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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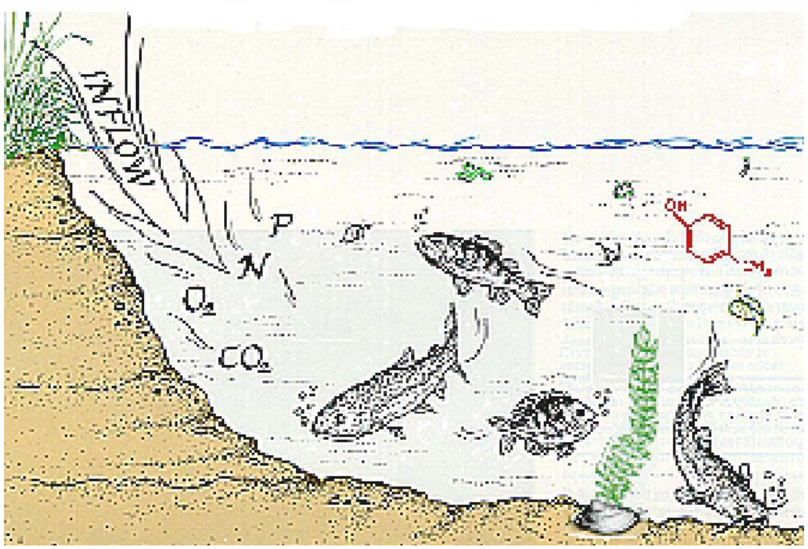


Lab 4: Application to Minnesota Rivers

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.**

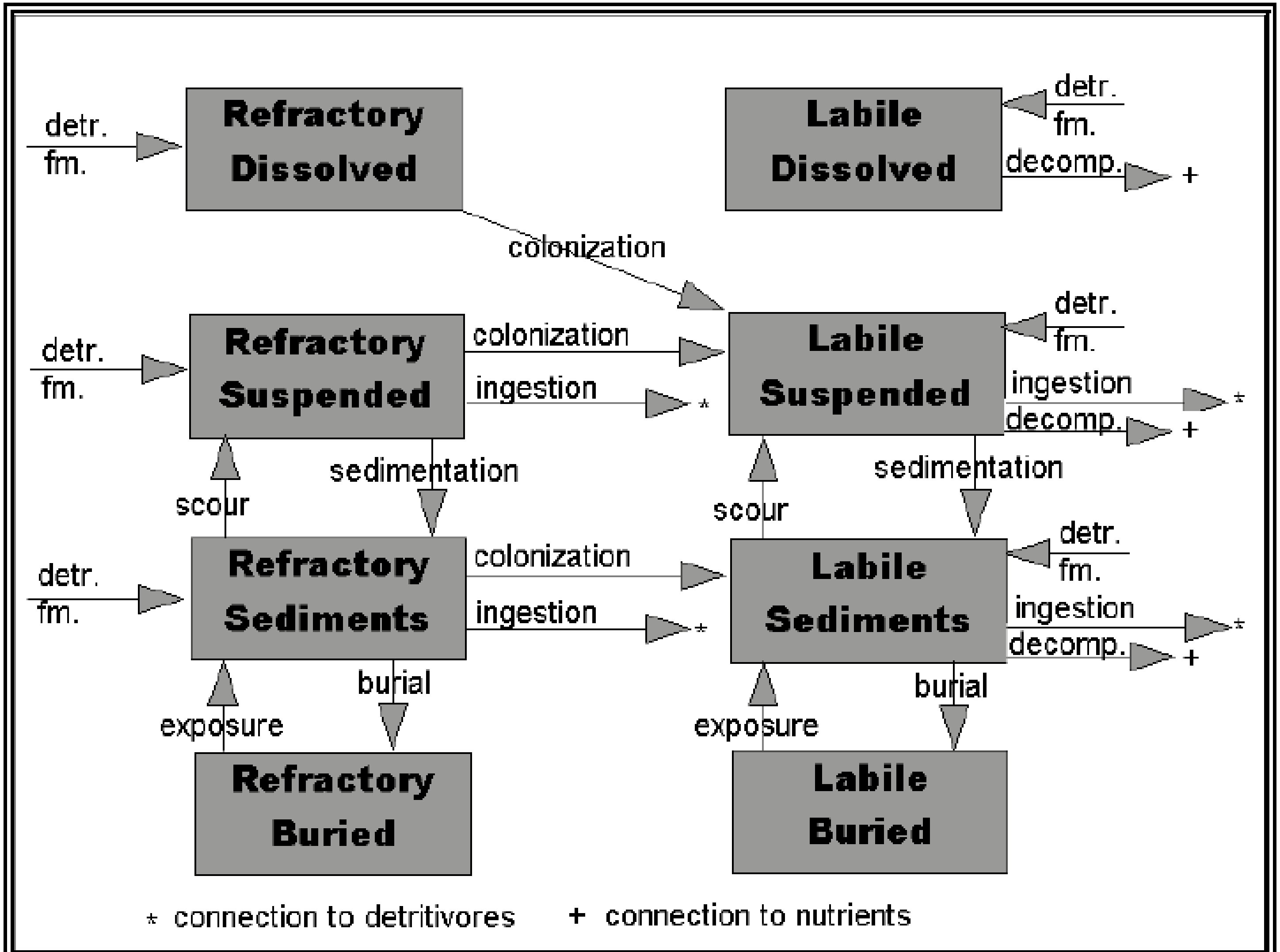
You can set up the simulations and let them run during the next lecture, then we will discuss the results.

Remineralization

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

Detritus Compartments in AQUATOX

Figure 54
Detritus Compartments in AQUATOX



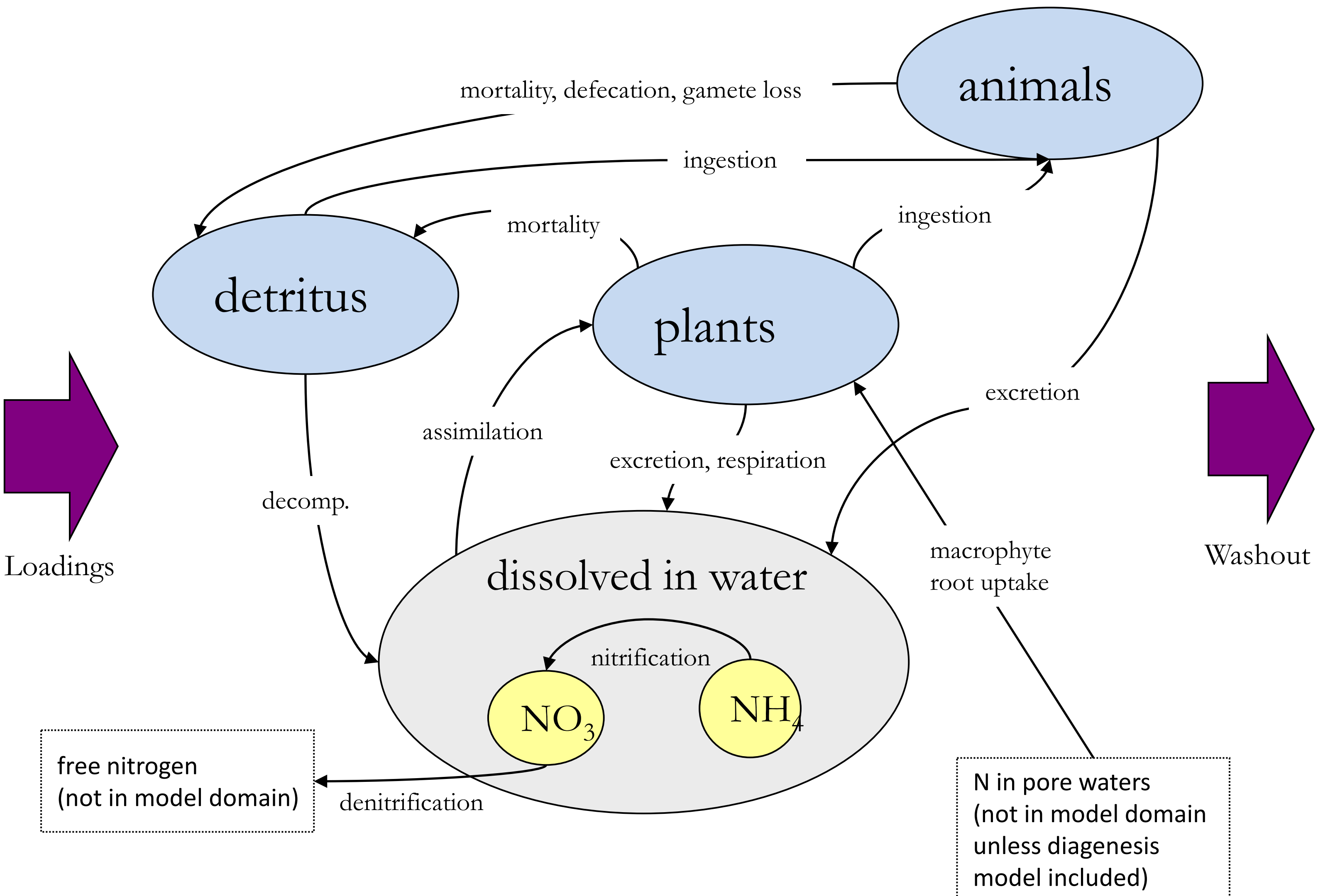
Variable Stoichiometry

- 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.

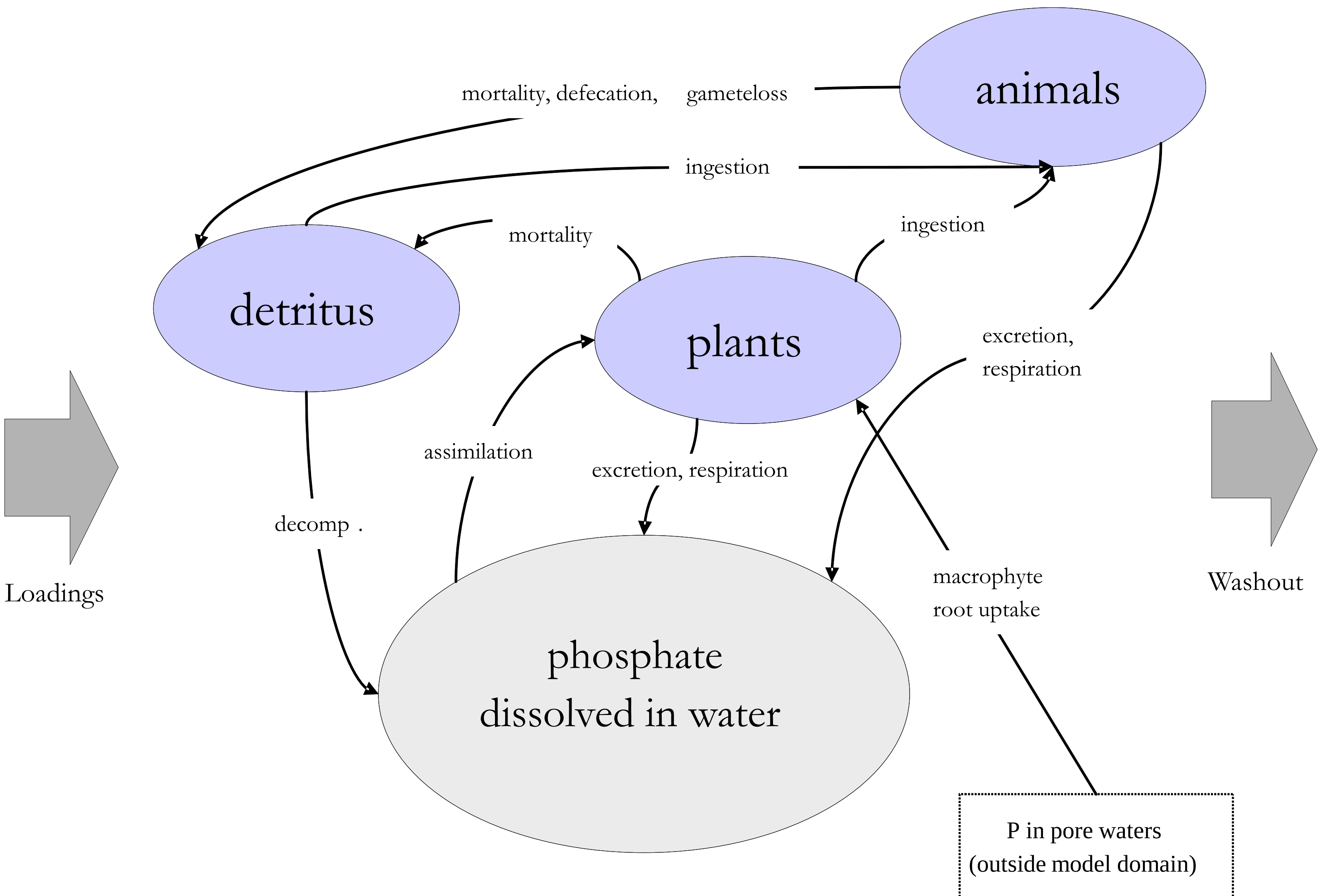
Default Nutrient to Organic Matter Ratios

Compartment	Frac. N (dry)	Frac. P (dry)	Reference
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)

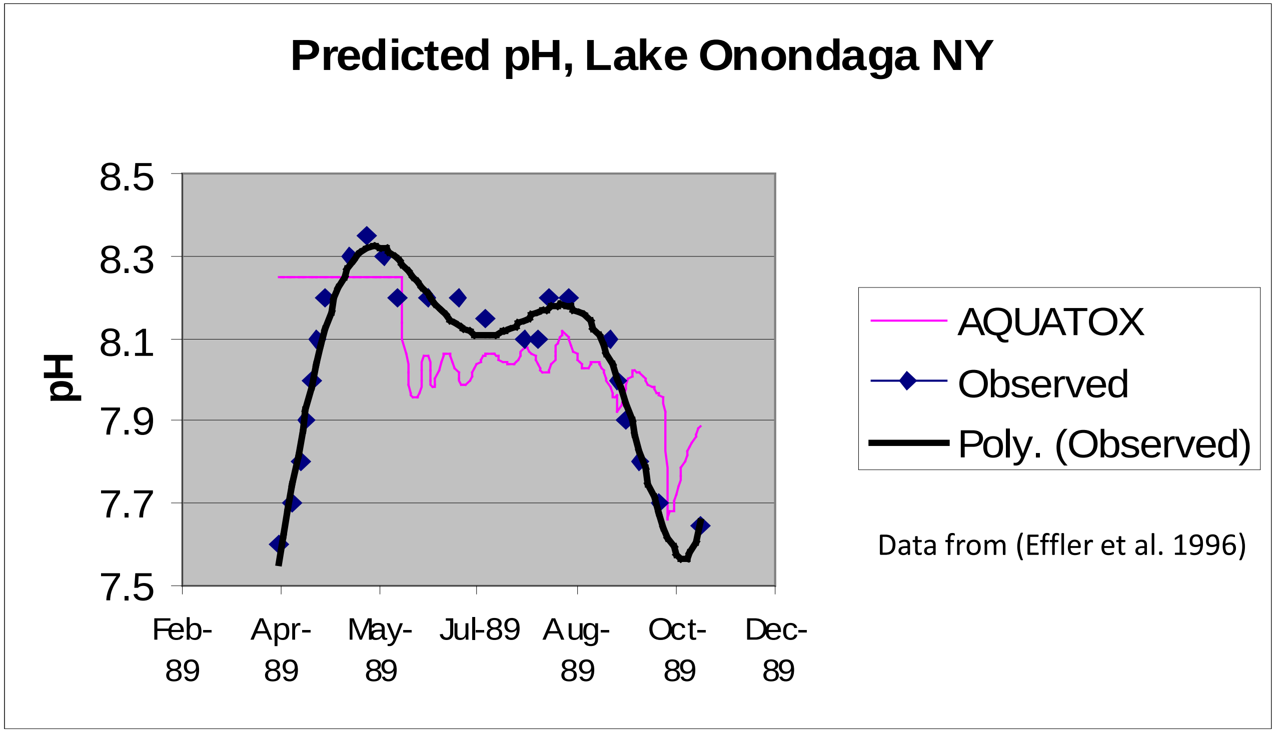


Nutrient Cycle in AQUATOX (Phosphorus)



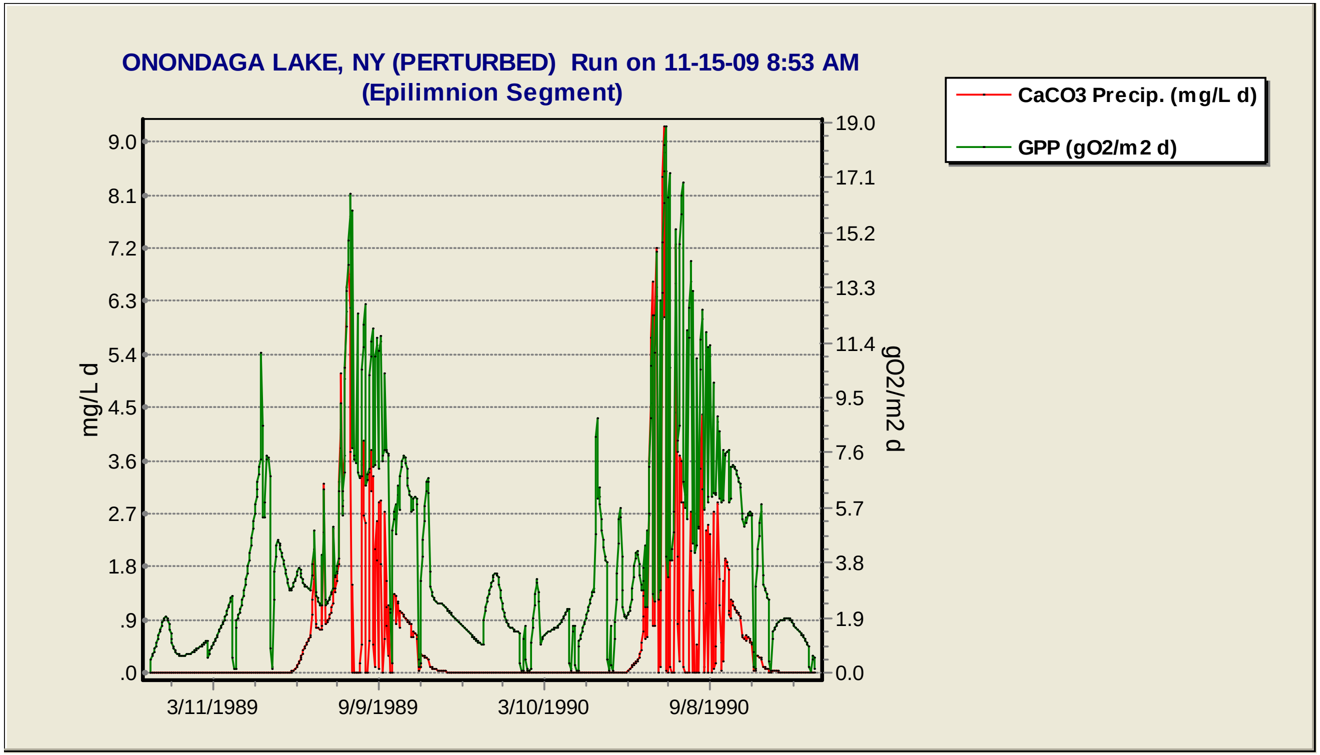
Dynamic pH also added to variable stoichiometry version:

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



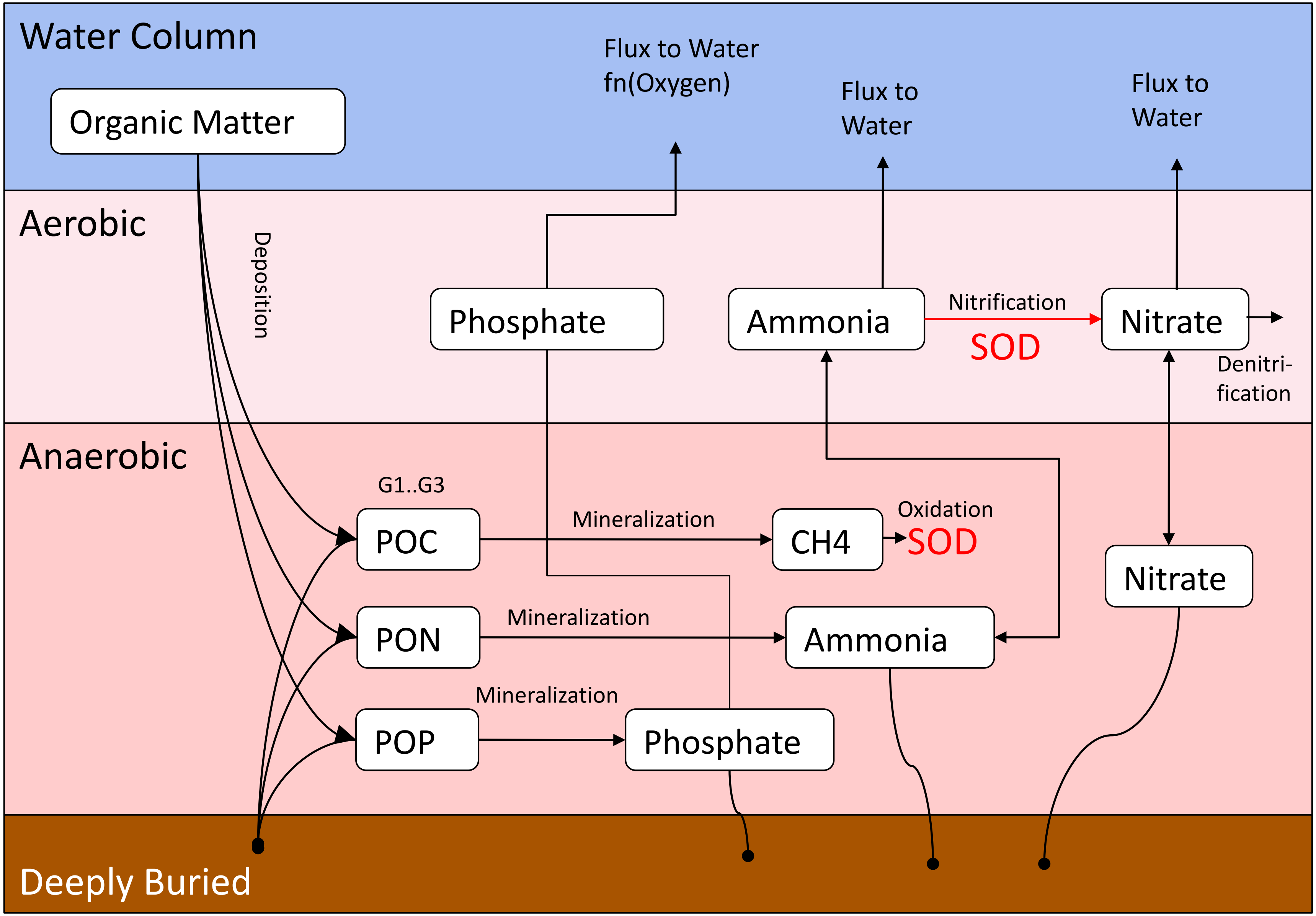
Calcium Carbonate Precipitation

- Predicted as a function of pH and algal type
  - When pH >=7.5, precipitation is predicted
  - Precipitation rate is dependent on photosynthesis rate (gross primary production) in some, but not all, plants
- $CaCO_3$ 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)

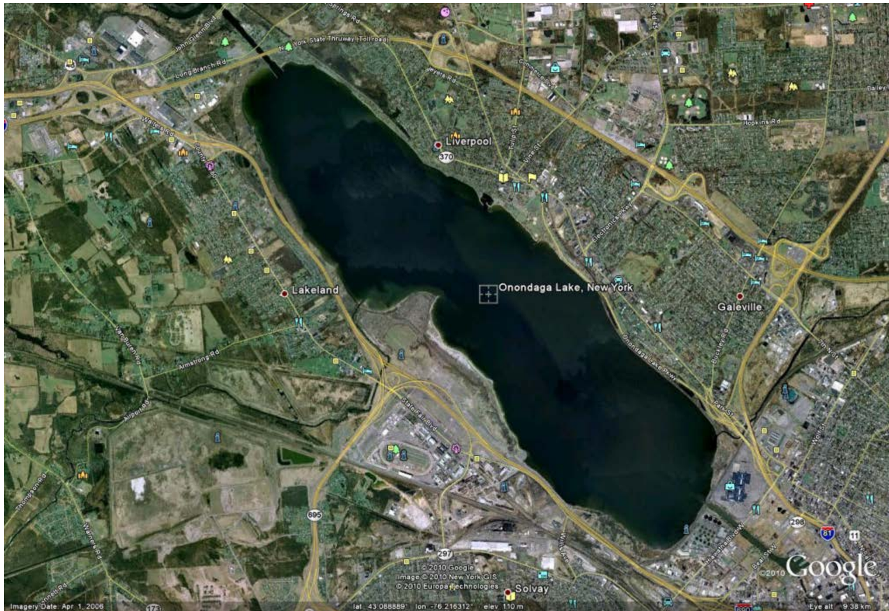


Key Points: Diagenesis Model

- 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
Diagenesis Only:						PON G2	147	g N/m3
frac G3 (nonreactive)	0.01					PON G3	0.7	g N/m3
						POP G1	6.7	g P/m3
Diagenesis Assumptions:						POP G2	14.7	g P/m3
						POP G3	0.07	g P/m3
P to Org, Refr	0.0002	frac dry						
N to Org, Refr	0.002	frac dry						
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

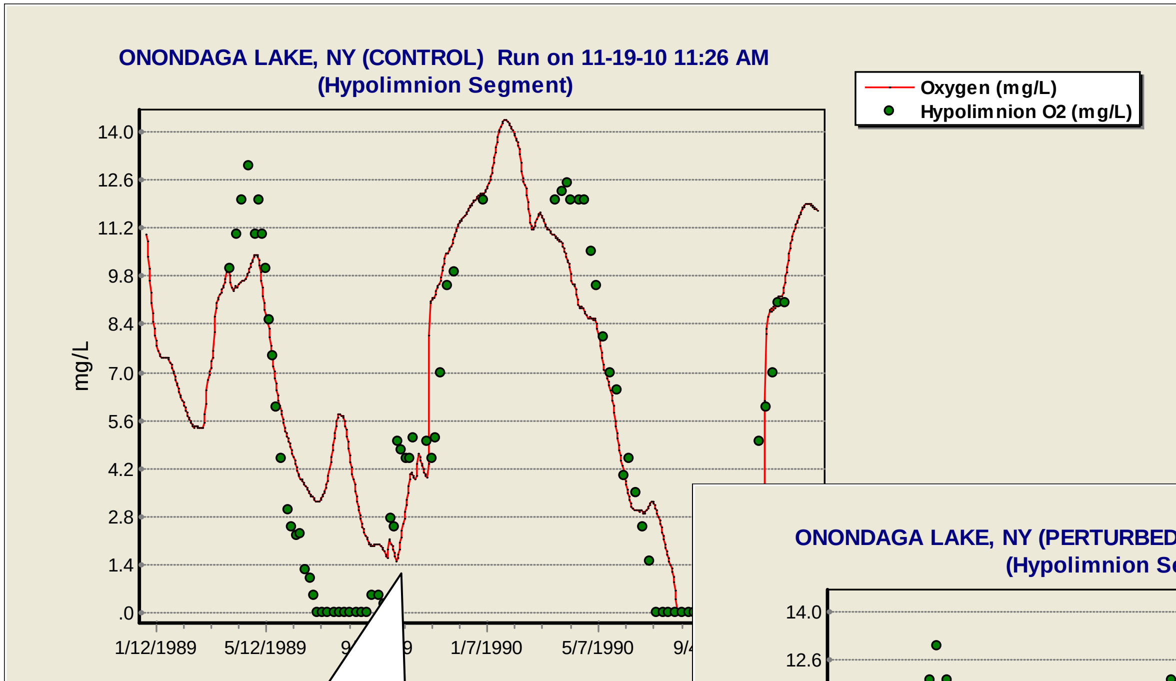
Edit Sediment Diagenesis Parameters

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	m2/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	

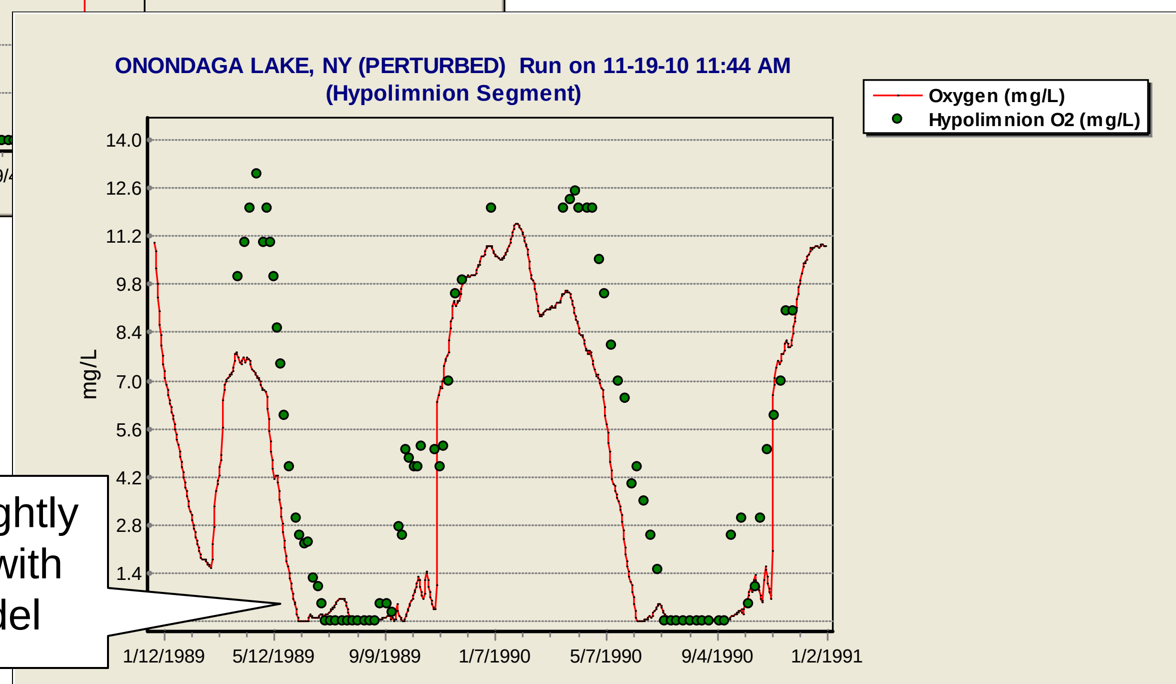
Copy to All Segments | Save Table to Excel | Help | Cancel | OK

Copy Diagenesis Parameters

Results are Improved



Hypoxia not predicted before addition of diagenesis



Perhaps even slightly “overpredicted” with diagenesis model

AQUATOX also simulates:

