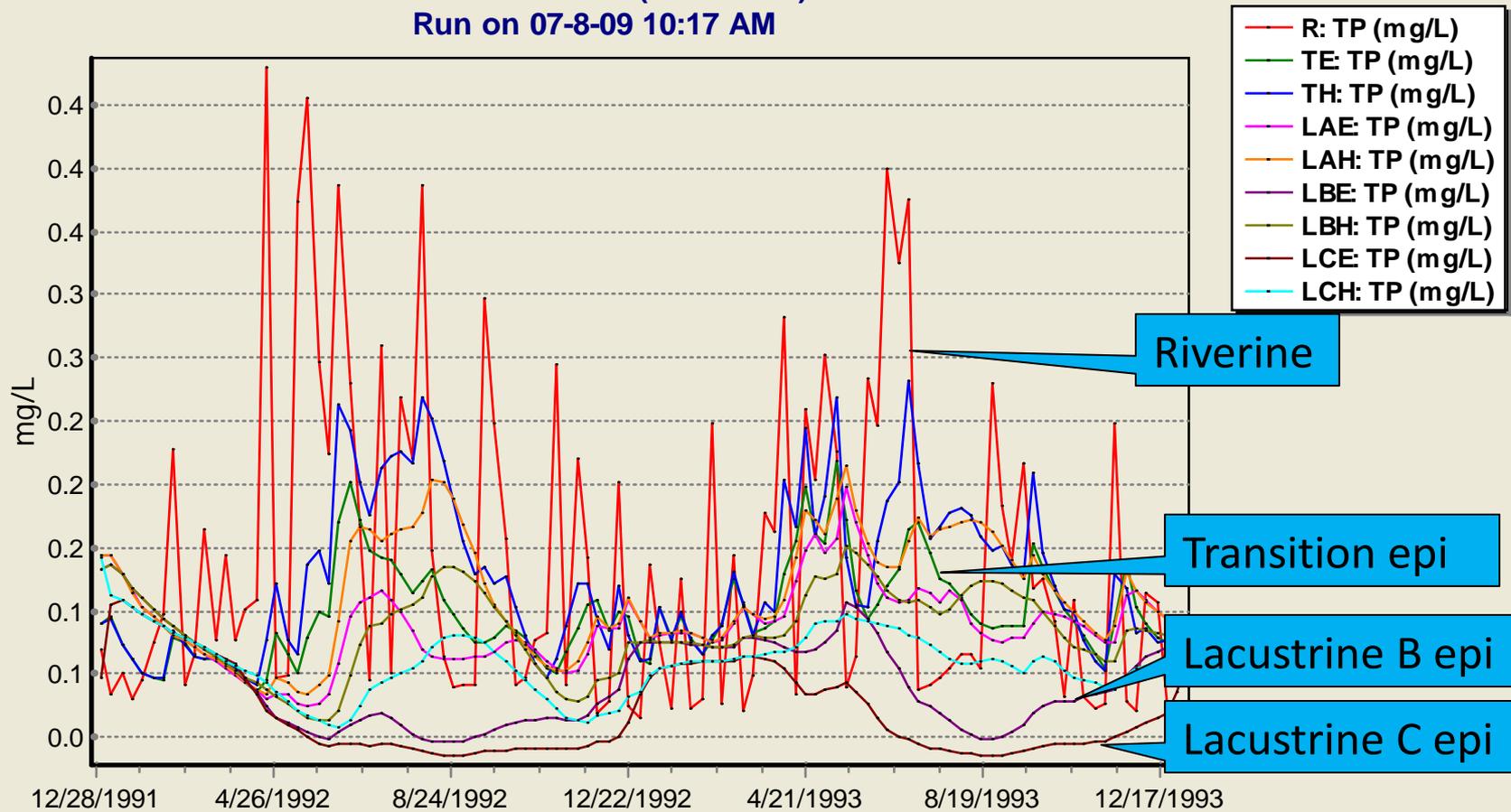
# Storm-water plume, algae-rich riverine segment

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

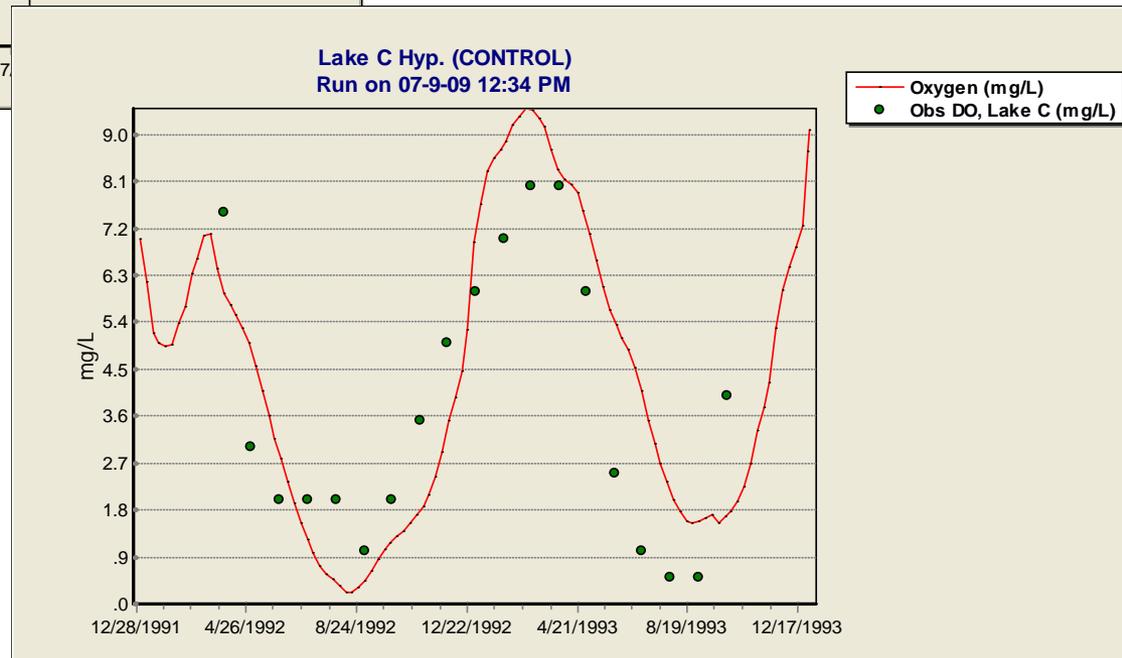
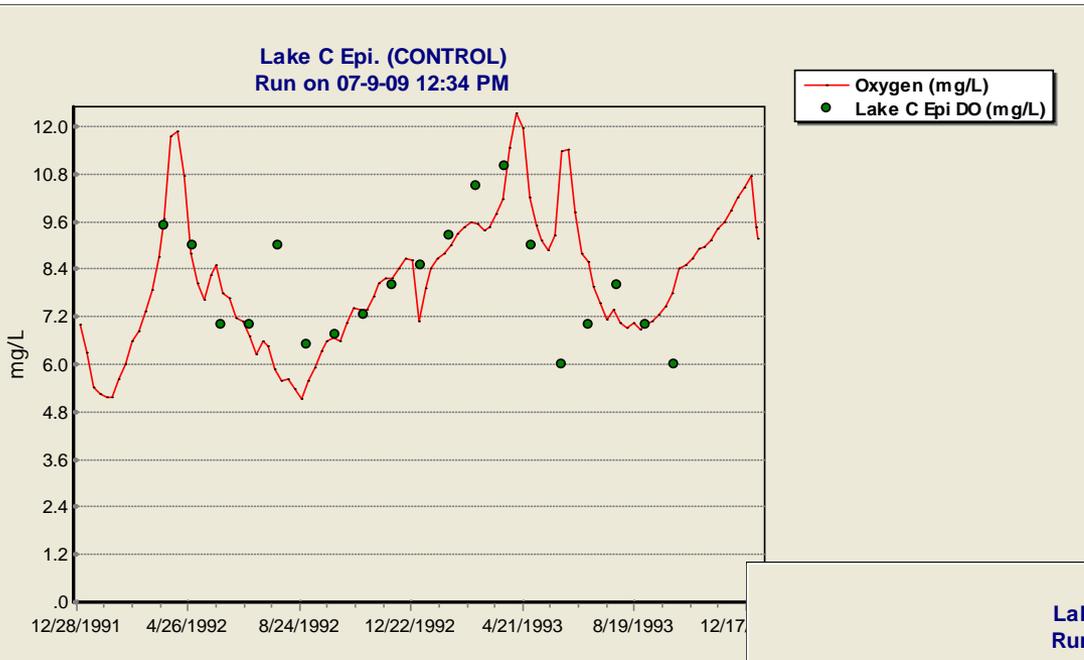


# Total phosphorus in water column decreases toward dam; loss to sediments is simulated

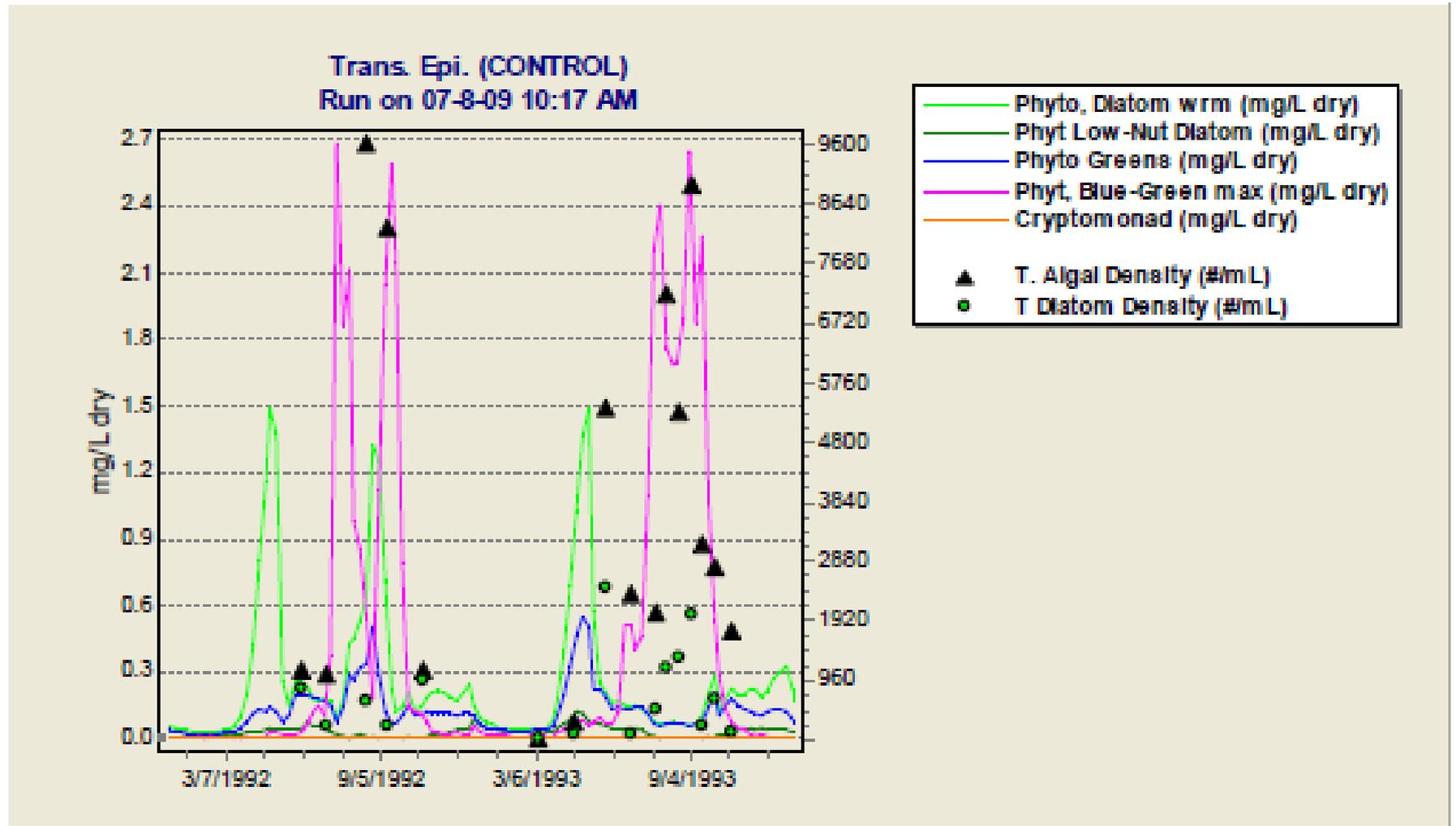
Tenkiller Linked (CONTROL)  
Run on 07-8-09 10:17 AM



# Simulated and observed dissolved oxygen in Lacustrine C

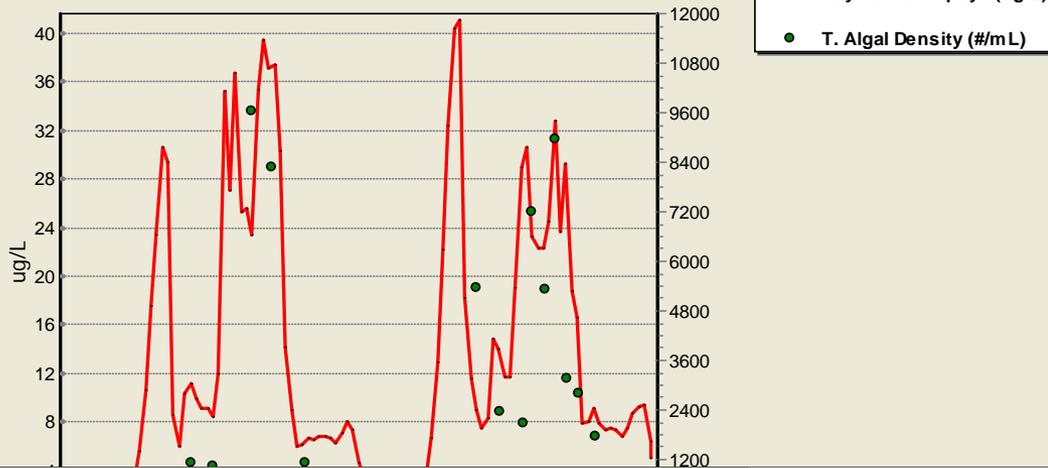


# Simulated & observed algal composition in epilimnetic Transition

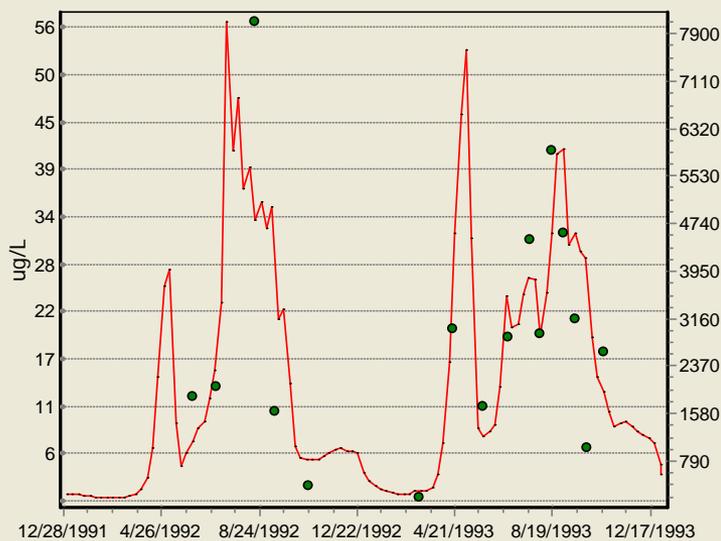


# Simulated chlorophyll *a* and observed algal density in Transition and Lacustrine A and B

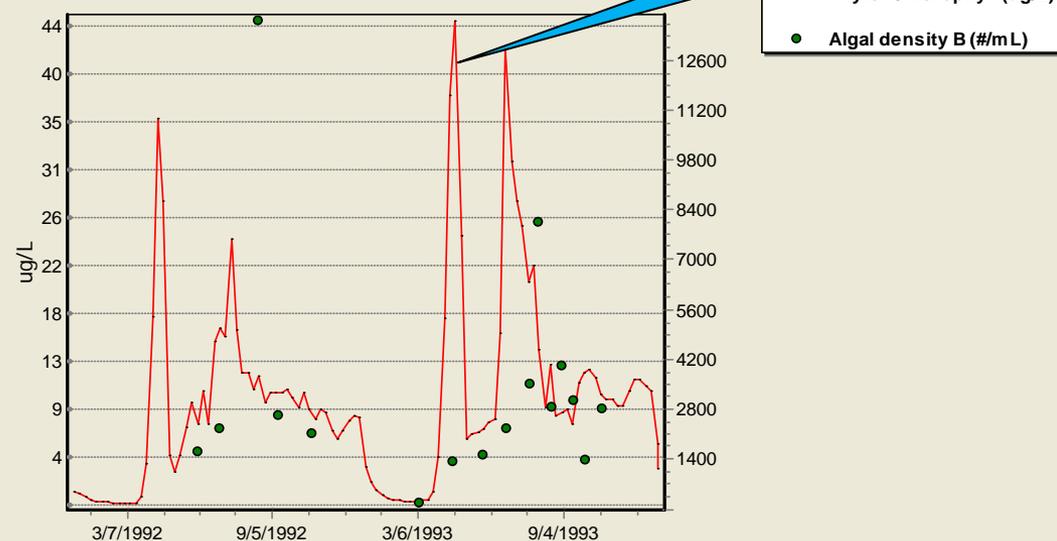
Trans. Epi. (CONTROL)  
Run on 07-9-09 12:34 PM



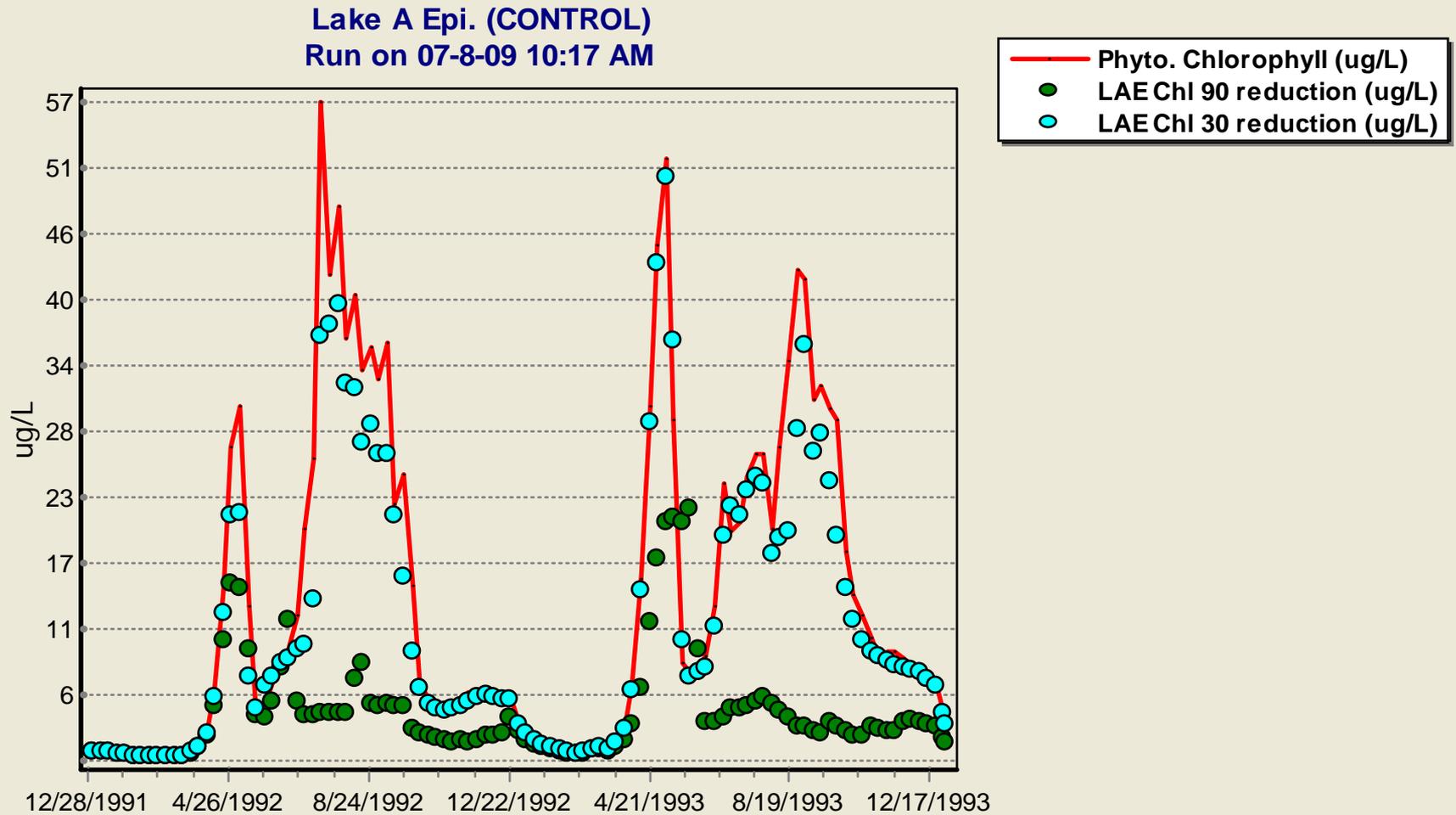
Lake A Epi. (CONTROL)  
Run on 07-9-09 12:34 PM



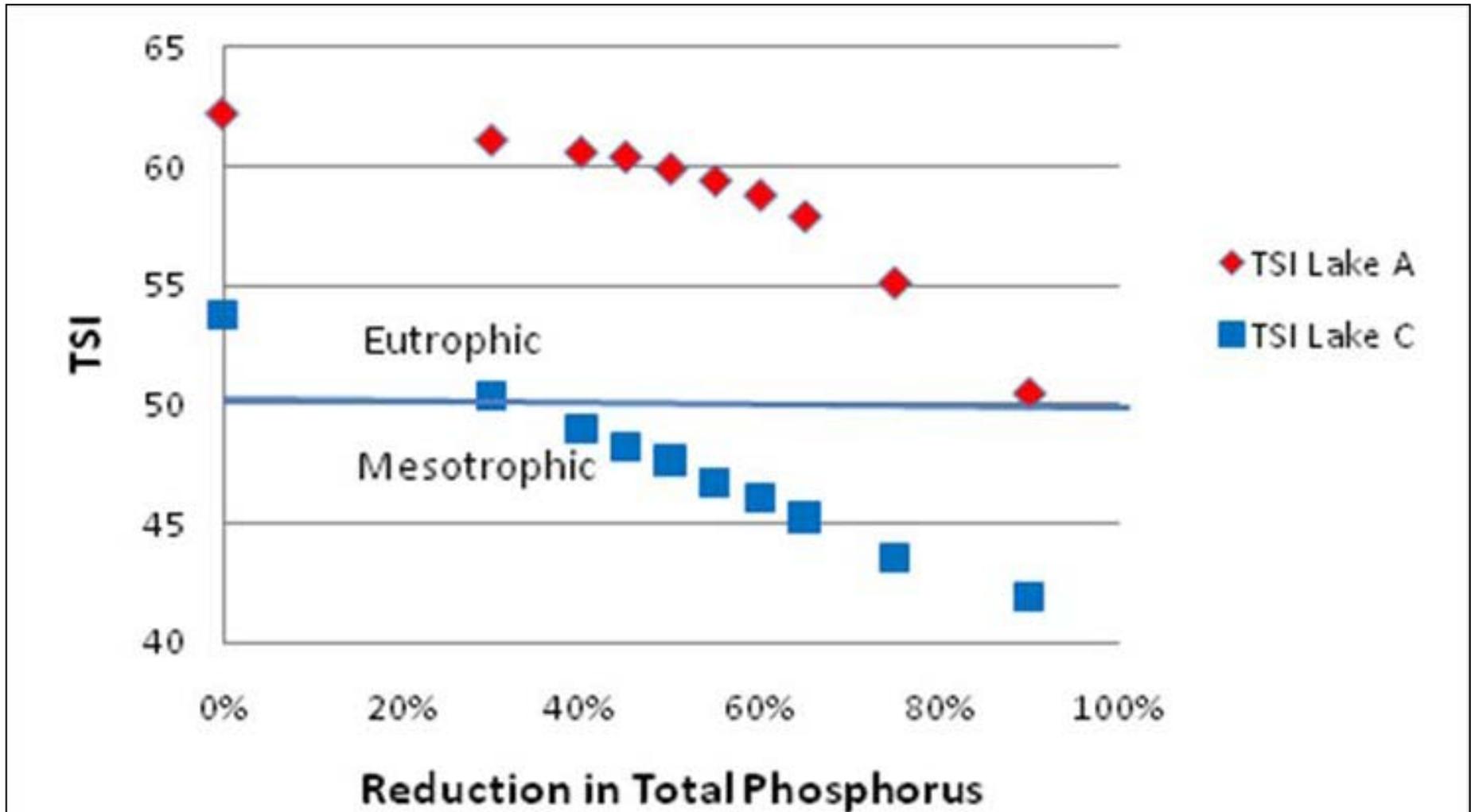
Lake B Epi. (CONTROL)  
Run on 07-9-09 12:34 PM