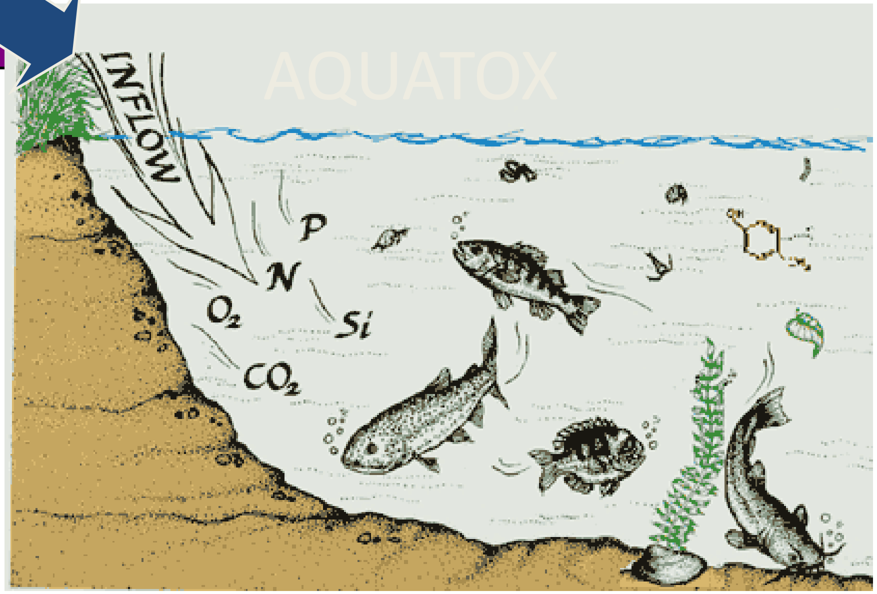
- Diel oxygen
- Effects of low dissolved oxygen
- Ammonia toxicity

AQUATOX as a Part of BASINS

Integration of tools

AQUATOX BASINS Linkage

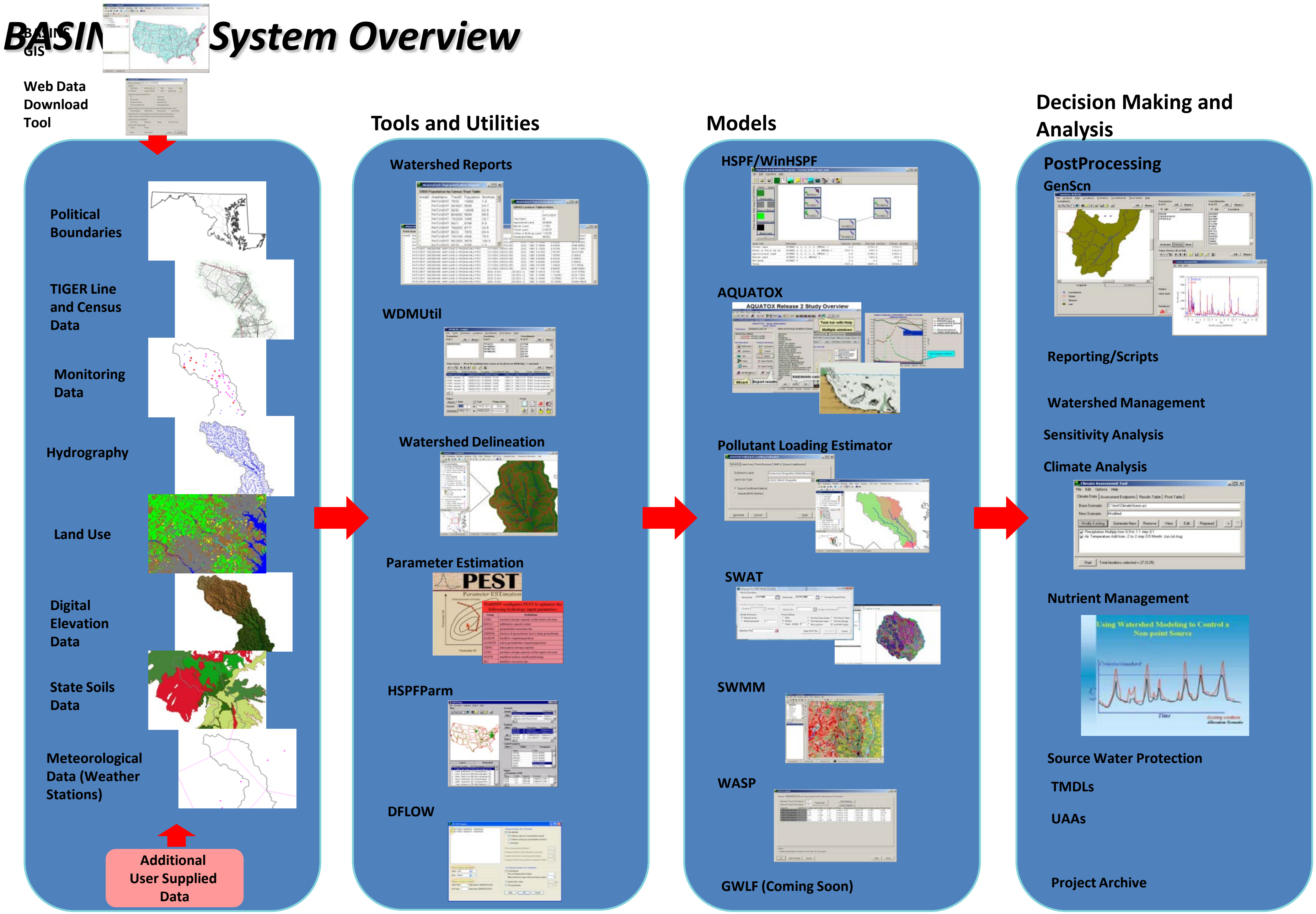
Integrates point/nonpoint source analysis with effects on receiving water and biota



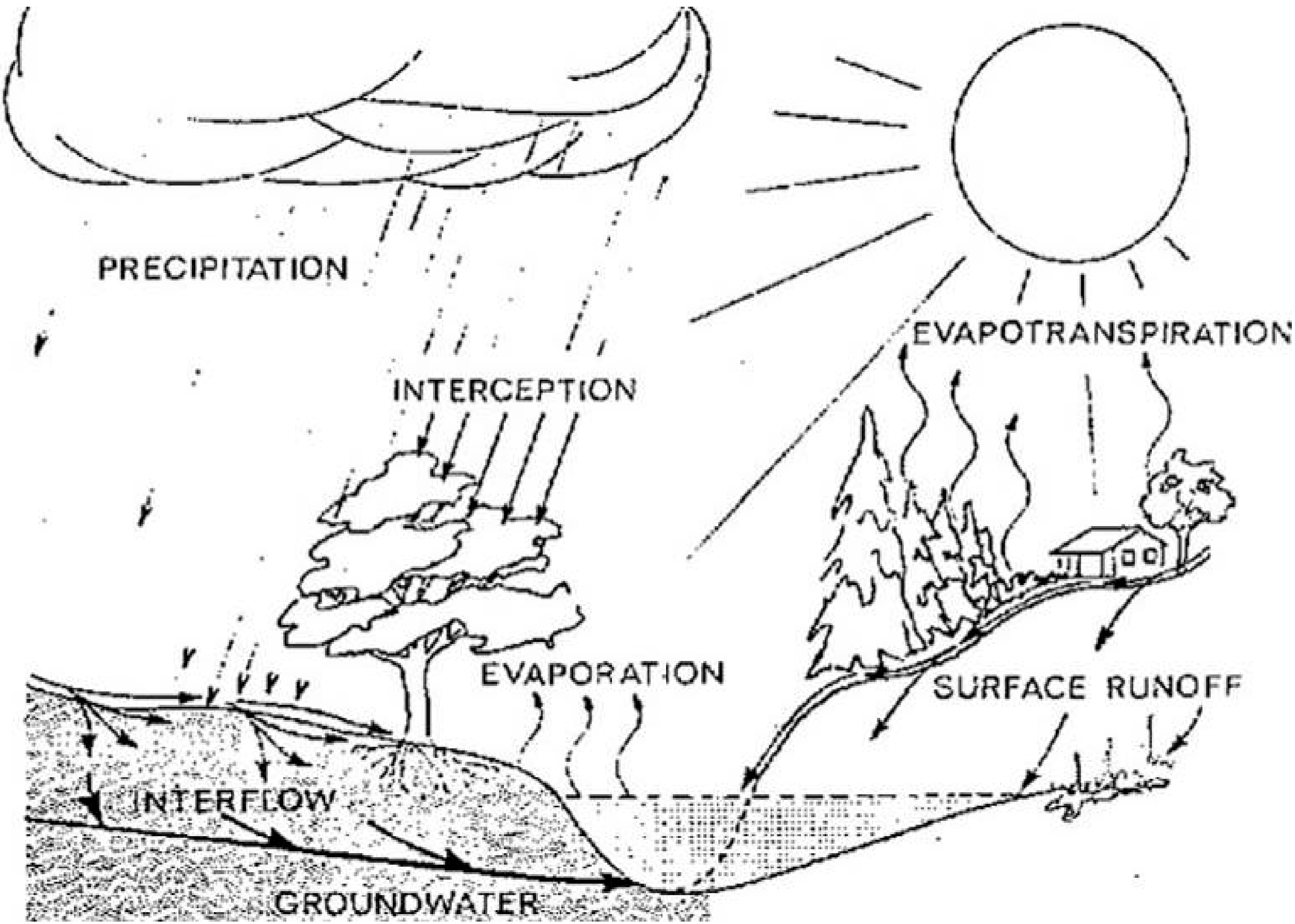
Provides time series loading data and GIS information to AQUATOX

Creates AQUATOX simulations using physical characteristics of BASINS watershed

BASINS System Overview



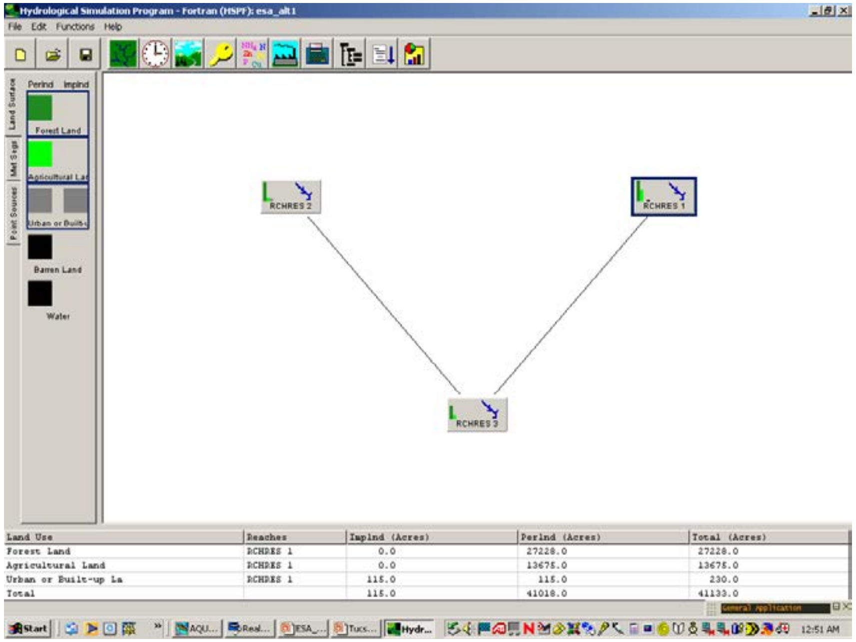
Simplified Hydrologic Model



WinHSPF

Hydrologic **S**imulation **P**rogram–**F**ORTRAN

- 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)**

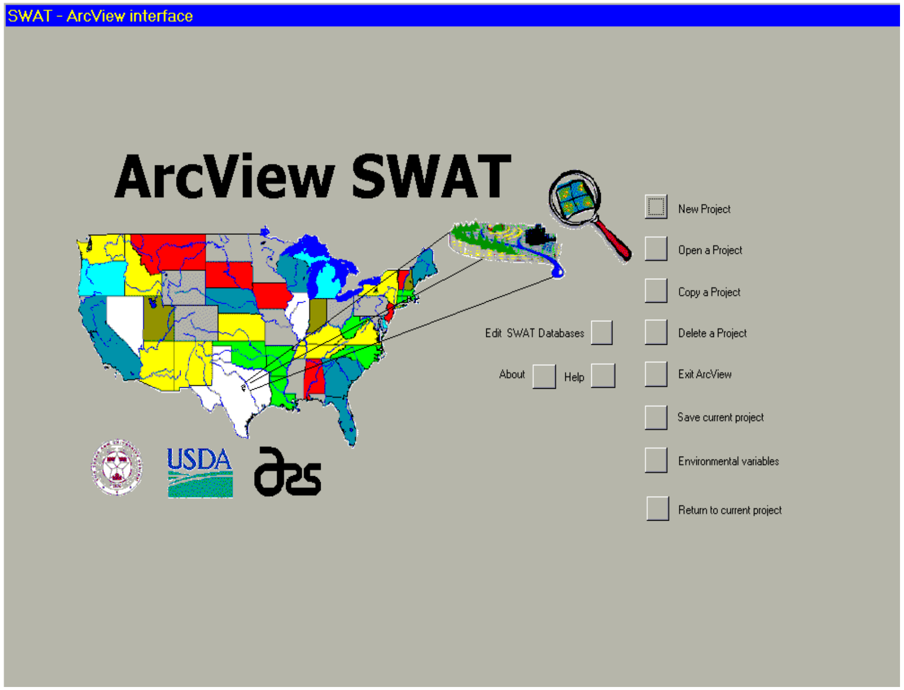


Note: red indicates parameter that may be loaded into AQUATOX

SWAT

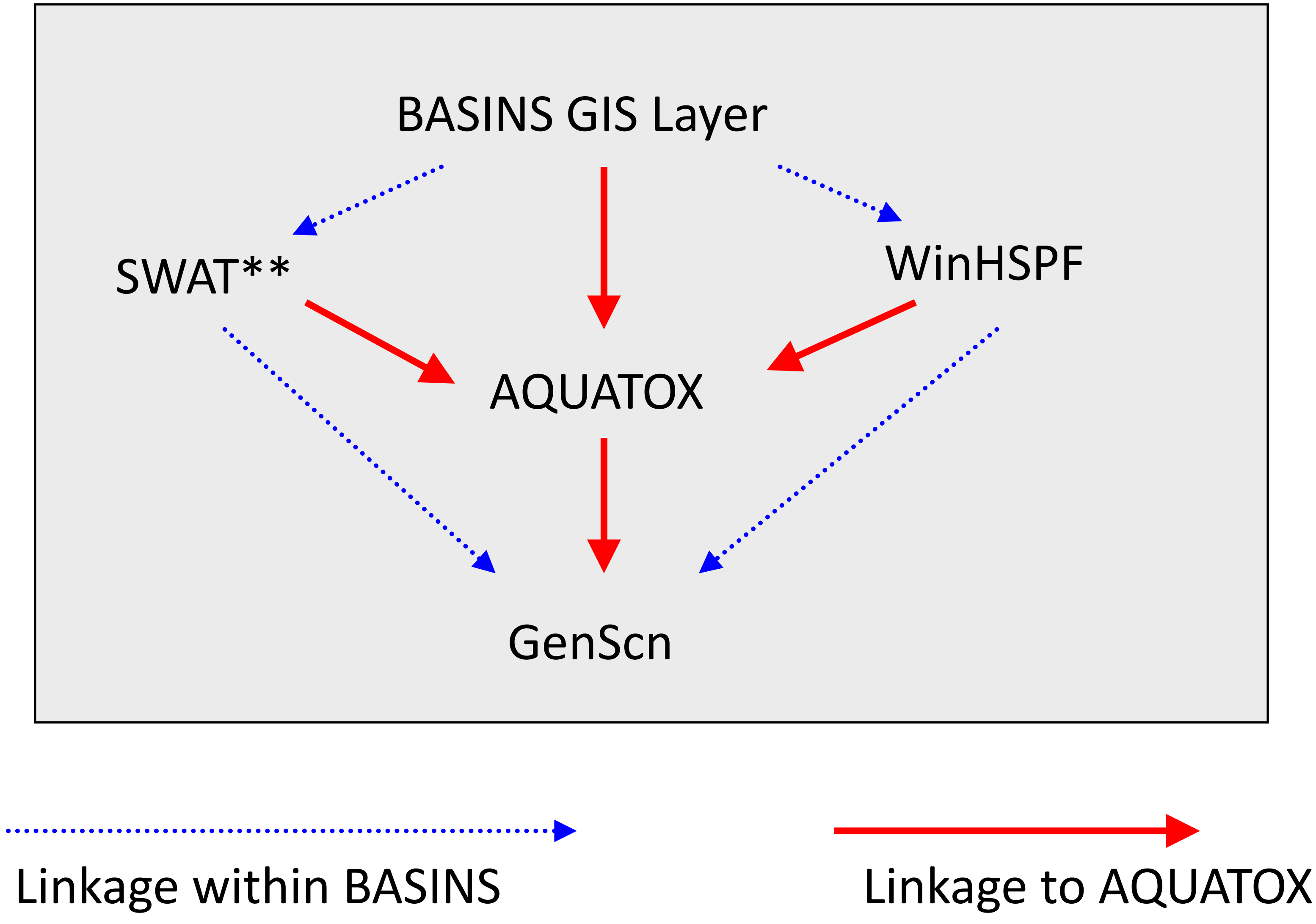
Soil and Water Assessment Tool

- 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



*(**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

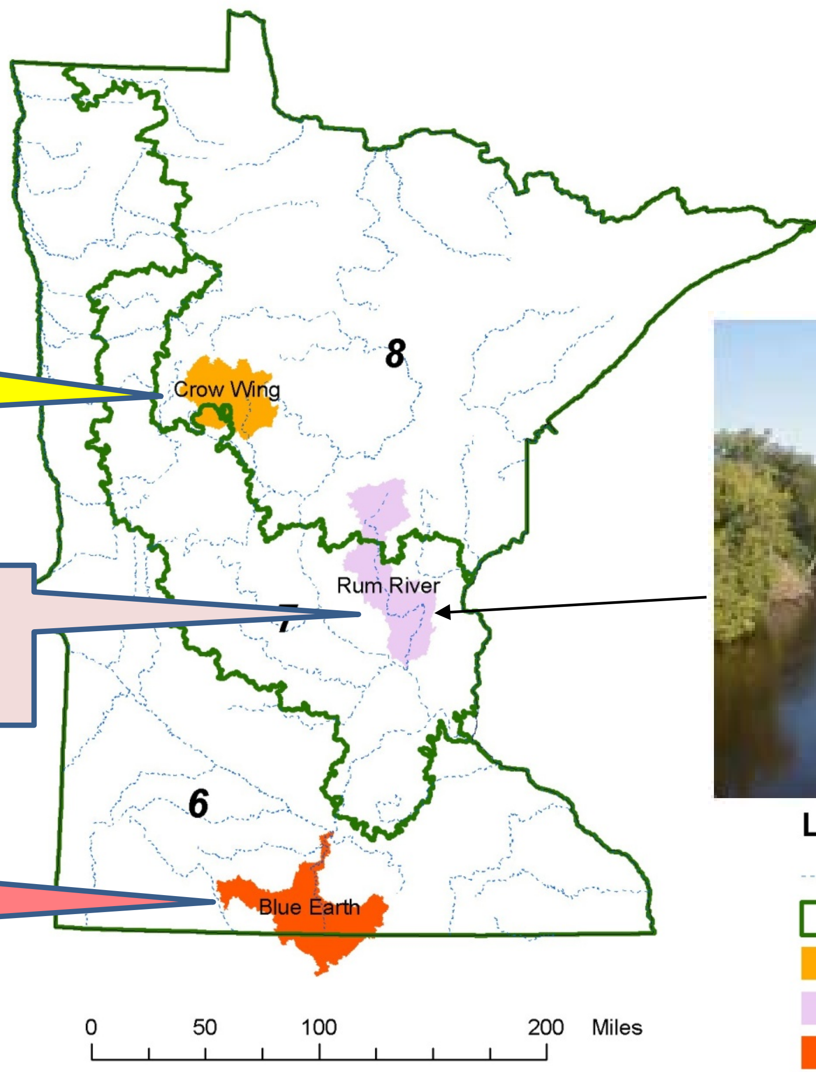
- 2008 peer review suggests AQUATOX is suited to support existing approaches used to develop water quality standards and criteria
  - One tool among many that should be used in a weight- of-evidence approach
- AQUATOX enables the evaluation of multiple stressor scenarios
  - What is the most important 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

Low nutrient
low turbidity

Moderate nutrient
moderate turbidity

High nutrient
high turbidity

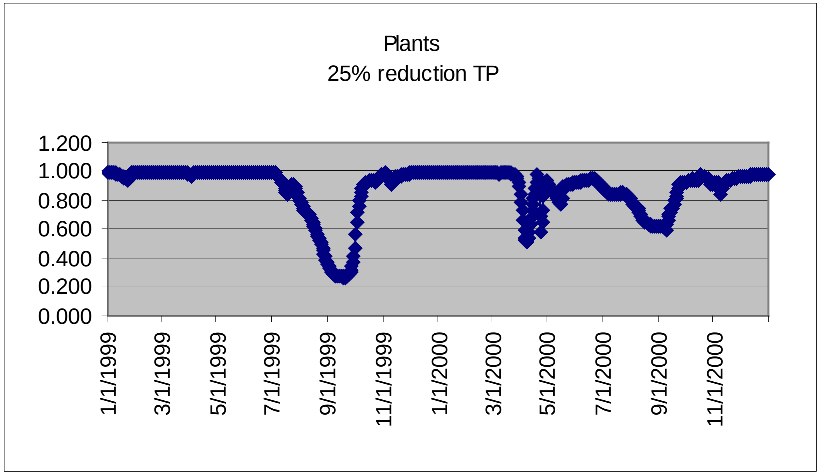


Example Nutrient Analyses from Minnesota

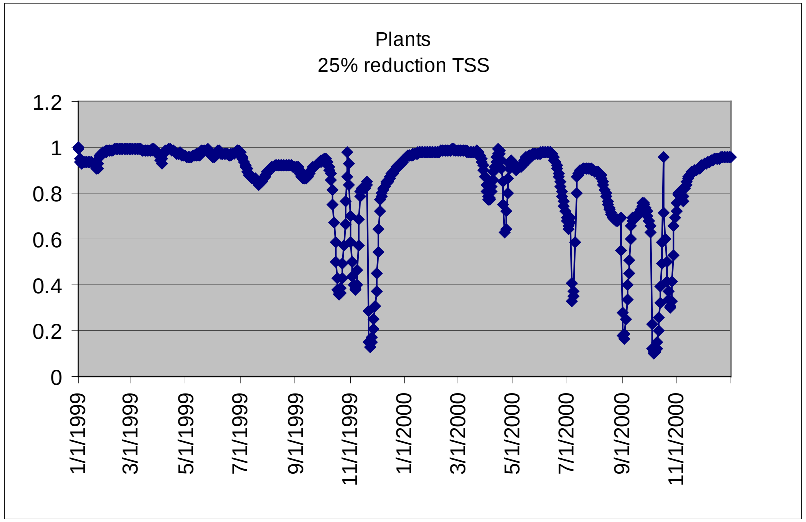
- Calibrated AQUATOX across nutrient gradient
- Set up HSPF, linked loadings to AQUATOX
- Ran iterative simulations with various nutrient reductions
- Applied 2 ways of developing nutrient target
  - Method #1: Accept existing chl *a* target, use AQUATOX to get corresponding TP level
  - Method #2: Use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

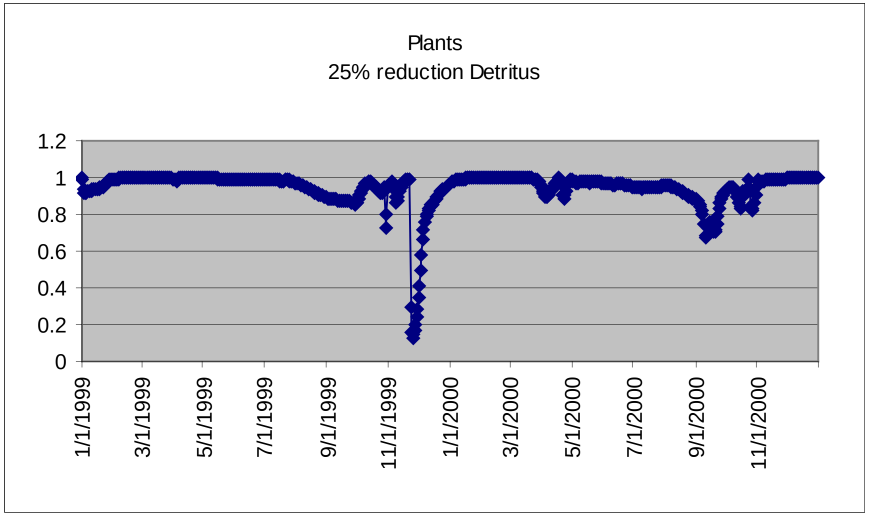
Step 1: Stressor ID using Biotic Index

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
- NO3 and NH3 reductions had little effect





Step 2: Run AQUATOX with multiple load reduction scenarios.

Calculate and compare Mean TP and Chl a

Baseline condition

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 criteria	***118.13***	***7.85***

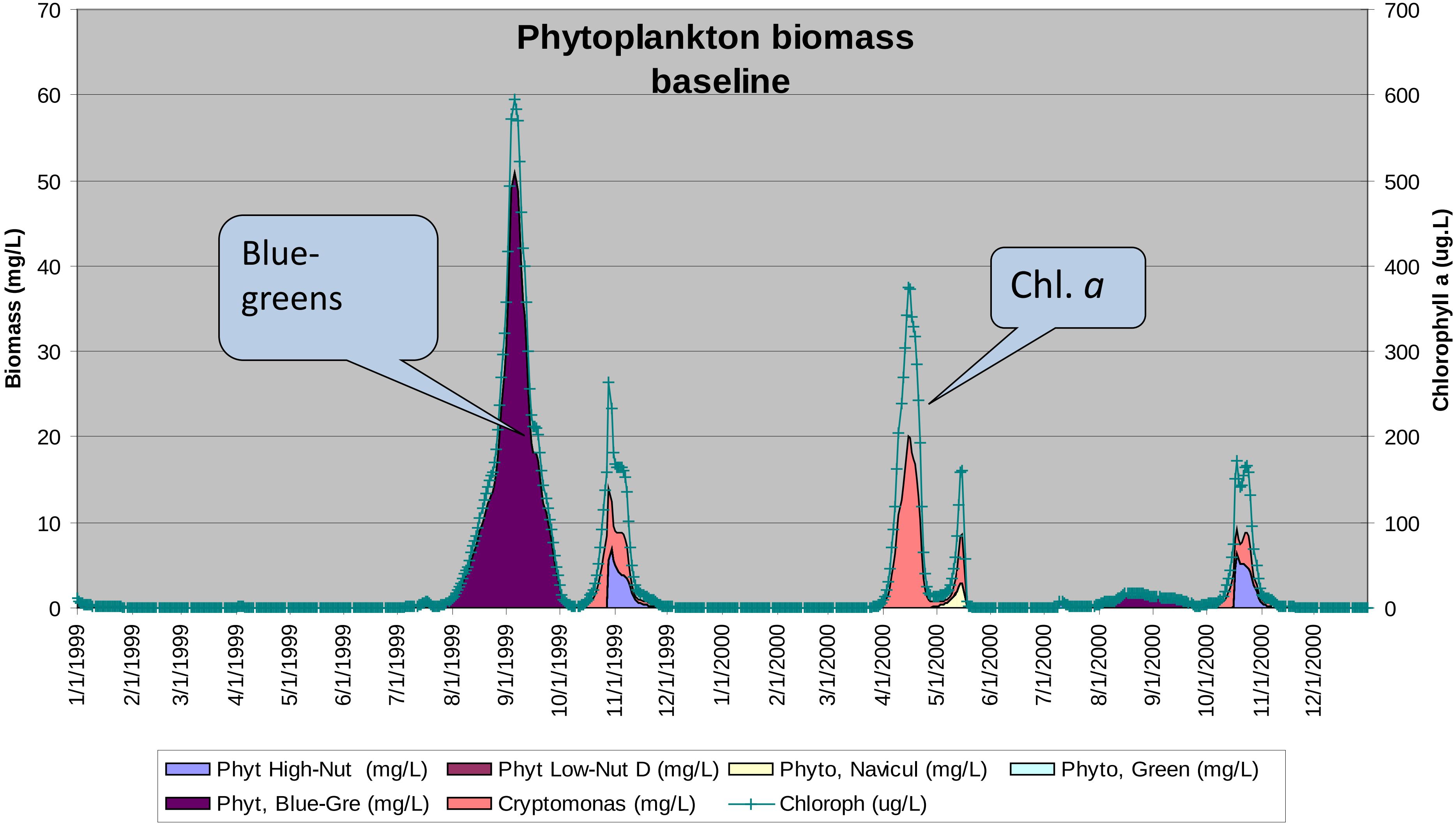
Step 3a: Water Quality Target Development Method #1

- 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?

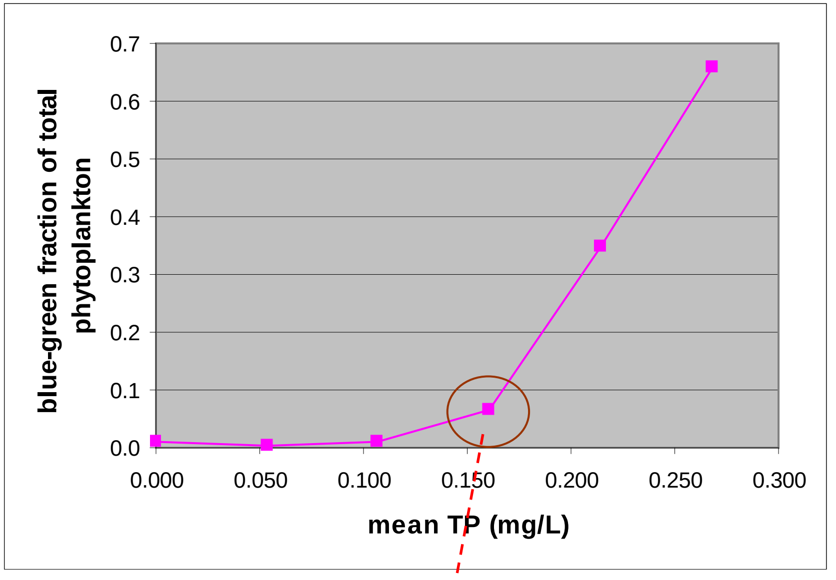
Algal Composition Changes Seasonally and from year to year



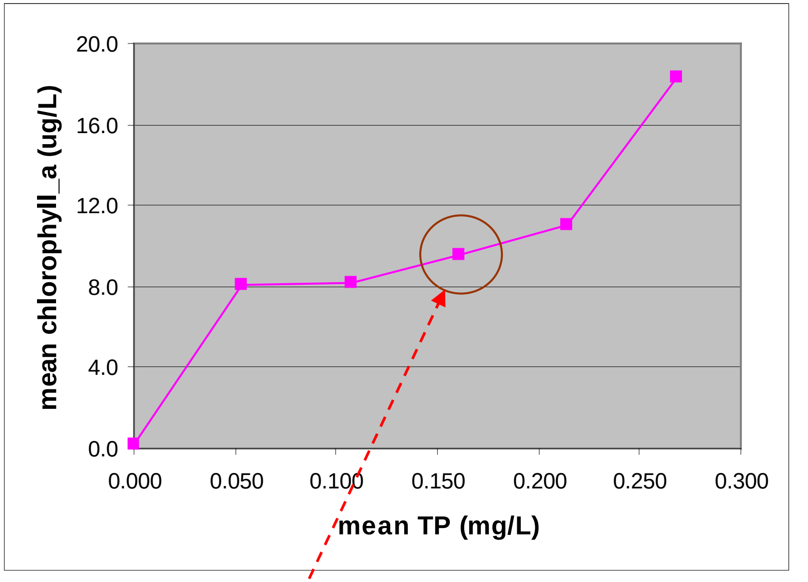
Target Development

- <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



<u>Inflection point</u> – 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).
  - 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.