# 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



# Lab 5 – Analysis of the Nutrient Status of DeGray Lake, Arkansas

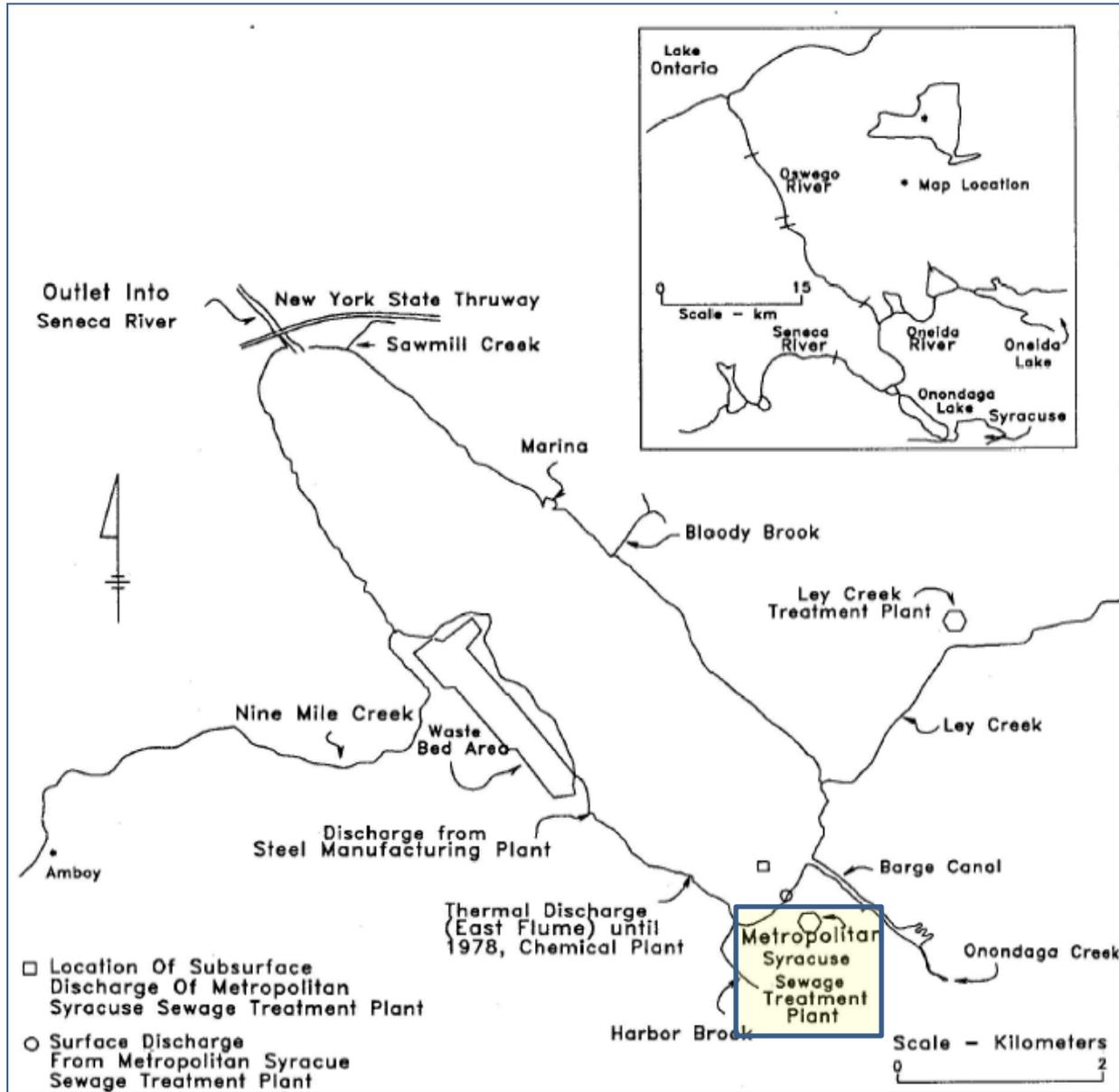


# Lake Onondaga, NY

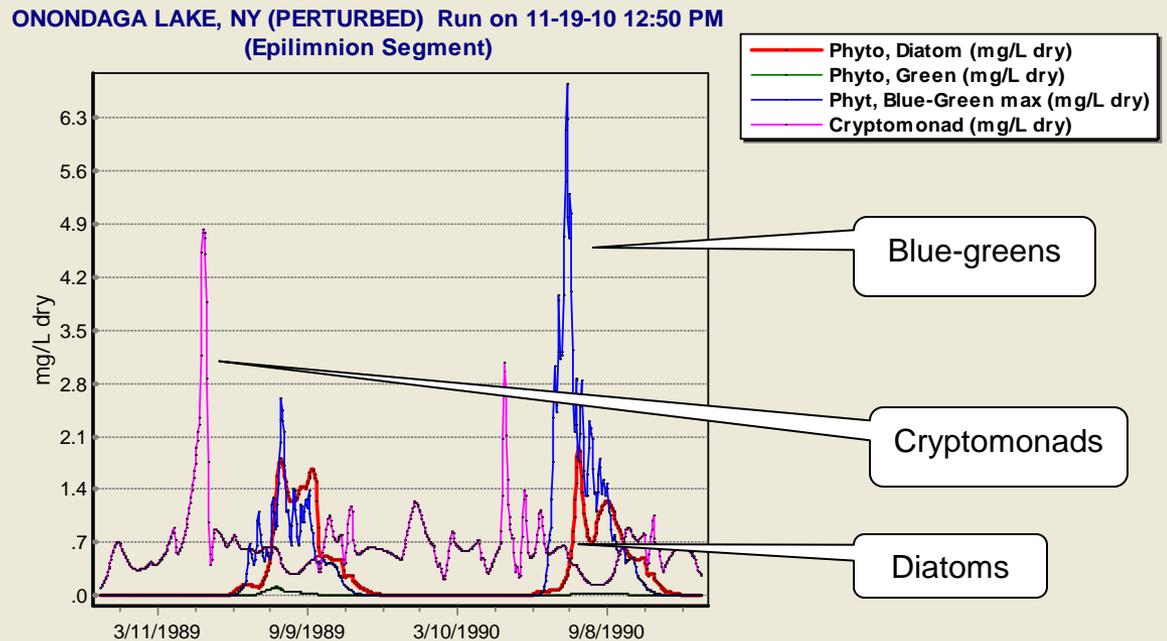
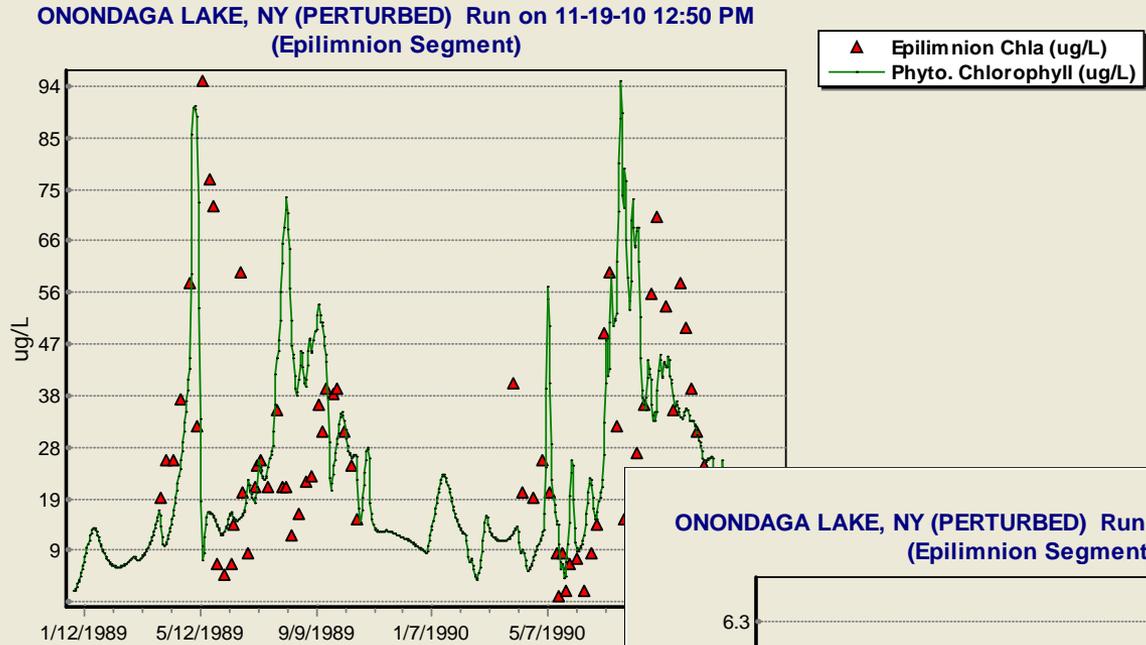
## Validation and Application

- 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

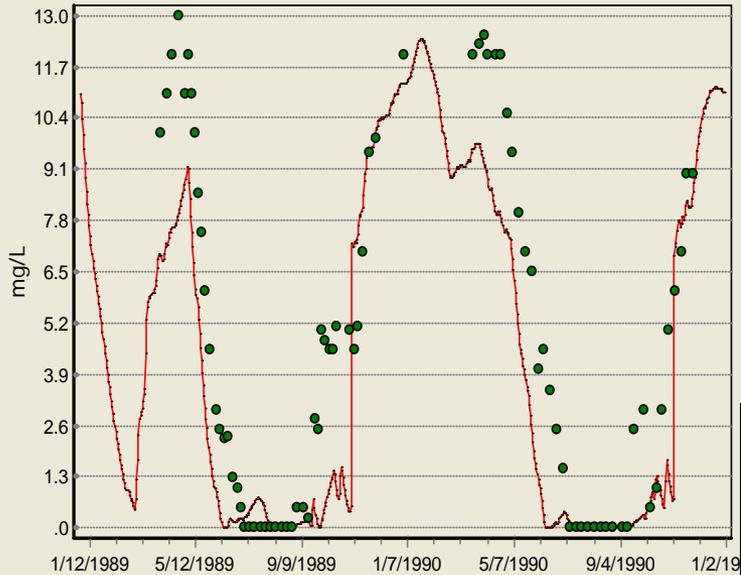


# Lake Onondaga was very productive with succession of algal groups

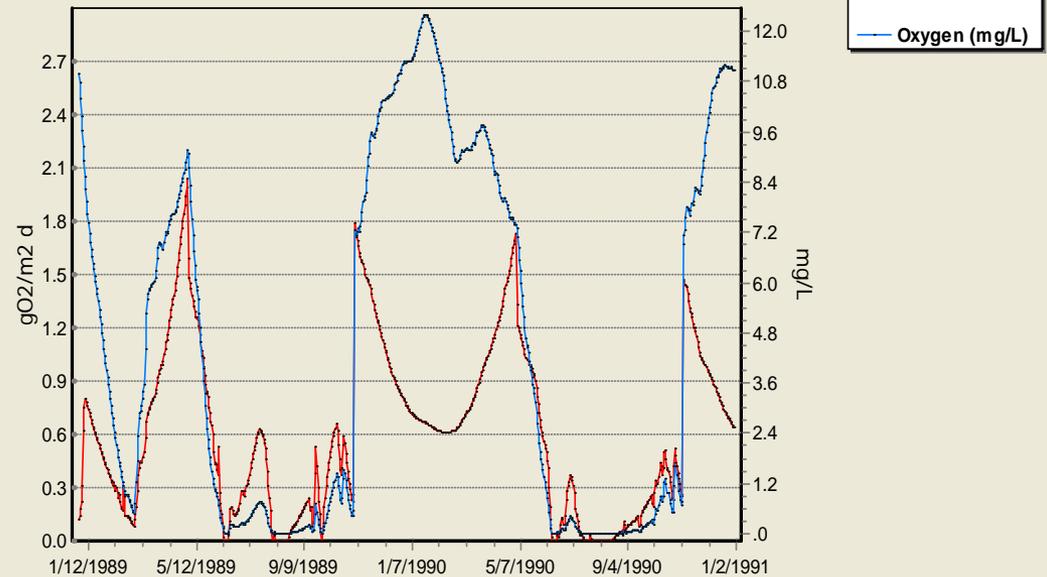


# Hypolimnion goes anoxic with high SOD

ONONDAGA LAKE, NY (PERTURBED) Run on 11-19-10 12:50 PM  
(Hypolimnion Segment)

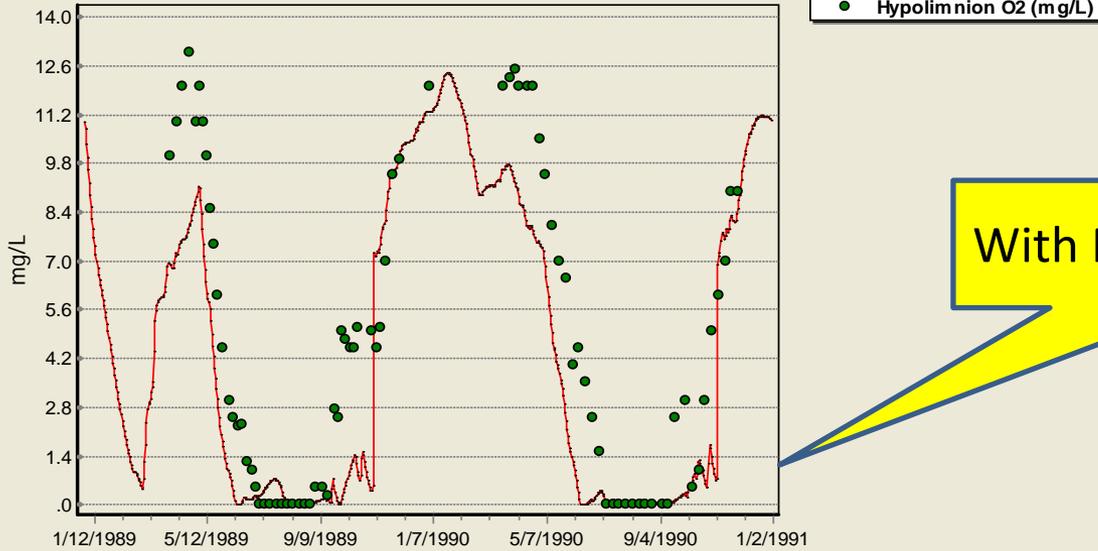


ONONDAGA LAKE, NY (PERTURBED) Run on 11-19-10 12:50 PM  
(Hypolimnion Segment)



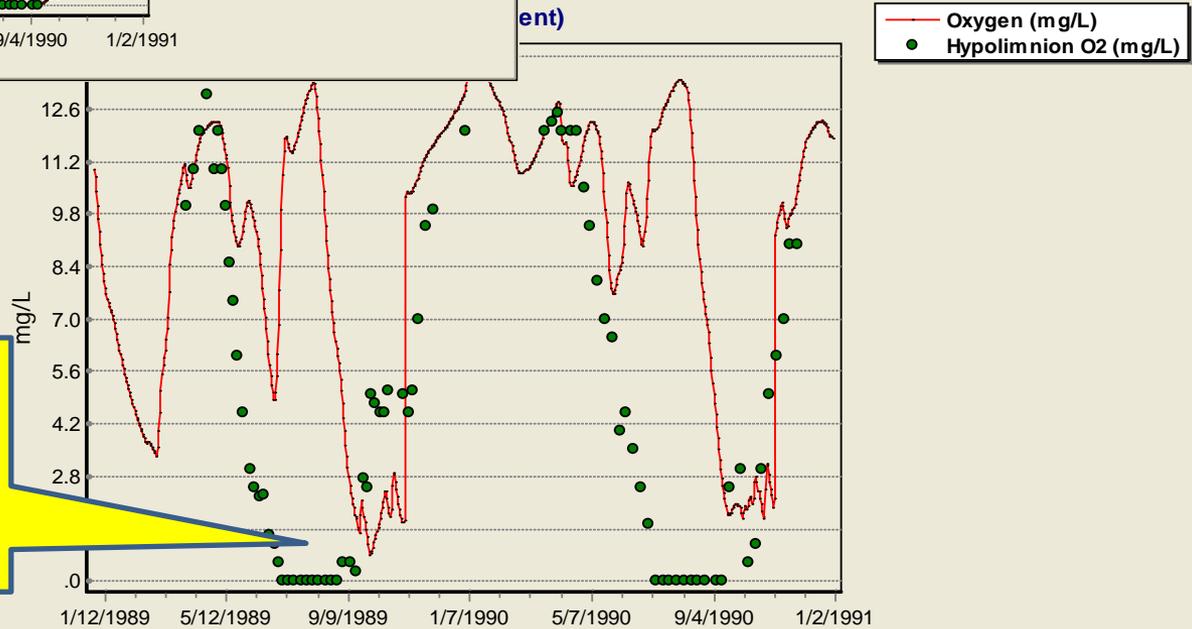
# What if Metro WWTP effluent were diverted?

ONONDAGA LAKE, NY (PERTURBED) Run on 10-9-09 11:38 AM  
(Hypolimnion Segment)



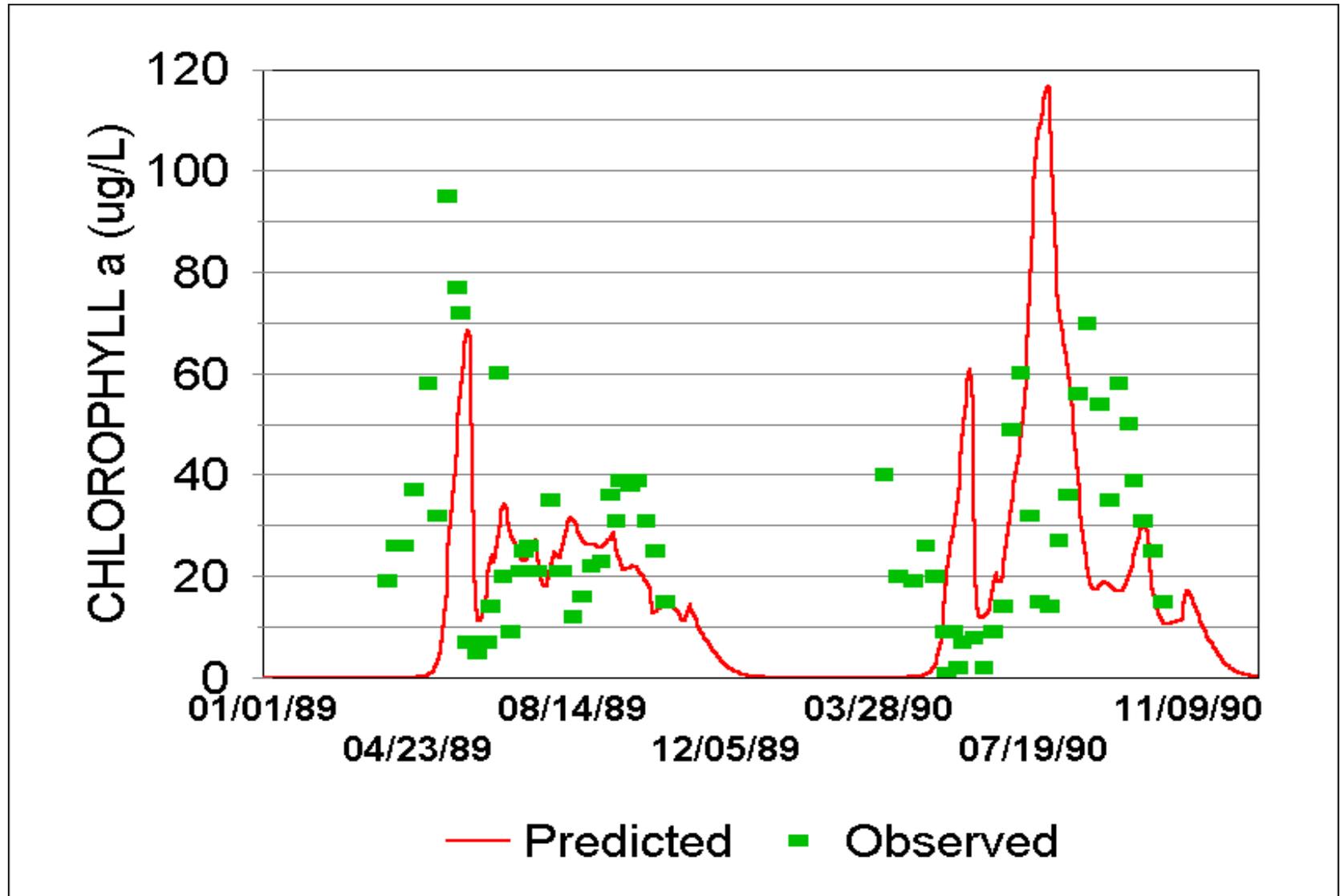
With Metro effluent

Run on 10-9-09 11:49 AM  
(entire)

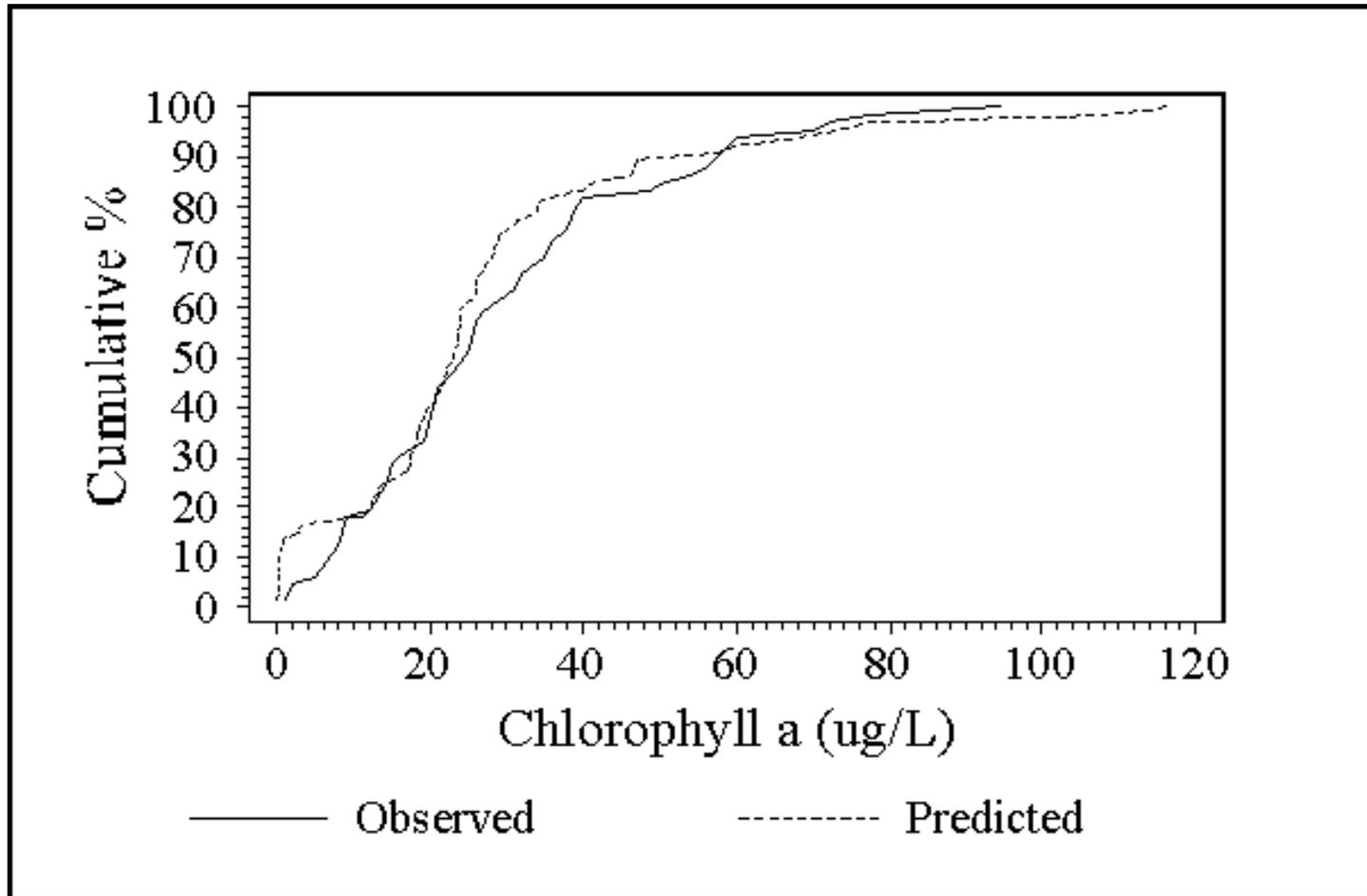


With Metro diversion,  
anoxia does not occur

# Validation of AQUATOX with Lake Onondaga Data—visual test



# Validation with chlorophyll a in Lake Onondaga, NY



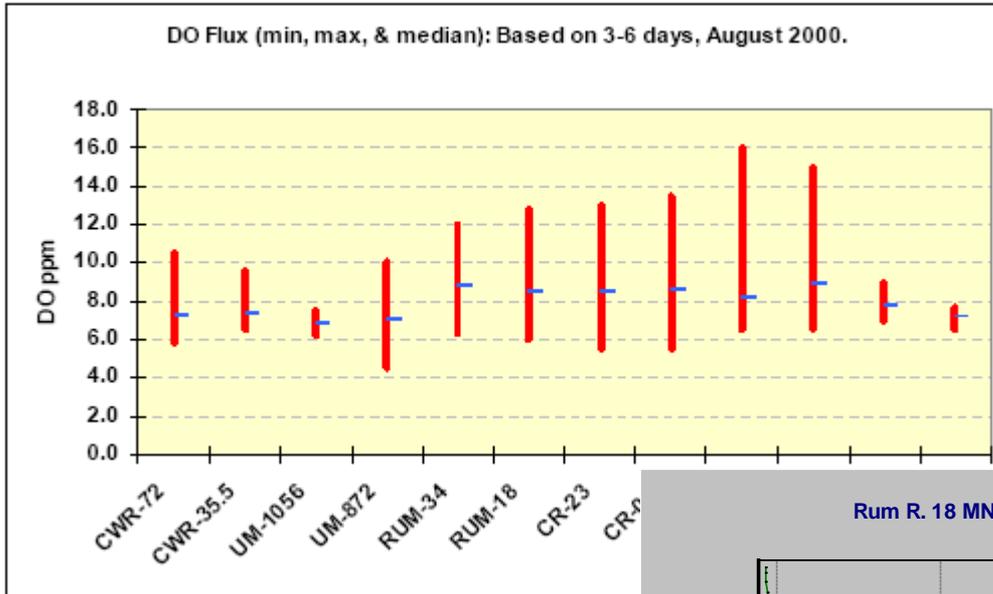
Kolmogorov-Smirnov p statistic = 0.319 (not significantly different)

# Miscellaneous Nutrient-related Topics

- Diel oxygen
- Effects of low dissolved oxygen
- Ammonia toxicity

# Diel Oxygen, Light; Hourly time-step

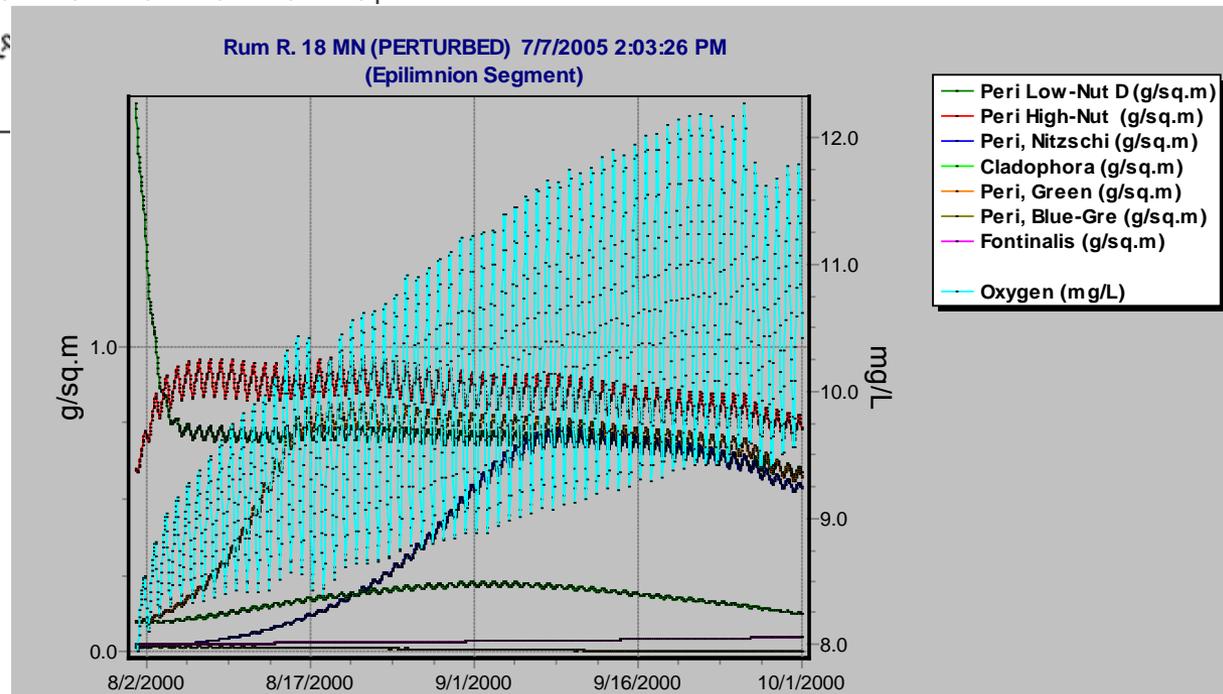
Figure 4. Dissolved oxygen flux based on continuous measurement.