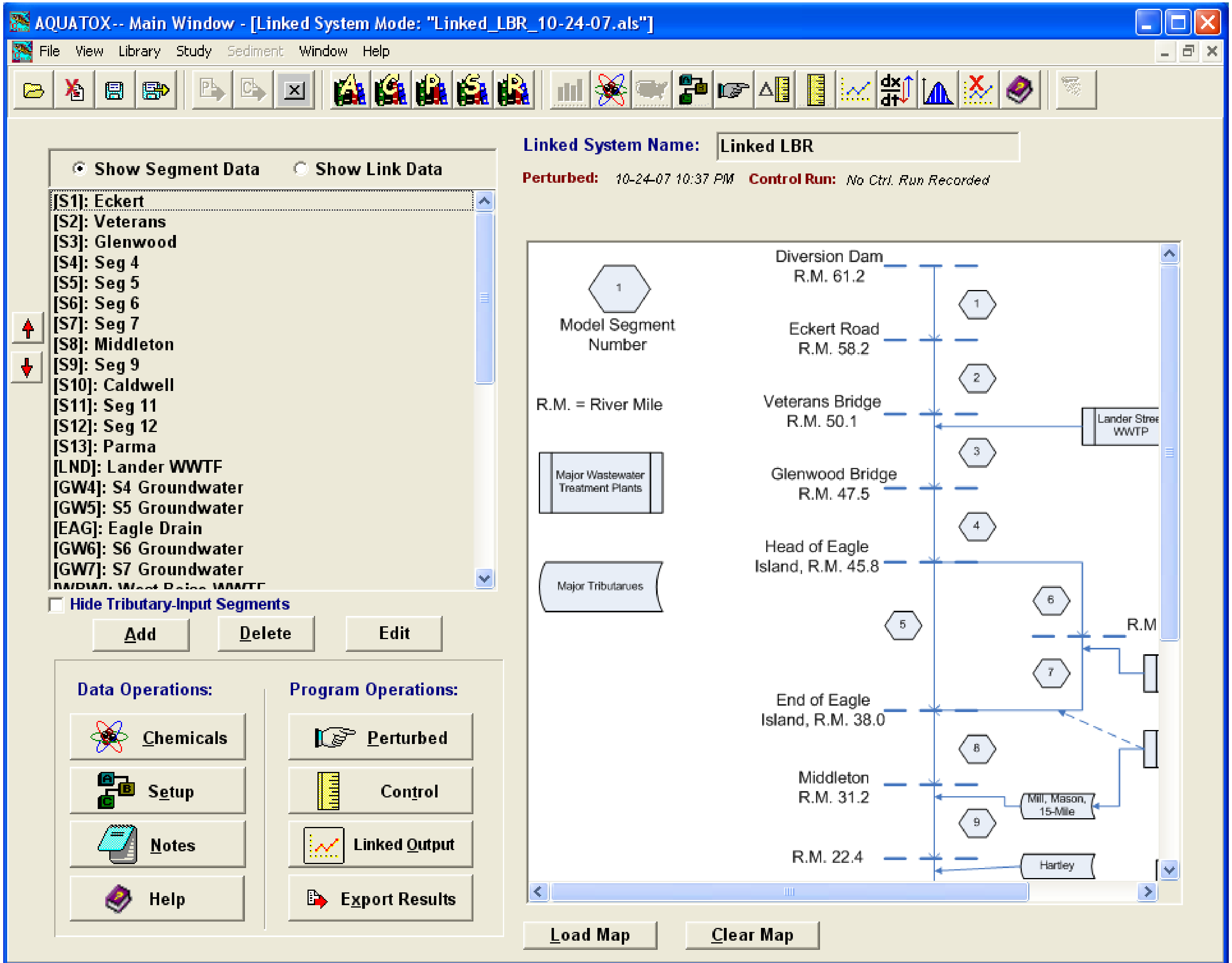
Other Possible Analyses

- 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



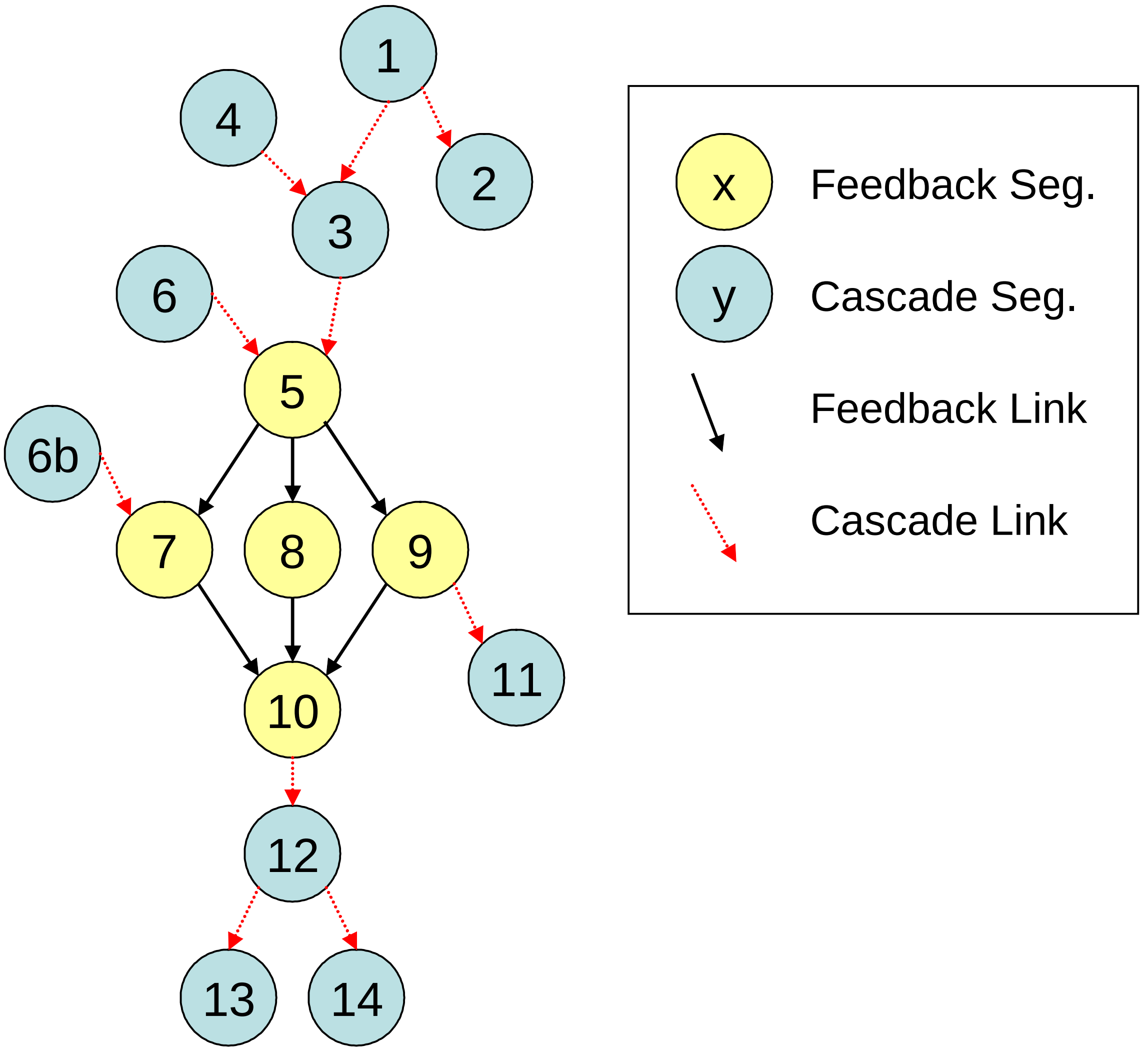
Cascade & Feedback Linkages

<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

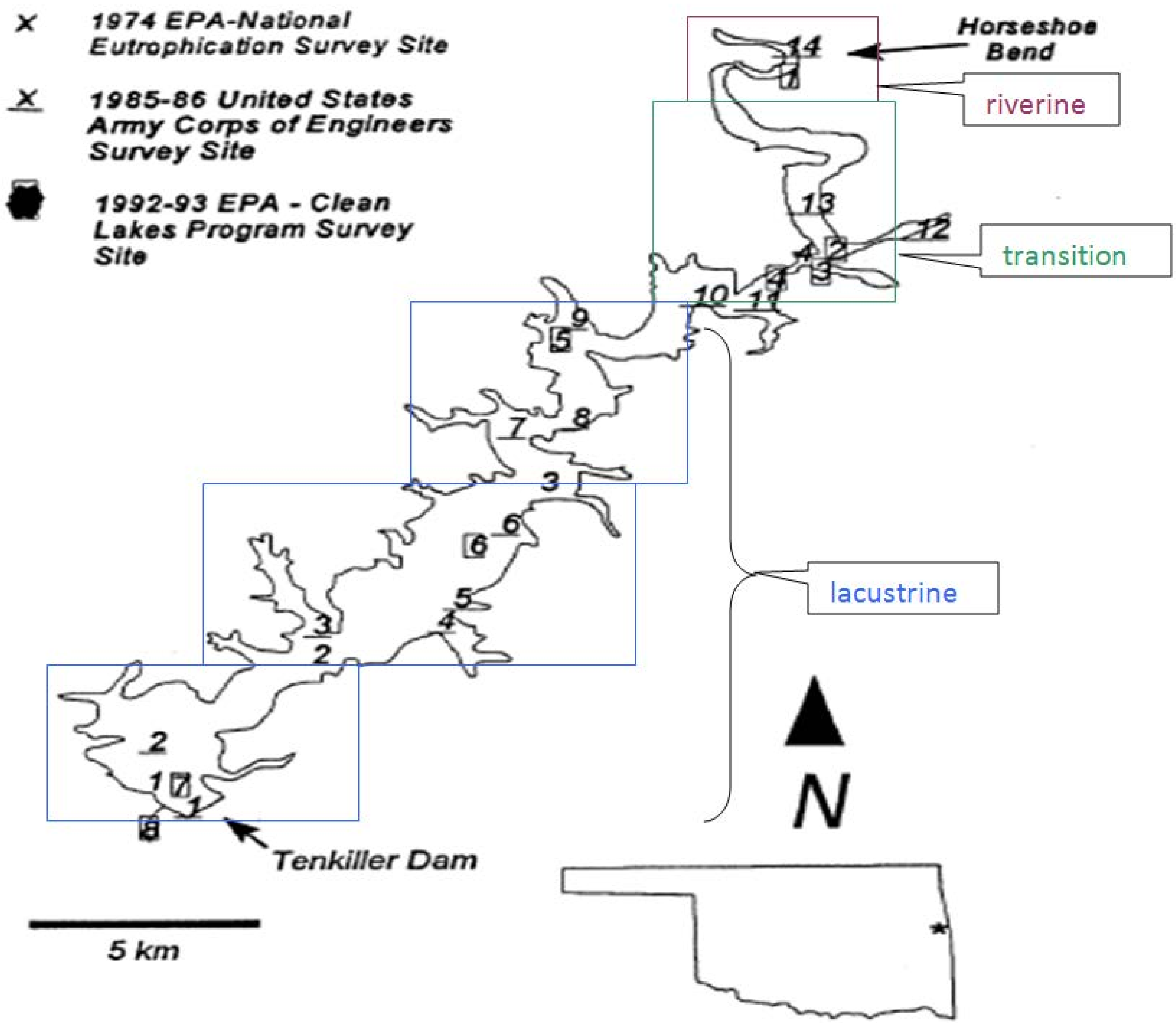
Interface Demonstration to follow

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

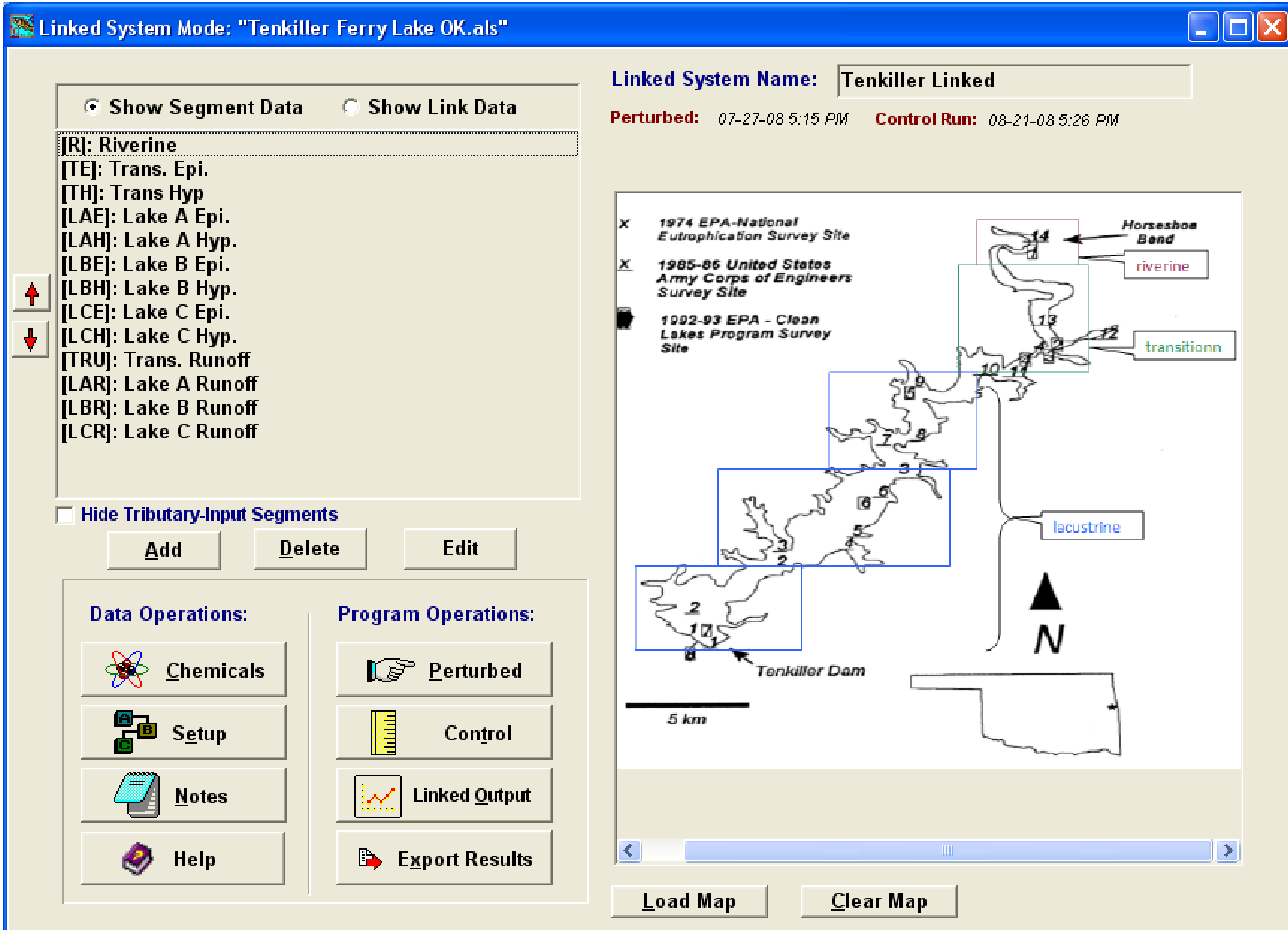
Tenkiller Lake, OK



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)

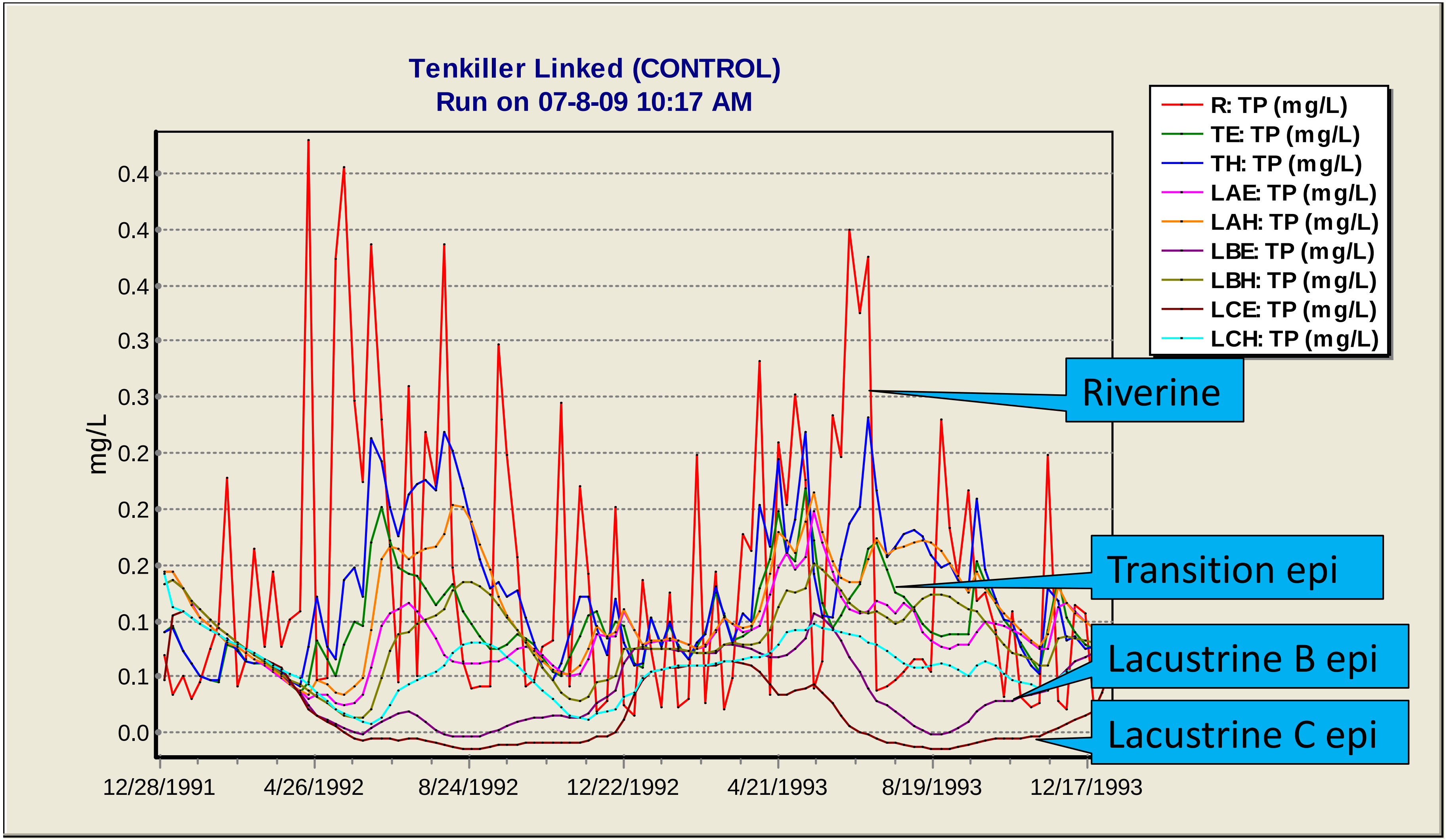
Tenkiller Lake OK



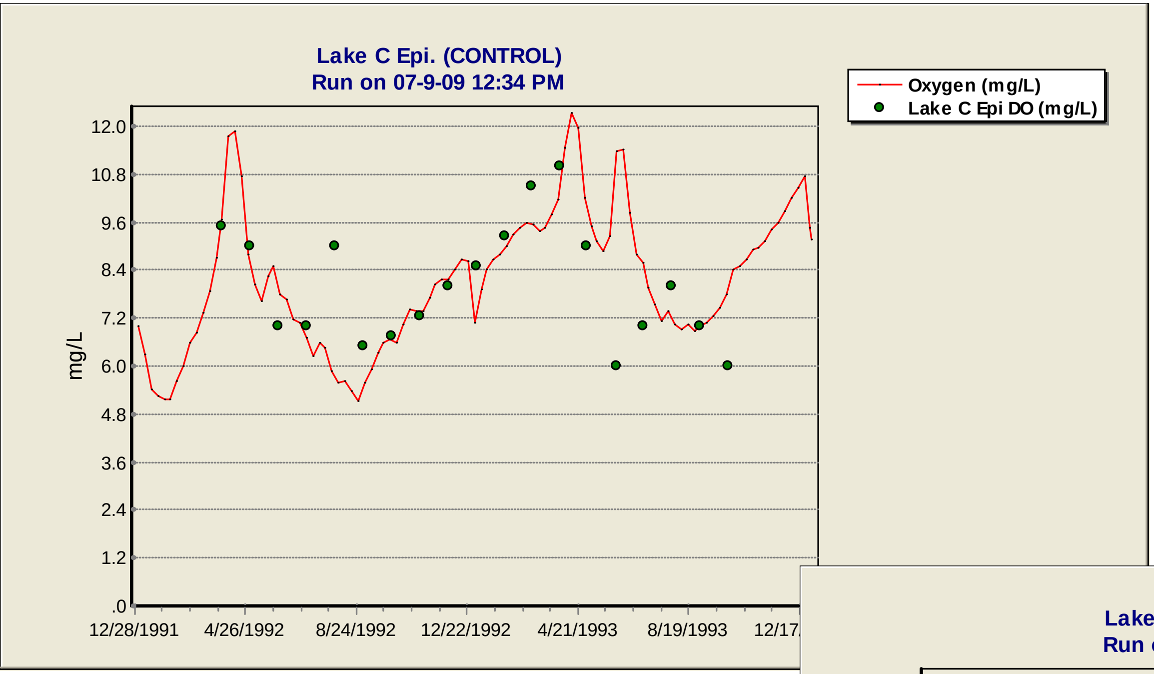
Storm-water plume, algae-rich riverine segment

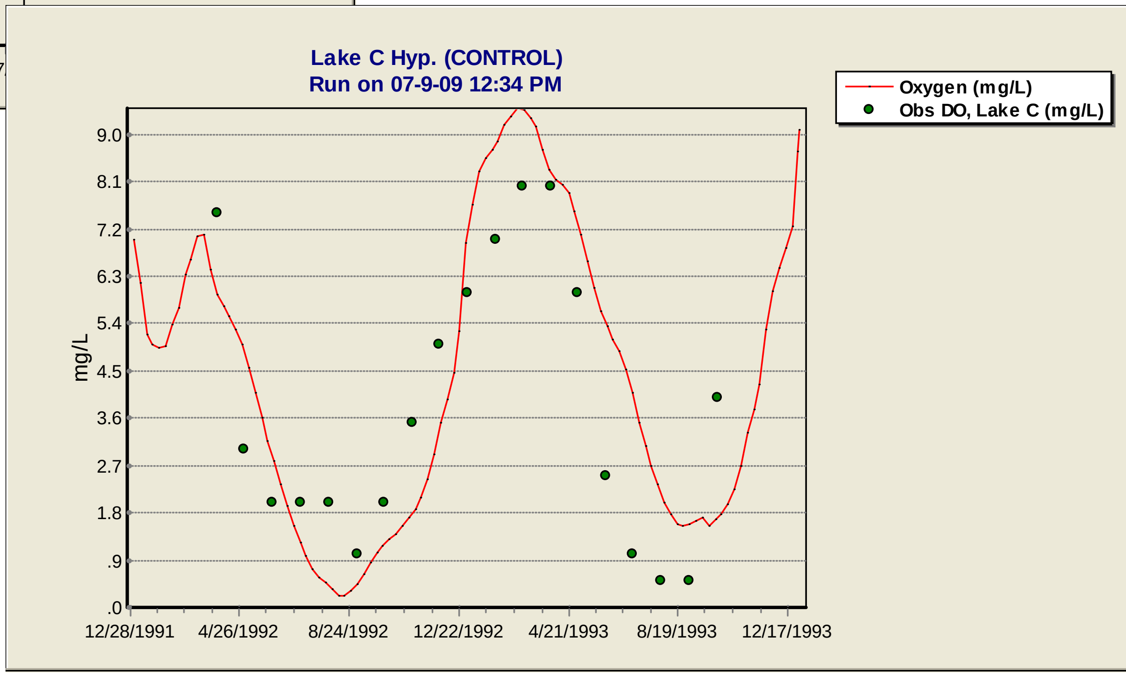
duckweed (*Lemna* sp.) forms surface scum at the interface

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

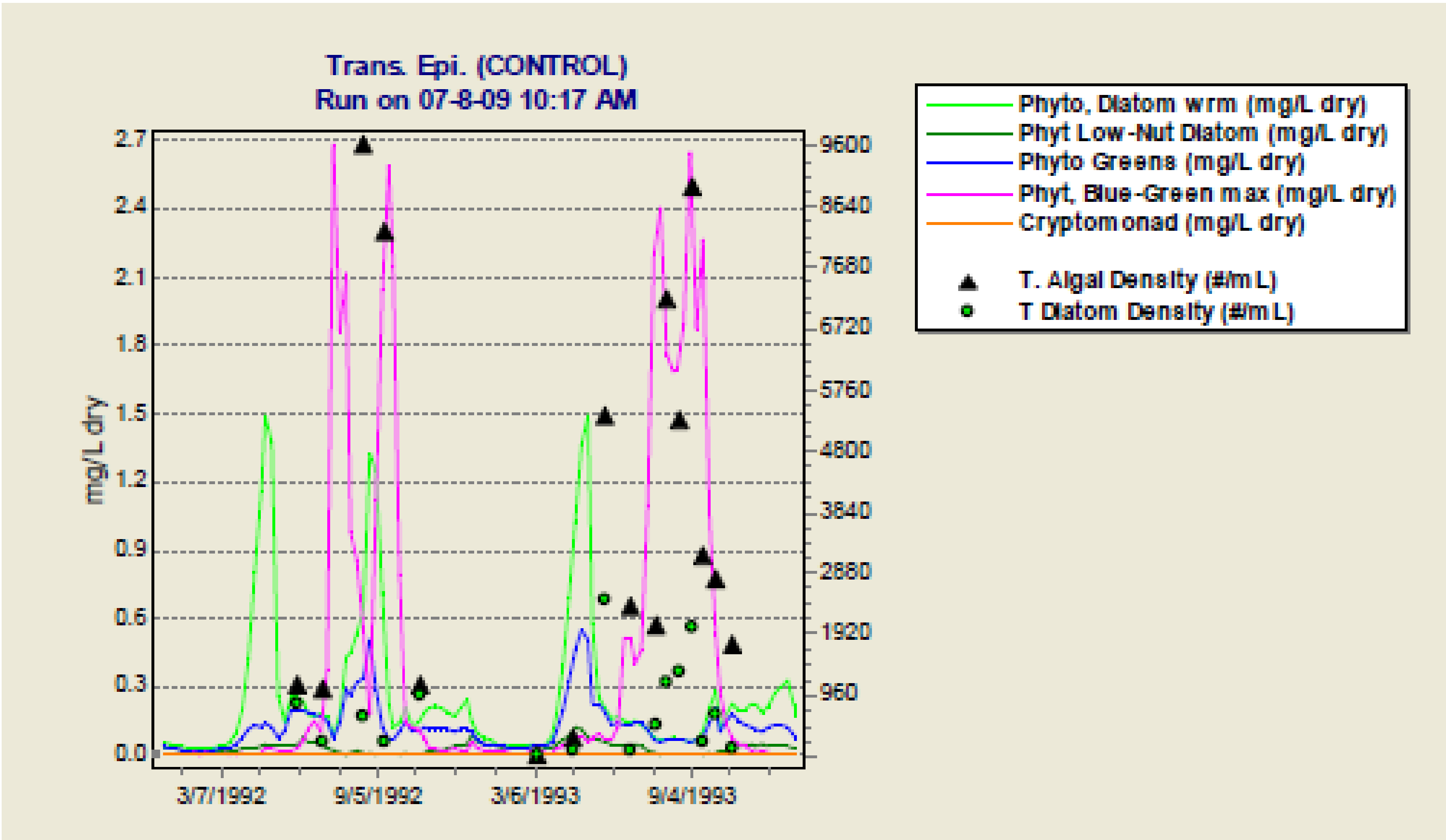


Simulated and observed dissolved oxygen in Lacustrine C

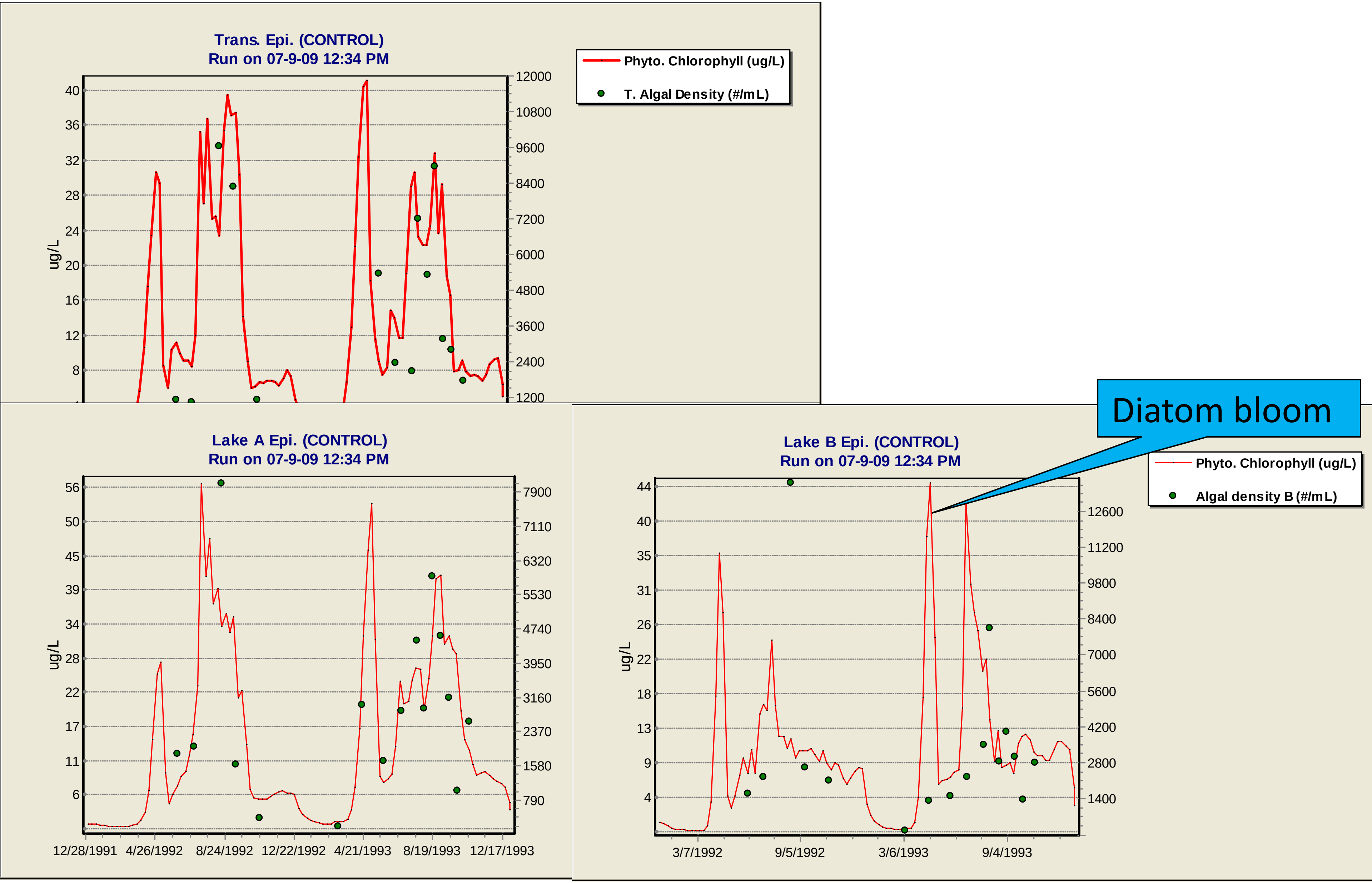




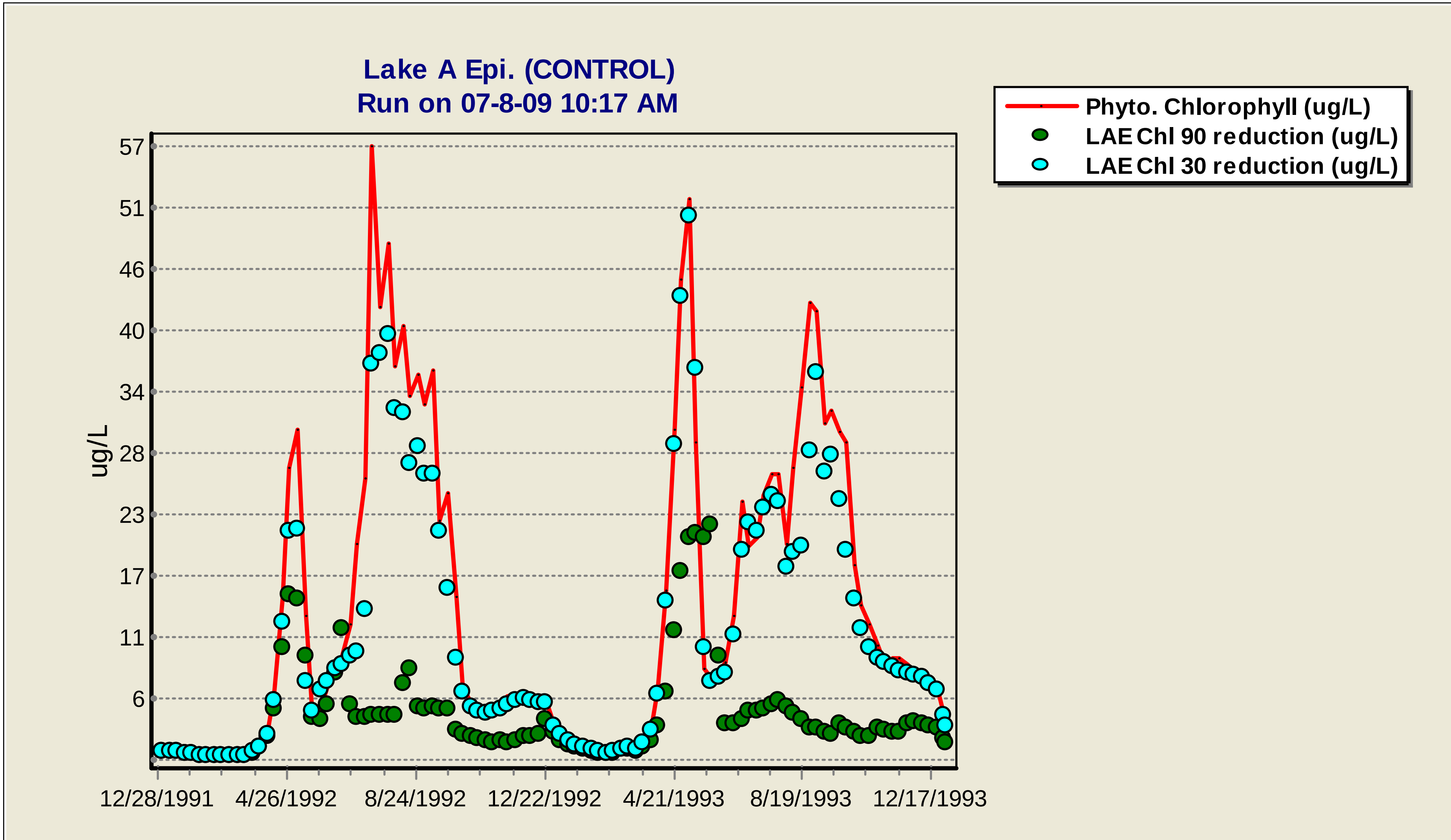
Simulated & observed algal composition in epilimnetic Transition