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

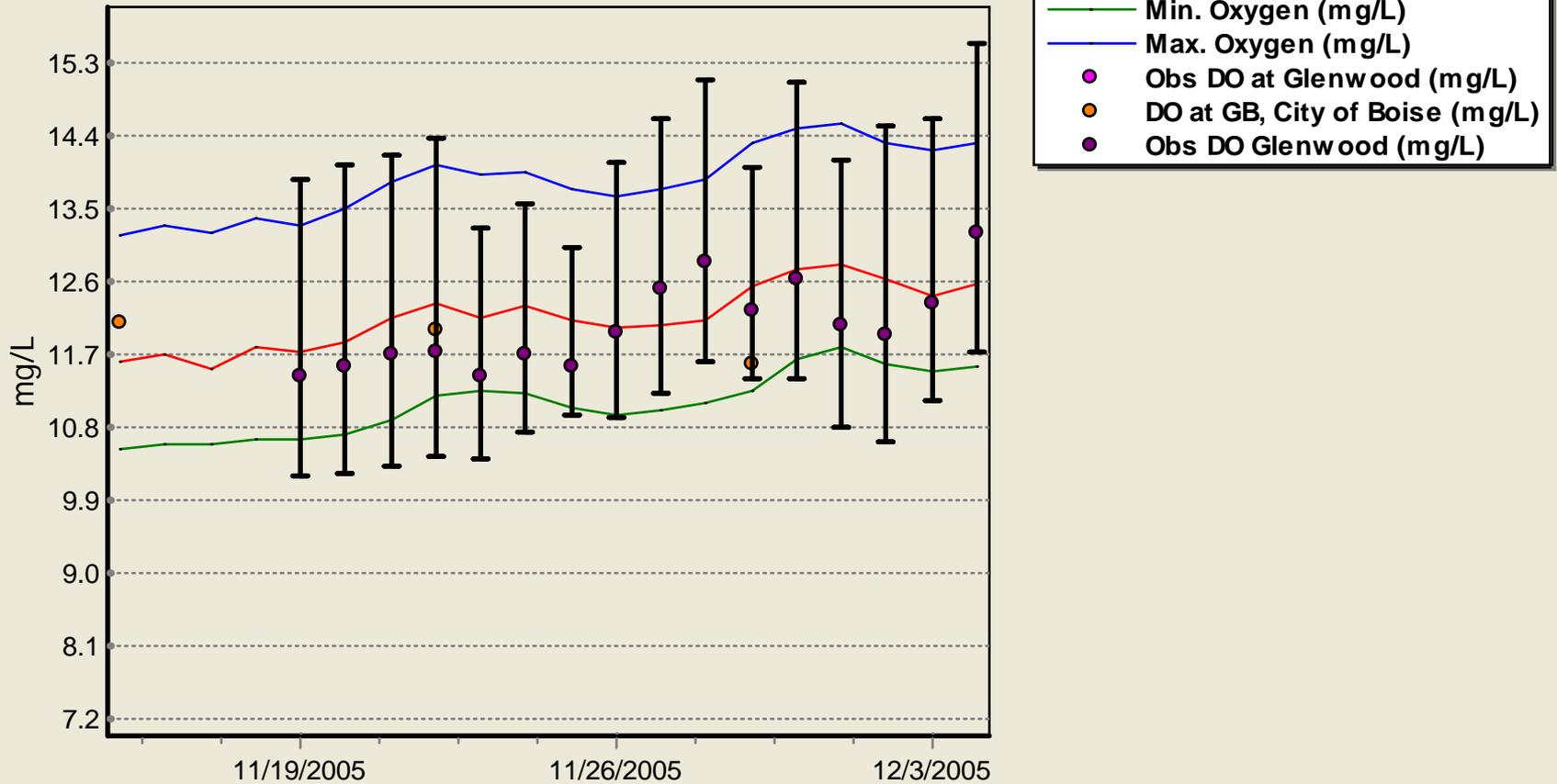


Monitoring data indicate that oxygen levels fluctuate daily



# Diel Oxygen, Hourly Time-step

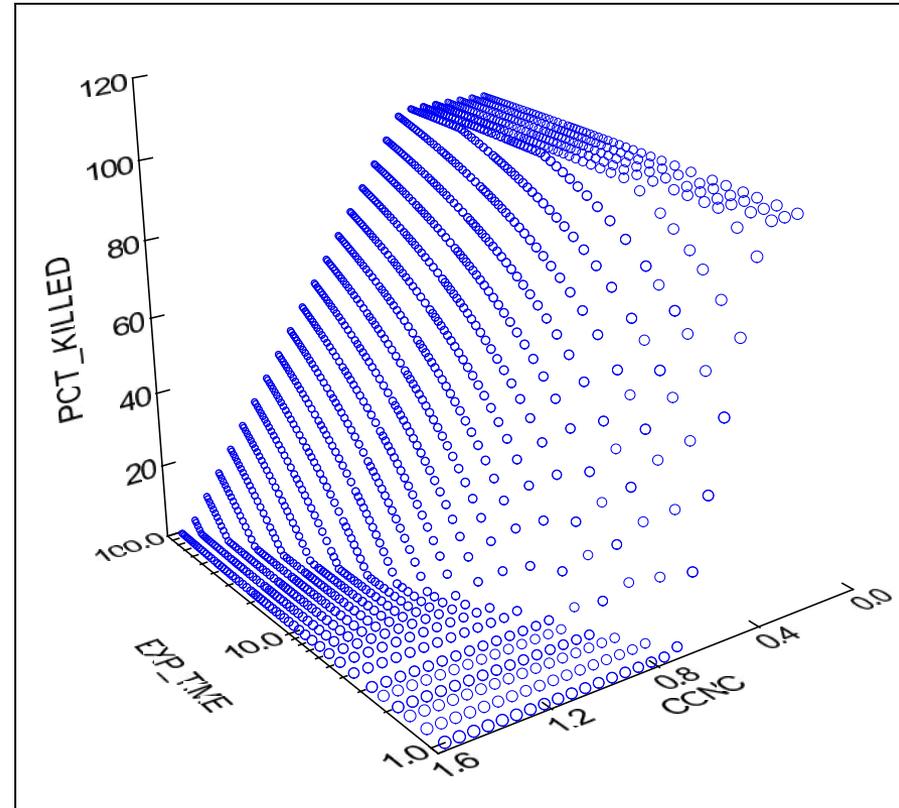
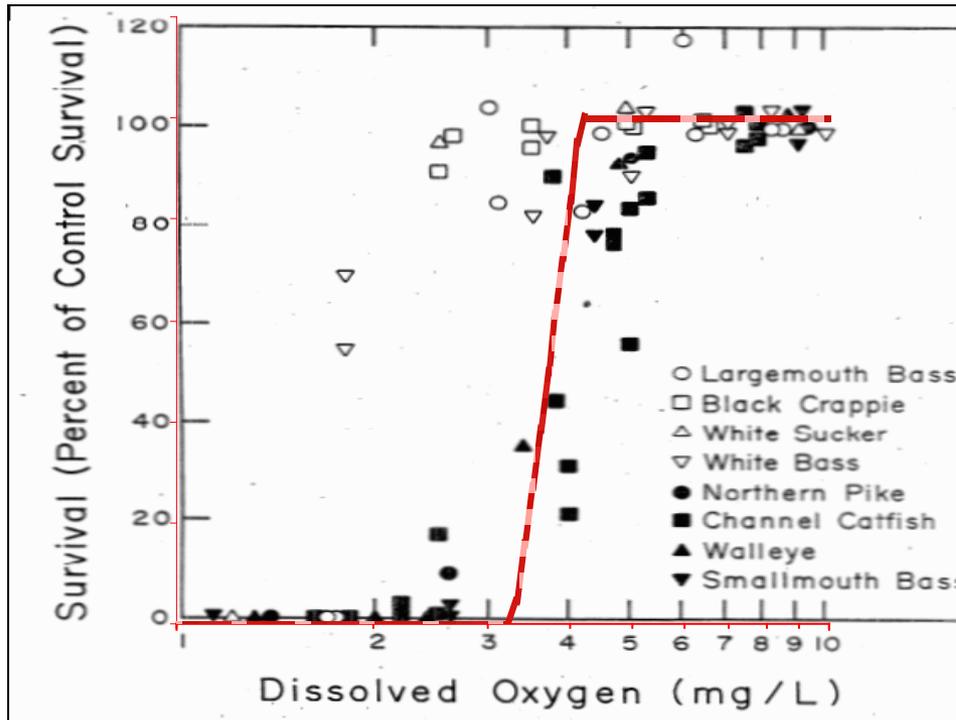
Seg 3 (PERTURBED)  
Run on 09-2-07 4:58 PM



# Low Oxygen Effects

Three dimensional model of effects is a function of exposure time and oxygen concentration.

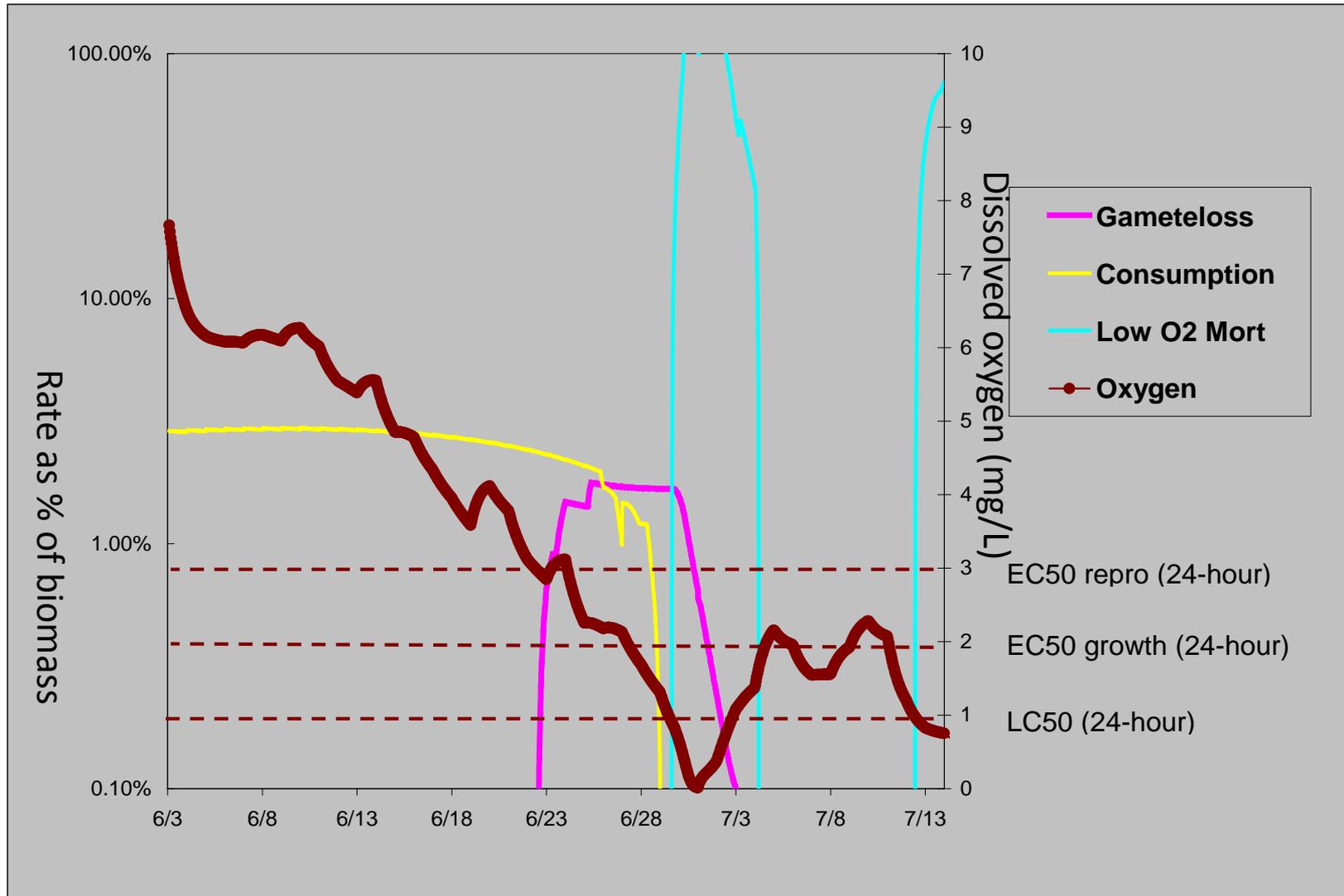
Species specific  $LC50_{24\text{-hour}}$  for  $O_2$  is required



Steep slope for effects matches available data well.  
(red line = model predictions with  $LC50_{24\text{-hour}}$  of 3.5 mg/L)

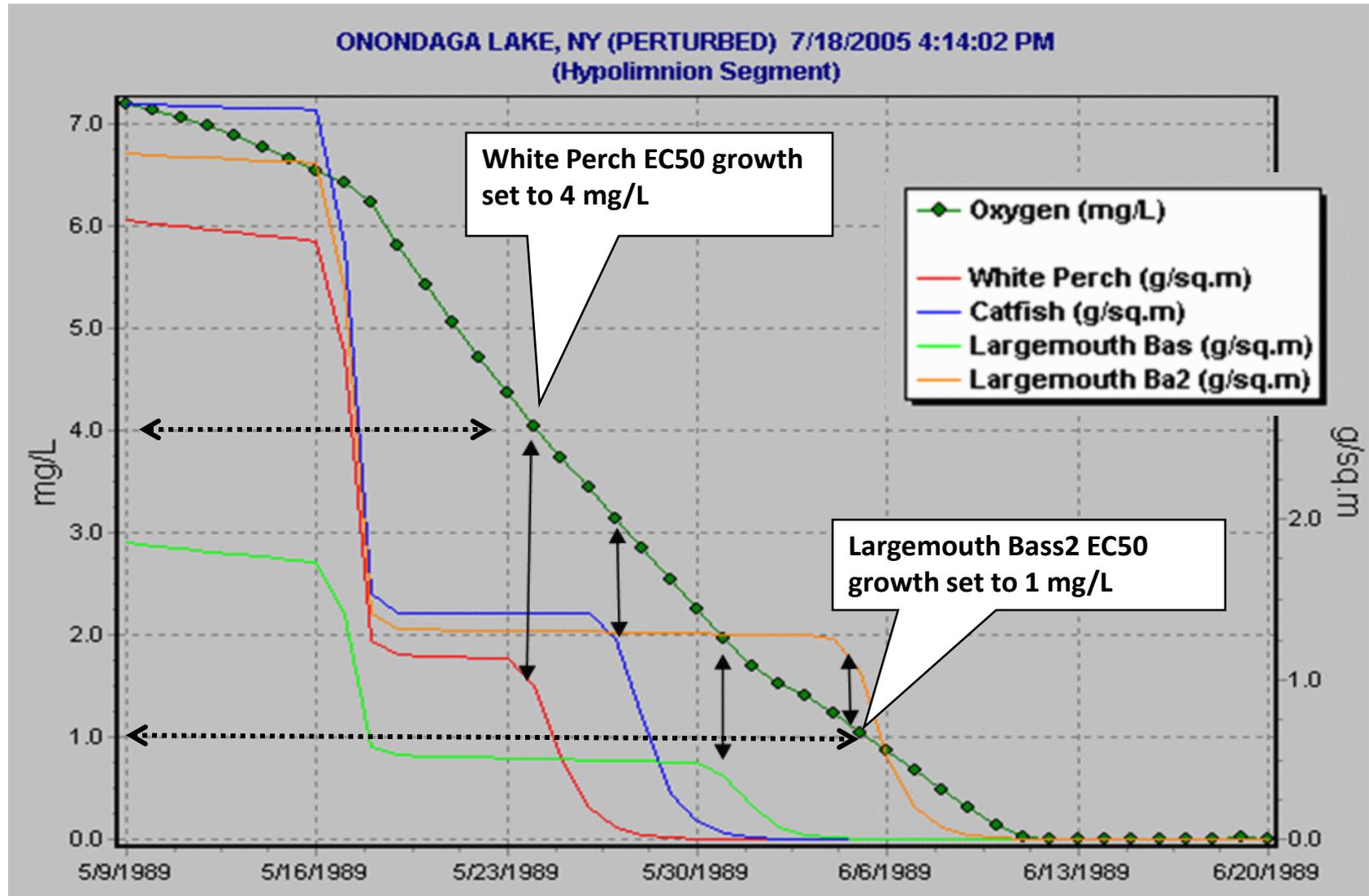
# Non-Lethal Low Oxygen Effects

EC50 reproduction and EC50 growth parameters affect timing



# Low O<sub>2</sub> Affects Timing of Migration from Hypolimnion

EC50 growth parameter is key



# Toxicity Due to Ammonia

Animal Specific Input Parameter Required:

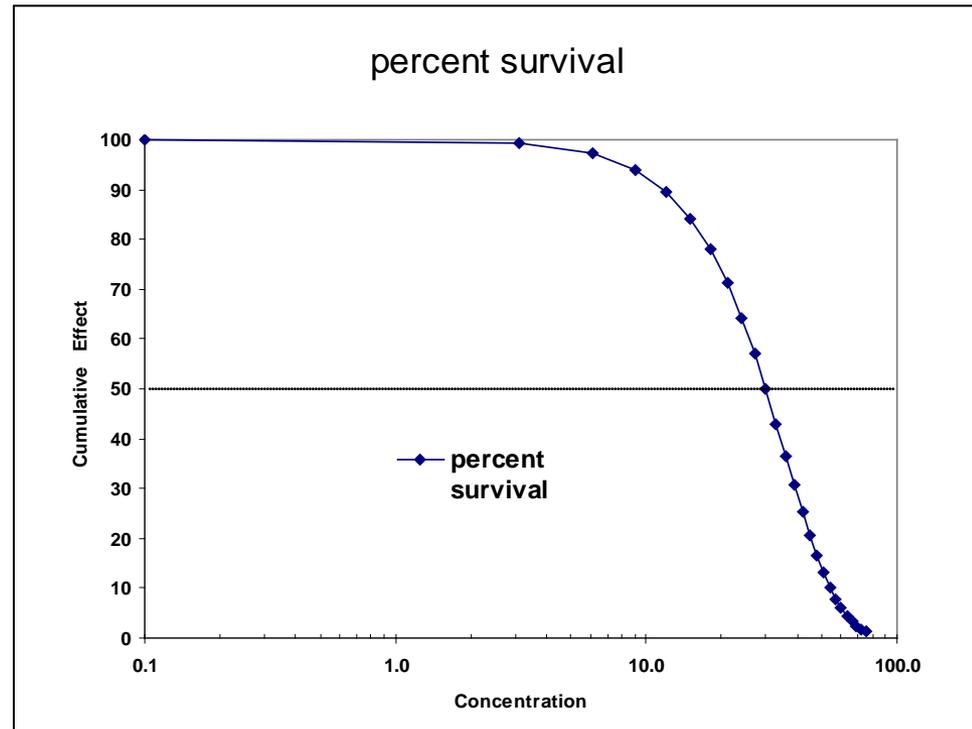
*Ammonia Toxicity:*

LC50, Total Ammonia (pH=8)  mg/L

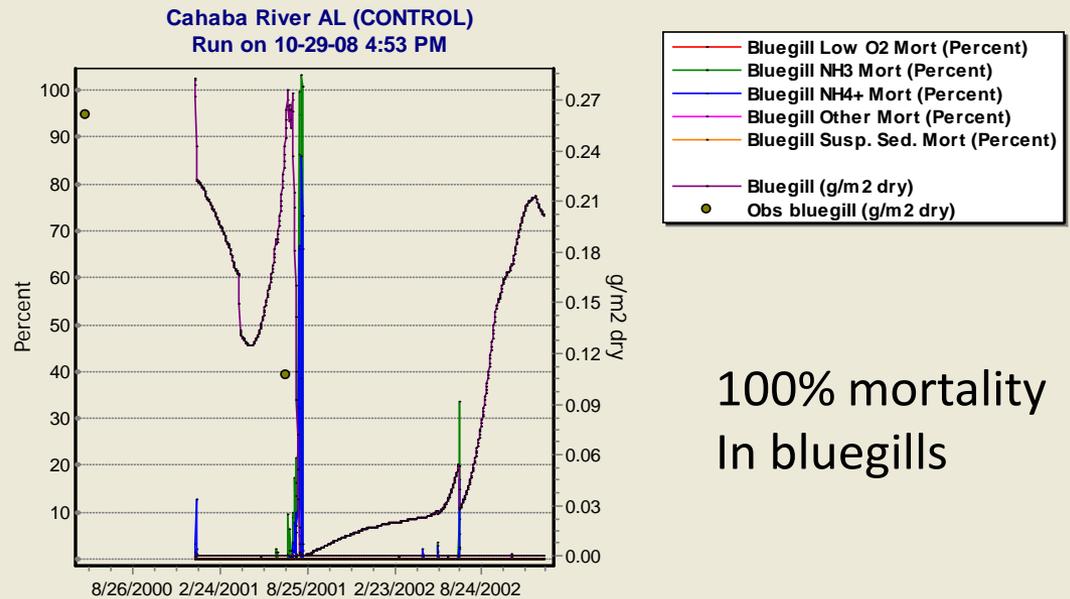
LC50 un-ionized and LC50 ionized calculated from LC50 total as a function of pH

External Toxicity Model Utilized:

- Effects from un-ionized and ionized ammonia are additive
- Un-ionized ammonia fraction calculated as a function of site pH and temperature



# Predicted ammonia toxicity in Cahaba River AL



# Sediment Effects Overview

- Mortality
- Reduction in feeding
- Stimulation of invertebrate drift
- Loss of spawning and protective habitat in interstices