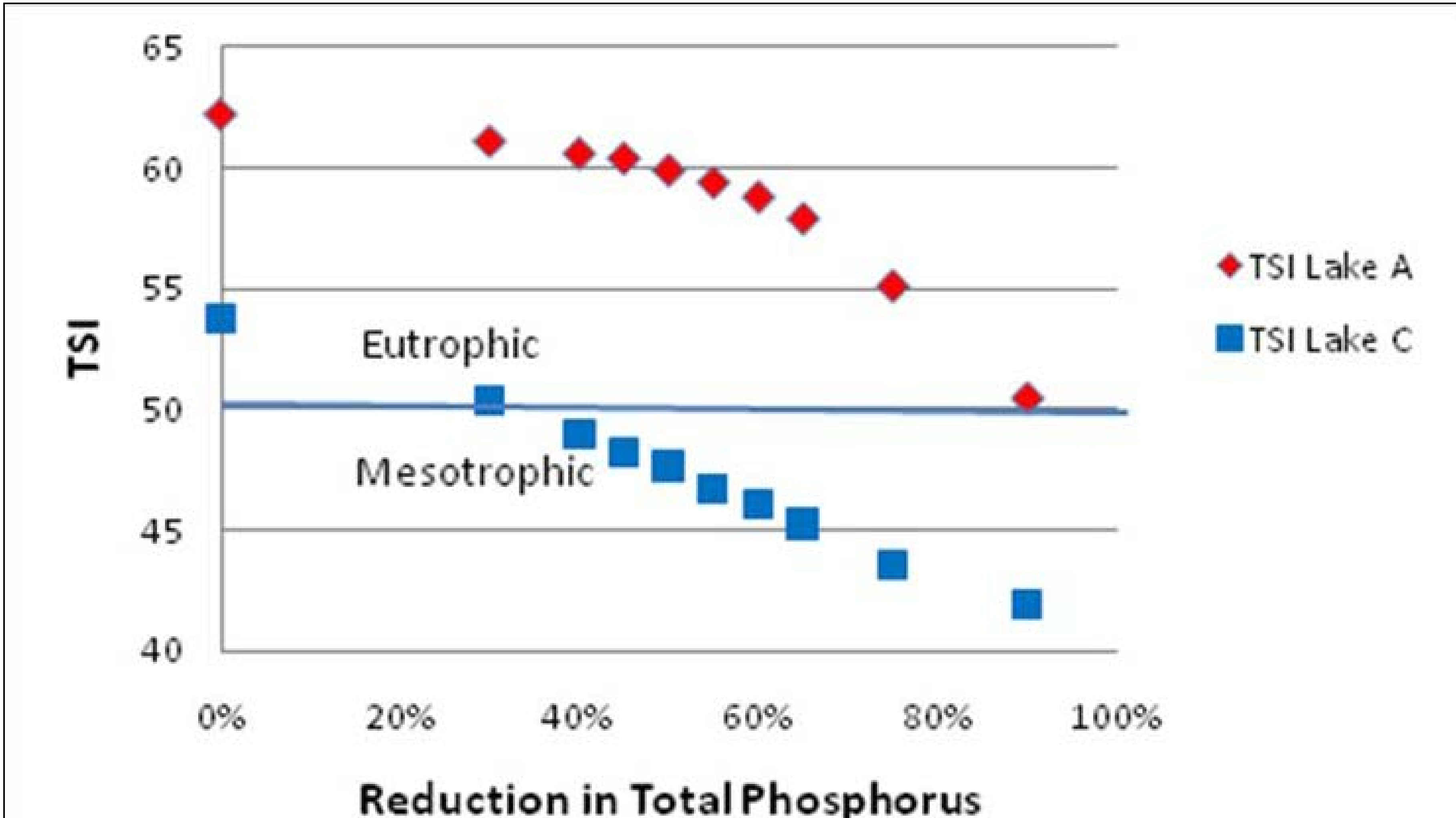
Simulated chlorophyll *a* and observed algal density in Transition and Lacustrine A and B



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

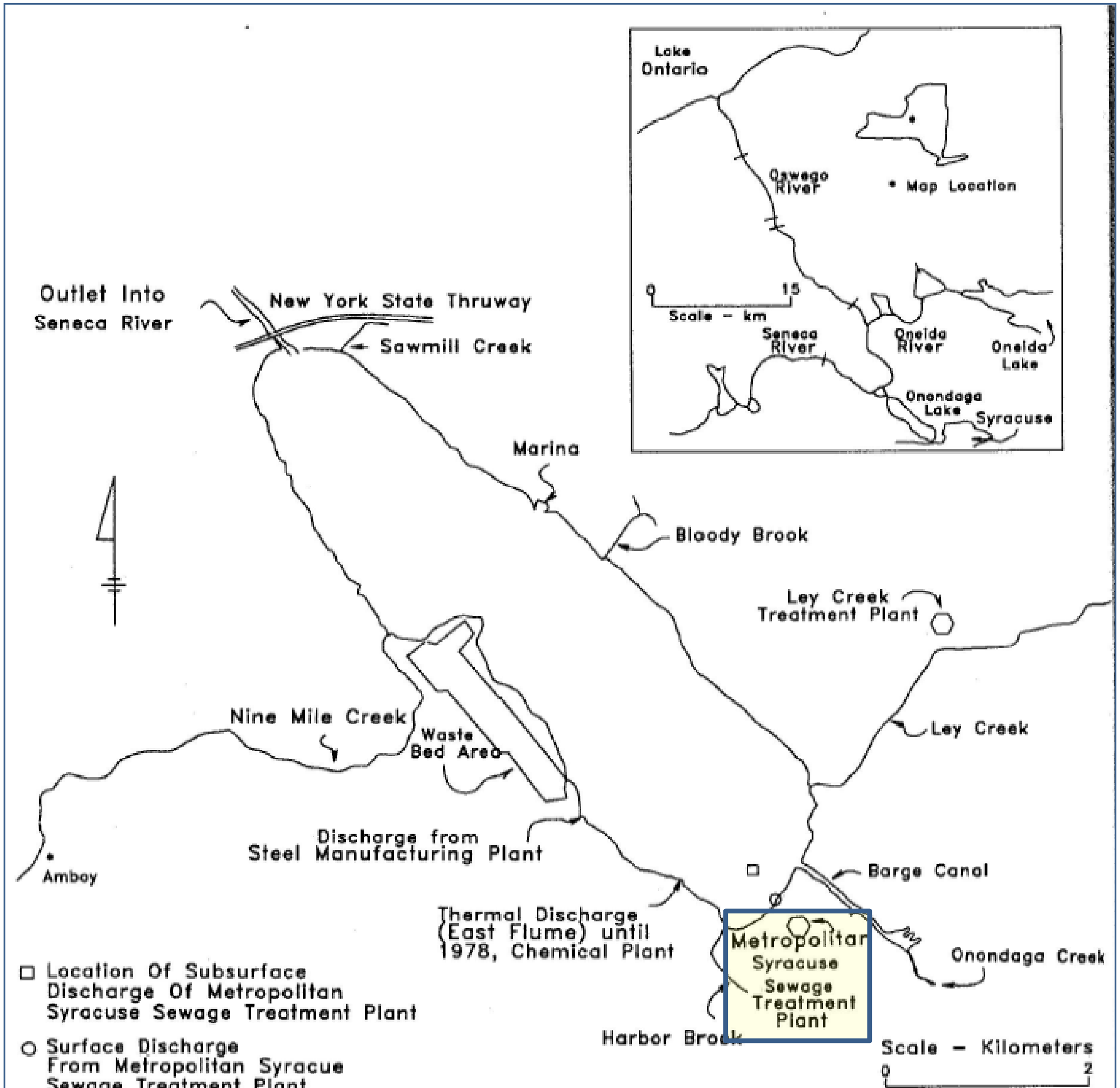


Lab 5 – Analysis of the Nutrient Status of DeGray Lake, Arkansas

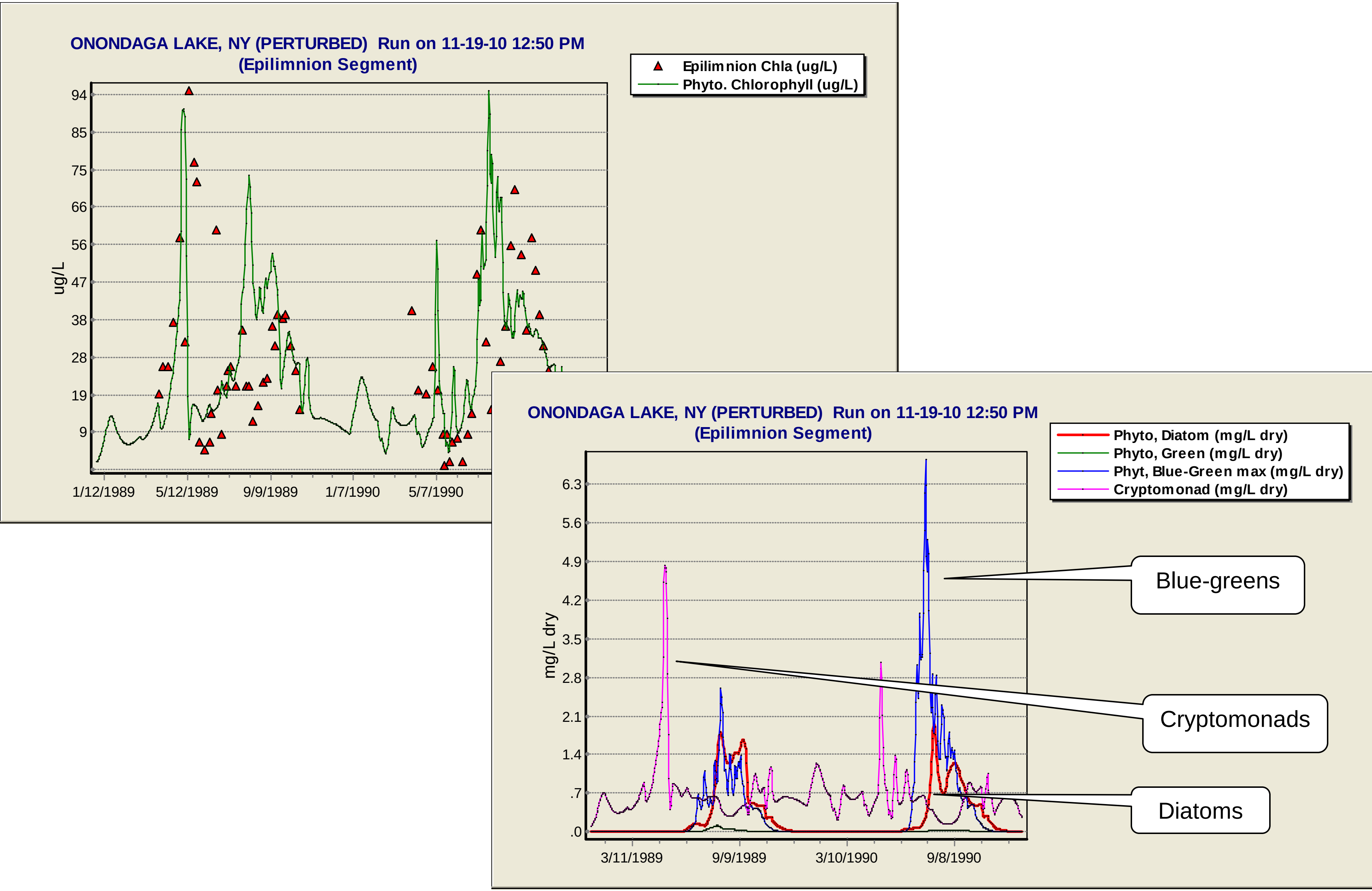
Lake Onondaga, NY
Validation and Application

- 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*

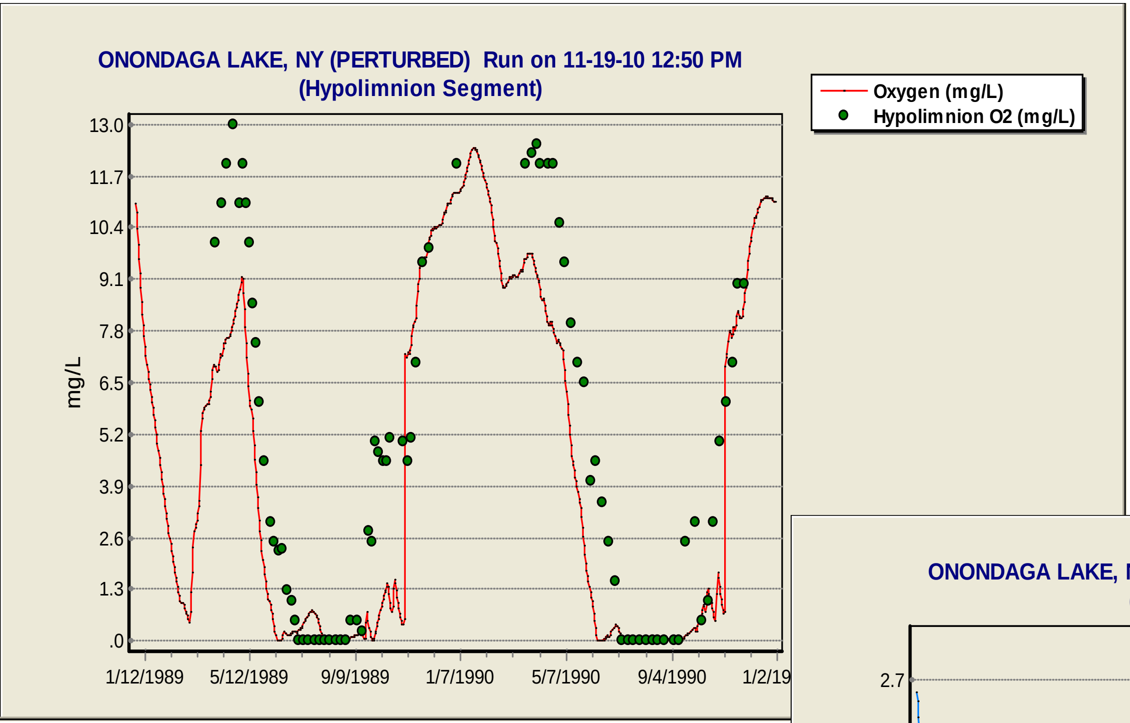
Lake Onondaga NY, heavily polluted

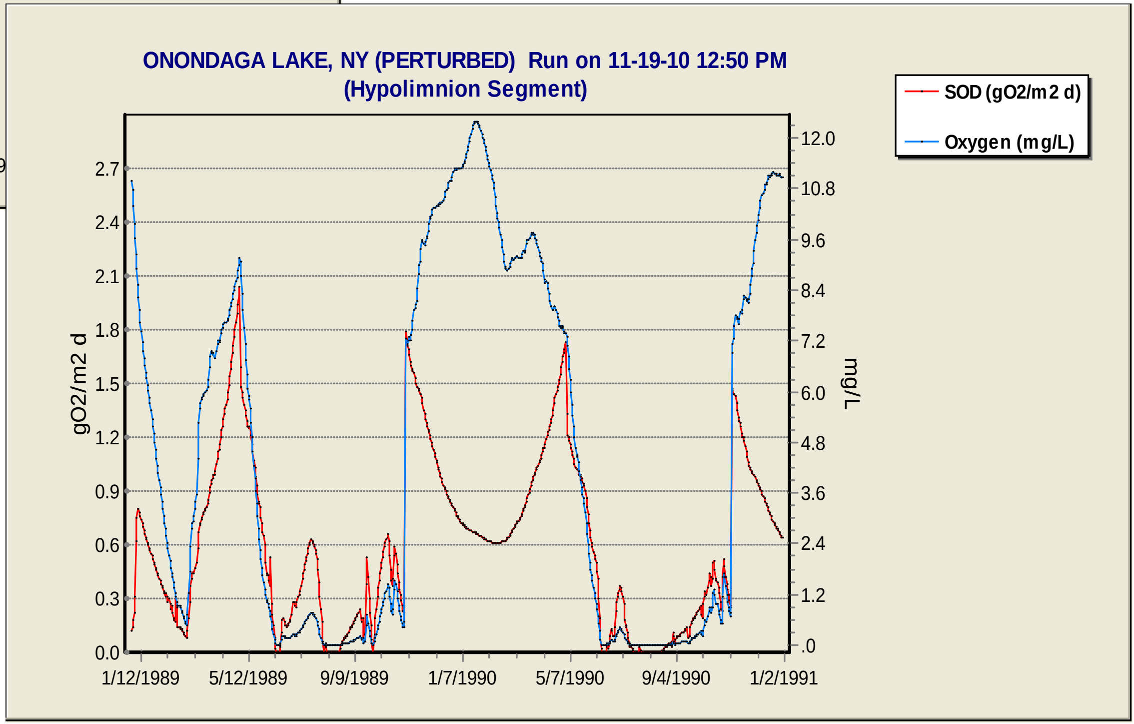


Lake Onondaga was very productive with succession of algal groups

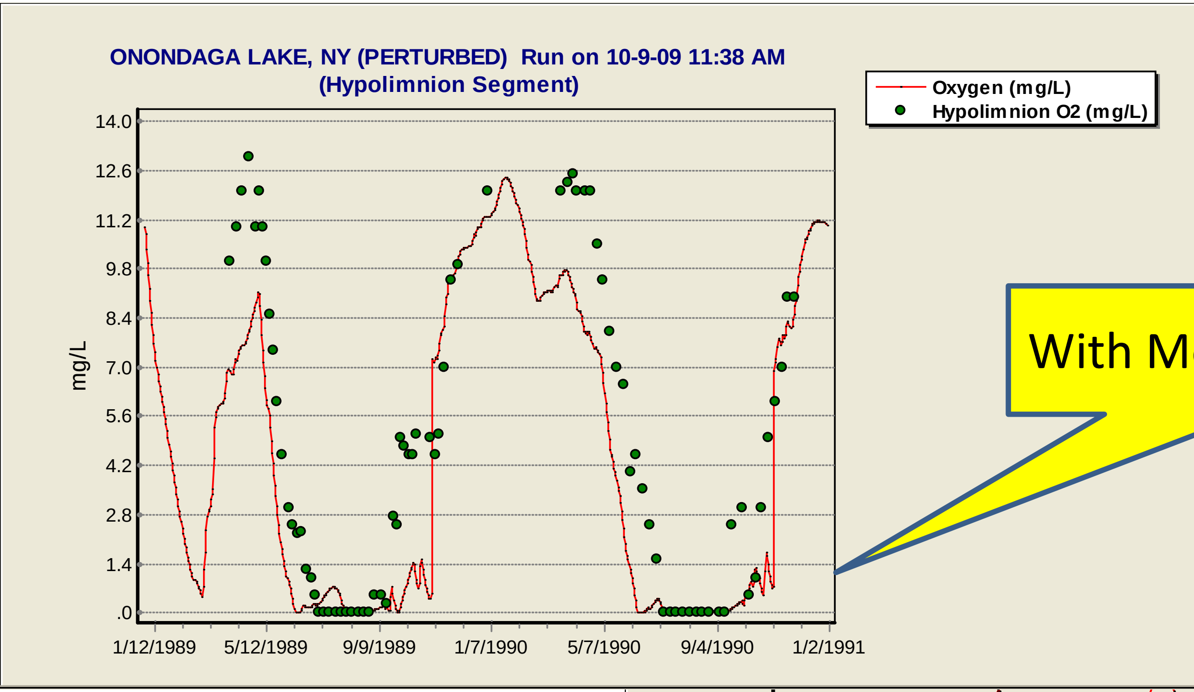


Hypolimnion goes anoxic with high SOD

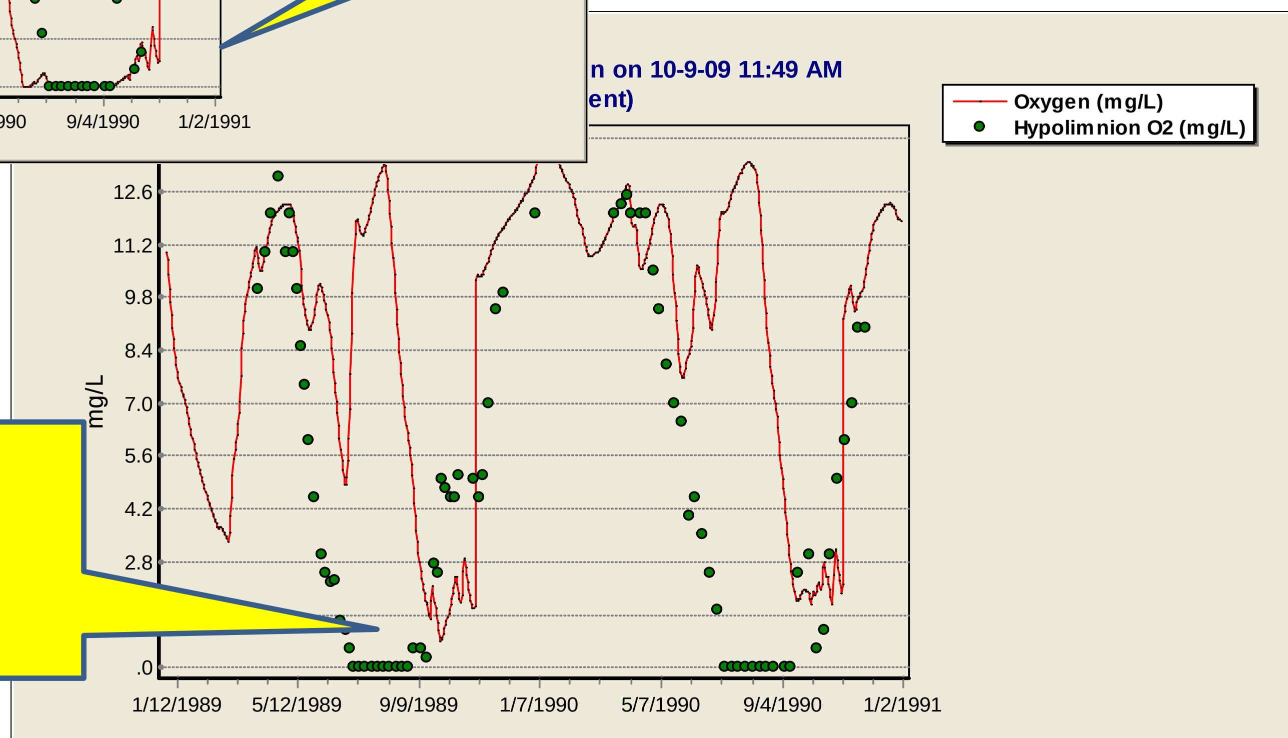




What if Metro WWTP effluent were diverted?

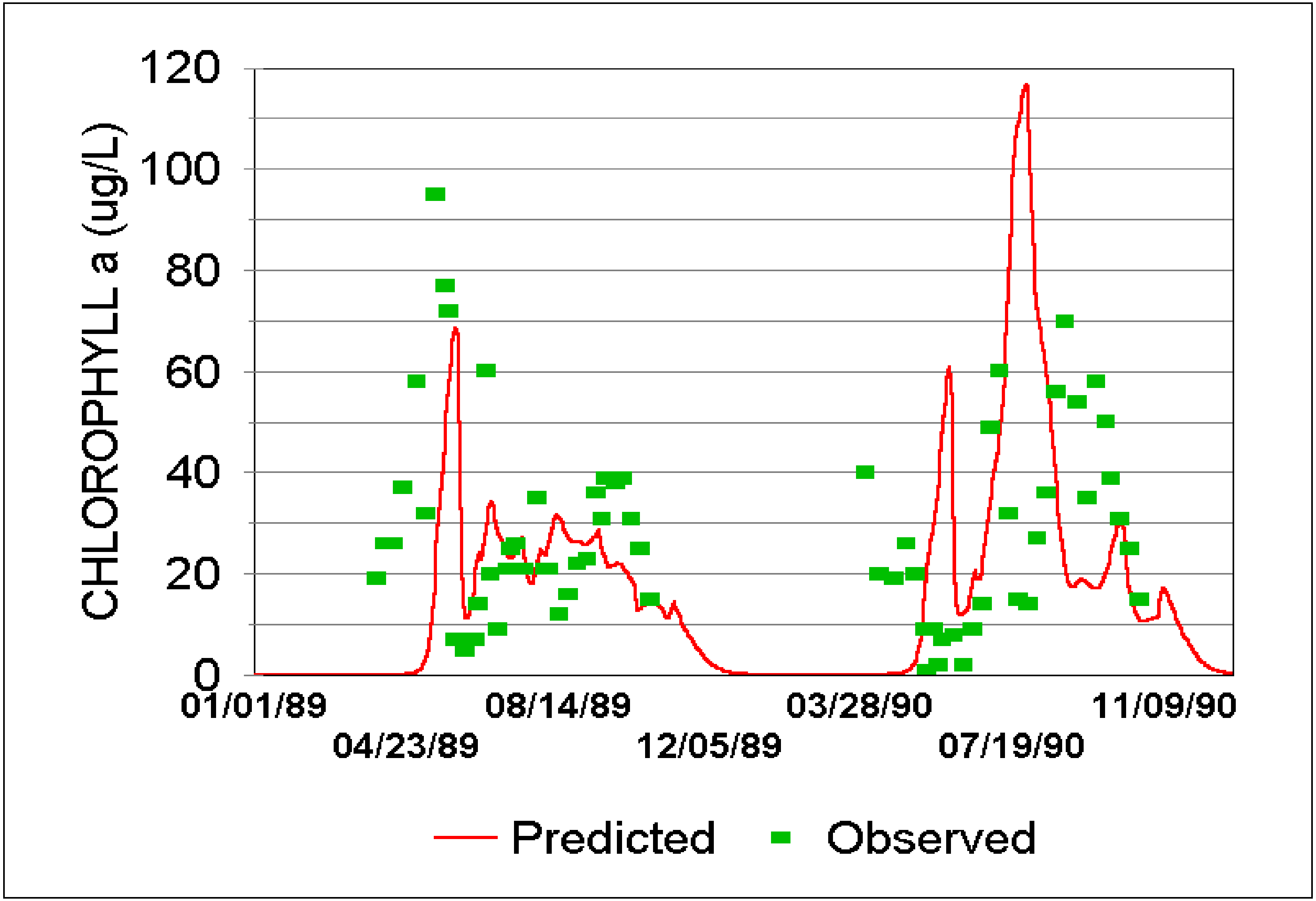


With Metro effluent

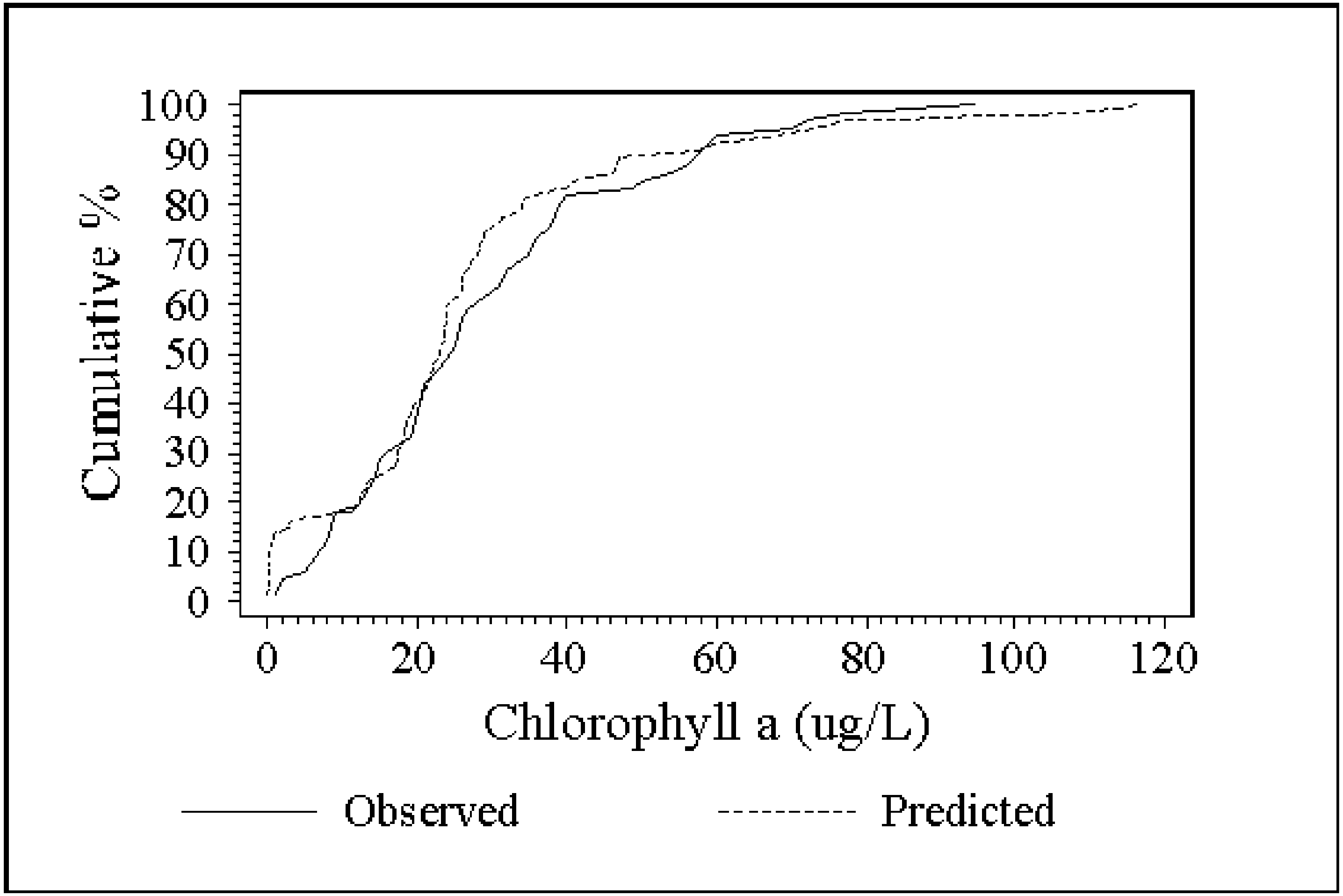


With Metro diversion, anoxia does not occur

Validation of AQUATOX with Lake Onondaga Data—visual test



Validation with chlorophyll a in Lake Onondaga, NY



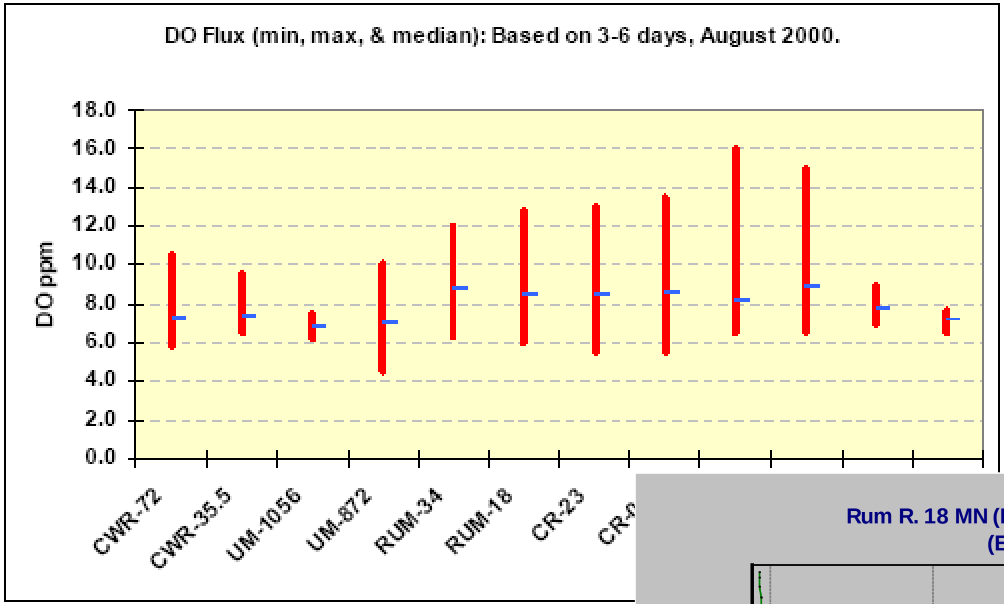
Kolmogorov-Smirnov p statistic = 0.319 (not significantly differe