# Suspended and bedded sediment effects

- Mortality

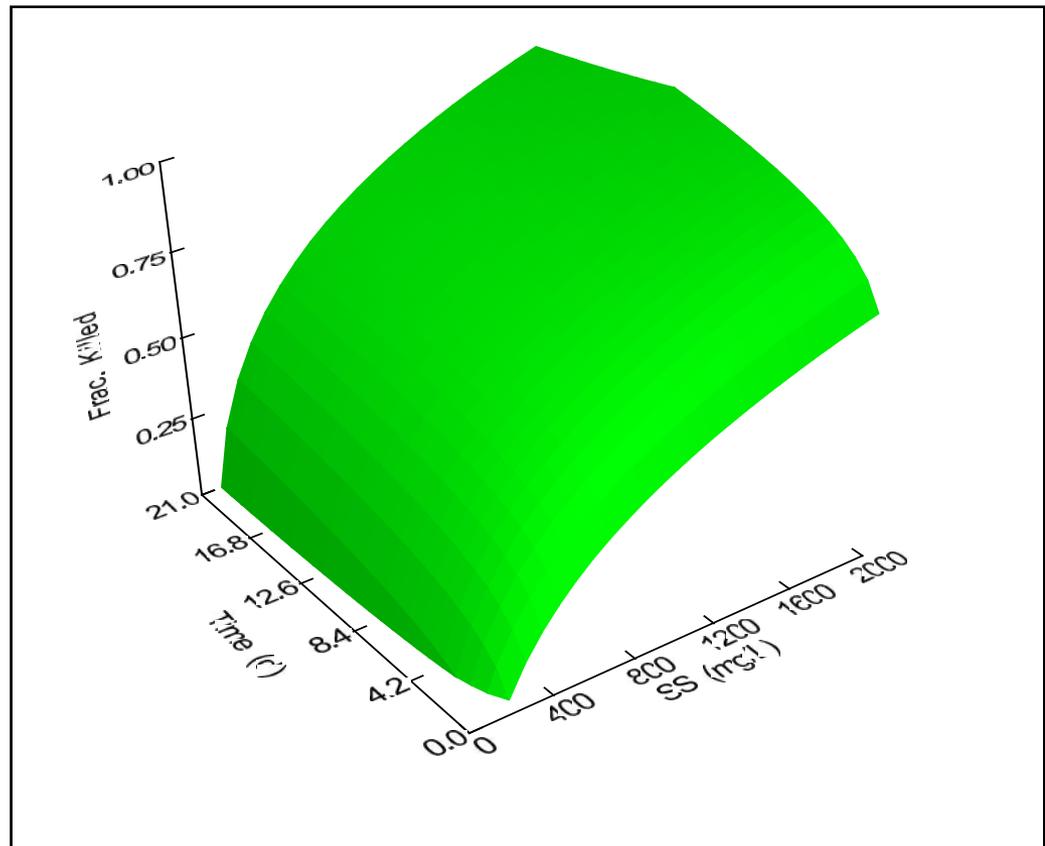
- Highly Sensitive

- Sensitive



- Intolerant

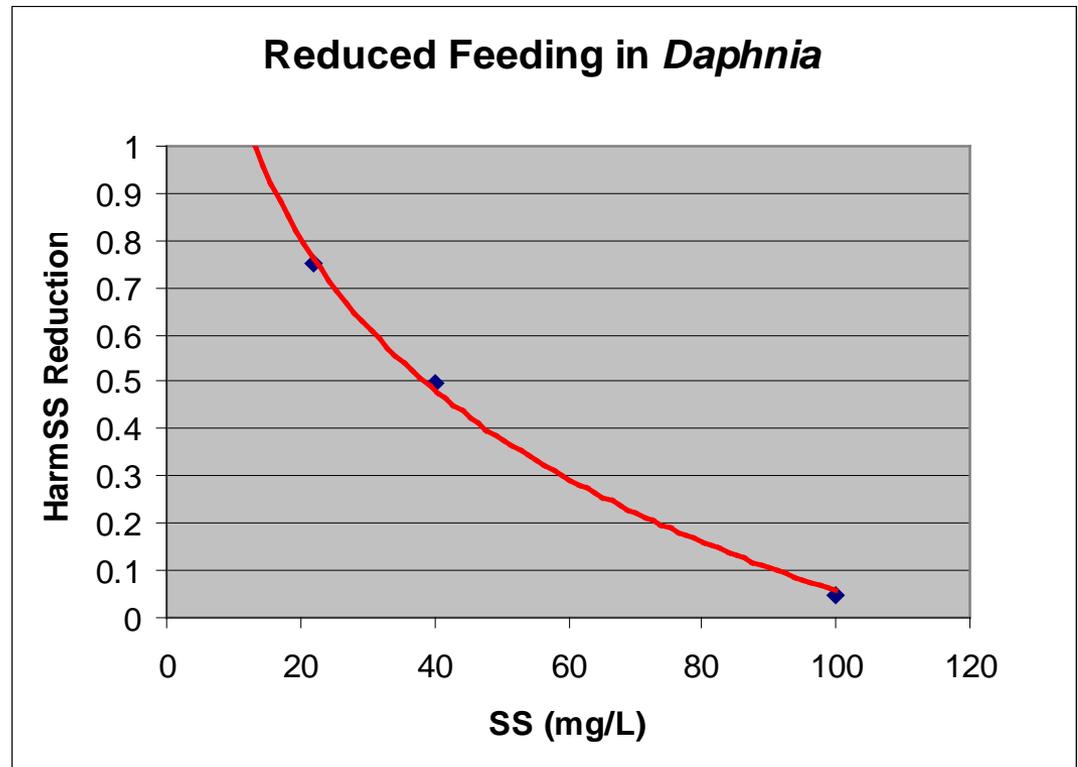
- Tolerant



# Suspended and bedded sediment effects

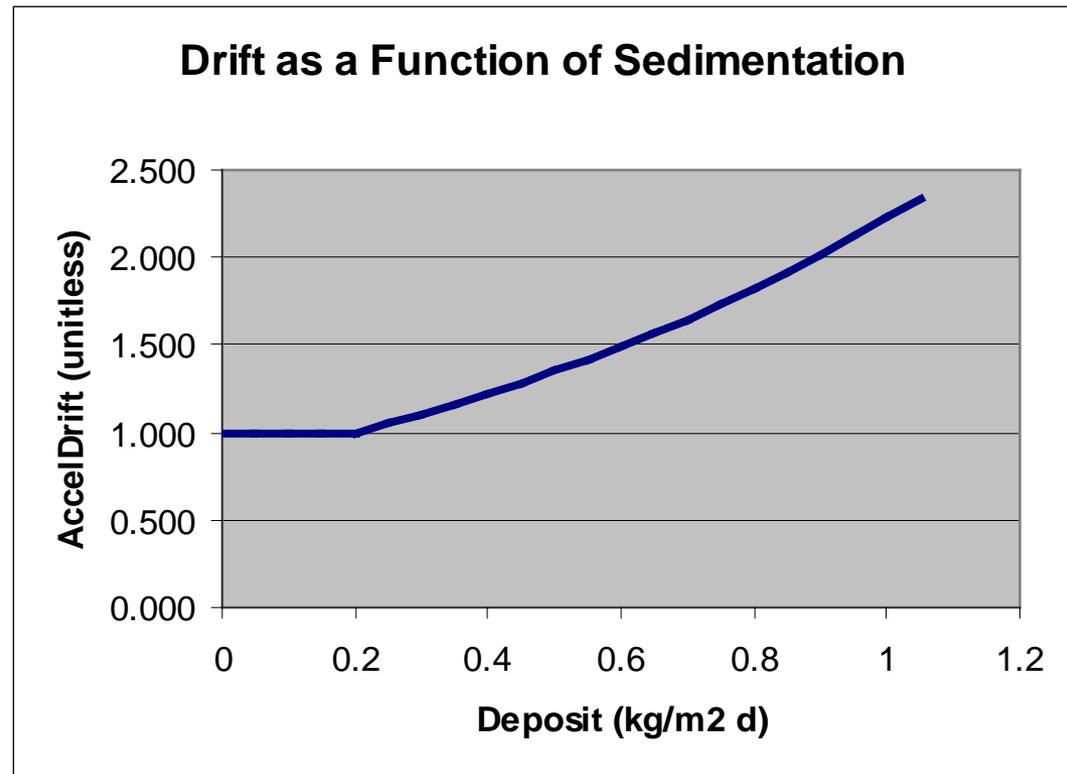
- Reduced Feeding

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



# Suspended and bedded sediment effects

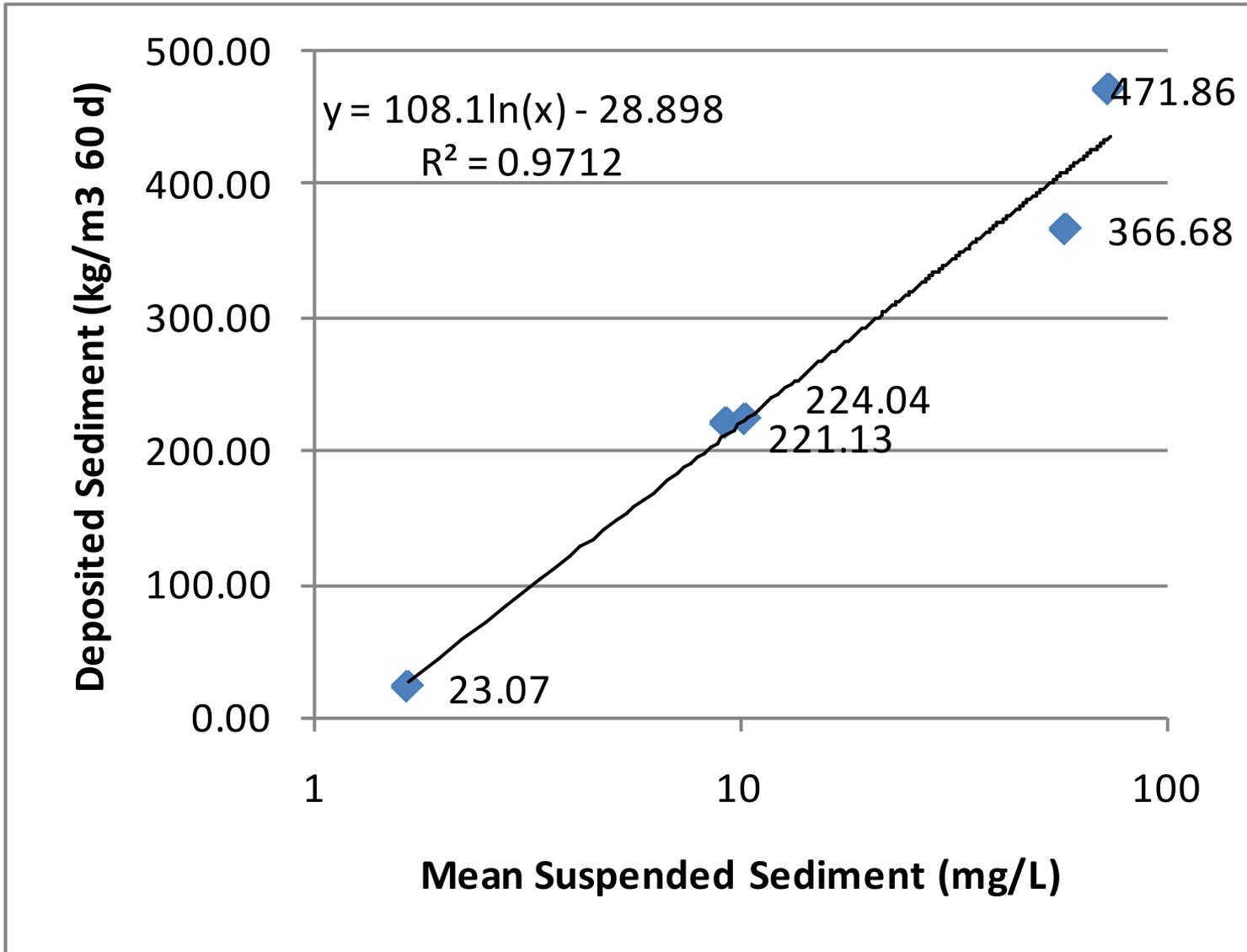
- Increased drift of benthos due to sedimentation



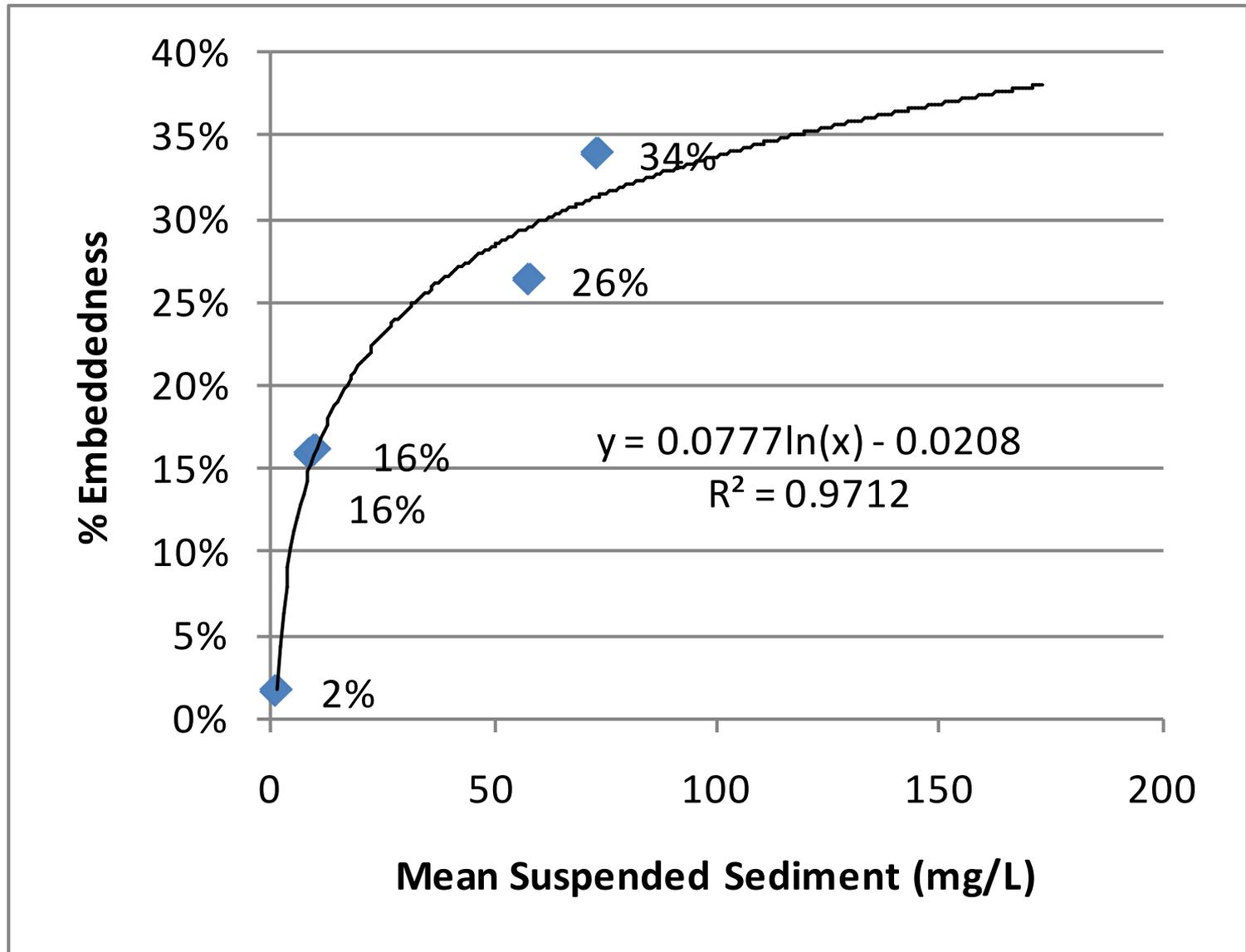
# Suspended and bedded sediment effects

- Deposition of fines and their effect on invertebrates and salmonid reproduction
  - Loss of spawning and protective habitat in interstices
  - Percent Embeddedness calculated as a function of 60-day average TSS

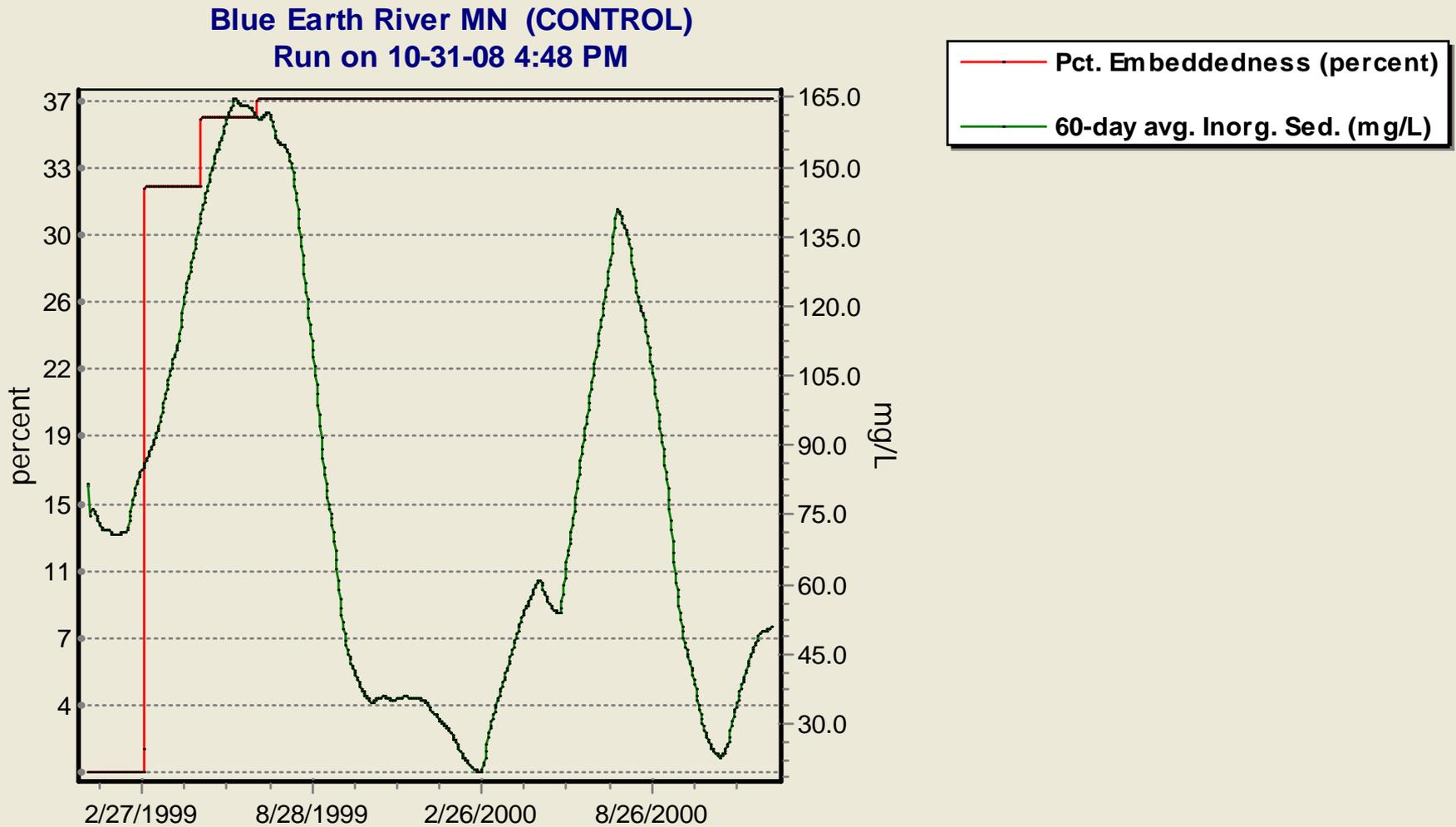
# Relationship of 60-day sedimentation to average TSS



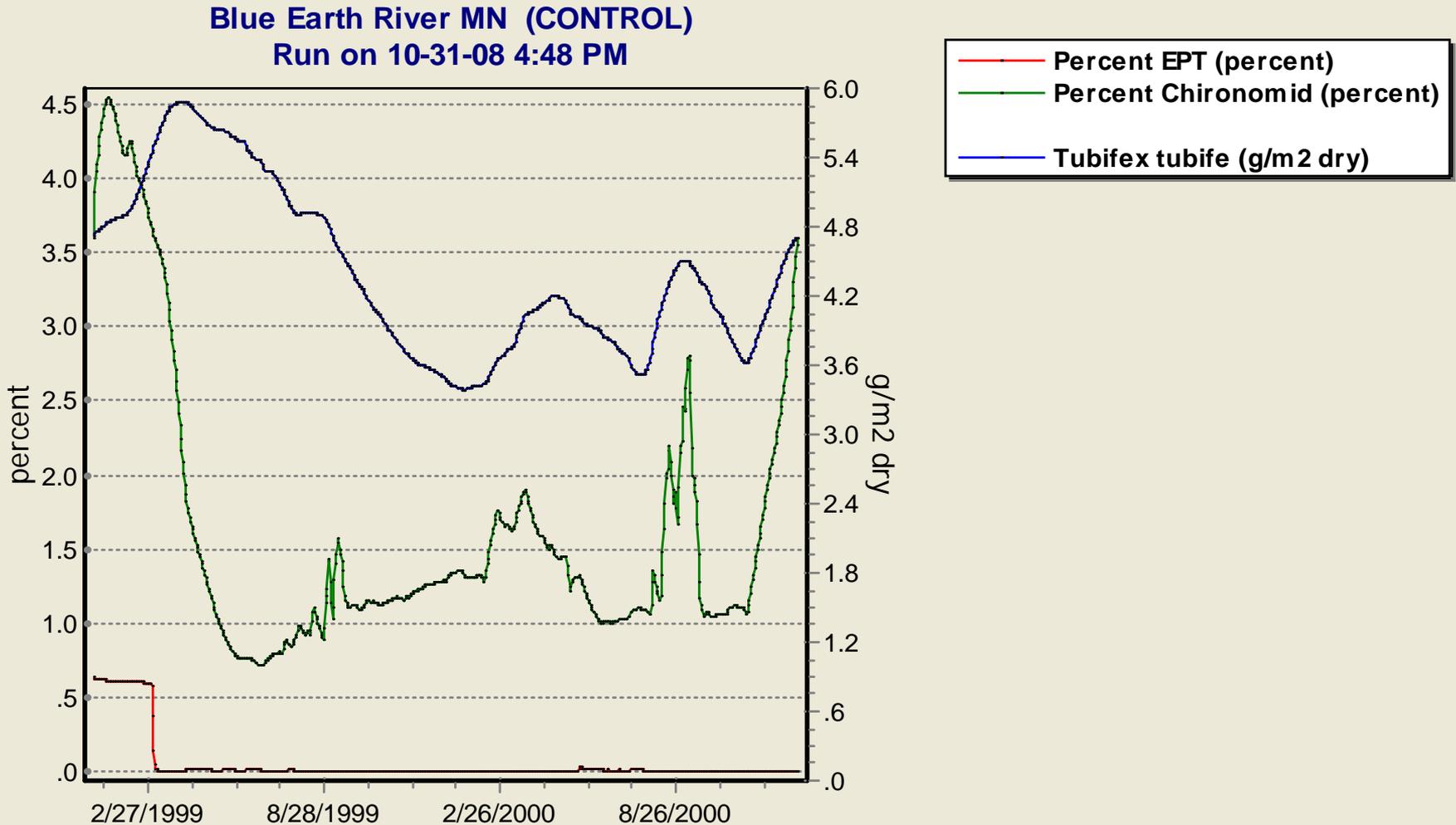
# Relationship of 60-day percent embeddedness to average TSS



# Computed % embeddedness and sedimentation are quite high in turbid Blue Earth River MN

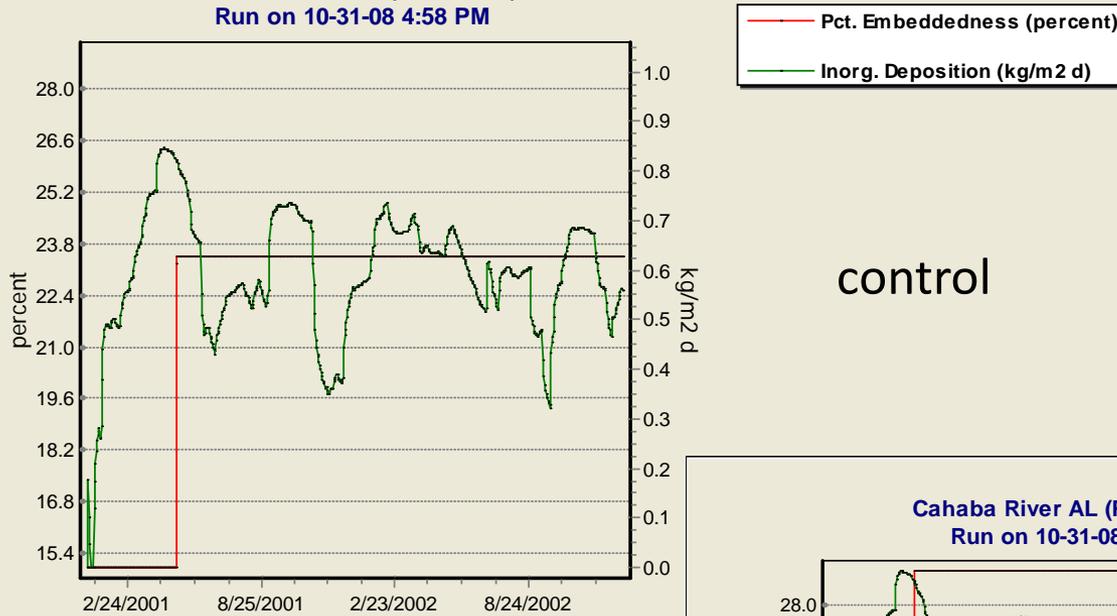


# Mayflies, stoneflies, & caddisflies (EPT) are sensitive to embeddedness; chironomids & oligochaetes are not

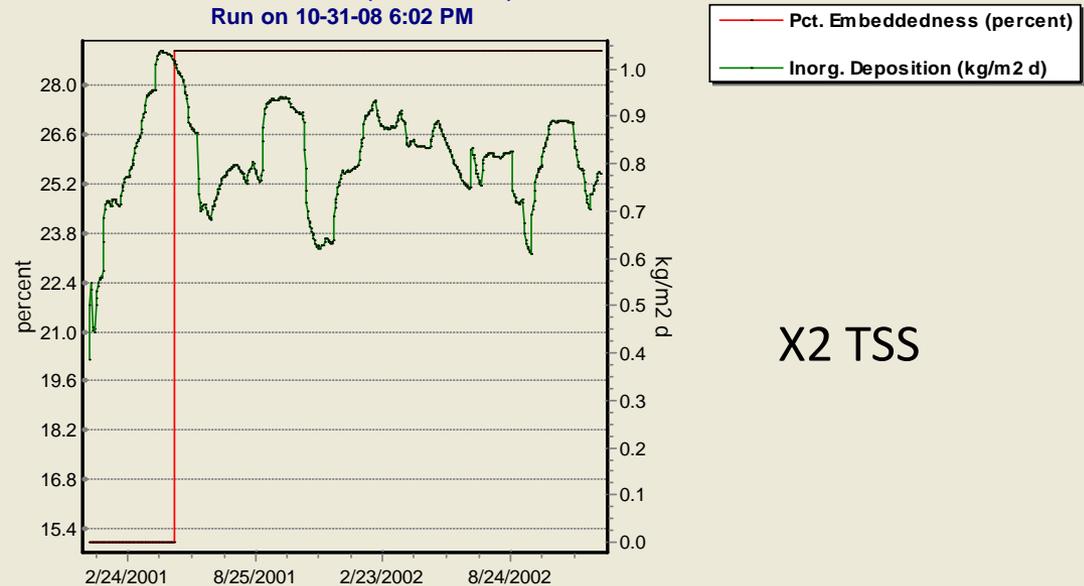


# Doubling TSS increases embeddedness in Cahaba River, AL

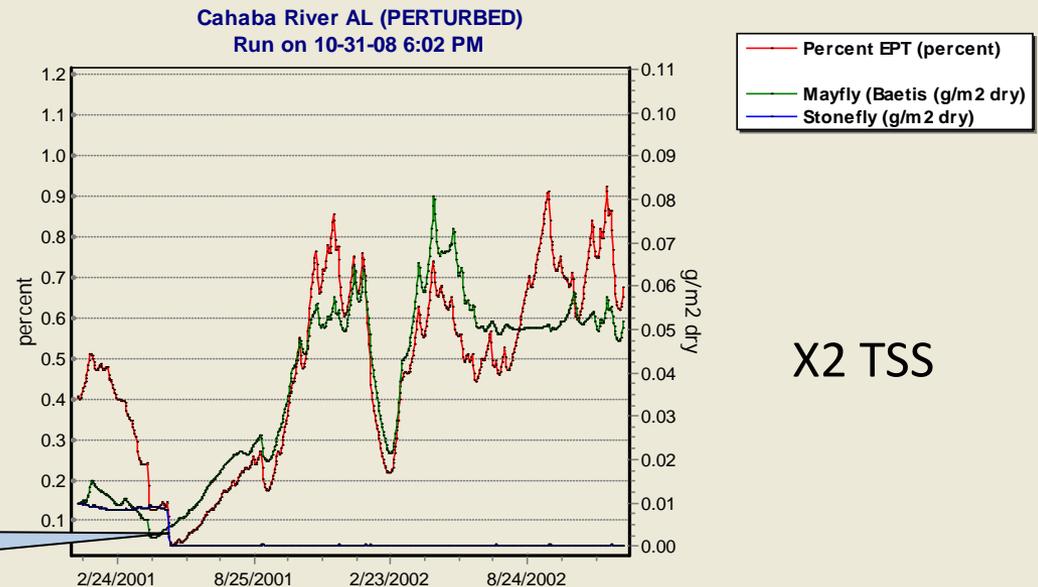
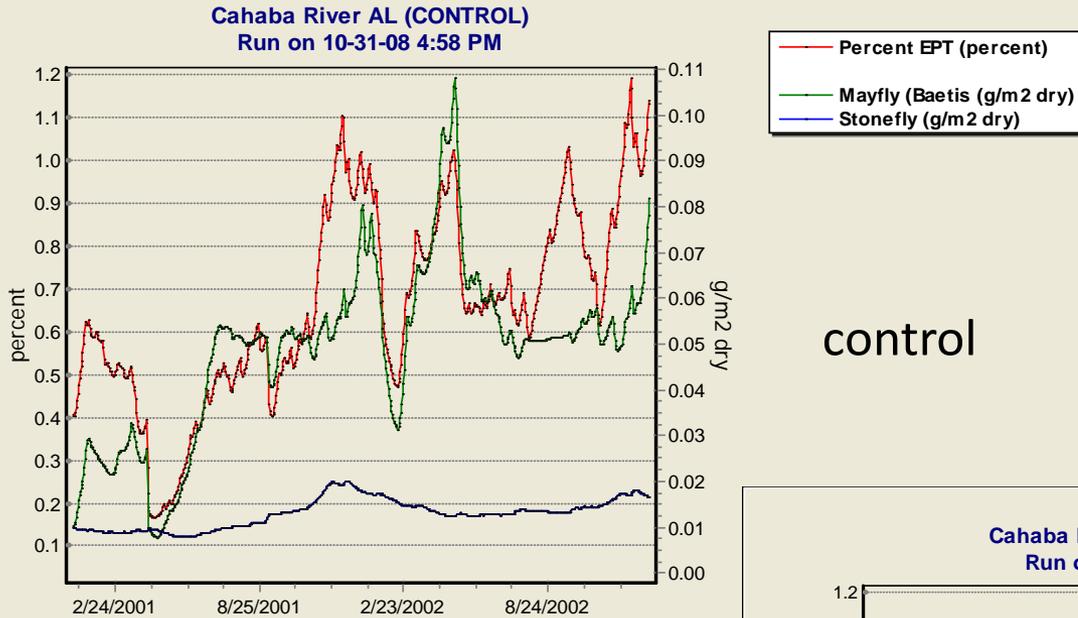
Cahaba River AL (CONTROL)  
Run on 10-31-08 4:58 PM