Miscellaneous Nutrient-related Topics

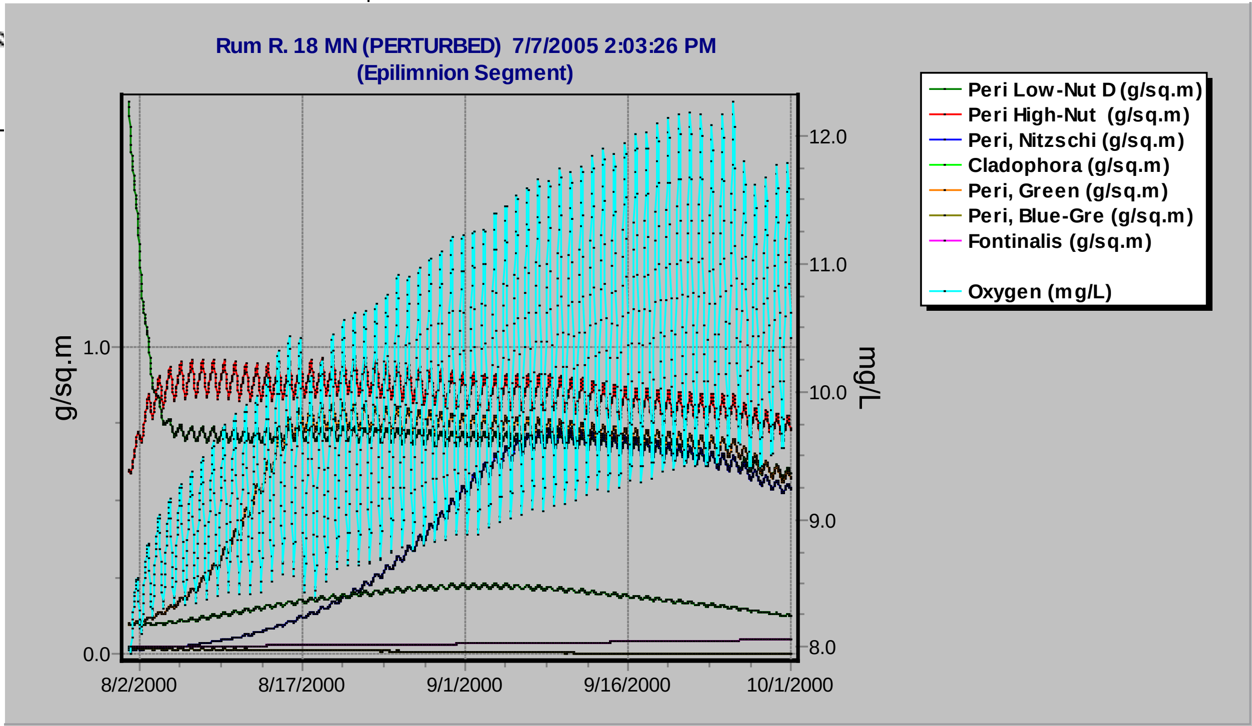
- Diel oxygen
- Effects of low dissolved oxygen
- Ammonia toxicity

Diel Oxygen, Light; Hourly time-step

Figure 4. Dissolved oxygen flux based on continuous measurement.

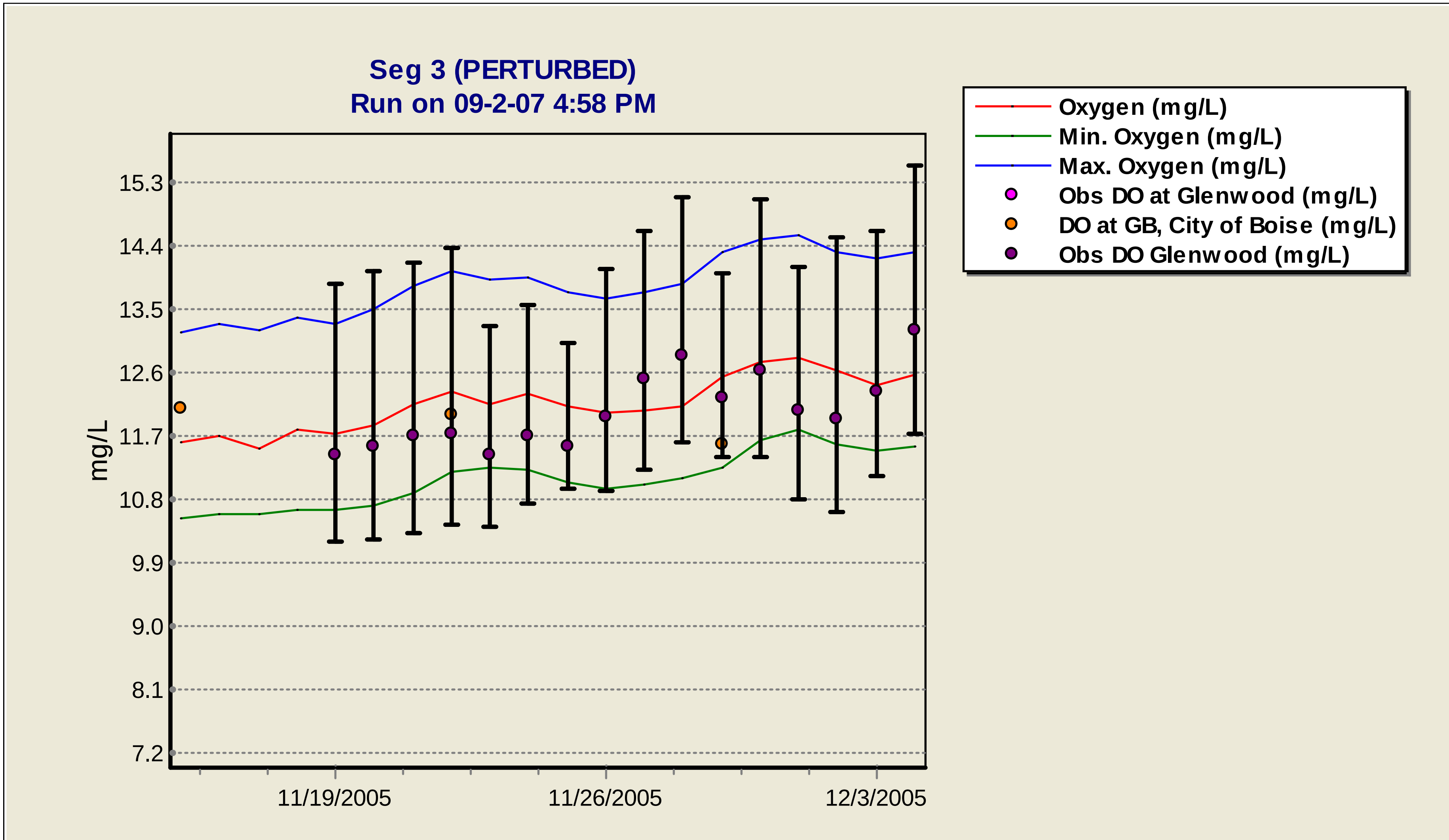


AQUATOX can now run with an hourly time-step including hourly light inputs. This results in a simulation of oxygen concentrations on an hourly basis



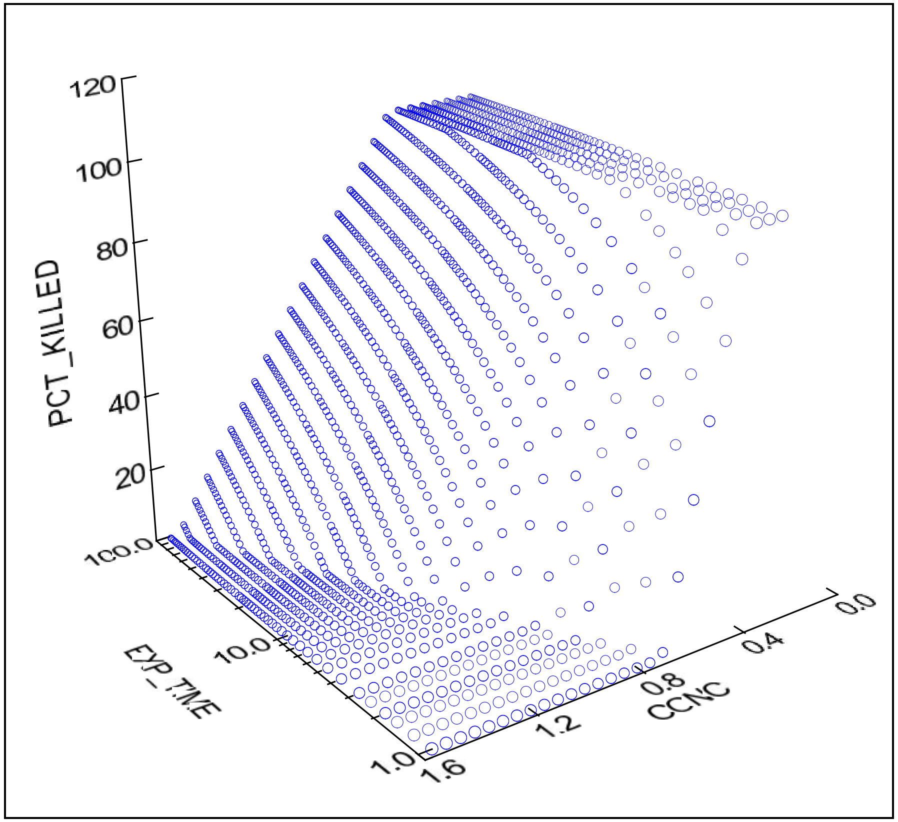
Monitoring data indicate that oxygen
levels fluctuate daily

Diel Oxygen, Hourly Time-step

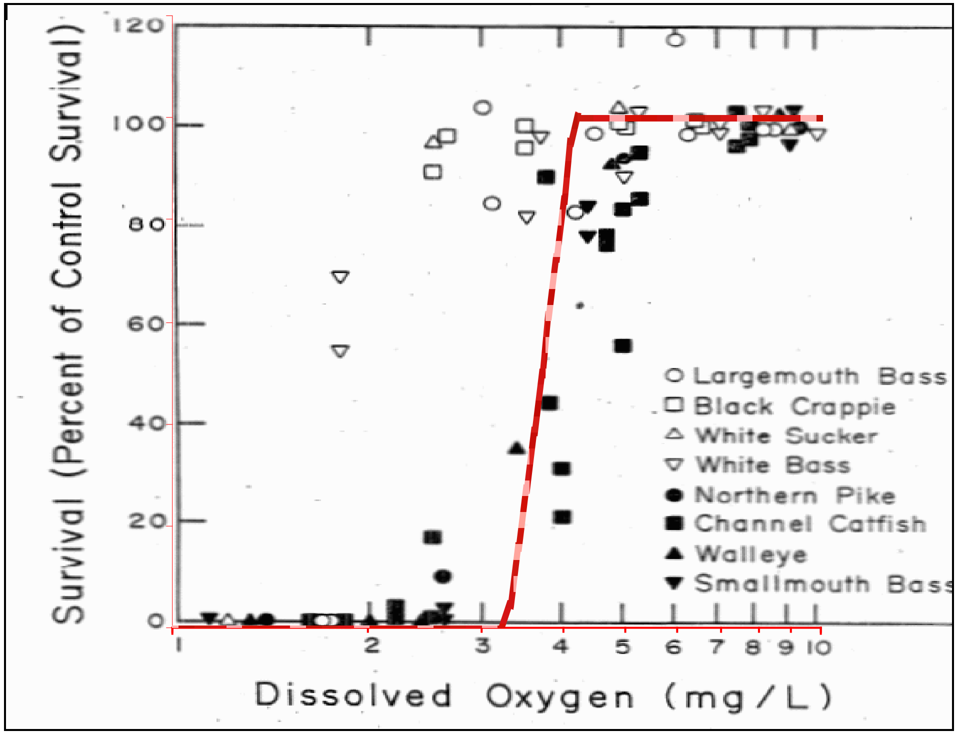


Low Oxygen Effects

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



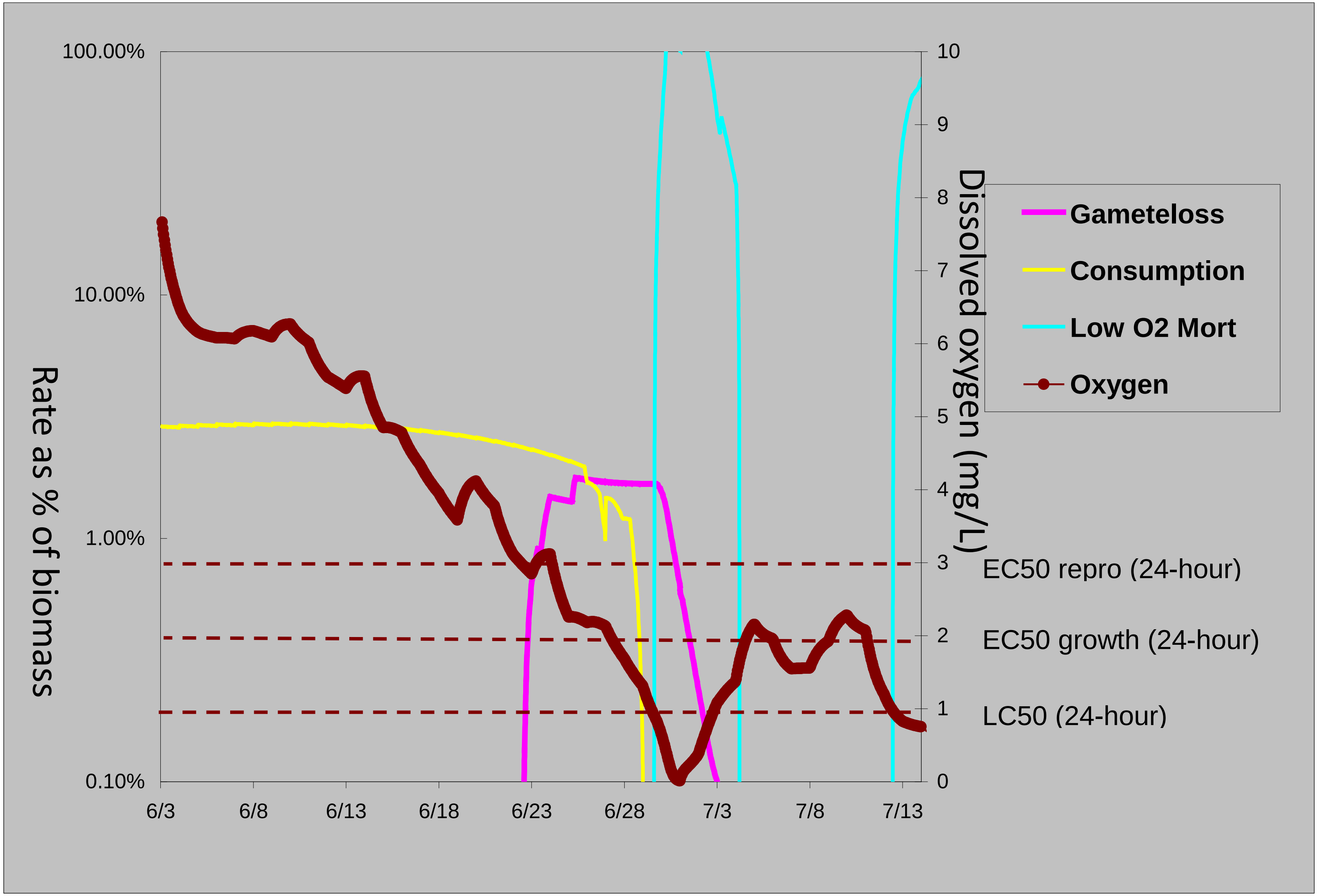
Species specific $LC50_{24\text{-hour}}$ for O_2 is required



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

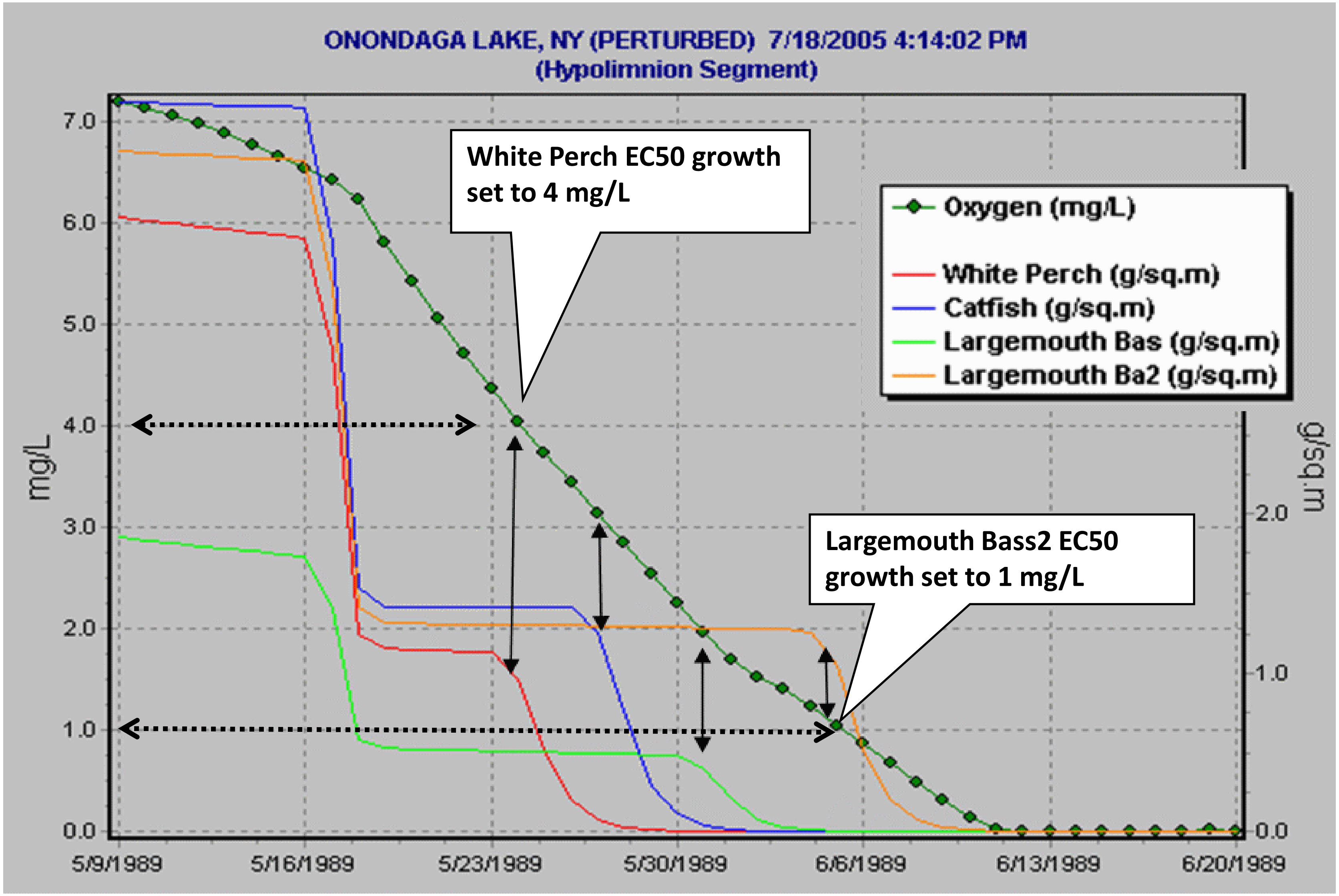
Non-Lethal Low Oxygen Effects

EC50 reproduction and EC50 growth parameters affect timing



Low O_2 Affects Timing of Migration from Hypolimnion

EC50 growth parameter is key



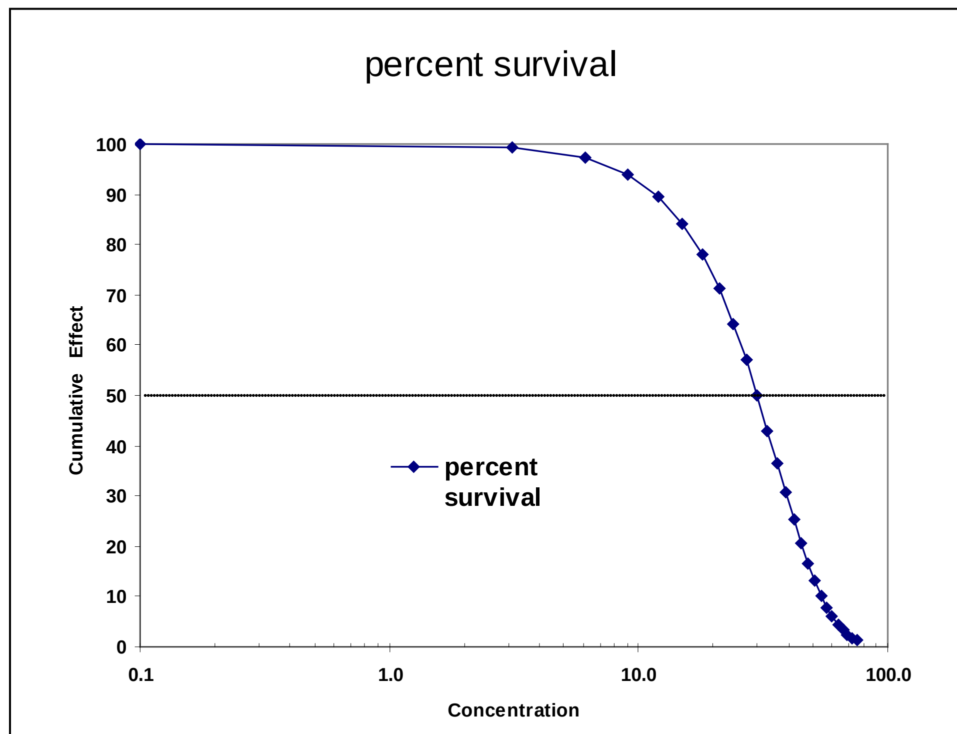
Toxicity Due to Ammonia

Animal Specific Input Parameter Required:

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

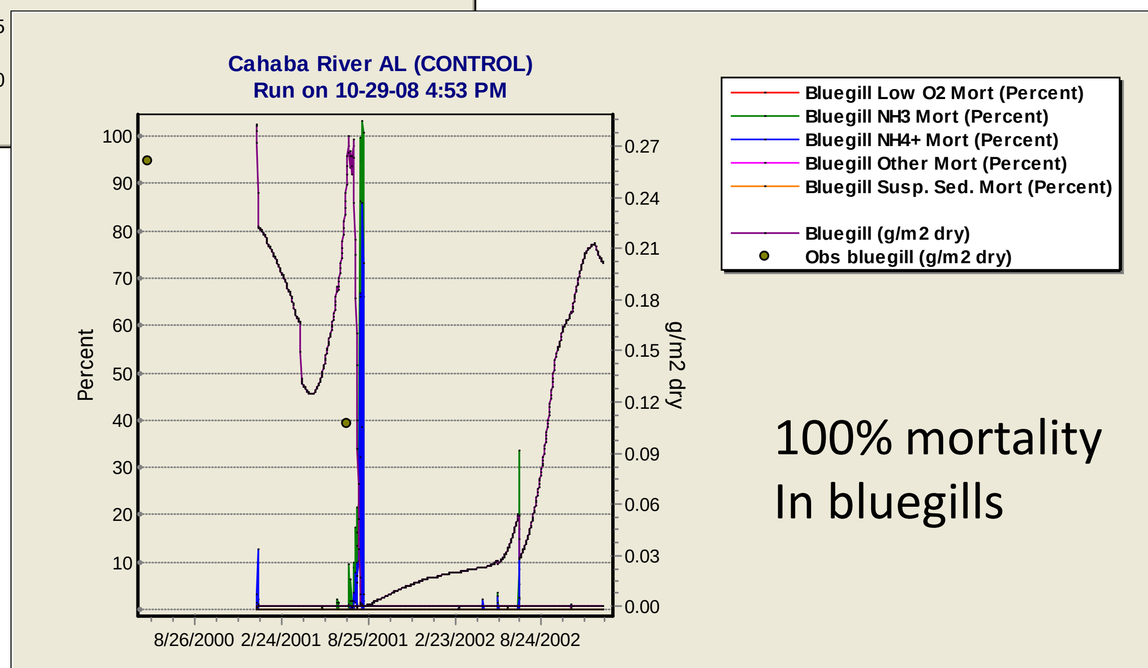
External Toxicity Model Utilized:

- 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

1% mortality in mussels



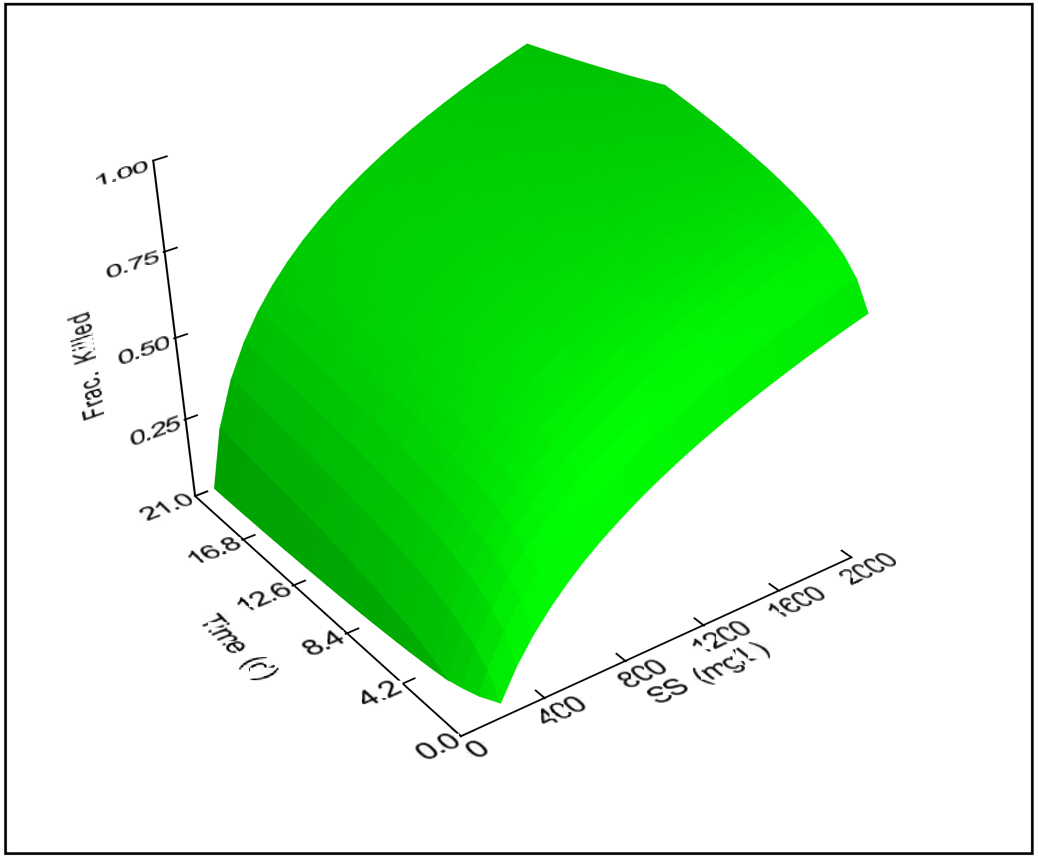
100% mortality
In bluegills

Sediment Effects Overview

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

Suspended and bedded sediment effects

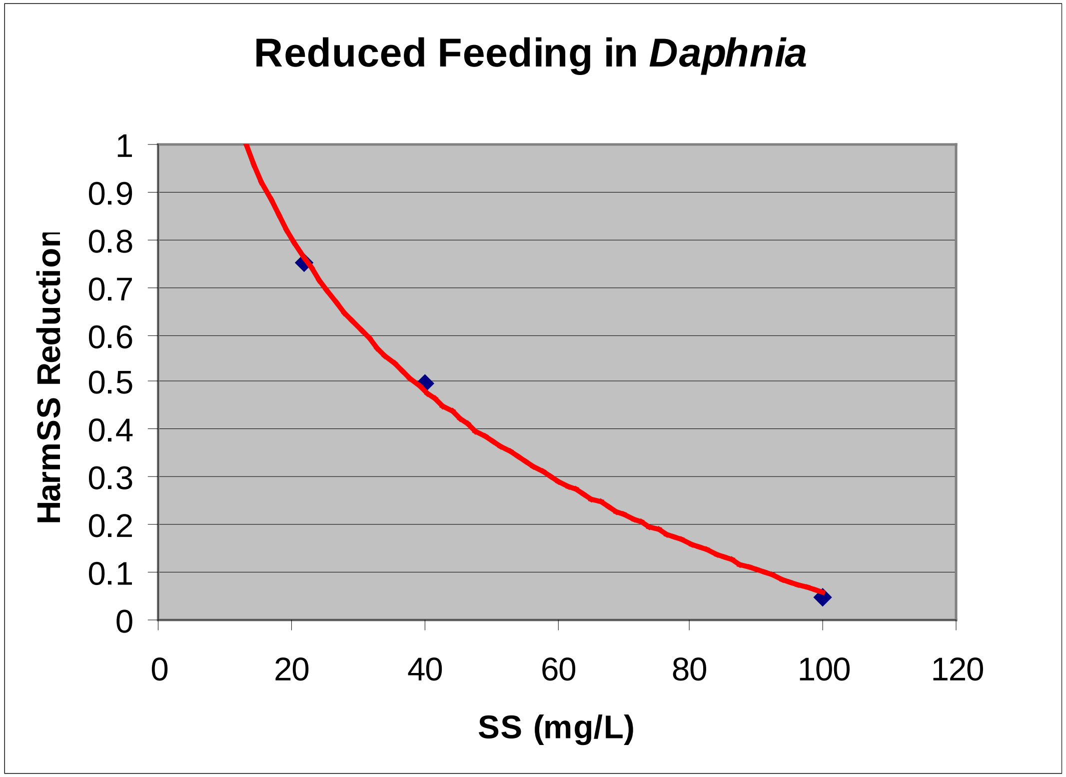
- Mortality
  - Highly Sensitive
  - Sensitive
  - Intolerant
  - Tolerant



Suspended and bedded sediment effects

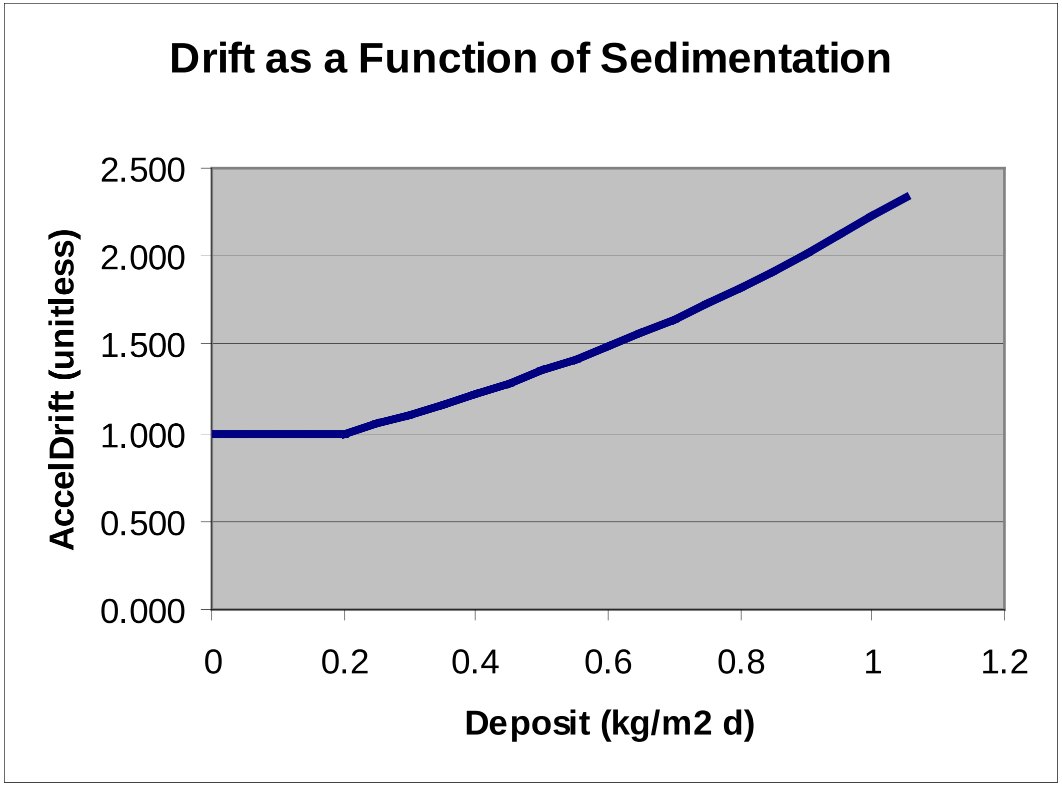
- Reduced Feeding

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



Suspended and bedded sediment effects

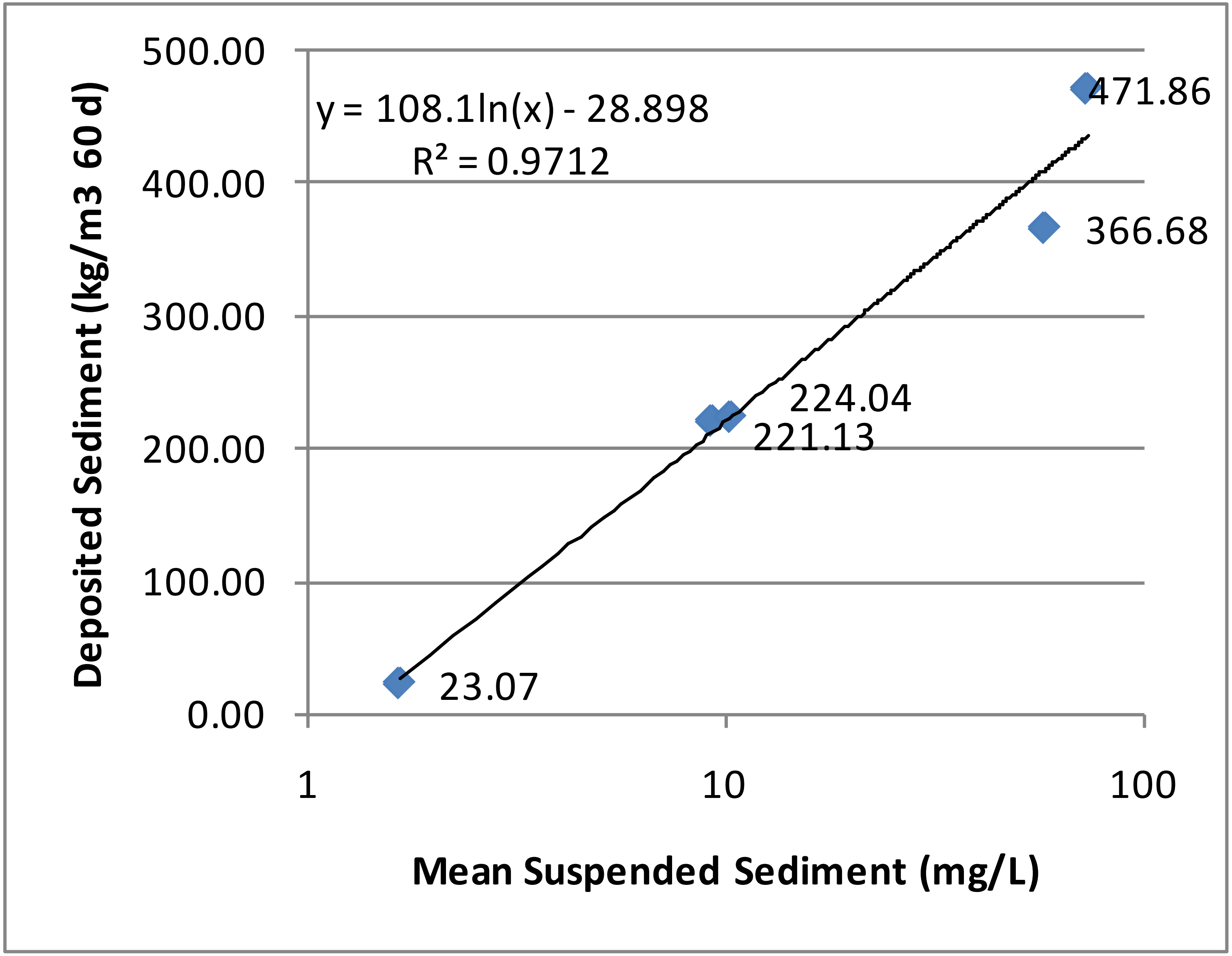
- Increased drift of benthos due to sedimentation



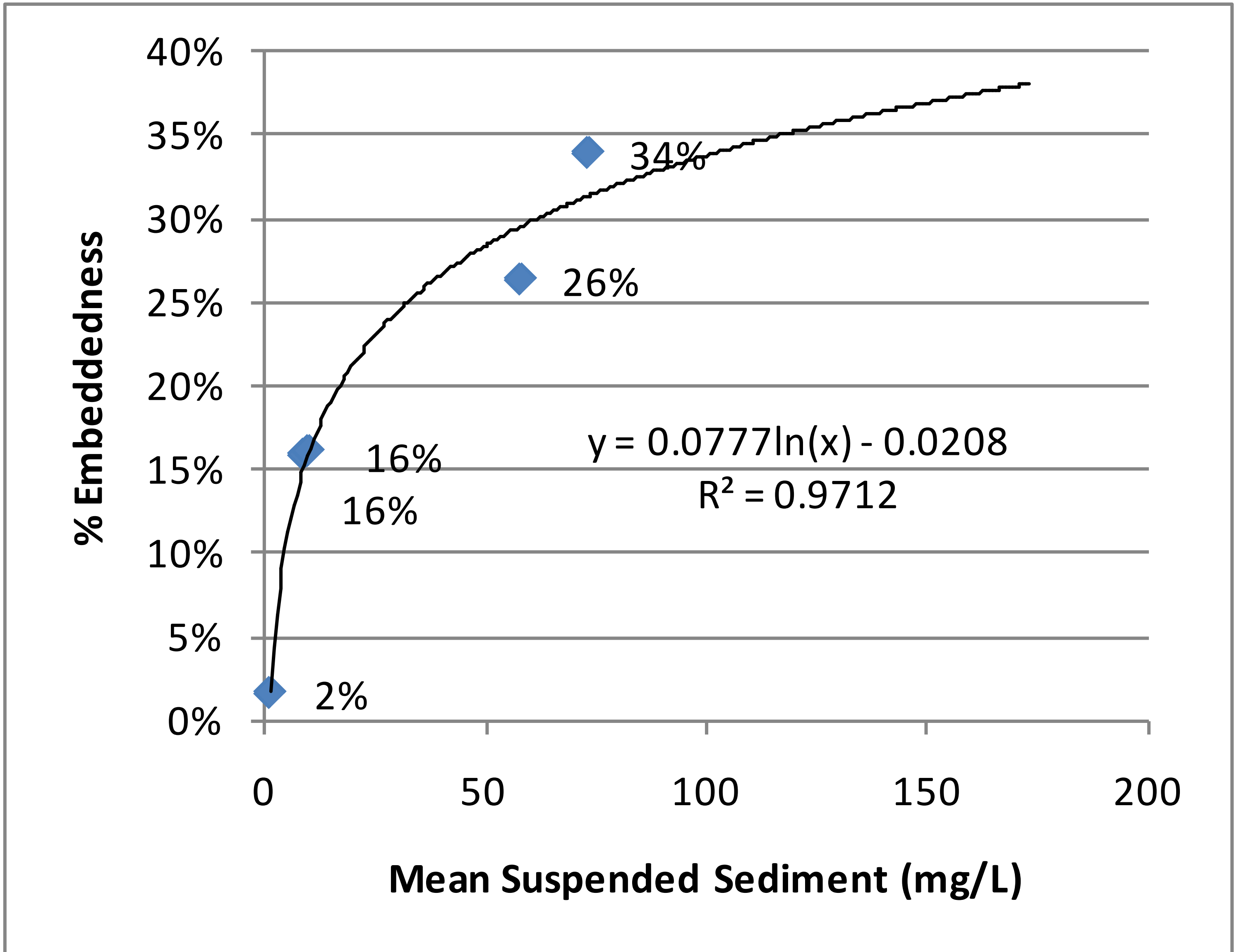
Suspended and bedded sediment effects

- 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

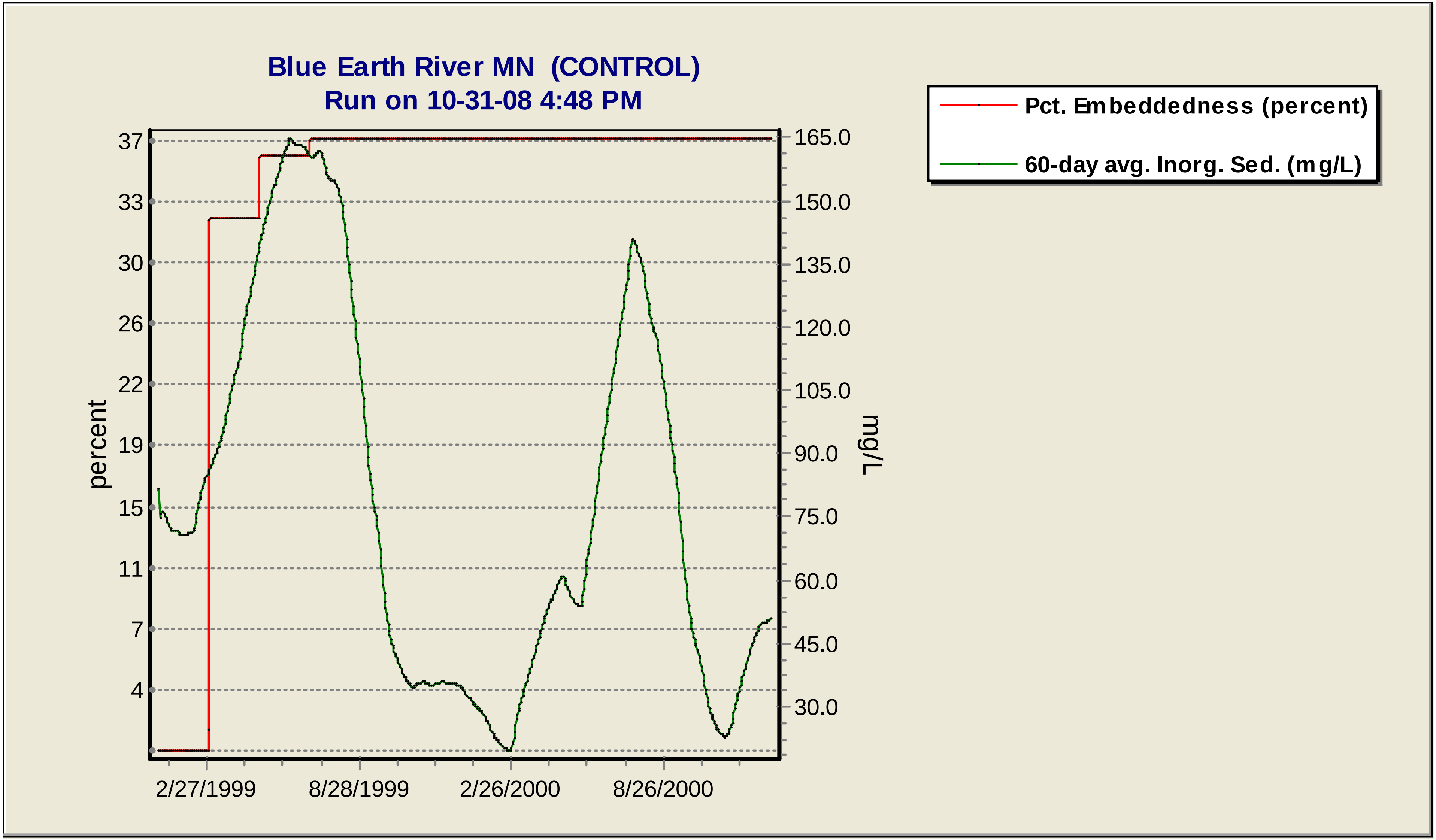
Relationship of 60-day sedimentation to average TSS



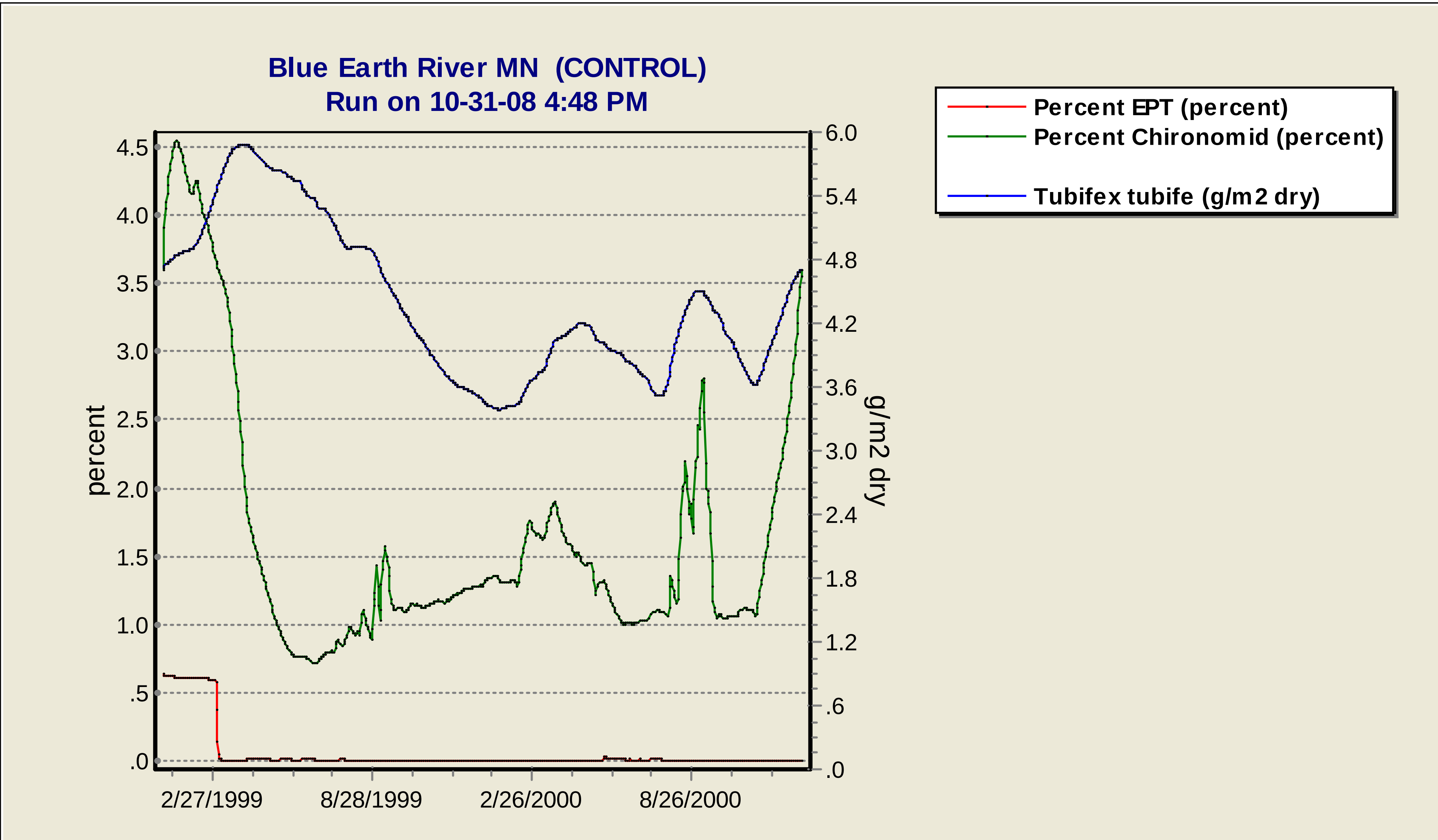
Relationship of 60-day percent embeddedness to average TSS



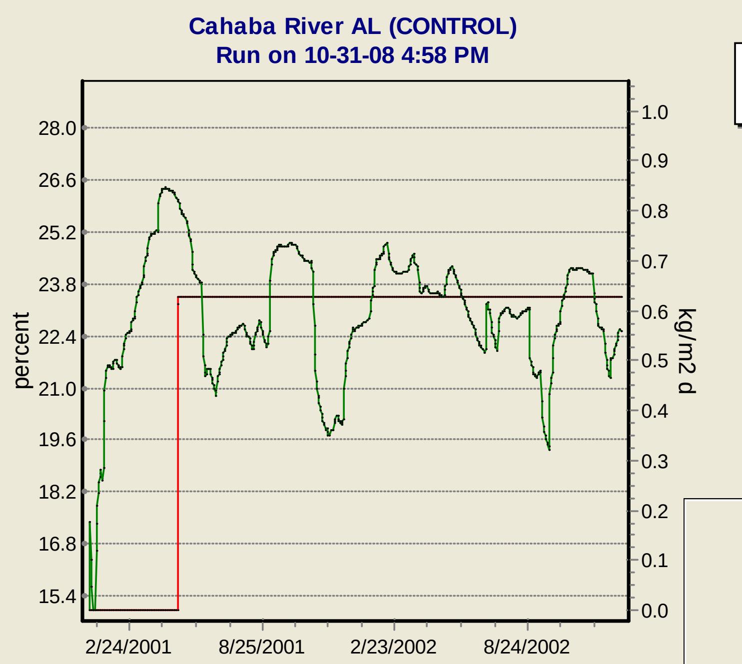
Computed % embeddedness and sedimentation are quite high in turbid Blue Earth River MN



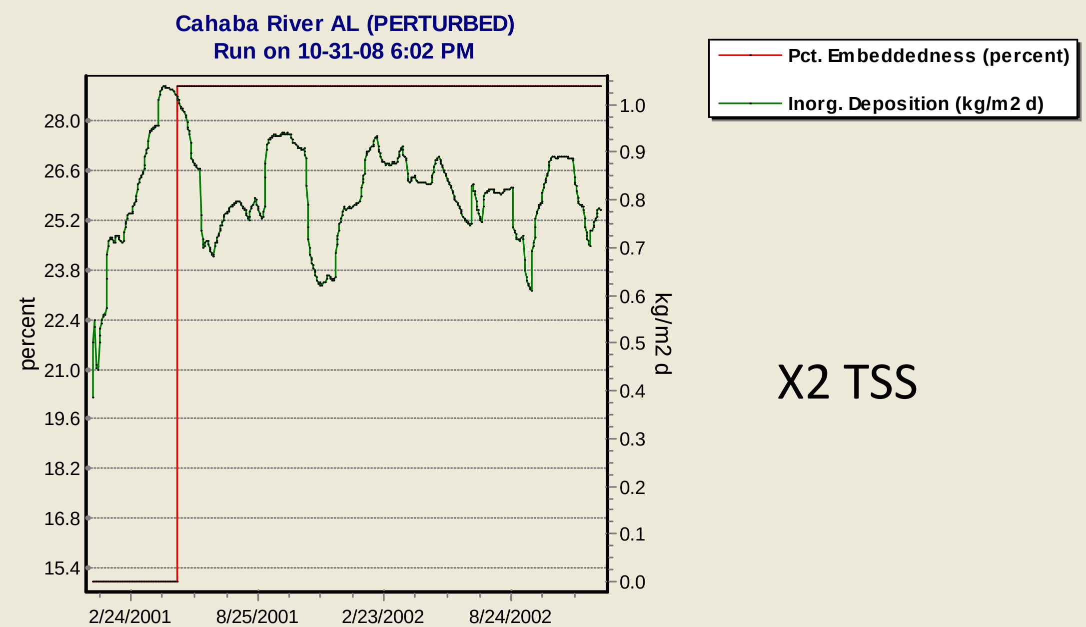
Mayflies, stoneflies, & caddisflies (EPT) are sensitive to embeddedness; chironomids & oligochaetes are not



Doubling TSS increases embeddedness in Cahaba River, AL

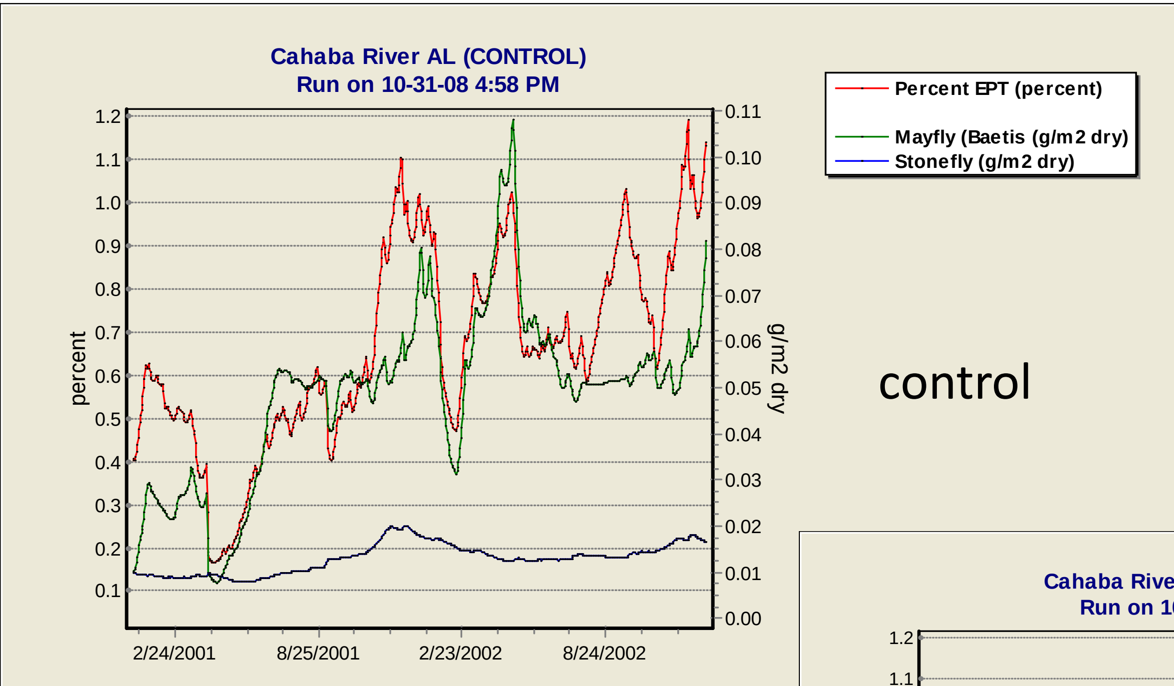


control

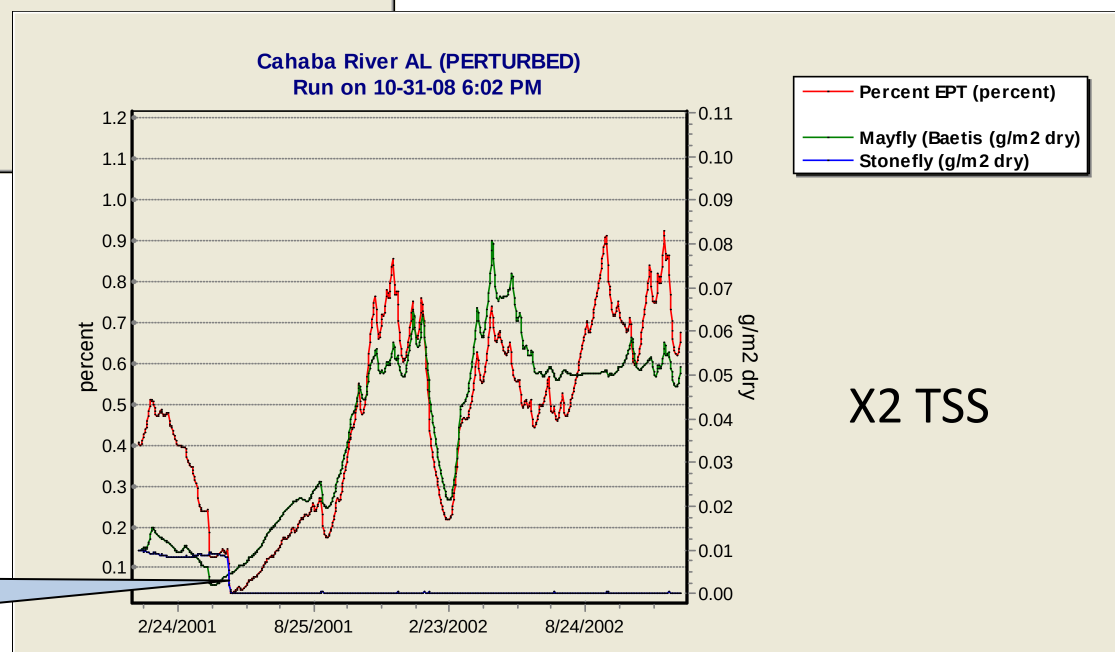


X2 TSS

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



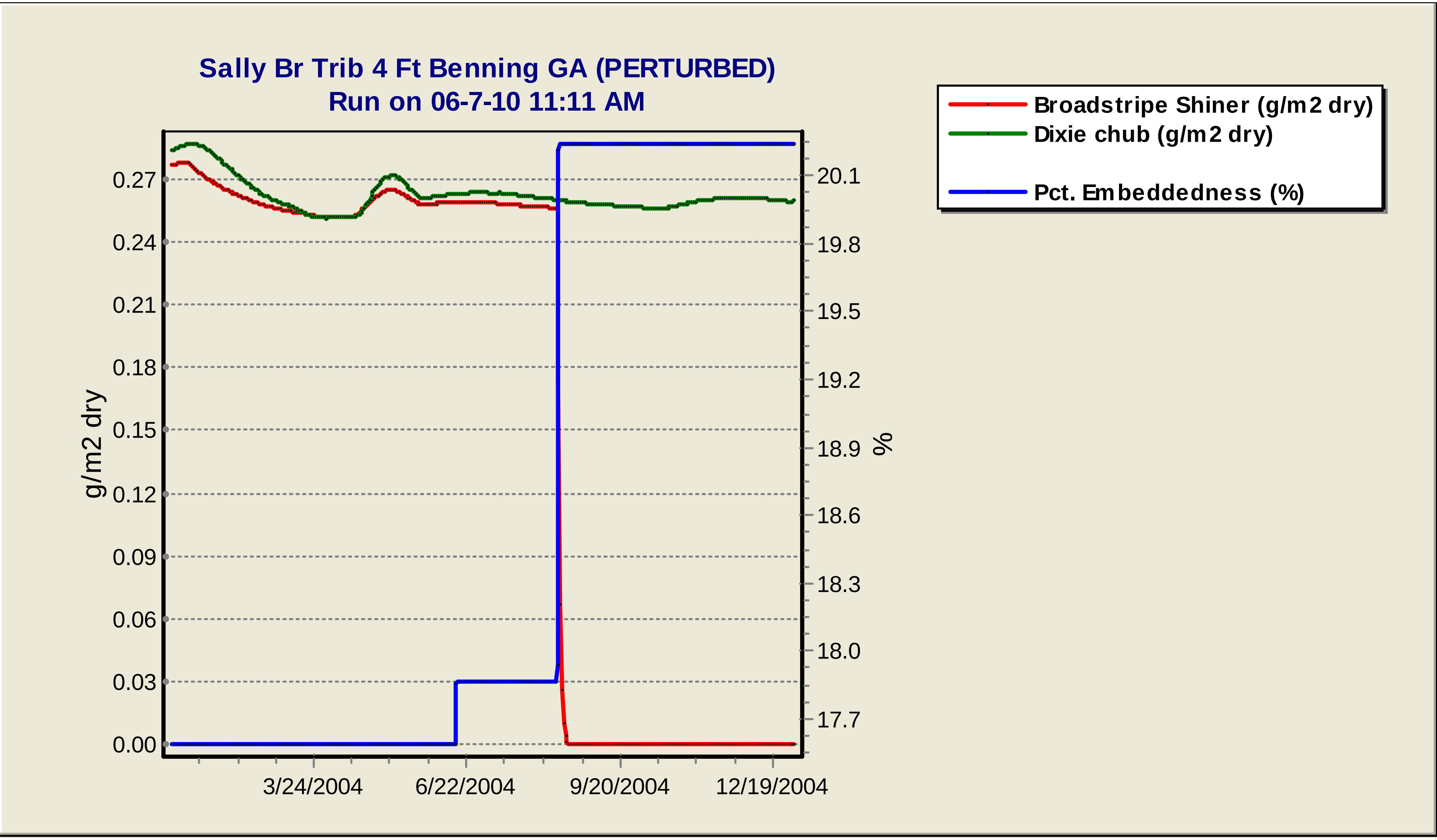
control



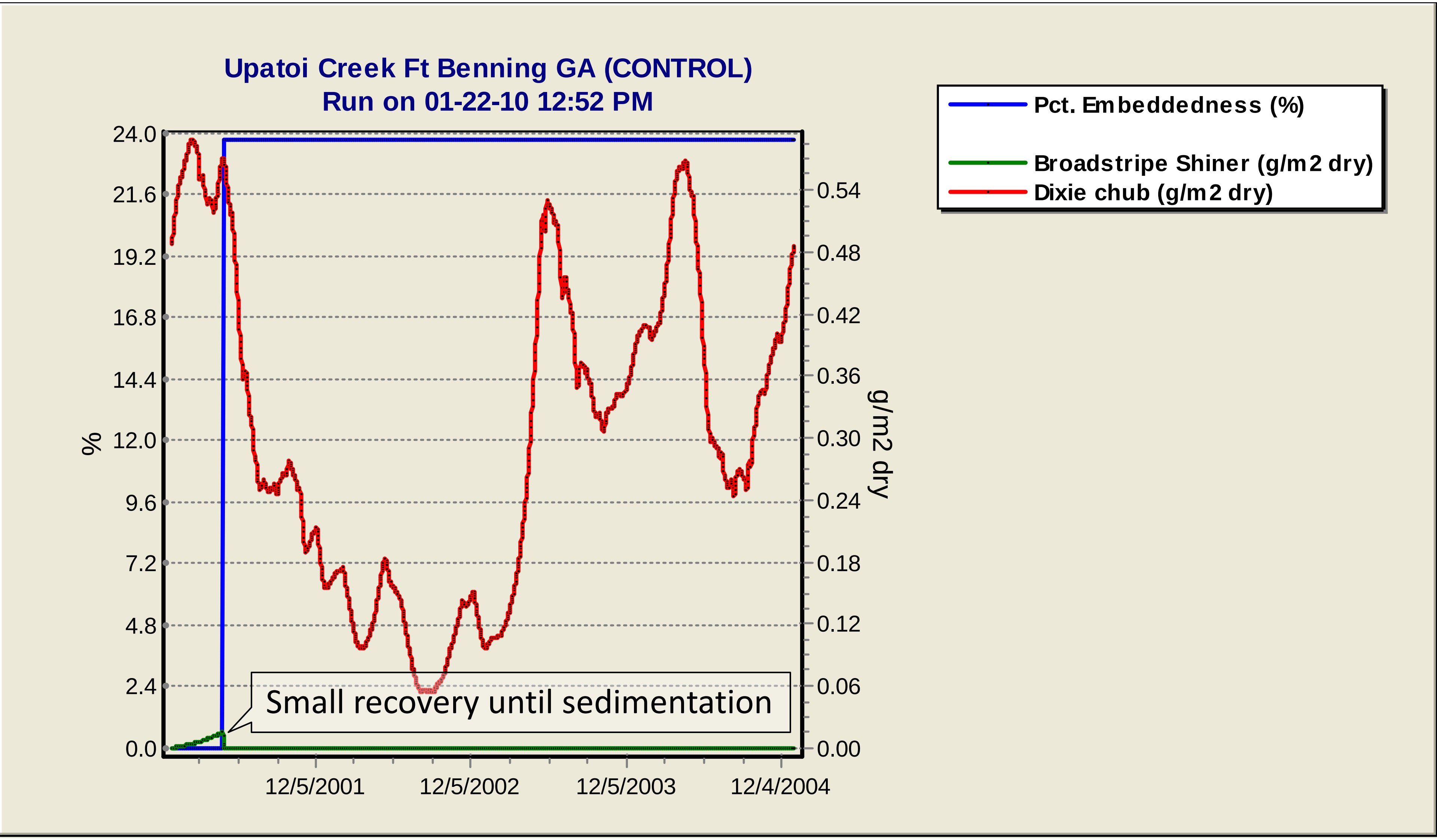
X2 TSS

stoneflies crash

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



Broadstripe shiner is excluded from another creek due to embeddedness



Lab 6: Analysis of Plant Control in "Clear Lake CA"

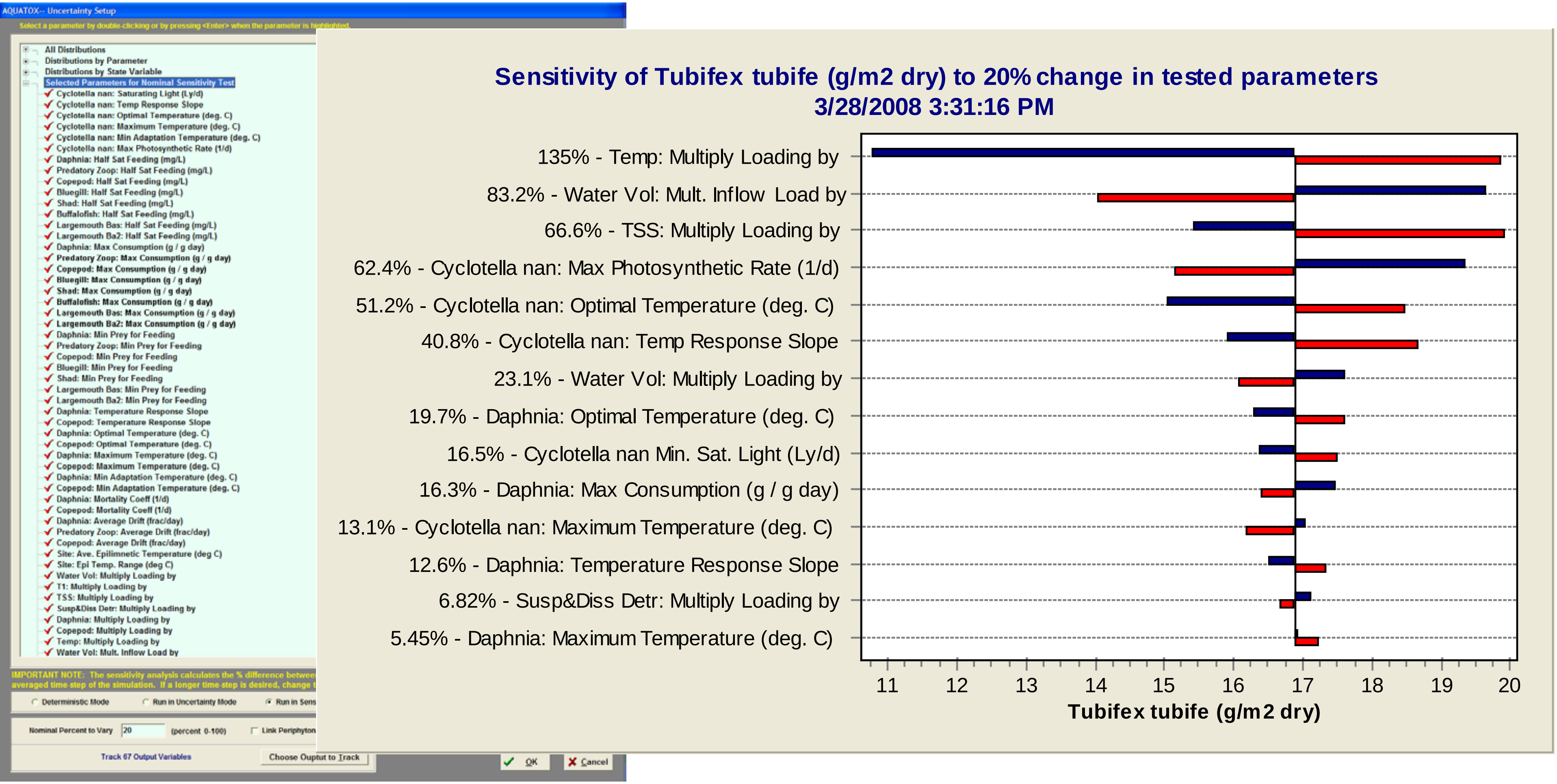
- Run control for 3 years
- Add *Hydrilla*
- Run perturbed
- Use difference graph to assess impacts of *Hydrilla*
    - animals
    - nutrients
- Interpret nutrients
    - *Technical Documentation*
    - mass balance plots
- Interpret blue-green algal response

Uncertainty and Nominal Range Sensitivity Analysis
Demonstration & Optional Lab

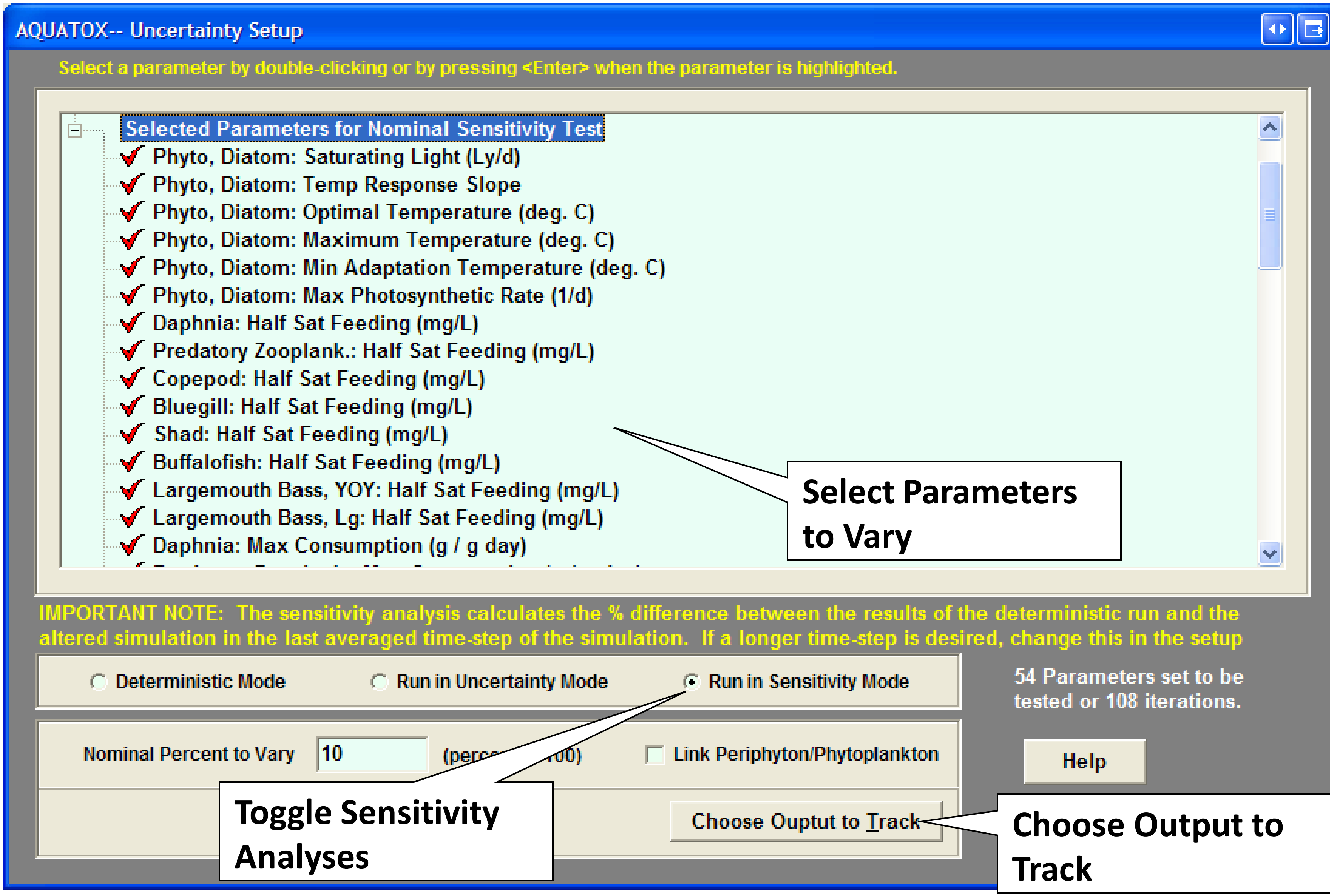
- “Sensitivity” refers to the variation in output of a mathematical model with respect to changes in the values of the model inputs (Saltelli, 2001).
- Sensitivity analysis provides a ranking of the model input assumptions with respect to their relative contribution to model output variability or uncertainty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

Coralville Sensitivity Analysis Demo

Demonstration of inputs and outputs from Coralville analysis



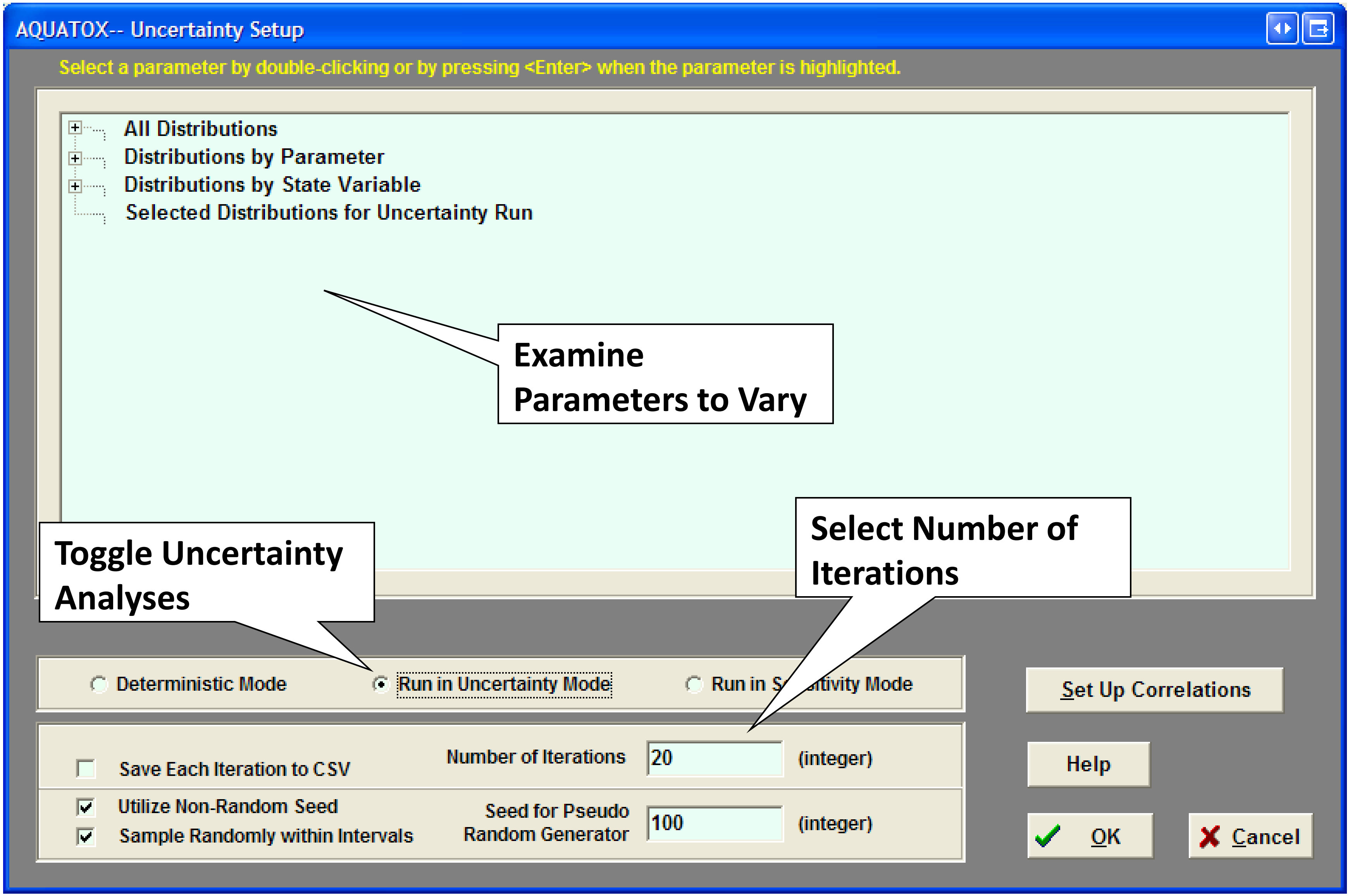
AQUATOX Sensitivity Screen



Uncertainty Analysis

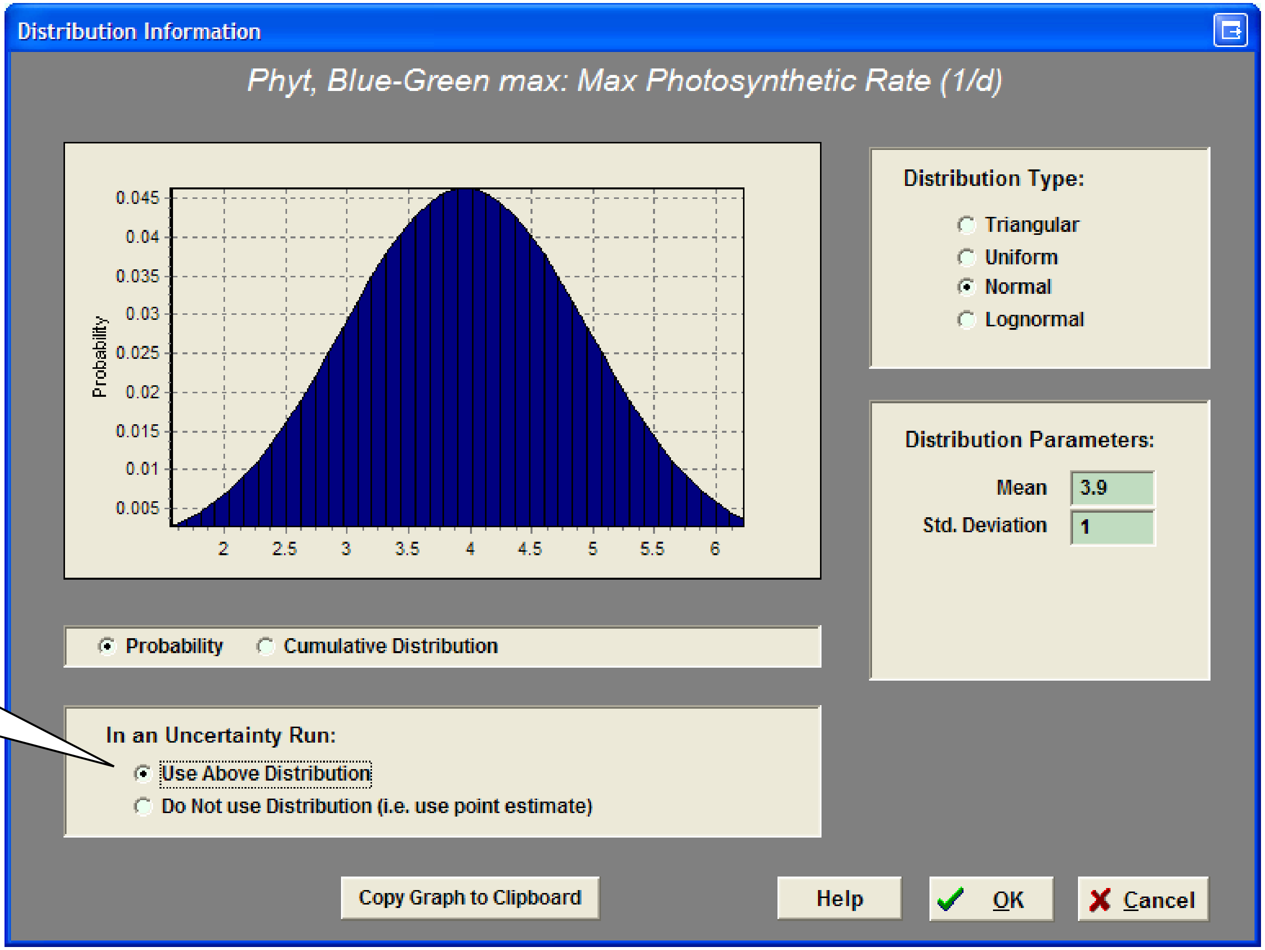
- Uncertainty analyses describe sources of incertitude and variability in model simulations
- There are many sources of uncertainty e.g.
  - parameter uncertainty
  - model uncertainty due to necessary simplification of real-world processes
- Monte Carlo analysis is a statistical sampling technique that 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



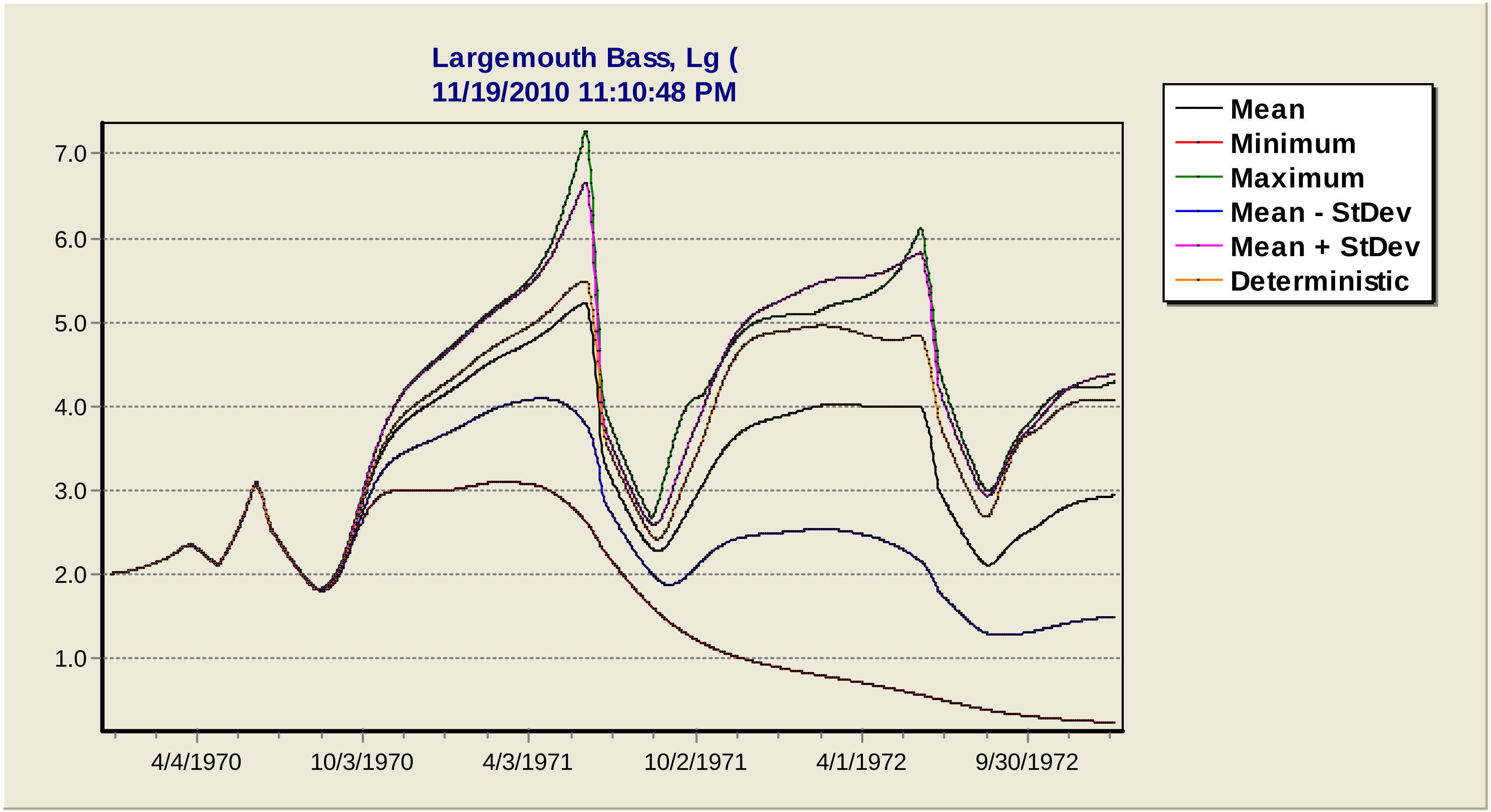
Select one or more Parameters to Vary

- 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.

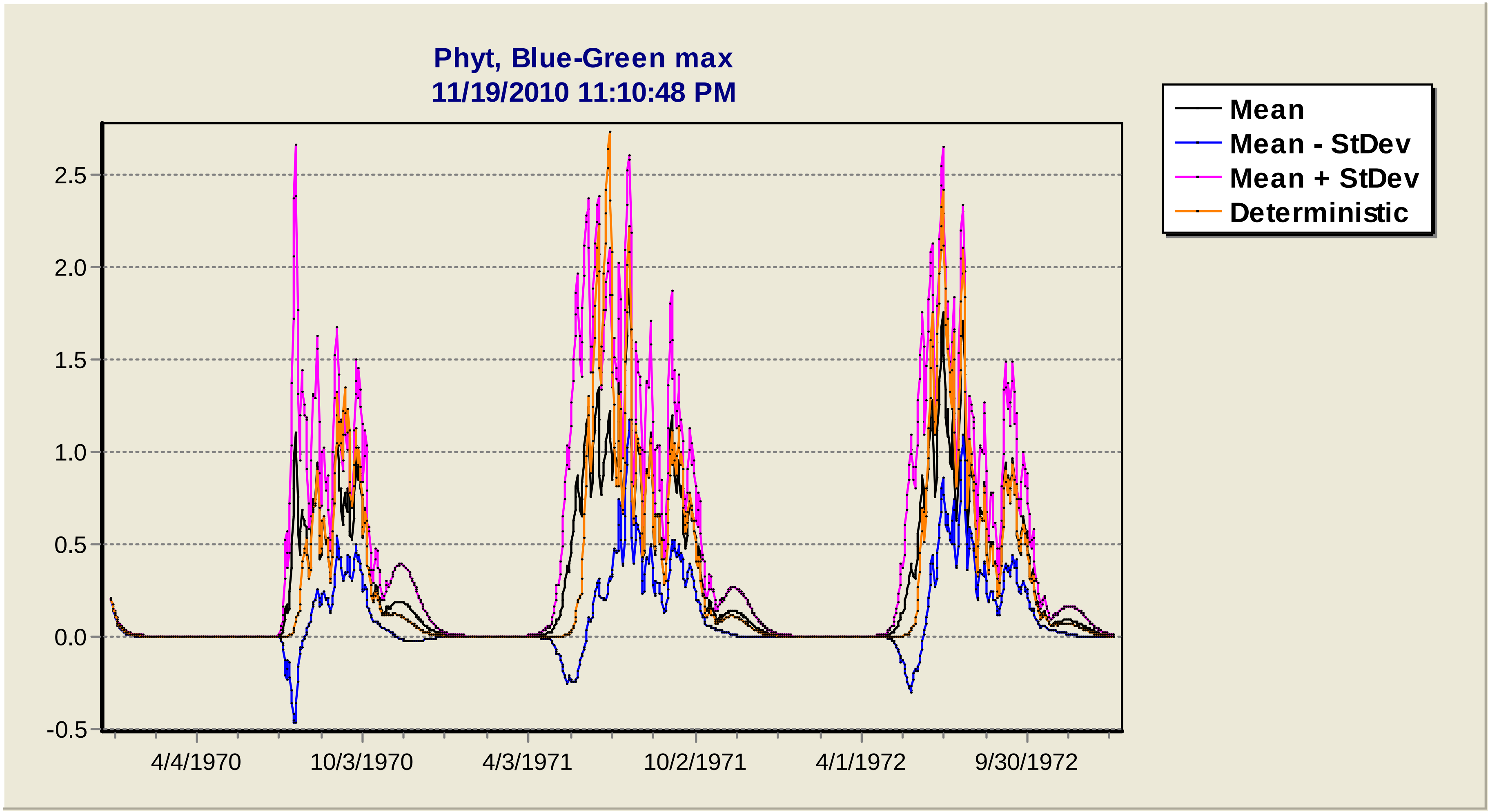


Choose whether to vary a parameter or keep as a constant "point estimate"