Cahaba River AL (PERTURBED)  
Run on 10-31-08 6:02 PM



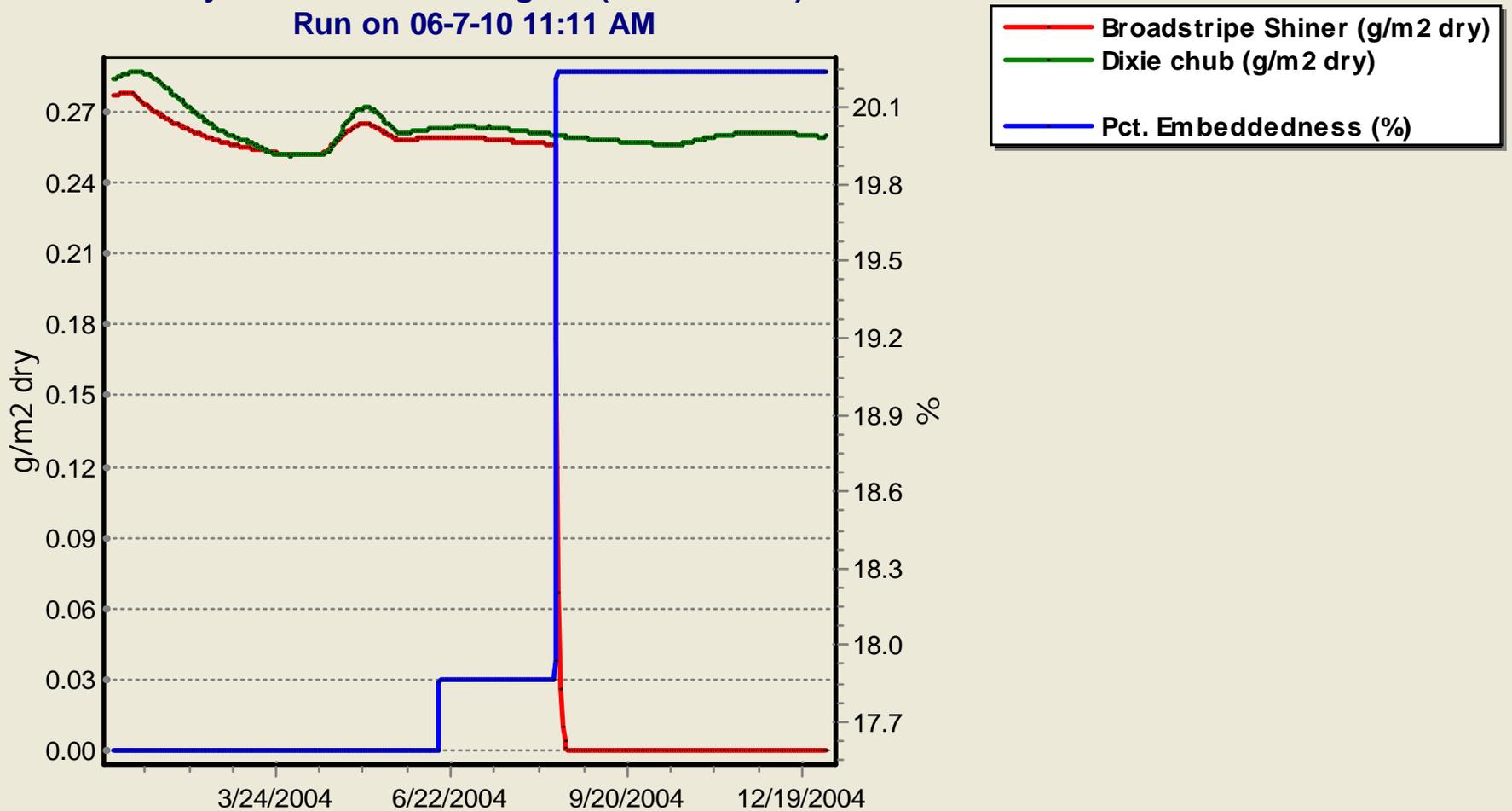
# Doubling TSS loadings adversely impacts insect community in Cahaba River, AL



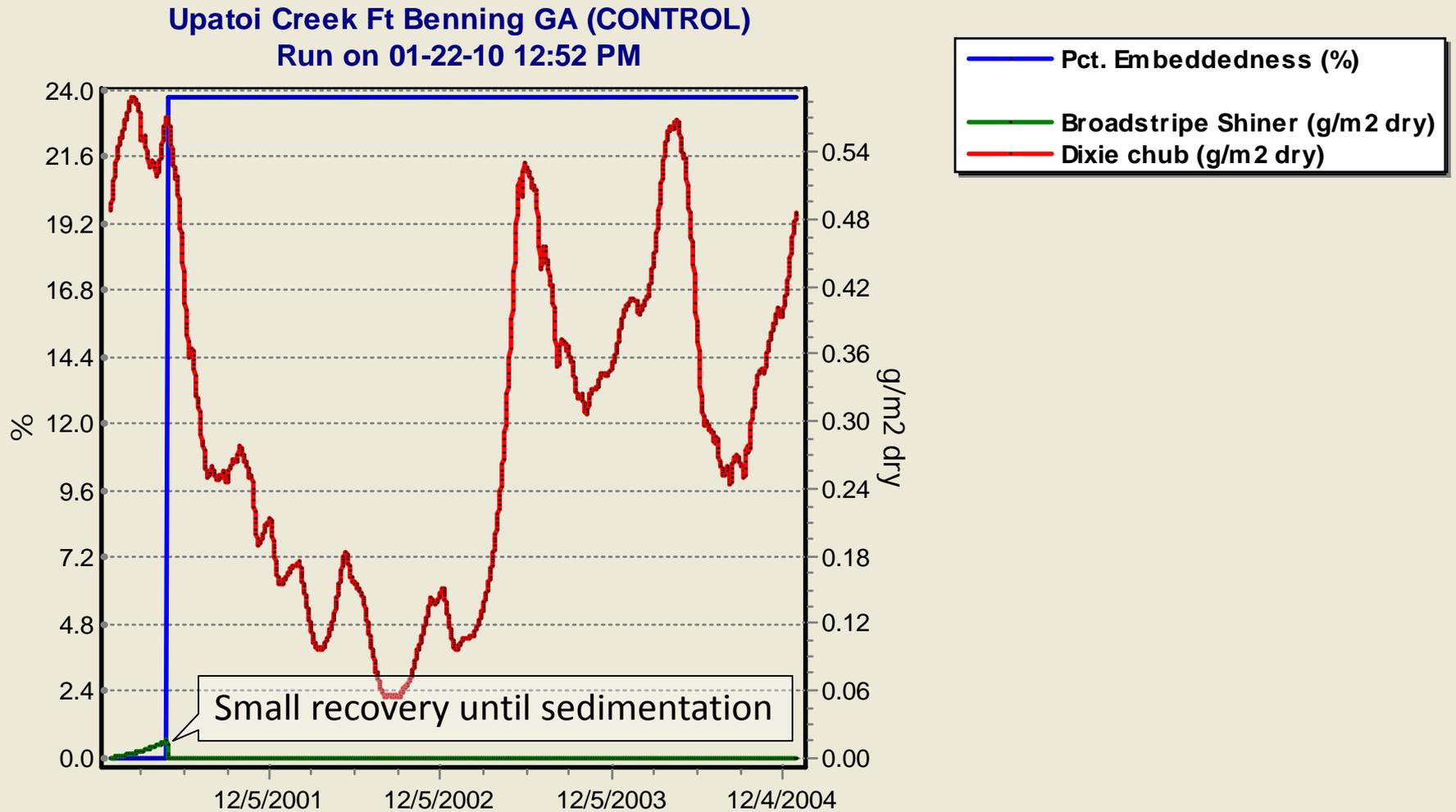
stoneflies crash

# Broadstripe shiner is sensitive to embeddedness; Dixie chub is not; otherwise they are similar

Sally Br Trib 4 Ft Benning GA (PERTURBED)  
Run on 06-7-10 11:11 AM



# Broadstripe shiner is excluded from another creek due to embeddedness



# Lab 6: Analysis of Plant Control in “Clear Lake CA”

- Run control for 3 years
- Add *Hydrilla*
- Run perturbed
- Use difference graph to assess impacts of *Hydrilla*
  - animals
  - nutrients
- Interpret nutrients
  - *Technical Documentation*
  - mass balance plots
- Interpret blue-green algal response

# Uncertainty and Nominal Range Sensitivity Analysis Demonstration & Optional Lab

- “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 for AQUATOX has been performed

# Coralville Sensitivity Analysis Demo

## Demonstration of inputs and outputs from Coralville analysis

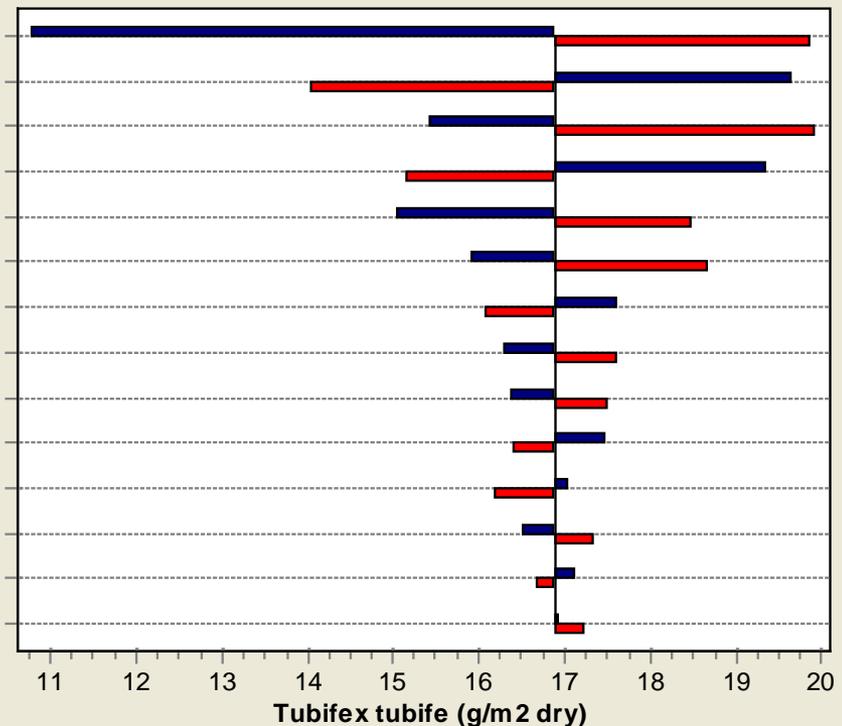
AQUATOX - Uncertainty Setup  
Select a parameter by double-clicking or by pressing <Enter> when the parameter is highlighted.

- All Distributions
- Distributions by Parameter
- Distributions by State Variable
- Selected Parameters for Nominal Sensitivity Test**
  - ✓ Cyclotella nan: Saturating Light (Ly/d)
  - ✓ Cyclotella nan: Temp Response Slope
  - ✓ Cyclotella nan: Optimal Temperature (deg. C)
  - ✓ Cyclotella nan: Maximum Temperature (deg. C)
  - ✓ Cyclotella nan: Min Adaptation Temperature (deg. C)
  - ✓ Cyclotella nan: Max Photosynthetic Rate (1/d)
  - ✓ Daphnia: Half Sat Feeding (mg/L)
  - ✓ Predatory Zoop: Half Sat Feeding (mg/L)
  - ✓ Copepod: Half Sat Feeding (mg/L)
  - ✓ Bluegill: Half Sat Feeding (mg/L)
  - ✓ Shad: Half Sat Feeding (mg/L)
  - ✓ Buffalo fish: Half Sat Feeding (mg/L)
  - ✓ Largemouth Bas: Half Sat Feeding (mg/L)
  - ✓ Largemouth Ba2: Half Sat Feeding (mg/L)
  - ✓ Daphnia: Max Consumption (g / g day)
  - ✓ Predatory Zoop: Max Consumption (g / g day)
  - ✓ Copepod: Max Consumption (g / g day)
  - ✓ Bluegill: Max Consumption (g / g day)
  - ✓ Shad: Max Consumption (g / g day)
  - ✓ Buffalo fish: Max Consumption (g / g day)
  - ✓ Largemouth Bas: Max Consumption (g / g day)
  - ✓ Largemouth Ba2: Max Consumption (g / g day)
  - ✓ Daphnia: Min Prey for Feeding
  - ✓ Predatory Zoop: Min Prey for Feeding
  - ✓ Copepod: Min Prey for Feeding
  - ✓ Bluegill: Min Prey for Feeding
  - ✓ Shad: Min Prey for Feeding
  - ✓ Largemouth Bas: Min Prey for Feeding
  - ✓ Largemouth Ba2: Min Prey for Feeding
  - ✓ Daphnia: Temperature Response Slope
  - ✓ Copepod: Temperature Response Slope
  - ✓ Daphnia: Optimal Temperature (deg. C)
  - ✓ Copepod: Optimal Temperature (deg. C)
  - ✓ Daphnia: Maximum Temperature (deg. C)
  - ✓ Copepod: Maximum Temperature (deg. C)
  - ✓ Daphnia: Min Adaptation Temperature (deg. C)
  - ✓ Copepod: Min Adaptation Temperature (deg. C)
  - ✓ Daphnia: Mortality Coeff (1/d)
  - ✓ Copepod: Mortality Coeff (1/d)
  - ✓ Daphnia: Average Drift (frac/day)
  - ✓ Predatory Zoop: Average Drift (frac/day)
  - ✓ Copepod: Average Drift (frac/day)
  - ✓ Site: Ave. Epilimnetic Temperature (deg. C)
  - ✓ Site: Epi Temp. Range (deg. C)
  - ✓ Water Vol: Multiply Loading by
  - ✓ TSS: Multiply Loading by
  - ✓ TSS: Multiply Loading by
  - ✓ Susp&Diss Deter: Multiply Loading by
  - ✓ Daphnia: Multiply Loading by
  - ✓ Copepod: Multiply Loading by
  - ✓ Temp: Multiply Loading by
  - ✓ Water Vol: Mult. Inflow Load by

### Sensitivity of Tubifex tubife (g/m2 dry) to 20% change in tested parameters

3/28/2008 3:31:16 PM

- 135% - Temp: Multiply Loading by
- 83.2% - Water Vol: Mult. Inflow Load by
- 66.6% - TSS: Multiply Loading by
- 62.4% - Cyclotella nan: Max Photosynthetic Rate (1/d)
- 51.2% - Cyclotella nan: Optimal Temperature (deg. C)
- 40.8% - Cyclotella nan: Temp Response Slope
- 23.1% - Water Vol: Multiply Loading by
- 19.7% - Daphnia: Optimal Temperature (deg. C)
- 16.5% - Cyclotella nan Min. Sat. Light (Ly/d)
- 16.3% - Daphnia: Max Consumption (g / g day)
- 13.1% - Cyclotella nan: Maximum Temperature (deg. C)
- 12.6% - Daphnia: Temperature Response Slope
- 6.82% - Susp&Diss Deter: Multiply Loading by
- 5.45% - Daphnia: Maximum Temperature (deg. C)



**IMPORTANT NOTE:** The sensitivity analysis calculates the % difference between averaged time step of the simulation, if a longer time step is desired, change it.

Deterministic Mode   
  Run in Uncertainty Mode   
  Run in Sens

Nominal Percent to Vary:  (percent 0-100)     Link Periphyton

Track 67 Output Variables    Choose Output to Track

# AQUATOX Sensitivity Screen

AQUATOX-- Uncertainty Setup

Select a parameter by double-clicking or by pressing <Enter> when the parameter is highlighted.

**Selected Parameters for Nominal Sensitivity Test**

- ✓ Phyto, Diatom: Saturating Light (Ly/d)
- ✓ Phyto, Diatom: Temp Response Slope
- ✓ Phyto, Diatom: Optimal Temperature (deg. C)
- ✓ Phyto, Diatom: Maximum Temperature (deg. C)
- ✓ Phyto, Diatom: Min Adaptation Temperature (deg. C)
- ✓ Phyto, Diatom: Max Photosynthetic Rate (1/d)
- ✓ Daphnia: Half Sat Feeding (mg/L)
- ✓ Predatory Zooplank.: Half Sat Feeding (mg/L)
- ✓ Copepod: Half Sat Feeding (mg/L)
- ✓ Bluegill: Half Sat Feeding (mg/L)
- ✓ Shad: Half Sat Feeding (mg/L)
- ✓ Buffalofish: Half Sat Feeding (mg/L)
- ✓ Largemouth Bass, YOY: Half Sat Feeding (mg/L)
- ✓ Largemouth Bass, Lg: Half Sat Feeding (mg/L)
- ✓ Daphnia: Max Consumption (g / g day)

**Select Parameters to Vary**

**IMPORTANT NOTE:** The sensitivity analysis calculates the % difference between the results of the deterministic run and the altered simulation in the last averaged time-step of the simulation. If a longer time-step is desired, change this in the setup

Deterministic Mode     Run in Uncertainty Mode     Run in Sensitivity Mode

Nominal Percent to Vary:  (percent of 100)     Link Periphyton/Phytoplankton

**Toggle Sensitivity Analyses**

**Choose Output to Track**

54 Parameters set to be tested or 108 iterations.

# Uncertainty Analysis

- Uncertainty analyses describe sources of uncertainty and variability in model simulations
- 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 the number of required iterations)

# AQUATOX Uncertainty Screen

The screenshot shows the 'AQUATOX-- Uncertainty Setup' dialog box. At the top, a yellow instruction bar reads: 'Select a parameter by double-clicking or by pressing <Enter> when the parameter is highlighted.' Below this is a tree view with four items: 'All Distributions', 'Distributions by Parameter', 'Distributions by State Variable', and 'Selected Distributions for Uncertainty Run'. A callout box labeled 'Examine Parameters to Vary' points to the tree view. Below the tree view are three radio buttons: 'Deterministic Mode', 'Run in Uncertainty Mode' (which is selected and has a dotted border), and 'Run in Sensitivity Mode'. A callout box labeled 'Toggle Uncertainty Analyses' points to these radio buttons. To the right of the radio buttons is a 'Set Up Correlations' button. Below the radio buttons are two rows of settings. The first row has a checkbox for 'Save Each Iteration to CSV' (unchecked), a text field for 'Number of Iterations' with the value '20' and '(integer)' to its right, and a 'Help' button. A callout box labeled 'Select Number of Iterations' points to the 'Number of Iterations' text field. The second row has two checked checkboxes: 'Utilize Non-Random Seed' and 'Sample Randomly within Intervals'. To their right are a text field for 'Seed for Pseudo Random Generator' with the value '100' and '(integer)' to its right, and 'OK' and 'Cancel' buttons. The 'OK' button has a green checkmark icon, and the 'Cancel' button has a red X icon.

**AQUATOX-- Uncertainty Setup**

Select a parameter by double-clicking or by pressing <Enter> when the parameter is highlighted.

- All Distributions
- Distributions by Parameter
- Distributions by State Variable
- Selected Distributions for Uncertainty Run

**Examine Parameters to Vary**

**Toggle Uncertainty Analyses**

Deterministic Mode     Run in Uncertainty Mode     Run in Sensitivity Mode

Save Each Iteration to CSV    Number of Iterations: 20 (integer)    **Help**

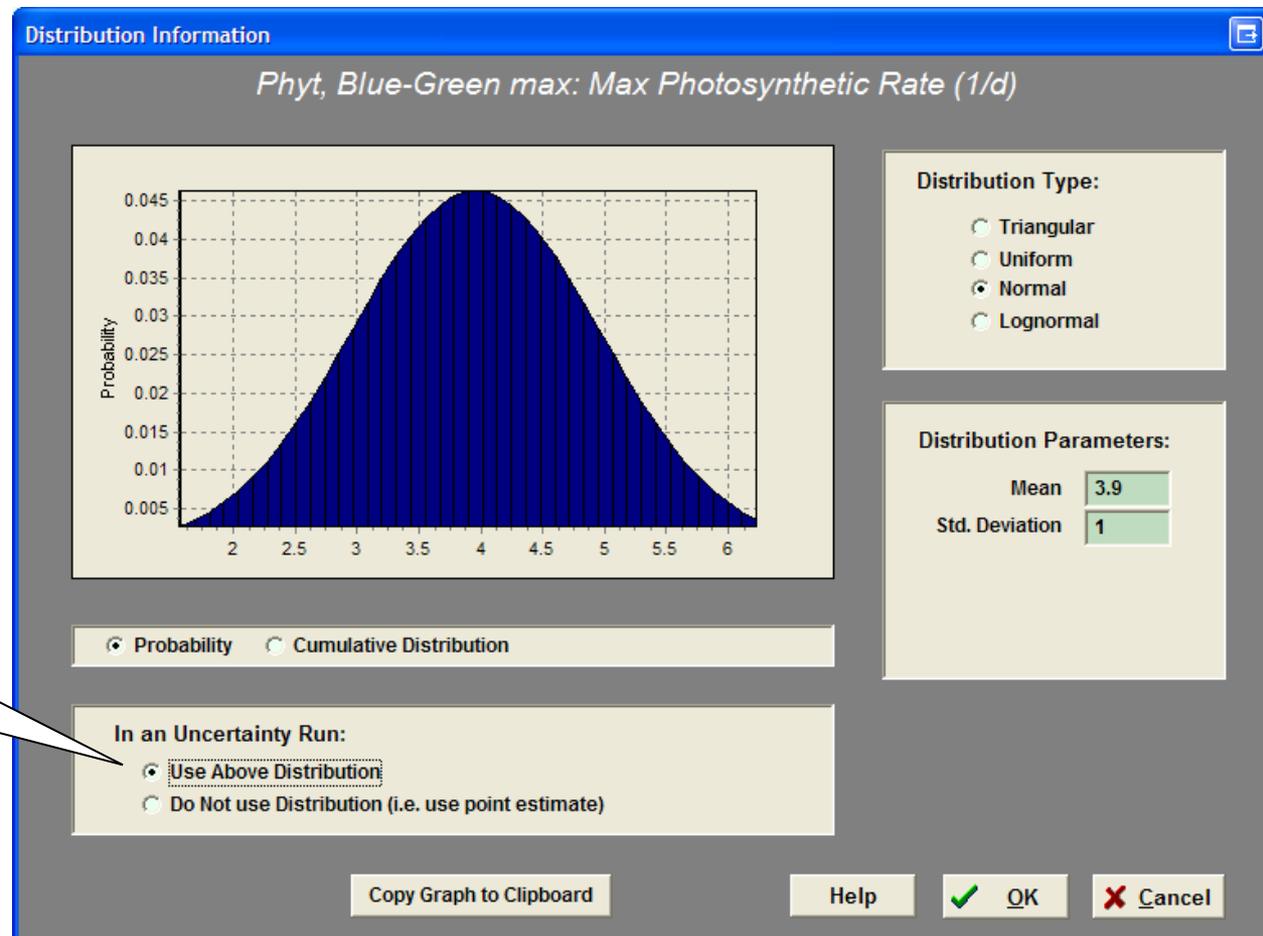
Utilize Non-Random Seed    Seed for Pseudo Random Generator: 100 (integer)     **OK**     **Cancel**

**Select Number of Iterations**

**Set Up Correlations**

# Select one or more Parameters to Vary

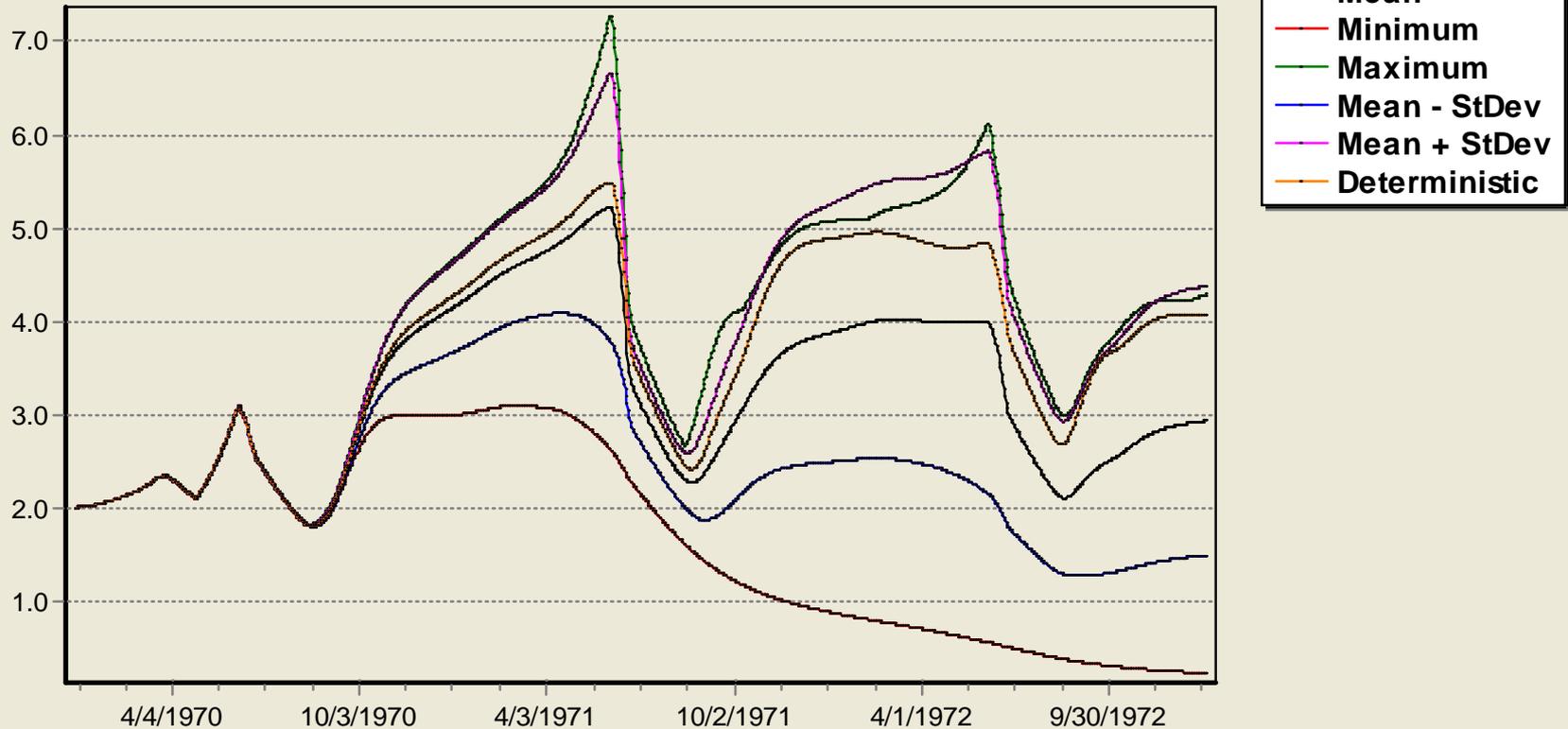
- Since blue-greens are important to this system, I will examine a parameter that affects phytoplankton, blue-greens.
- You may choose to make the same modification or choose your own variable to vary.



Choose whether to vary a parameter or keep as a constant "point estimate"

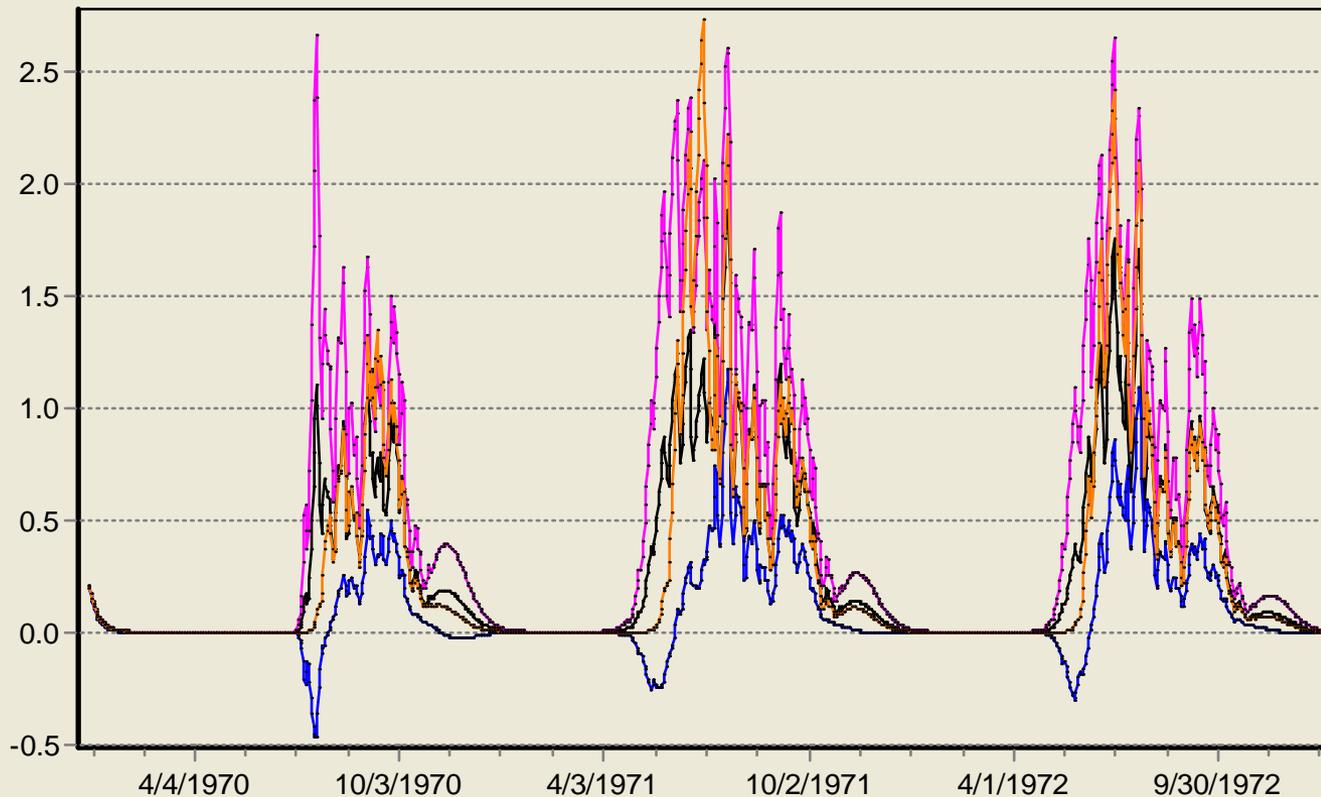
# Using the Uncertainty Tab on the Output Screen

Largemouth Bass, Lg (  
11/19/2010 11:10:48 PM



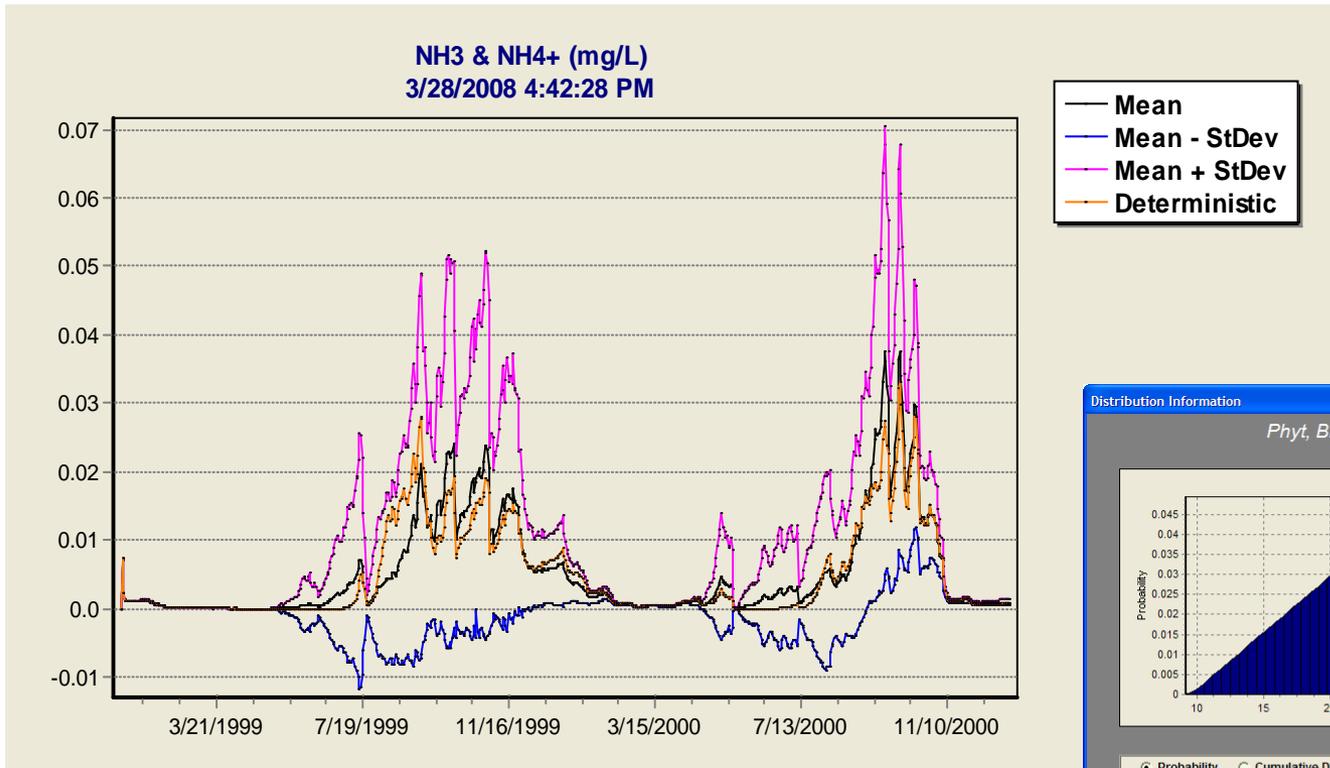
# Sensitivity of Blue-Greens

Phyt, Blue-Green max  
11/19/2010 11:10:48 PM



# Blue Earth Uncertainty Analysis Demo

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



Distribution Information

*Phyt, Blue-Gre: Optimal Temperature (deg. C)*

Distribution Type:

- Triangular
- Uniform
- Normal
- Lognormal

Distribution Parameters:

Most Likely	27
Minimum	9.17
Maximum	35.83

Probability  Cumulative Distribution

In an Uncertainty Run:

- Use Above Distribution
- Do Not use Distribution (i.e. use point estimate)

Help  OK  Cancel

# 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 (to follow)

# Chemical Derivatives Tend to be Complex

$$\begin{aligned} \frac{d\text{Toxicant}_{\text{Water}}}{dt} = & \text{Loading} + \sum_{\text{LabileDetr}} (\text{Decomposition}_{\text{LabileDetr}} \cdot \text{PPB}_{\text{LabileDetr}} \cdot 1e-6) \\ & + \sum \text{Desorption}_{\text{DetrTox}} + \sum \text{Depuration}_{\text{Org}} - \sum \text{Sorption}_{\text{DetrTox}} \\ & - \sum \text{GillUptake} - \text{MacroUptake} - \sum \text{AlgalUptake}_{\text{Alga}} \\ & - \text{Hydrolysis} - \text{Photolysis} - \text{MicrobialDegrdn} + \text{Volatilization} \\ & - \text{Discharge} + \text{Biotransform}_{\text{Microb In}} \pm \text{TurbDiff} \end{aligned}$$

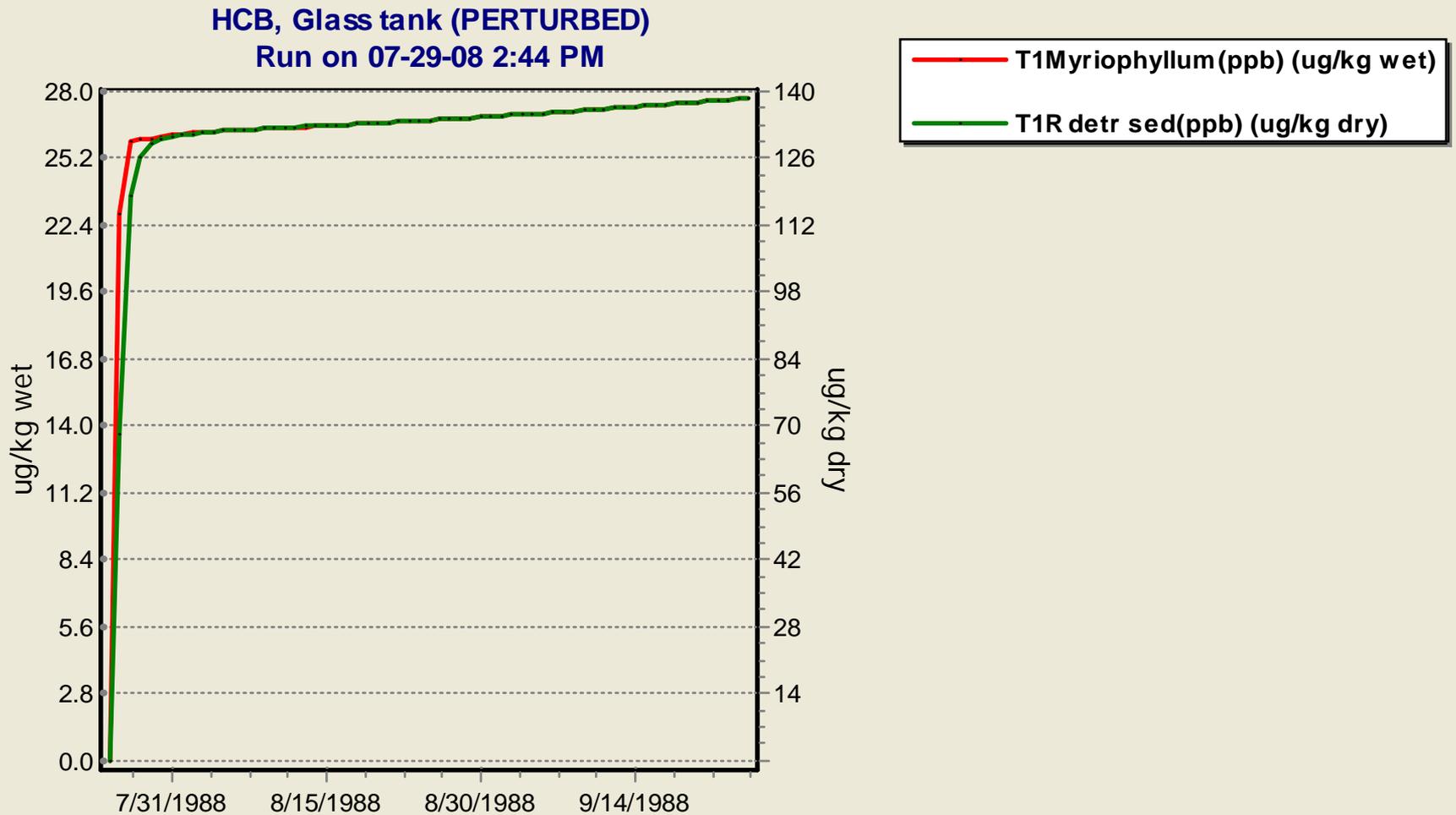
$$\begin{aligned} \frac{d\text{Toxicant}_{\text{Alga}}}{dt} = & \text{Loading} + \text{AlgalUptake} - \text{Depuration} \pm \text{TurbDiff} \\ & - (\text{Excretion} + \text{Washout} + \sum_{\text{Pred}} \text{Predation}_{\text{Pred, Alga}} + \text{Mortality} \\ & + \text{Sink} \pm \text{SinkToHypo}) \cdot \text{PPB}_{\text{Alga}} \cdot 1e-6 \pm \text{Biotransform}_{\text{Alga}} \end{aligned}$$

$$\begin{aligned} \frac{d\text{Toxicant}_{\text{Animal}}}{dt} = & \text{Loading} + \text{GillUptake} + \sum_{\text{Prey}} \text{DietUptake} \pm \text{TurbDiff} \\ & - (\text{Depuration} + \sum_{\text{Pred}} \text{Predation}_{\text{Pred, Animal}} + \text{Mortality} + \text{Recruit} \\ & \pm \text{Promotion} + \text{GameteLoss} + \text{Drift} + \text{Migration} + \text{EmergeInsect}) \\ & \cdot \text{PPB}_{\text{Animal}} \cdot 1e-6 \pm \text{Biotransform}_{\text{Animal}} \end{aligned}$$

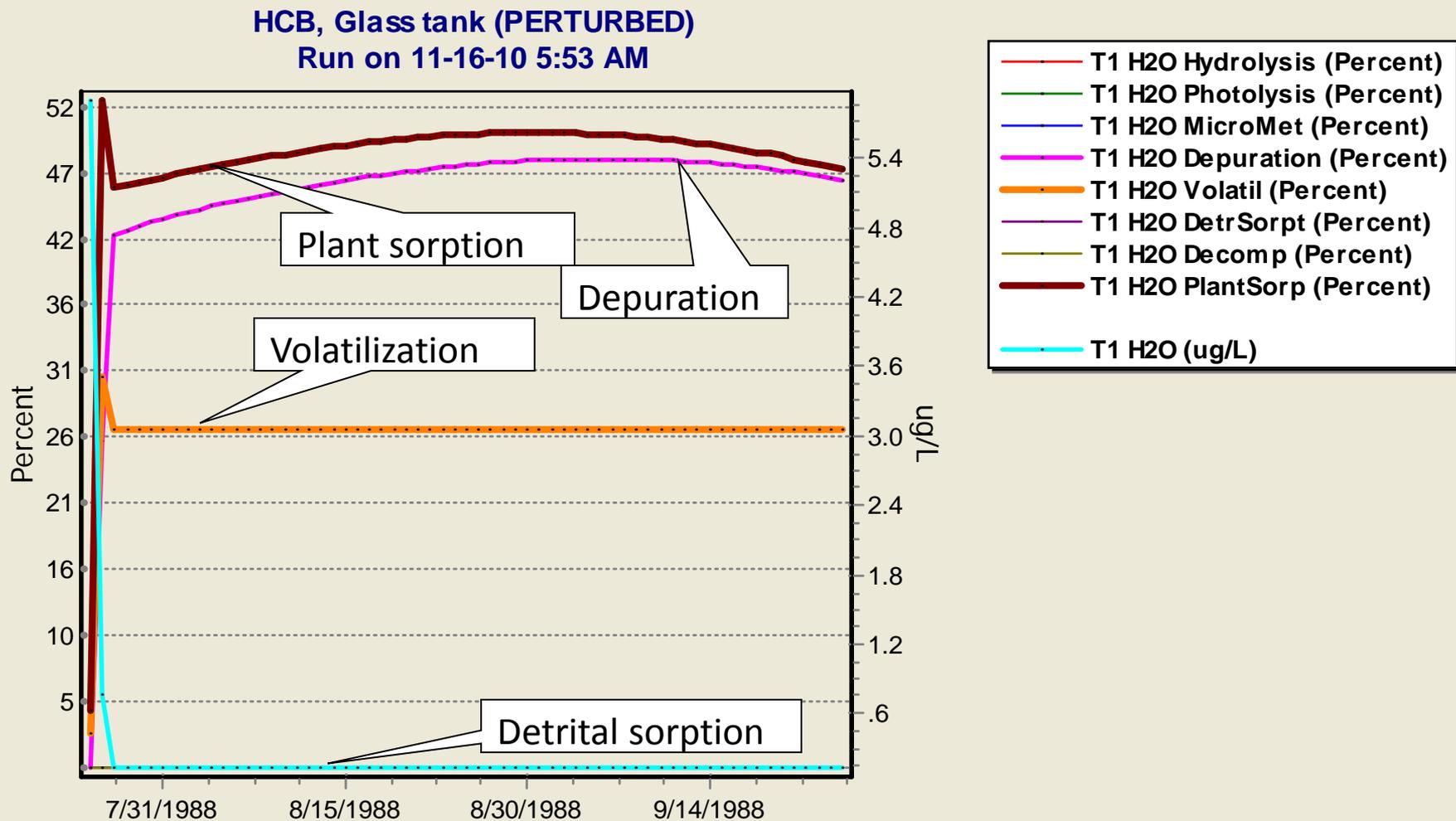
## HCB in tank

- 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



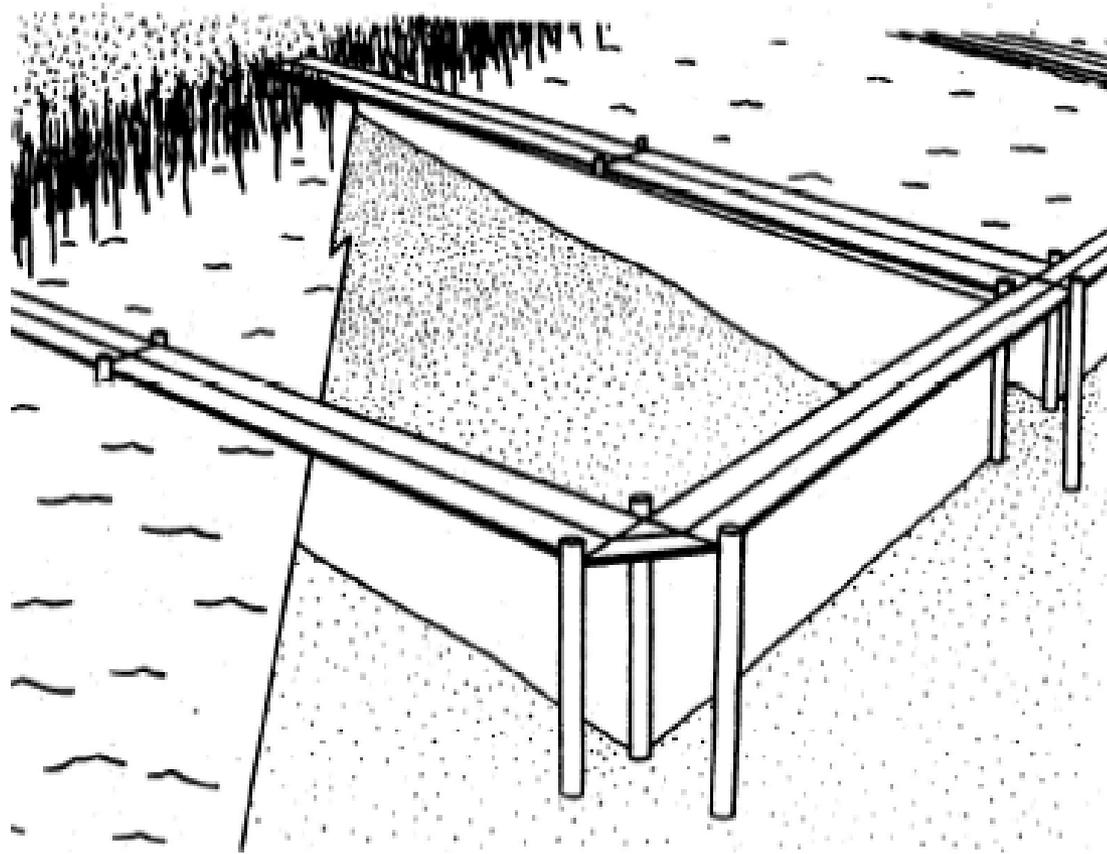
# HCB loss rates can be plotted, showing that sorption to detritus is negligible (due to mass)



# Chlorpyrifos in Pond

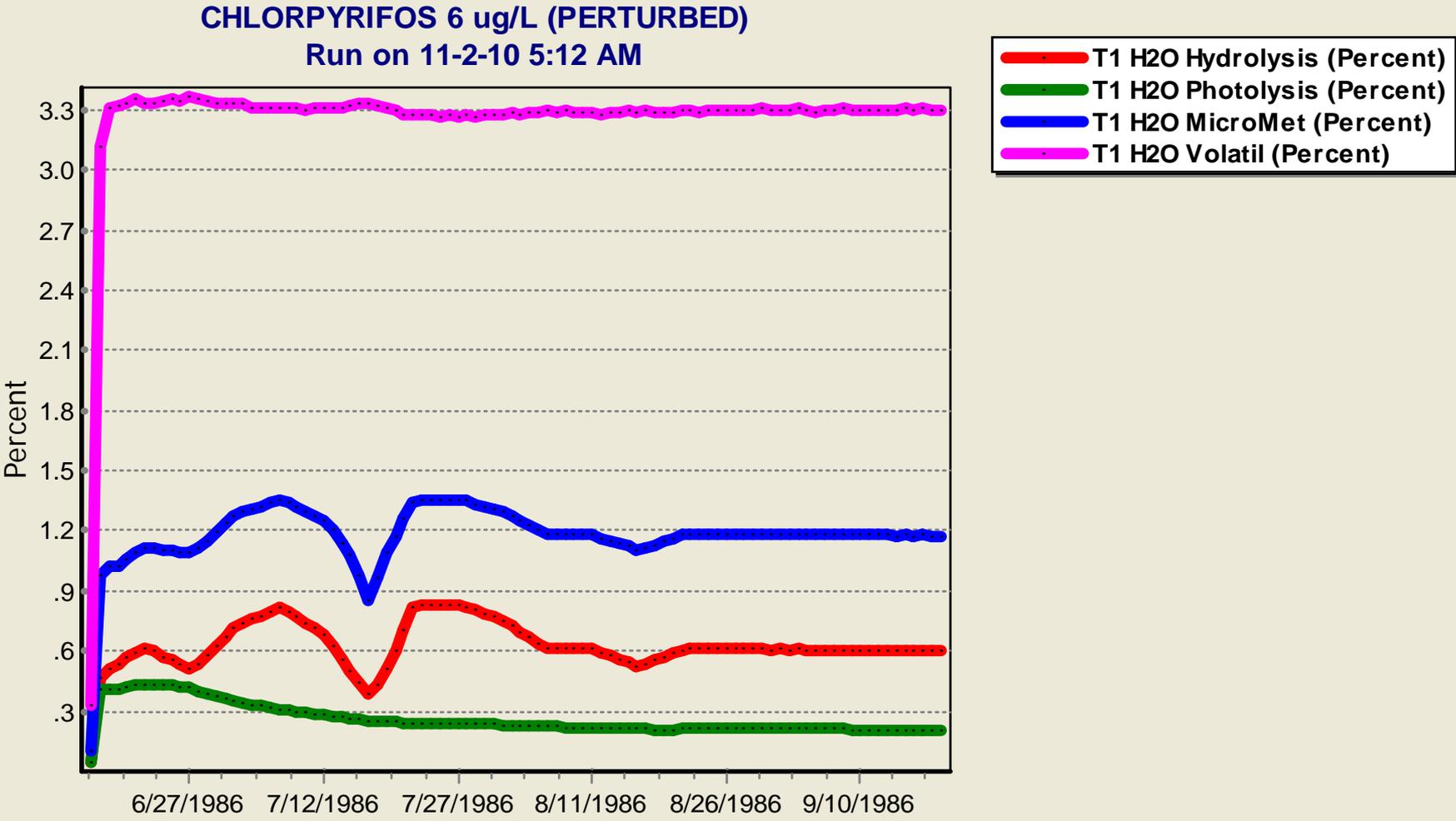
- Pond enclosure dosed with chlorpyrifos at EPA Duluth lab
- A single dose of chlorpyrifos is applied at the beginning of the simulation
- Additional biotic compartments
  - diatoms, greens, invertebrates,
  - sunfish, shiner

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

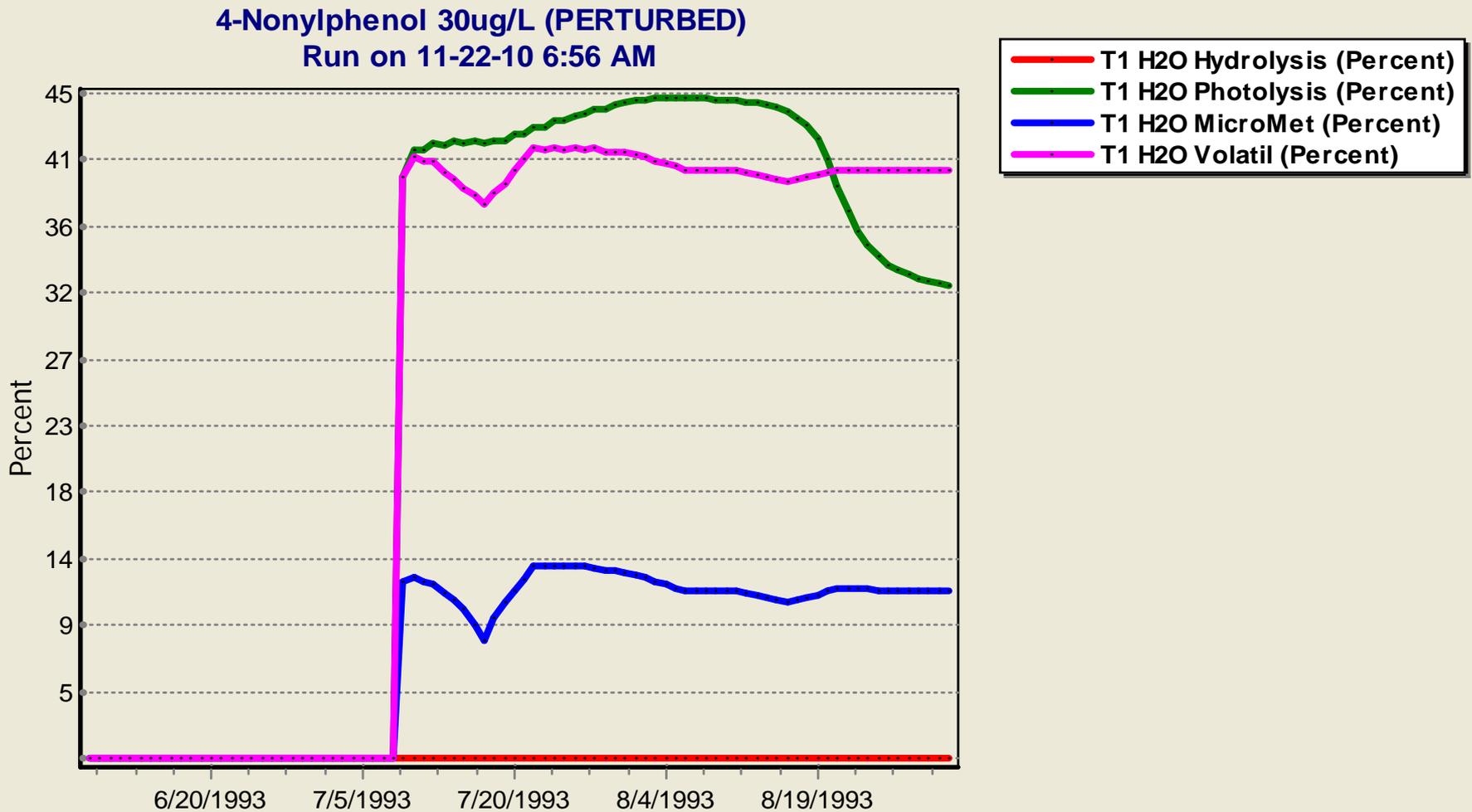


# Chemical rates may be tracked

## Predicted In-situ Degradation Rates for Chlorpyrifos in Pond



# Predicted In-situ Degradation Rates for Nonylphenol in the Same Pond are Quite Different



# Chemical fate clarified using half-Lives and DT95

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

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

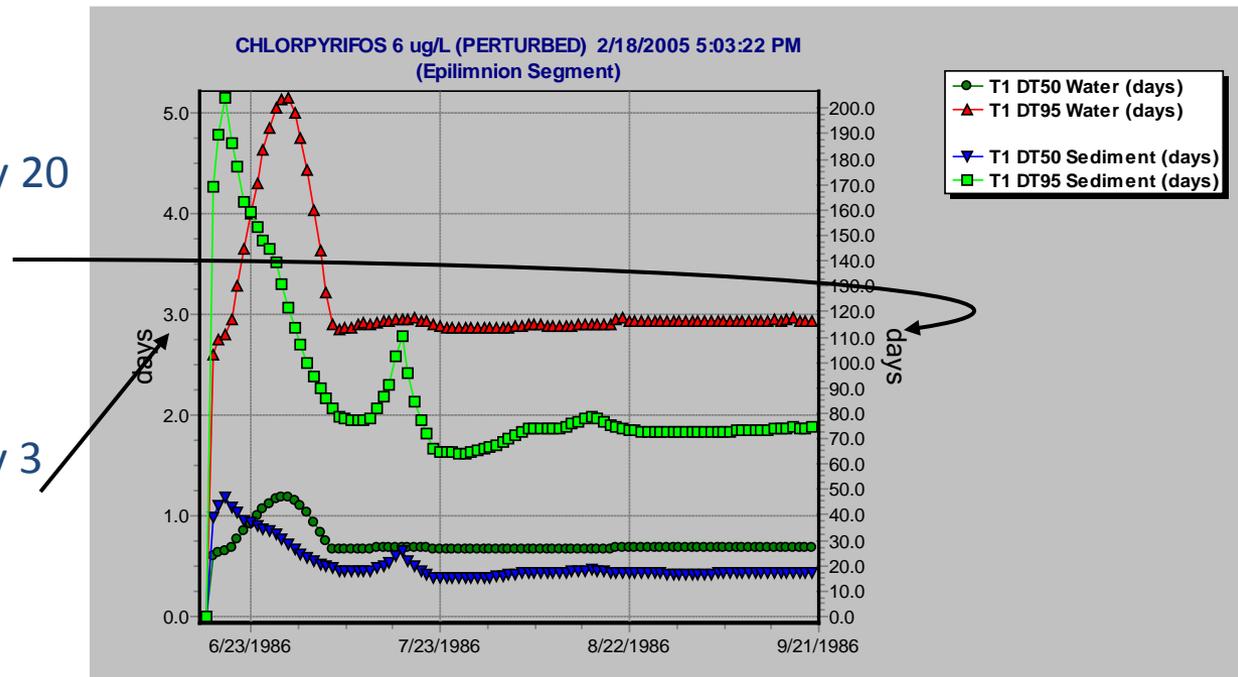
$$Loss_{Sed} = \frac{Microbial_{Sed} + Hydrolysis_{Sed} + Desorption}{Mass_{Sed}}$$

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



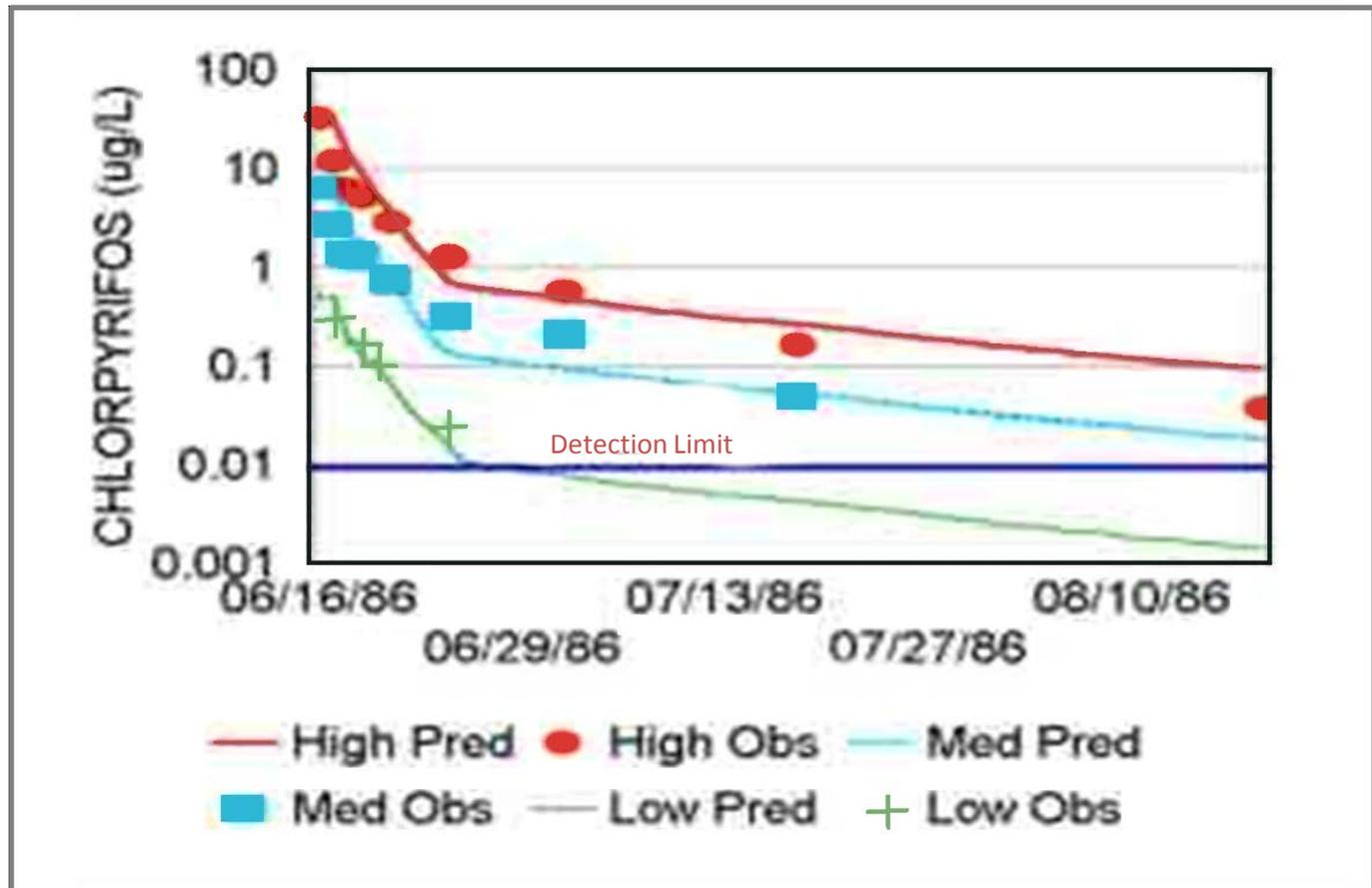
# Toxicant mass balance tracking

- 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

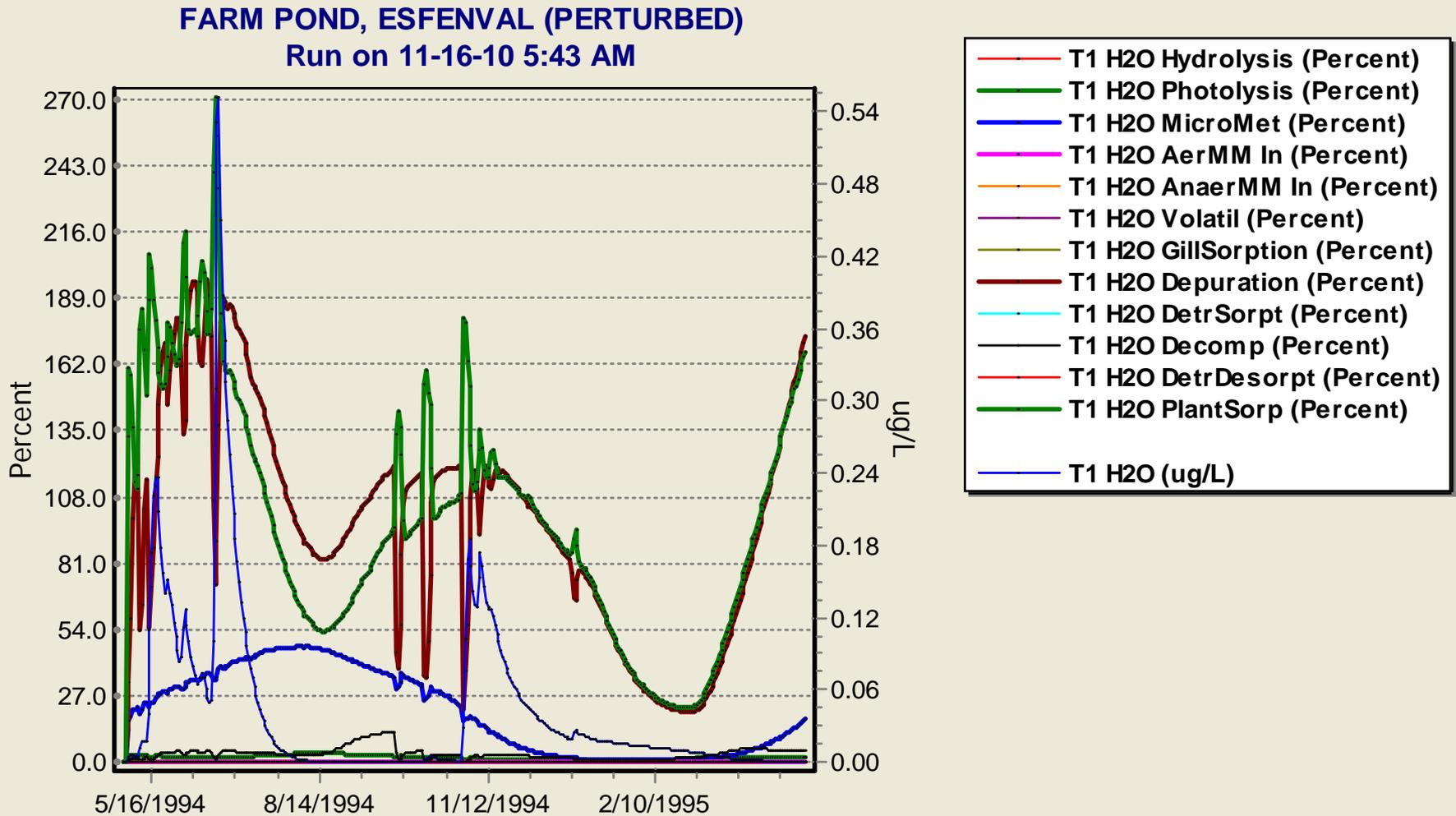


# Fate of Chlorpyrifos in the Duluth MN Pond was Predicted Successfully

Multiple Dosing Levels



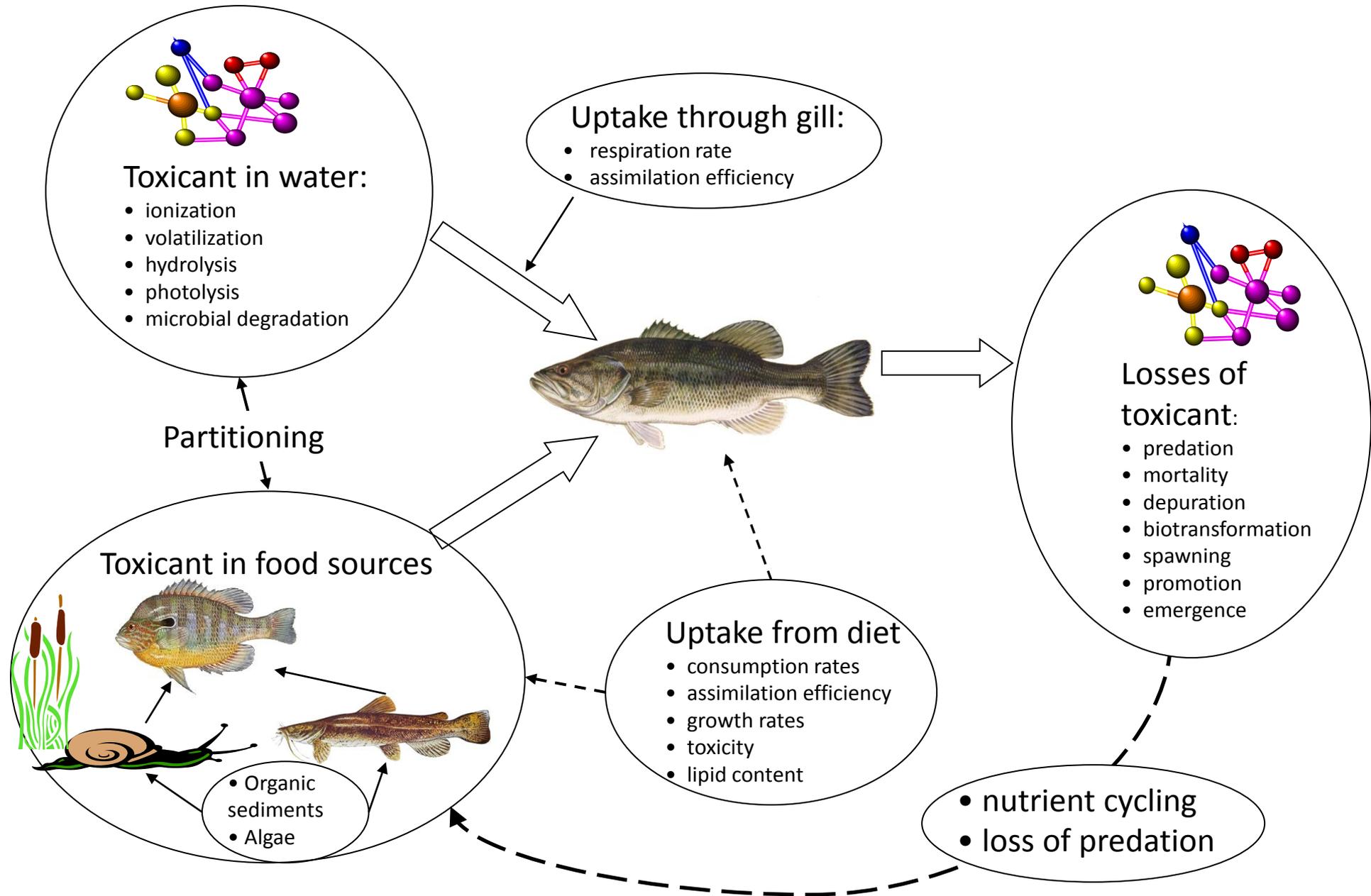
# Esfenvalerate in farm pond is taken up and depurated by phytoplankton and lost by microbial degradation



# 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) Bioconcentration Factor (BCF) model available

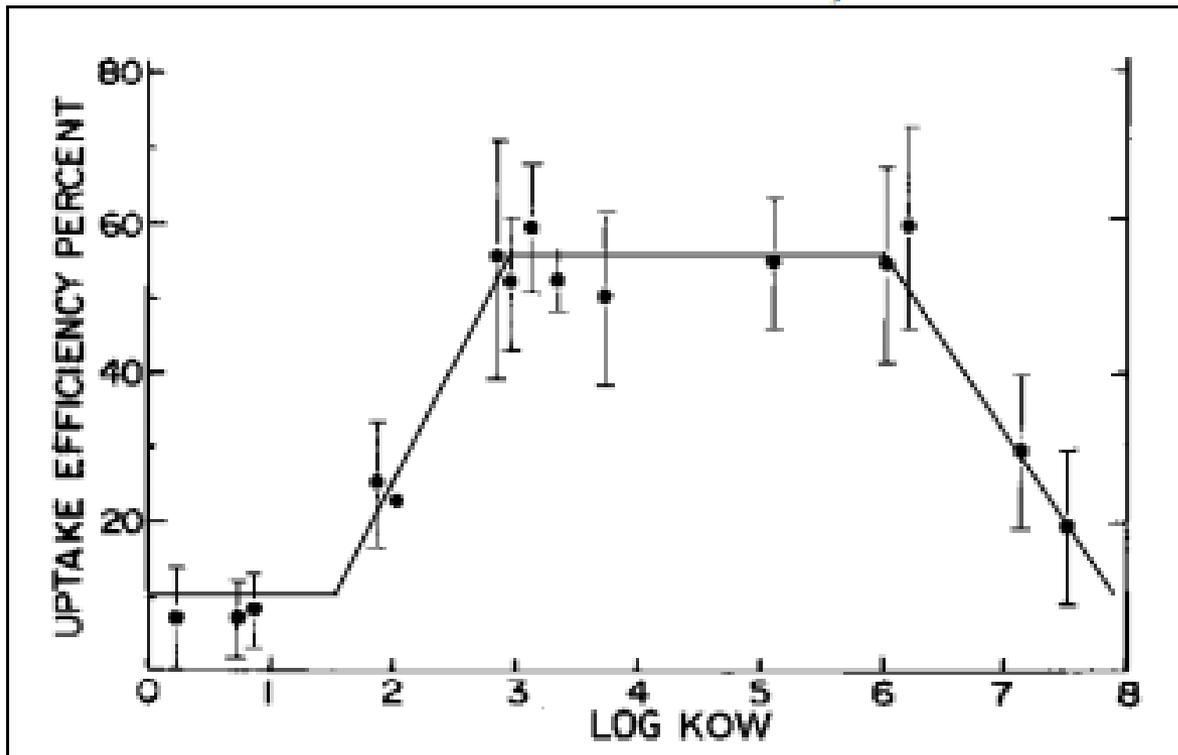
# Bioaccumulation in AQUATOX



# Gill Uptake is Function of Respiration and Efficiency of Toxicant Uptake

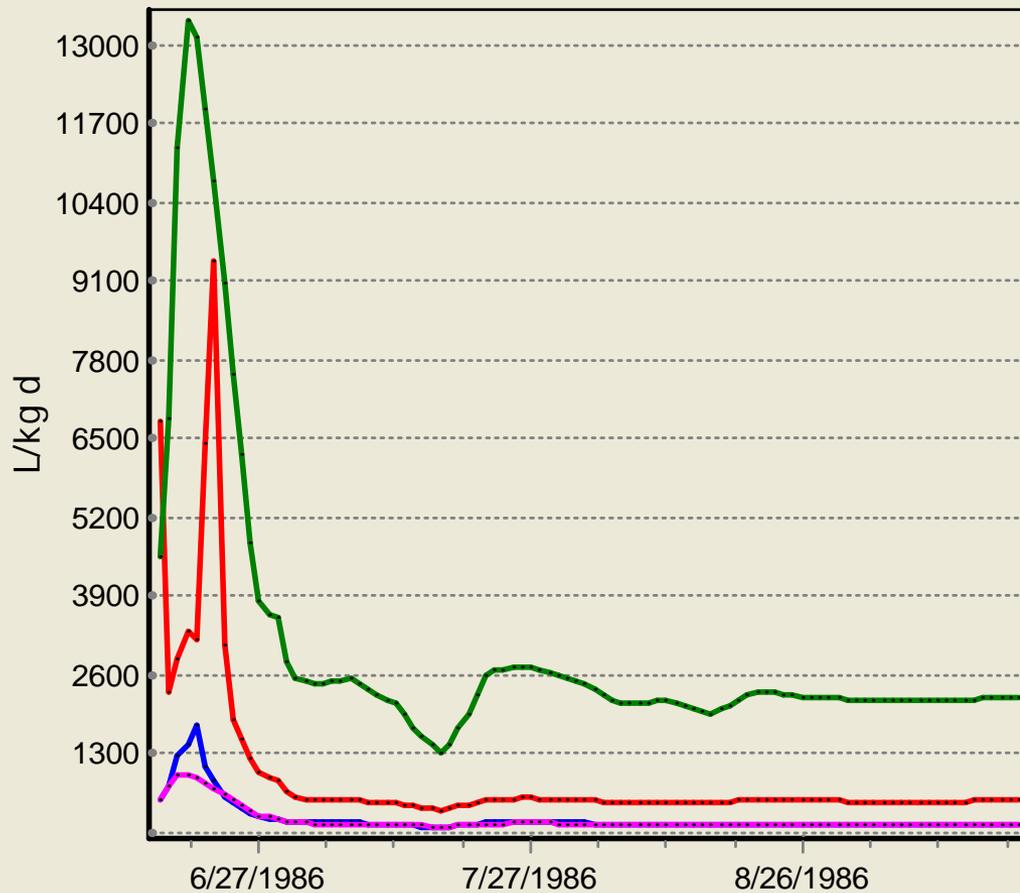
$$GillUptake = KUptake \cdot Toxicant_{Water} \cdot Frac_{WaterColumn}$$

$$KUptake = \frac{WEffTox \cdot Respiration \cdot O2Biomass}{Oxygen \cdot WEffO2}$$



# Chlorpyrifos Uptake Rates for Invertebrates and Fish in Pond

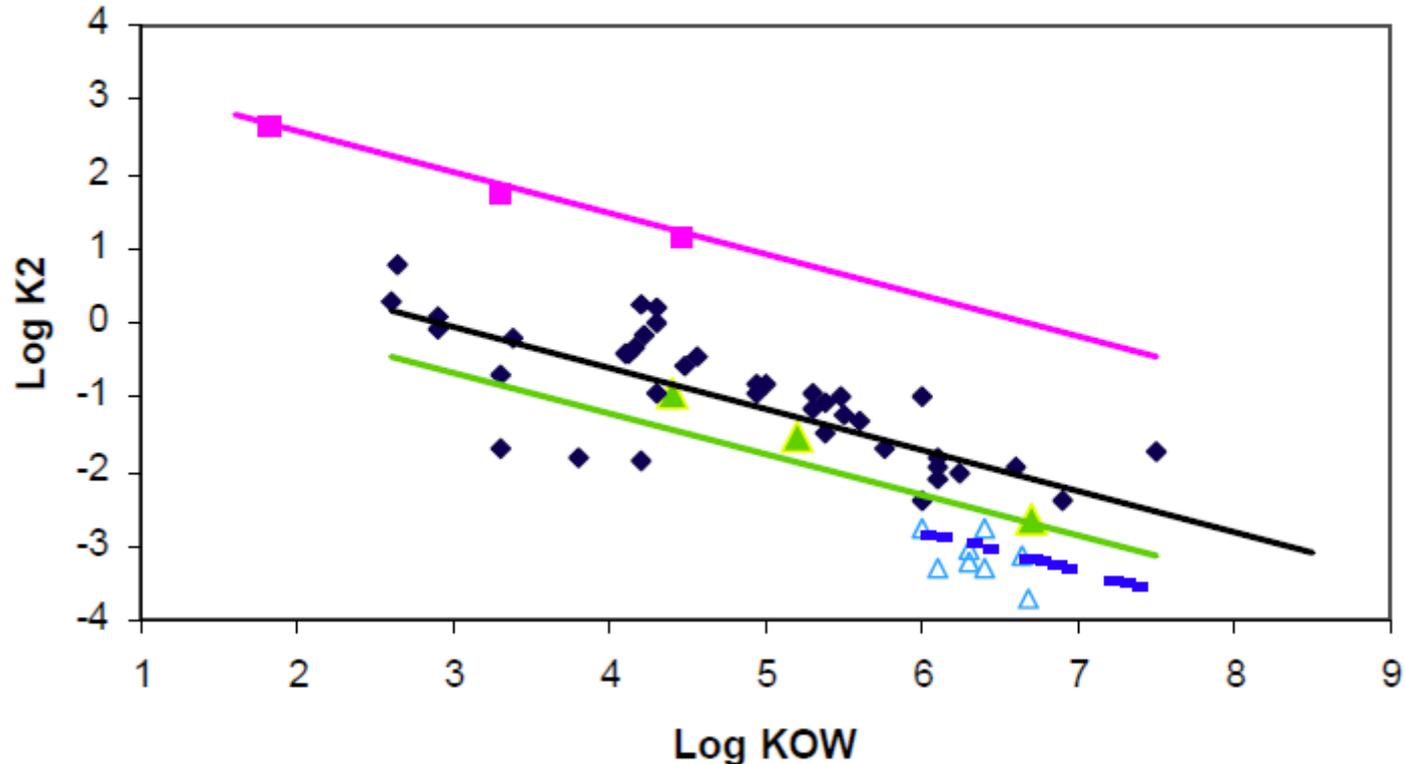
**CHLORPYRIFOS 6 ug/L (PERTURBED)**  
Run on 11-15-10 4:32 PM



- K1 T1Chironomid (L/kg d)
- K1 T1Daphnia (L/kg d)
- K1 T1Shiner (L/kg d)
- K1 T1Green Sunfish, Adult (L/kg d)

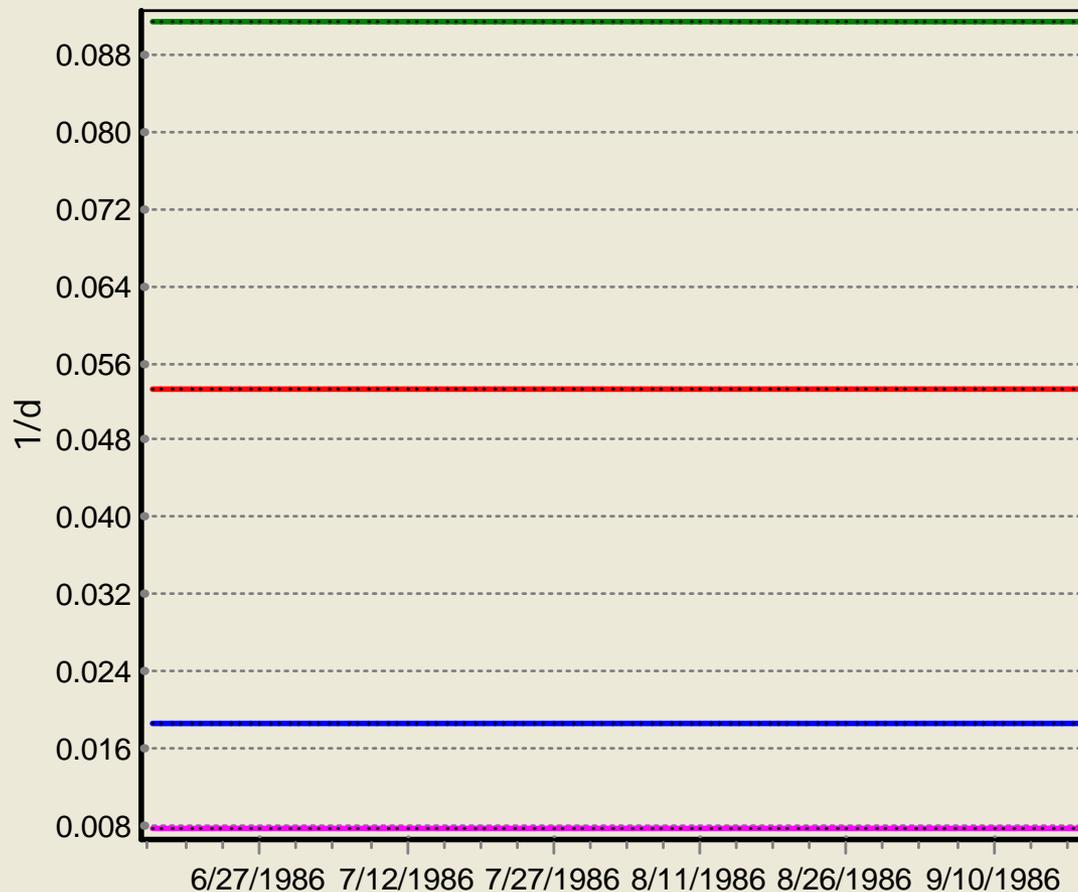
# Depuration Rate Constants for Invertebrates and Fish – Default Option

## K2 for Various Animals



# Chlorpyrifos Depuration Rate Constants for Invertebrates and Fish in Pond

**CHLORPYRIFOS 6 ug/L (PERTURBED)**  
**Run on 11-15-10 4:32 PM**



- K2 T1Chironomid (1/d)
- K2 T1Daphnia (1/d)
- K2 T1Shiner (1/d)
- K2 T1Green Sunfish, Adult (1/d)

# Alternative Chemical Uptake Model

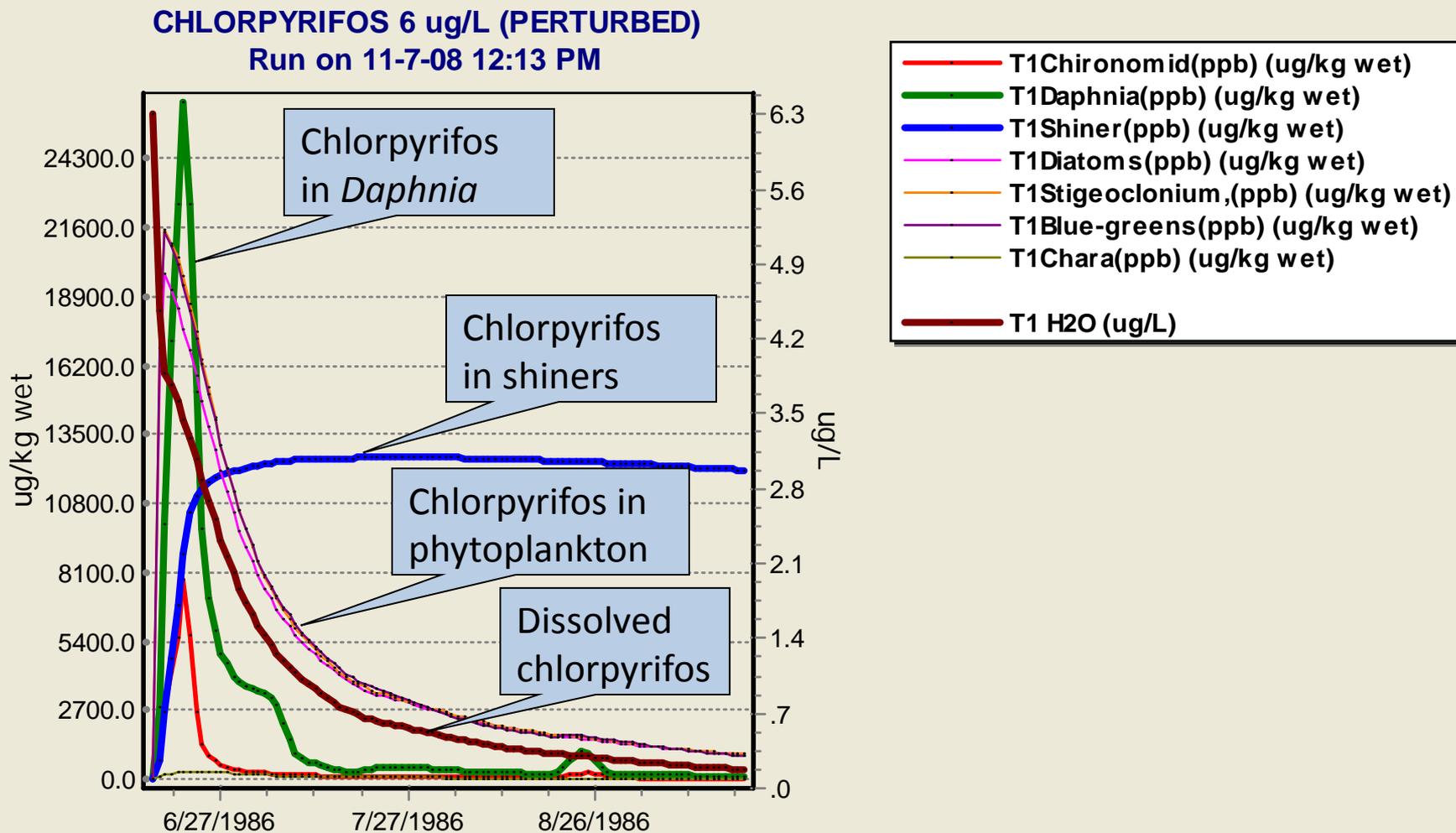
The user may enter **two** of the three factors defining uptake (BCF, K1, K2) and the third factor is calculated:

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

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

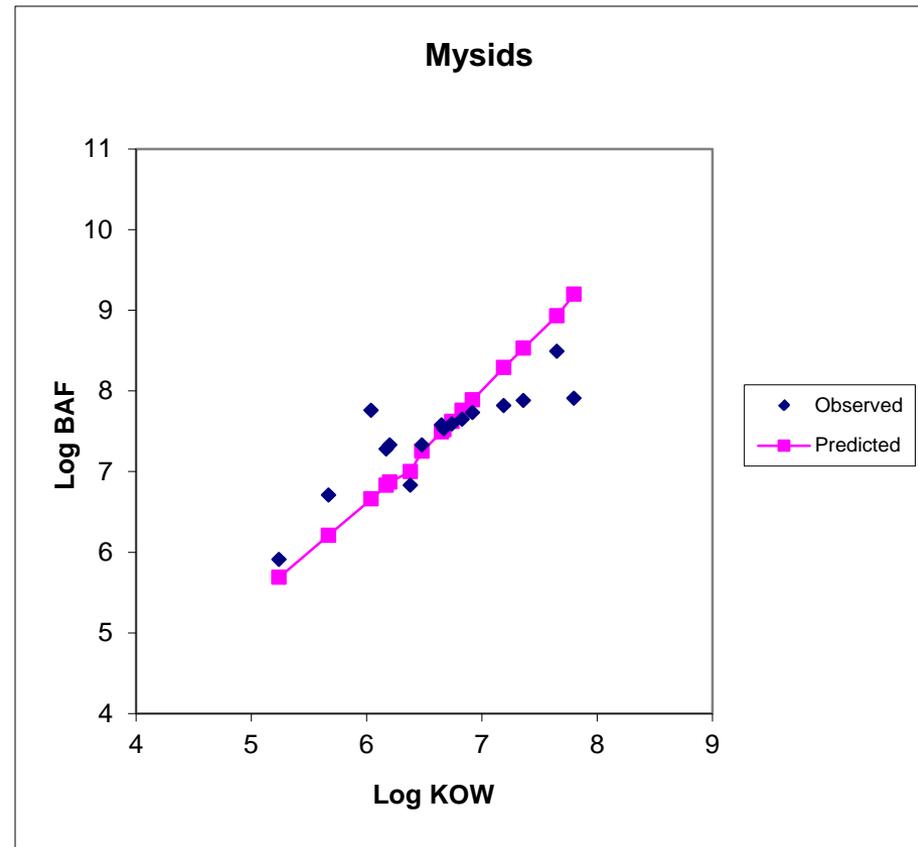
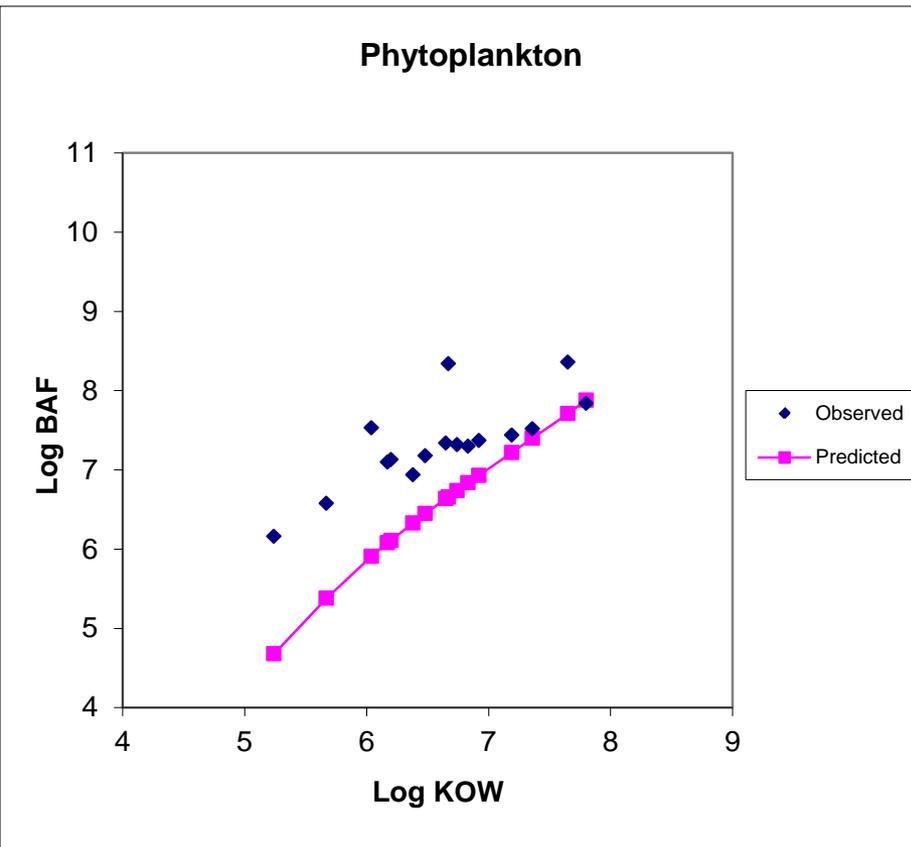
Dietary uptake of chemicals by animals is not affected by this alternative parameterization.

# Model can trace how the toxicant is partitioned in the biota



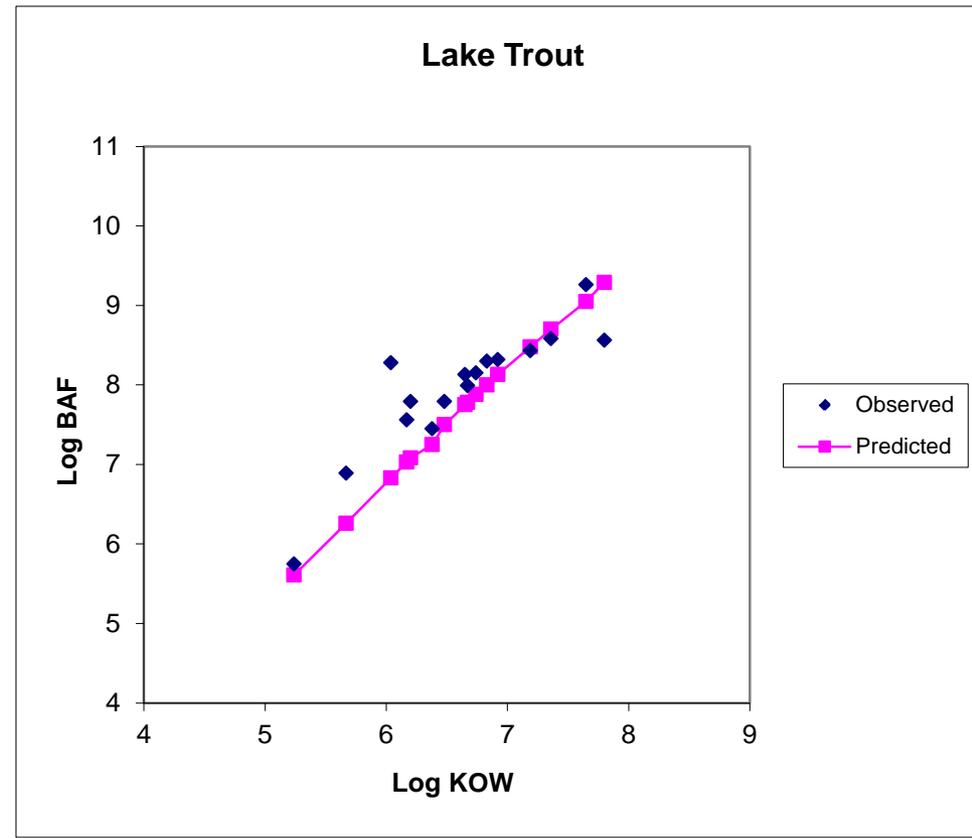
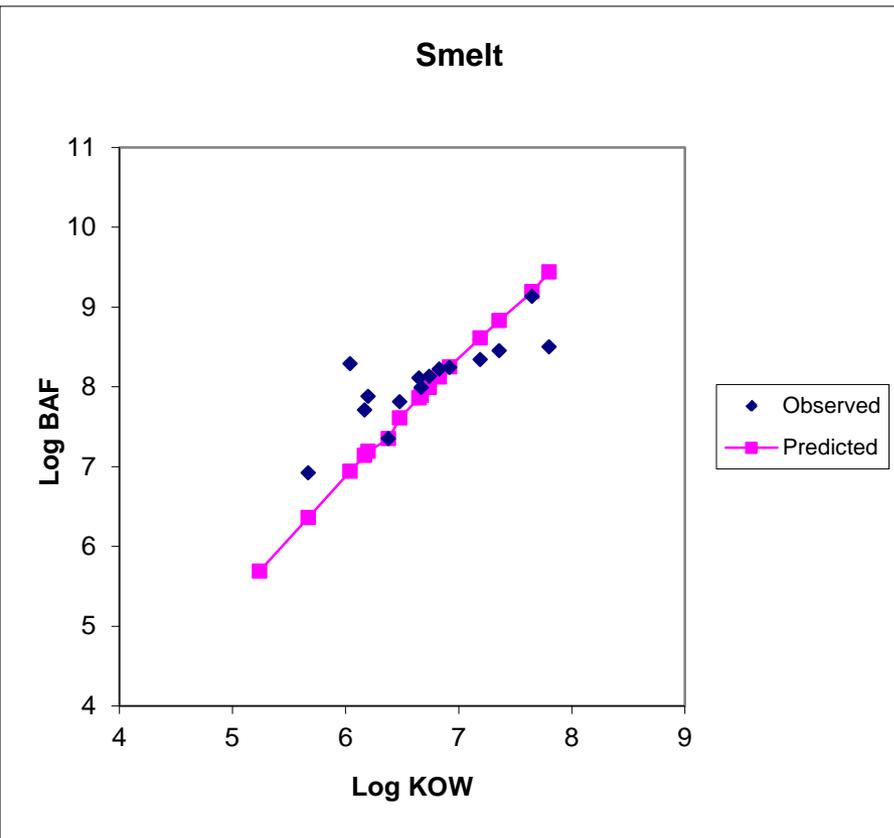
# Lake Ontario Bioaccumulation

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

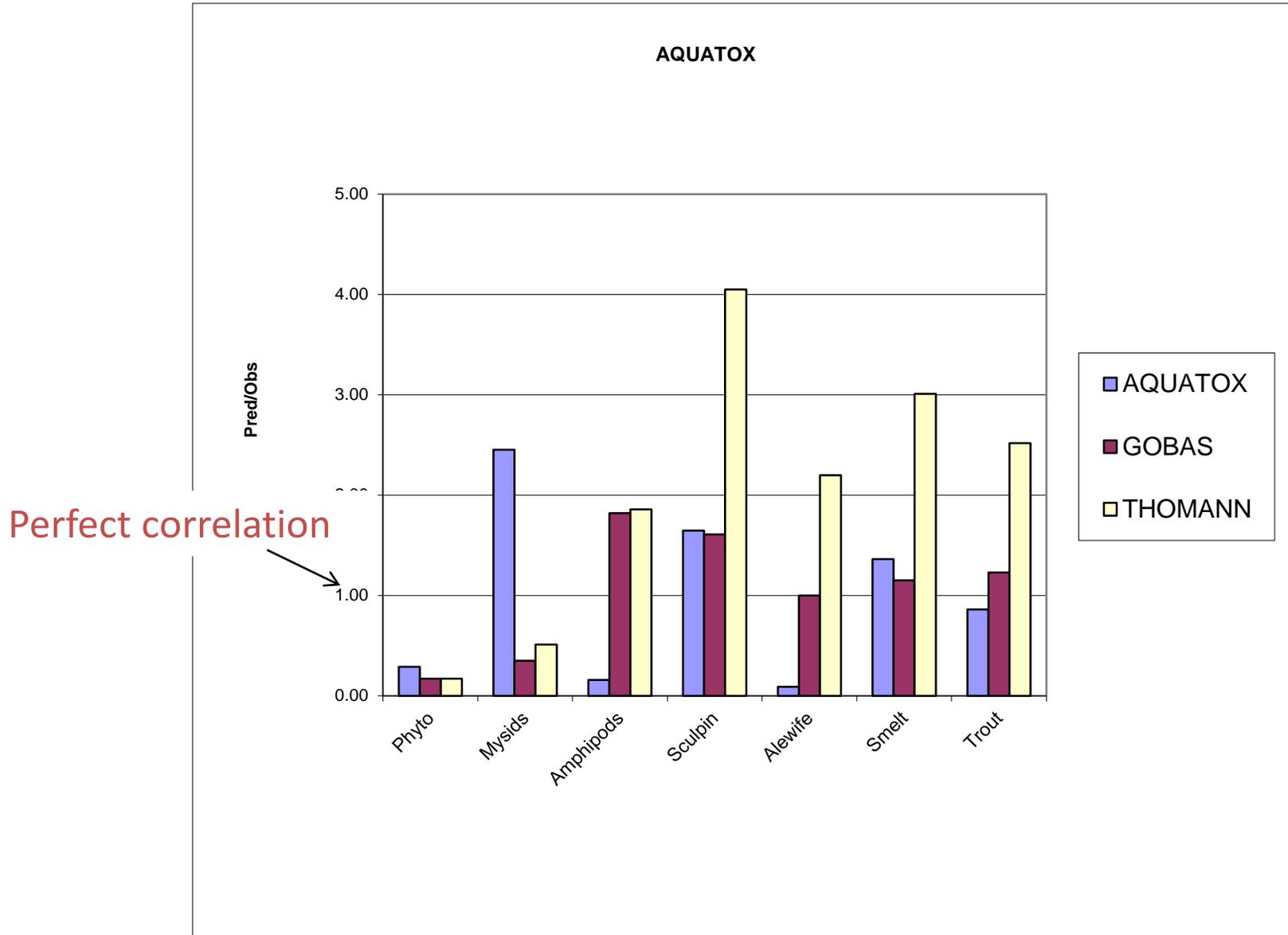


# Lake Ontario Bioaccumulation

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



# Lake Ontario BAF model comparison

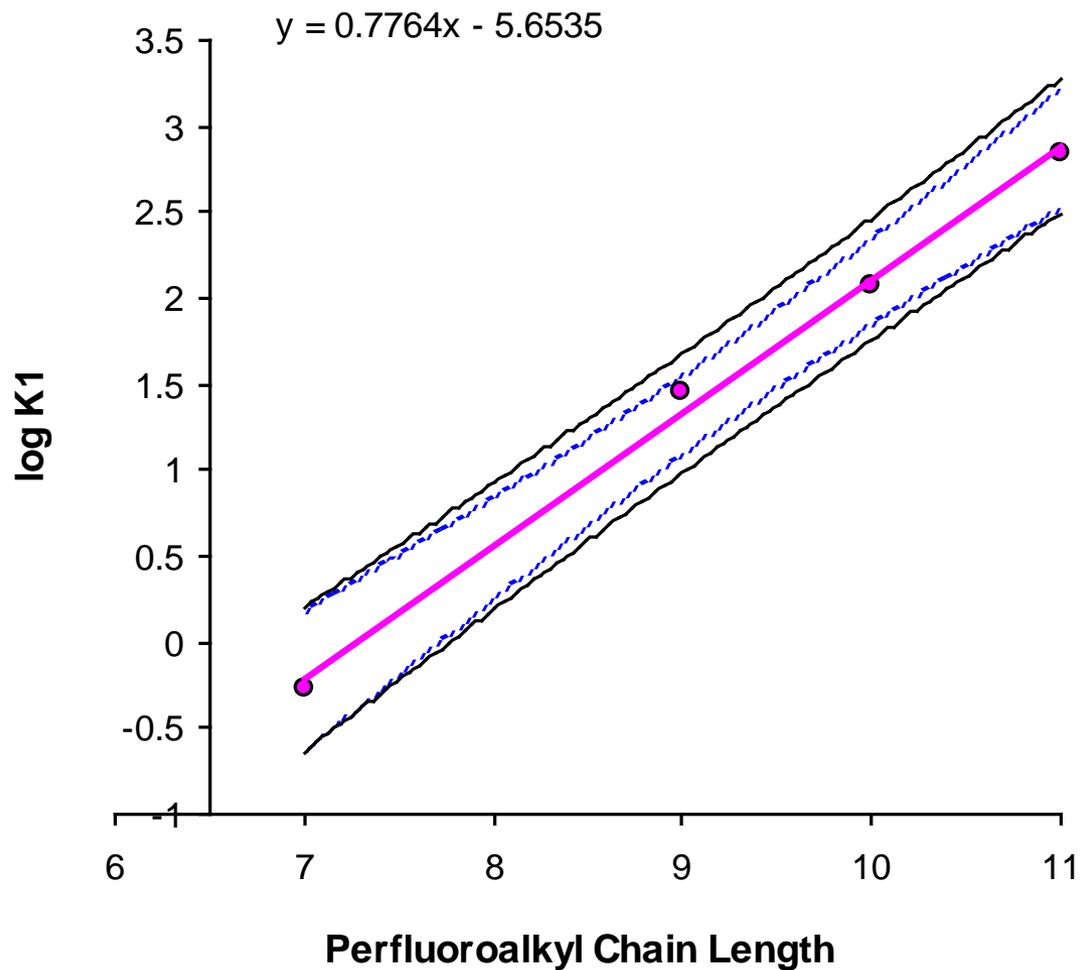


## Perfluorinated Surfactants (PFAs)

- 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

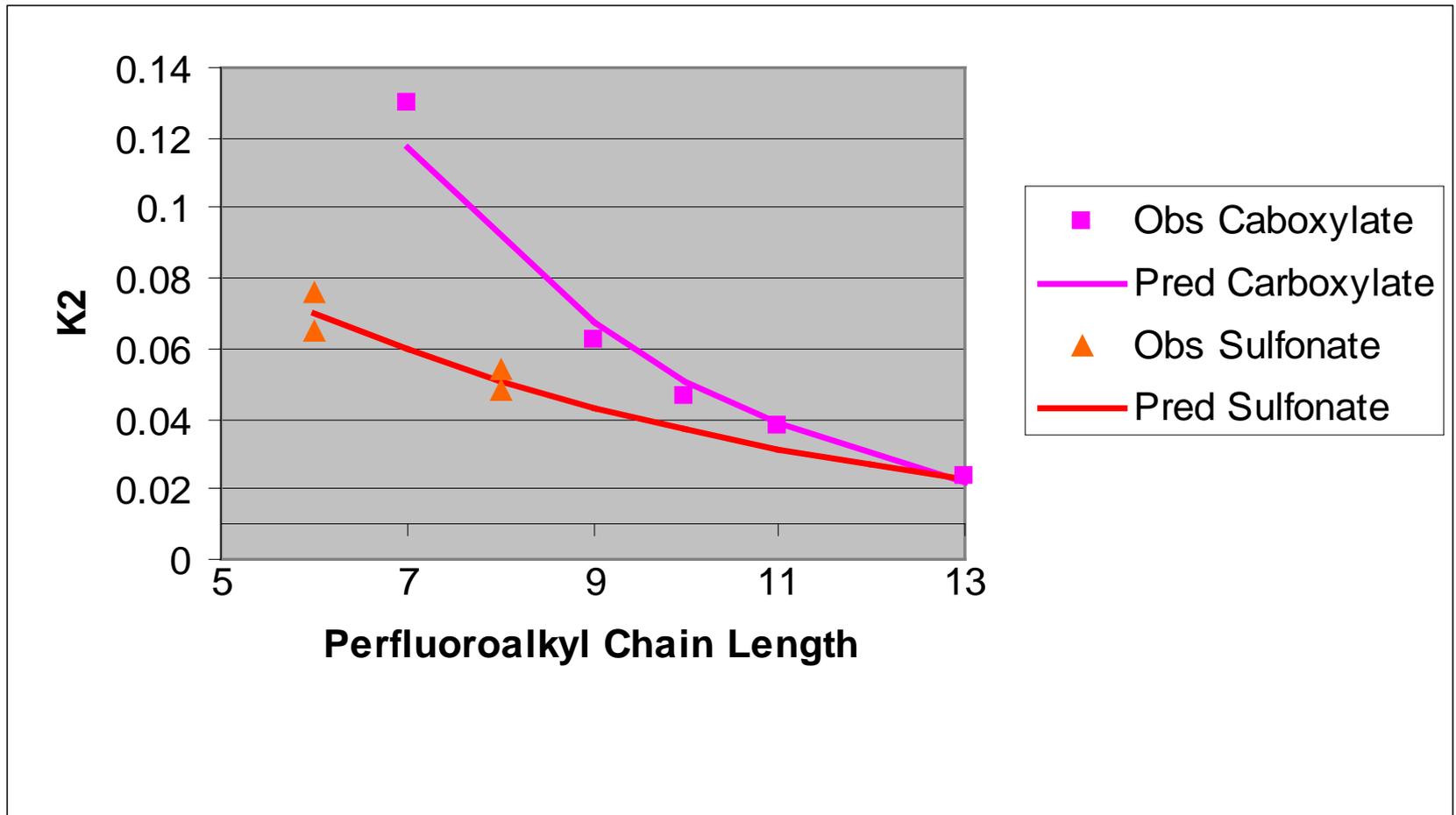
# Uptake of carboxylates can be predicted by chain length

*data from Martin et al., 2003*



# Depuration rate is also a function of chain length

*data from Martin et al., 2003*



# PFA Model Data Requirements

- Perflouralkyl Chain Length
- $K_{OM}$  for sediments
- BCF for algae
- BCF for macrophytes
- Toxicity Data (LC50s)

(Parameters provided for PFOS, PFOA)