Using the Uncertainty Tab on the Output Screen

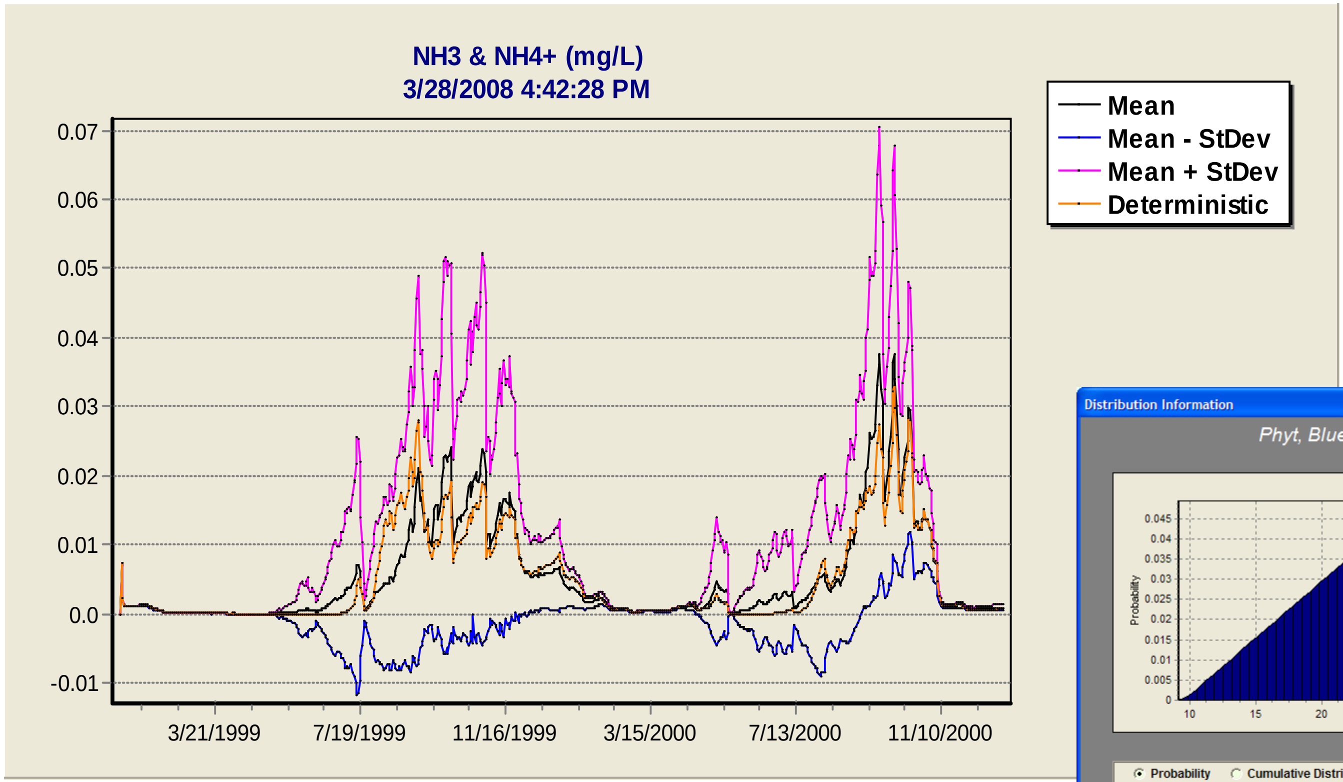


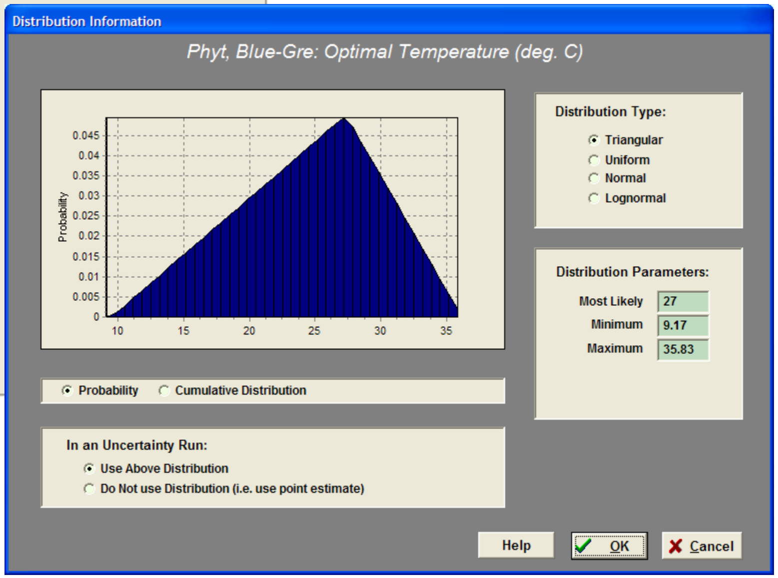
Sensitivity of Blue-Greens



Blue Earth Uncertainty Analysis Demo

Demonstration of inputs and outputs from Blue Earth River, MN





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

$$\frac{dToxicant_{Water}}{dt} = Loading + \sum_{LabileDetr}(Decomposition_{LabileDetr} \cdot PPB_{LabileDetr} \cdot 1e-6) + \sum Desorption_{DetrTox} + \sum Depuration_{Org} - \sum Sorption_{DetrTox} - \sum GillUptake - MacroUptake - \sum AlgalUptake_{Alga} - Hydrolysis - Photolysis - MicrobialDegrdn + Volatilization - Discharge + Biotransform_{Microb\ In} \pm TurbDiff$$

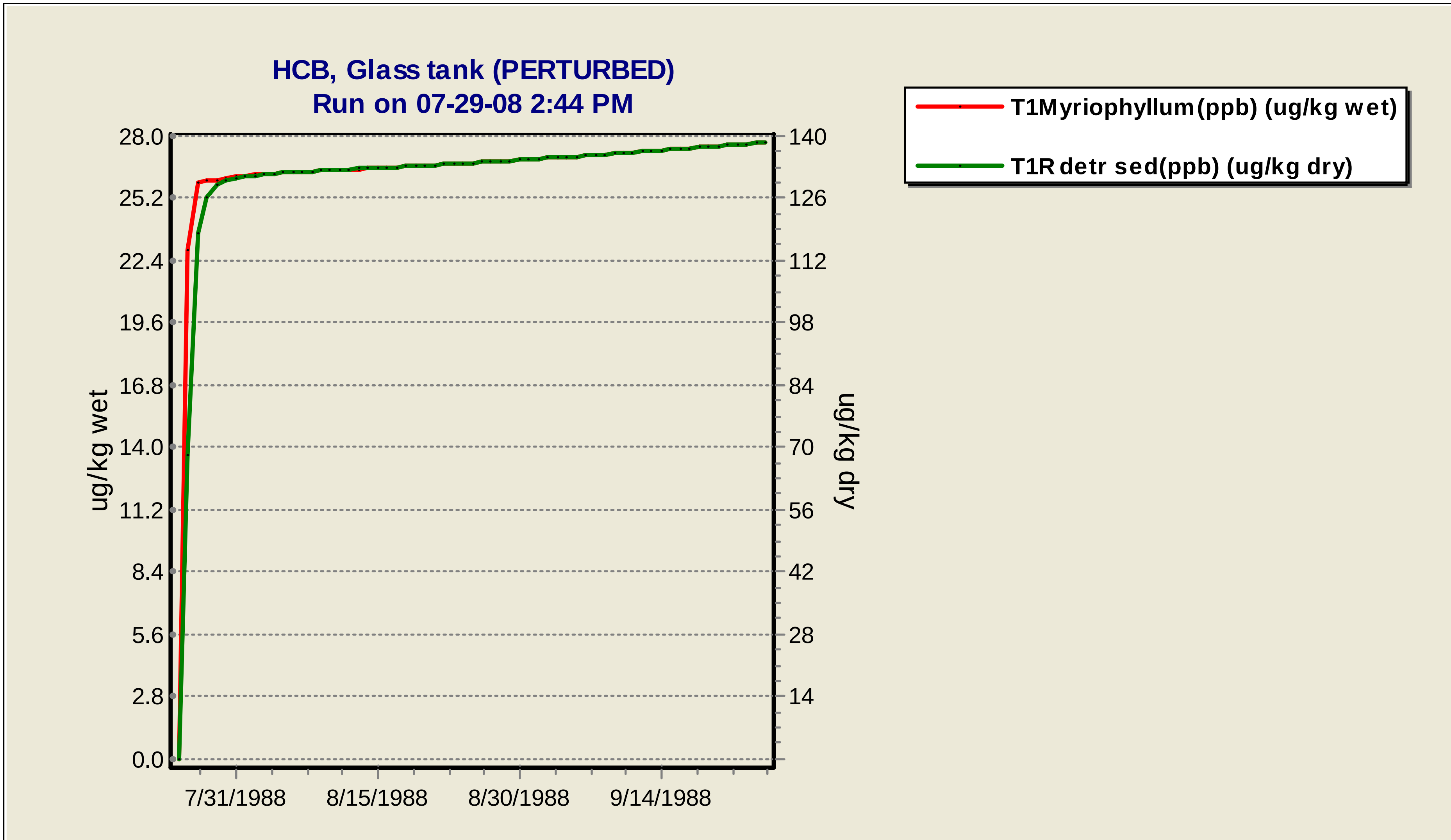
$$\frac{dToxicant_{Alga}}{dt} = Loading + AlgalUptake - Depuration \pm TurbDiff - (Excretion + Washout + \sum_{Pred} Predation_{Pred,\ Alga} + Mortality + Sink \pm SinkToHypo) \cdot PPB_{Alga} \cdot 1e-6 \pm Biotransform_{Alga}$$

$$\frac{dToxicant_{Animal}}{dt} = Loading + GillUptake + \sum_{Prey} DietUptake \pm TurbDiff - (Depuration + \sum_{Pred} Predation_{Pred,\ Animal} + Mortality + Recruit \pm Promotion + GameteLoss + Drift + Migration + EmergeInsect) \cdot PPB_{Animal} \cdot 1e-6 \pm Biotransform_{Animal}$$

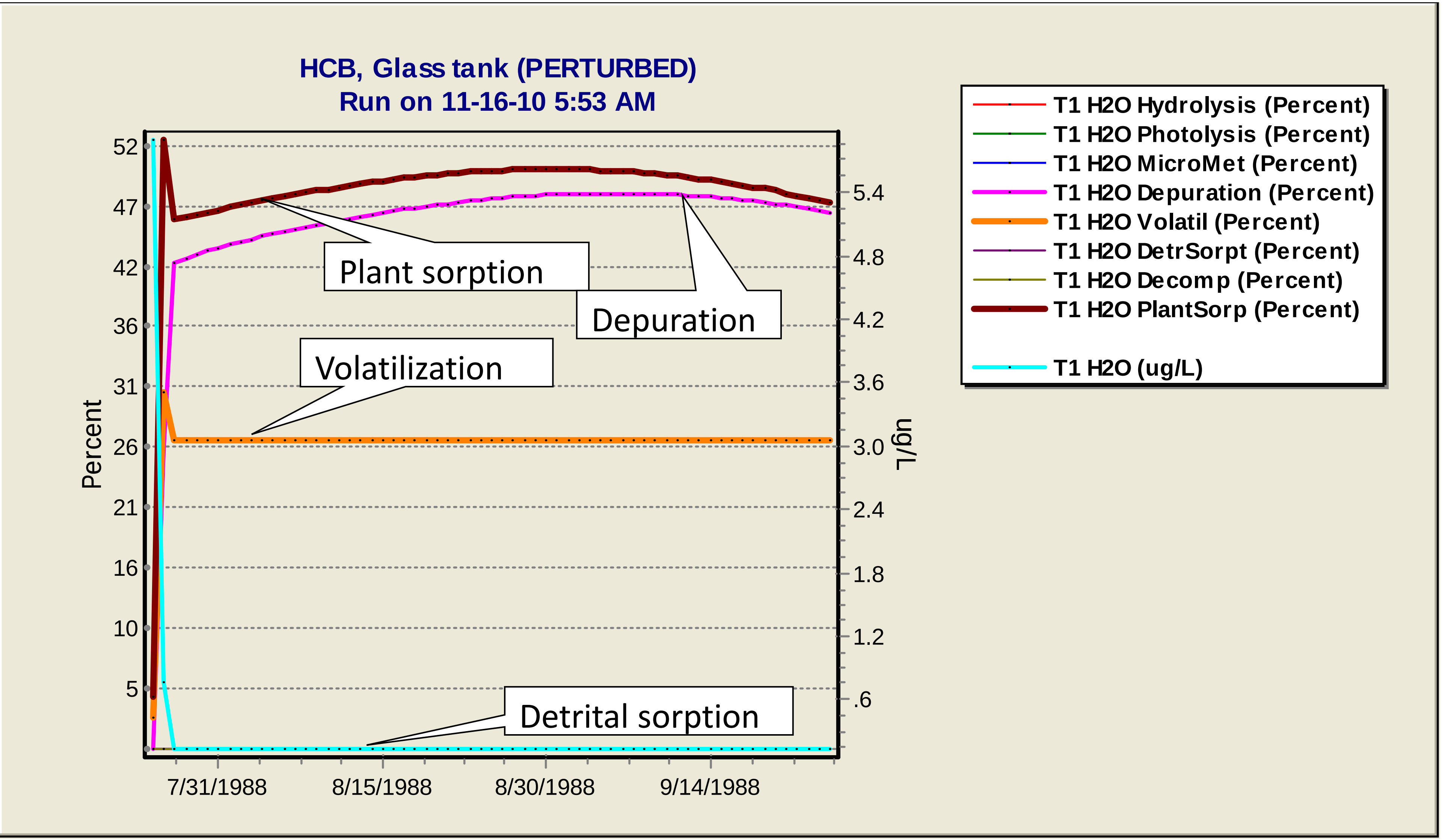
HCB in tank

- 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



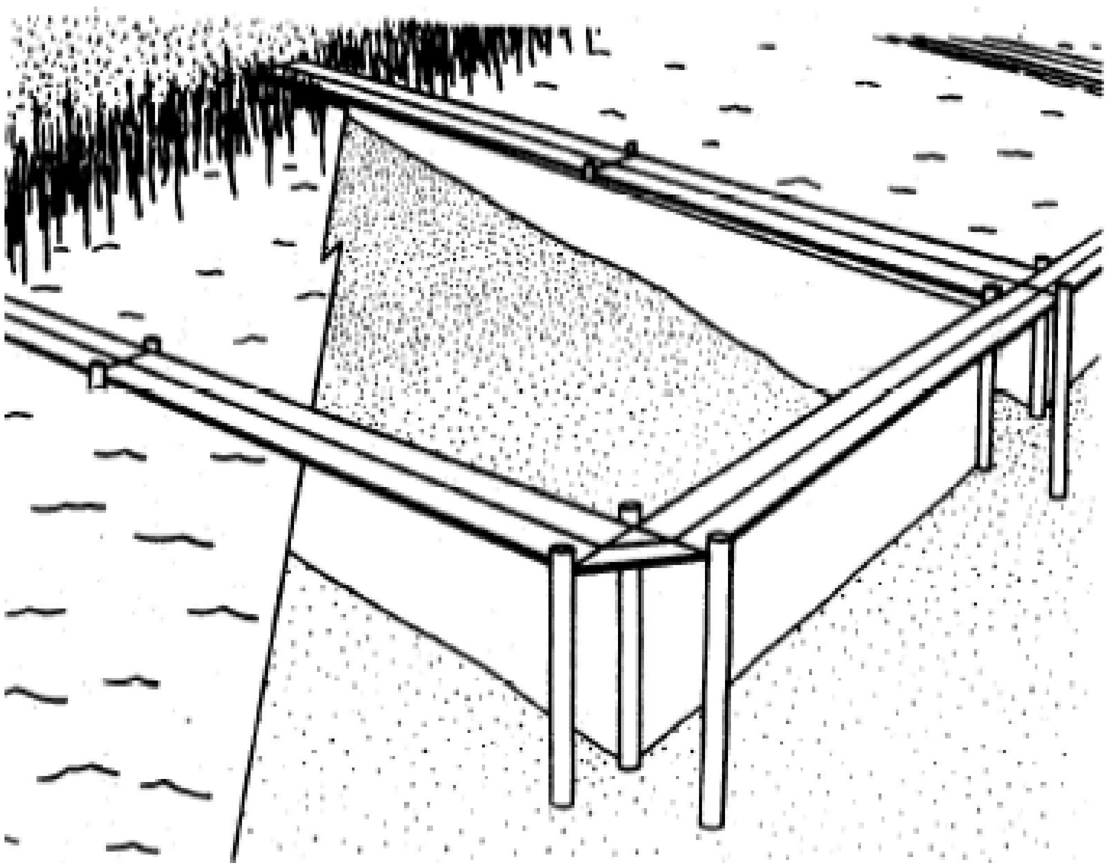
HCB loss rates can be plotted, showing that sorption to detritus is negligible (due to mass)



Chlorpyrifos in Pond

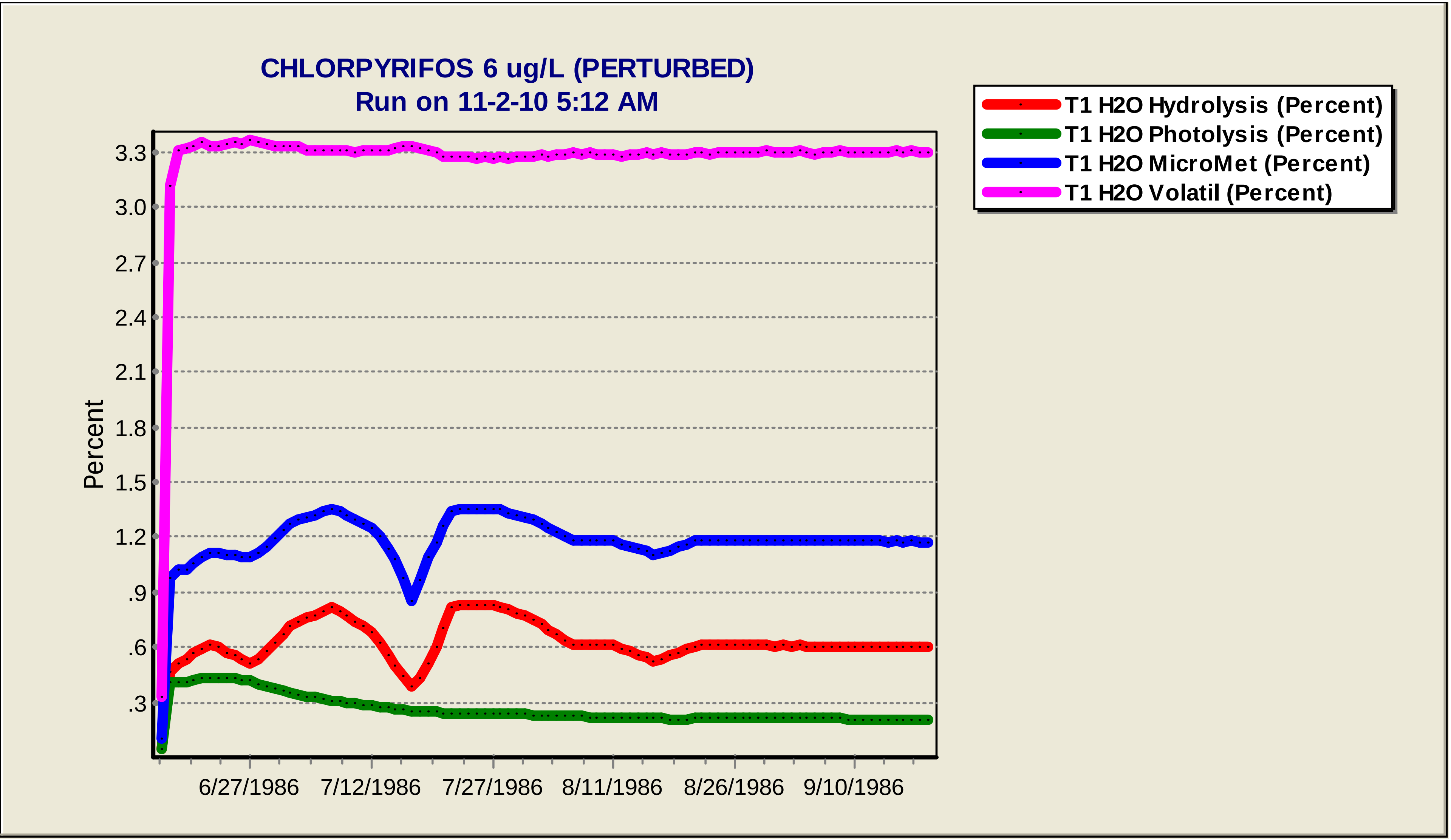
- Pond enclosure dosed with chlorpyrifos at EPA Duluth lab
- A single dose of chlorpyrifos is applied at the beginning of the simulation
- Additional biotic compartments
  - diatoms, greens, invertebrates,
  - sunfish, shiner

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

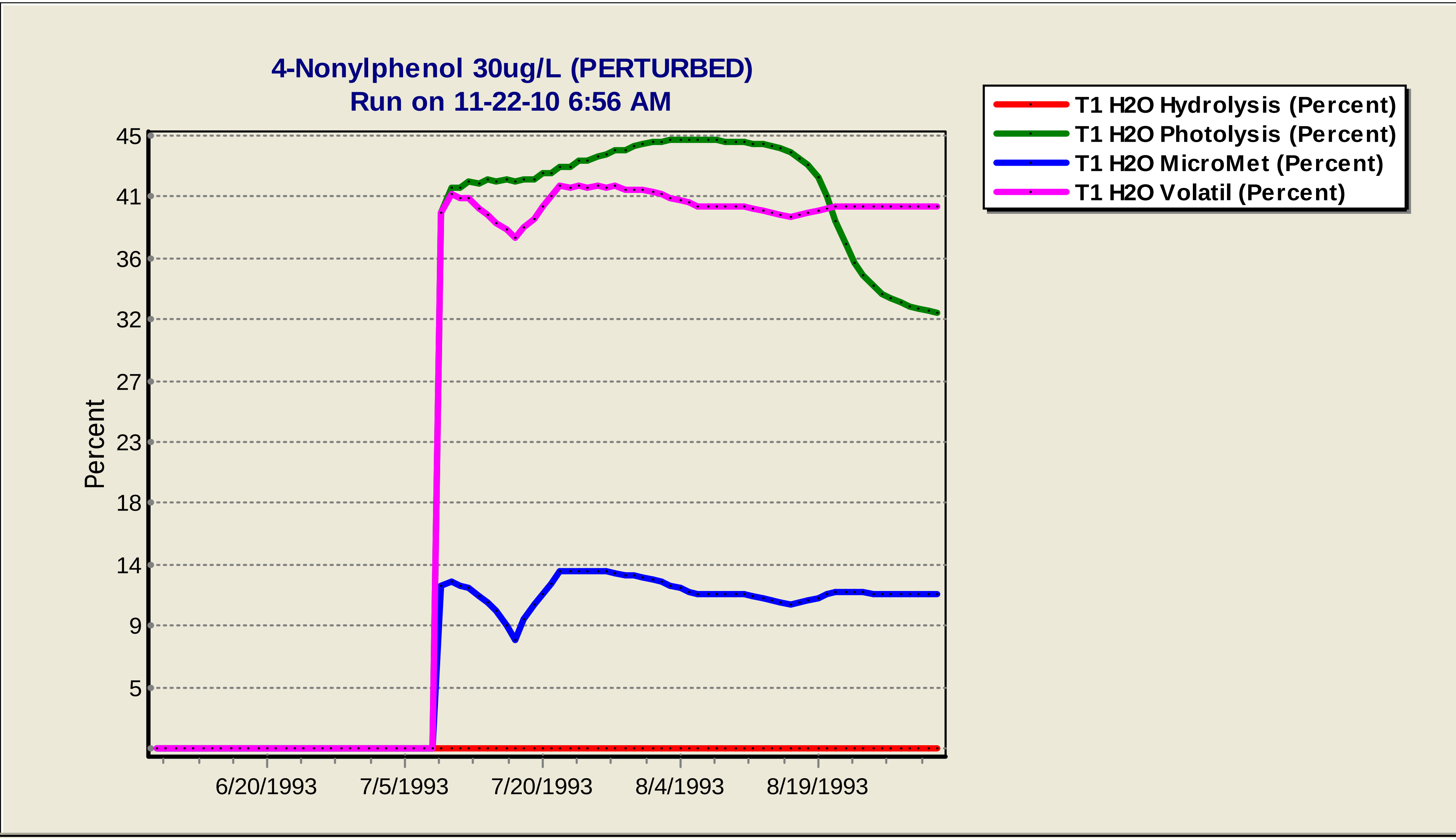


Chemical rates may be tracked

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

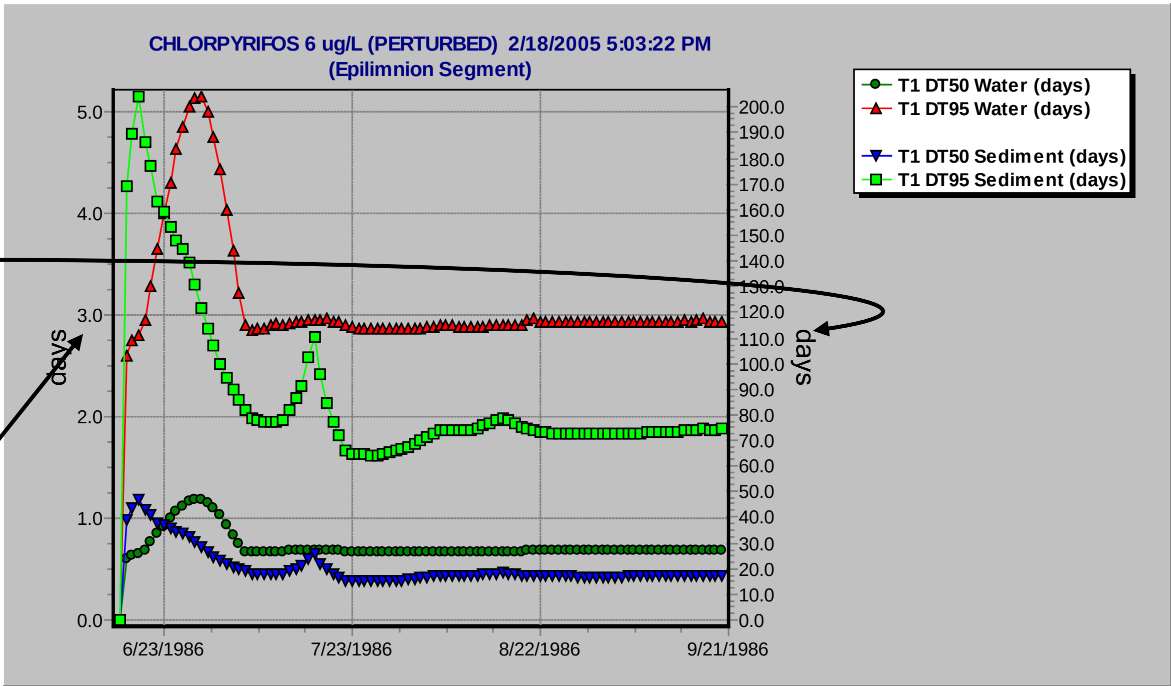
$$Loss_{Water} = \frac{Hydrolysis_{Water} + Photolysis + Microbial_{Water} + Washout + Volat. + Sorption}{Mass_{Water}}$$

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

For this Chlorpyrifos Study:

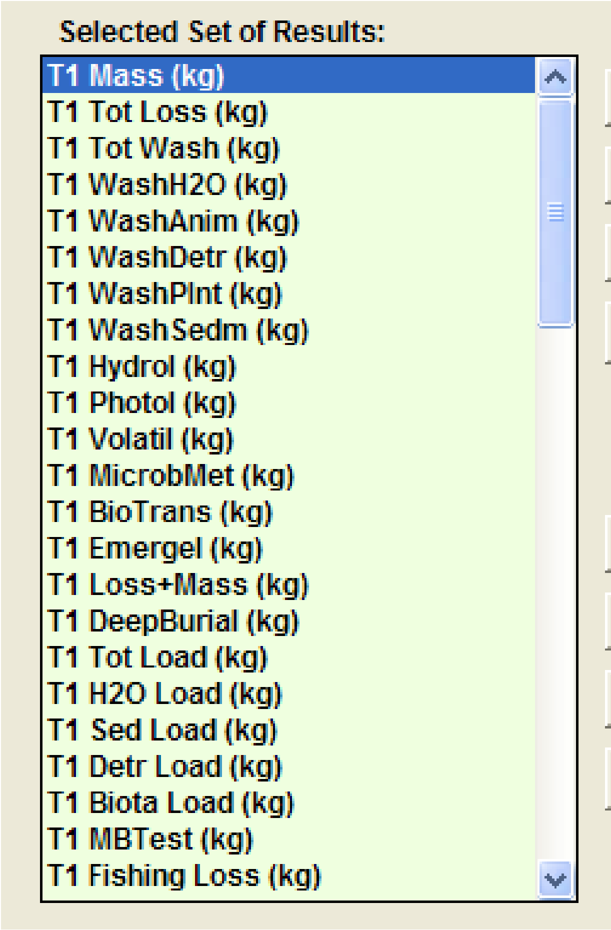
Half-life in Sediment of roughly 20 days
DT95 of roughly 75 days

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



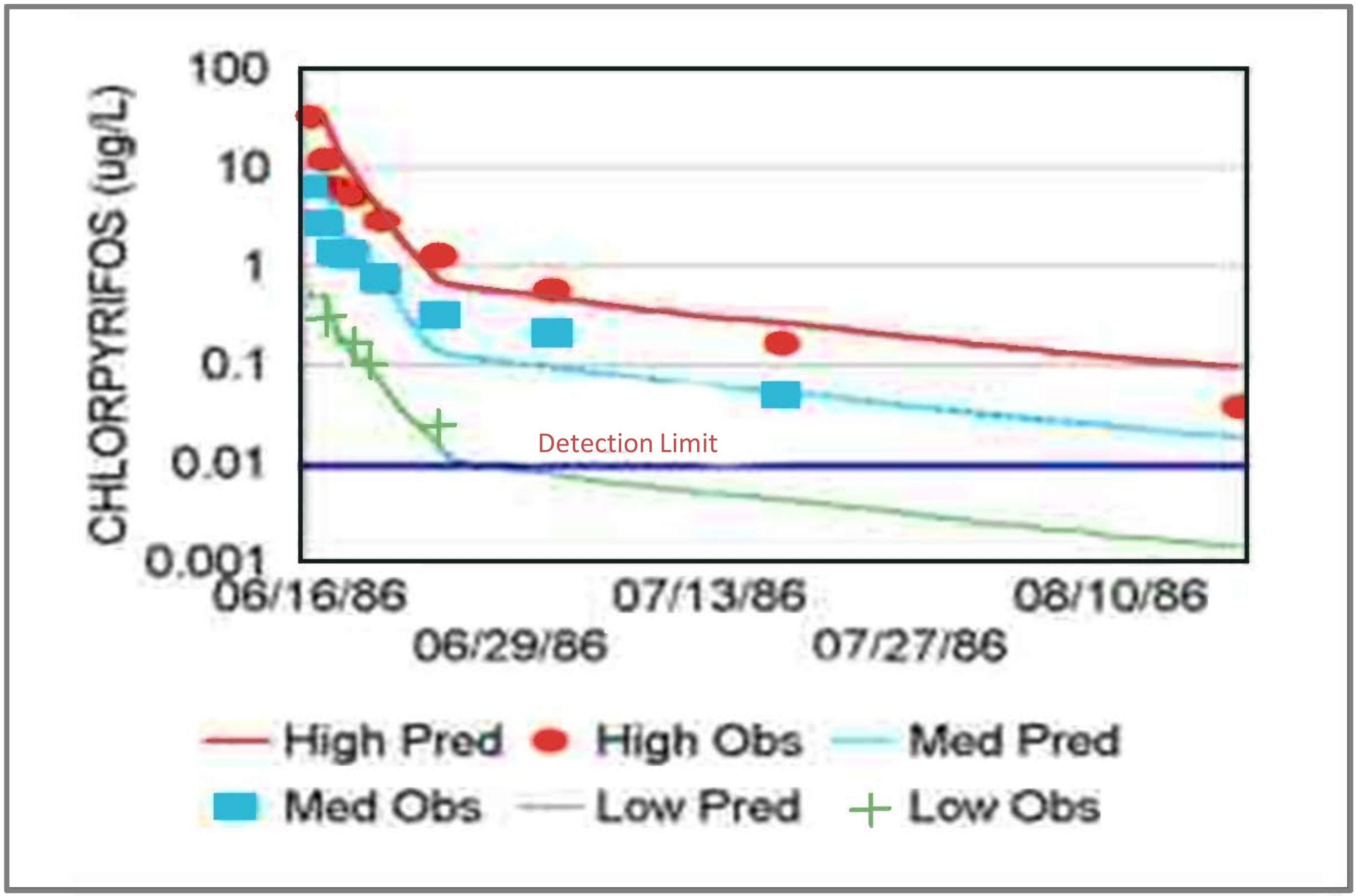
Toxicant mass balance tracking

- 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

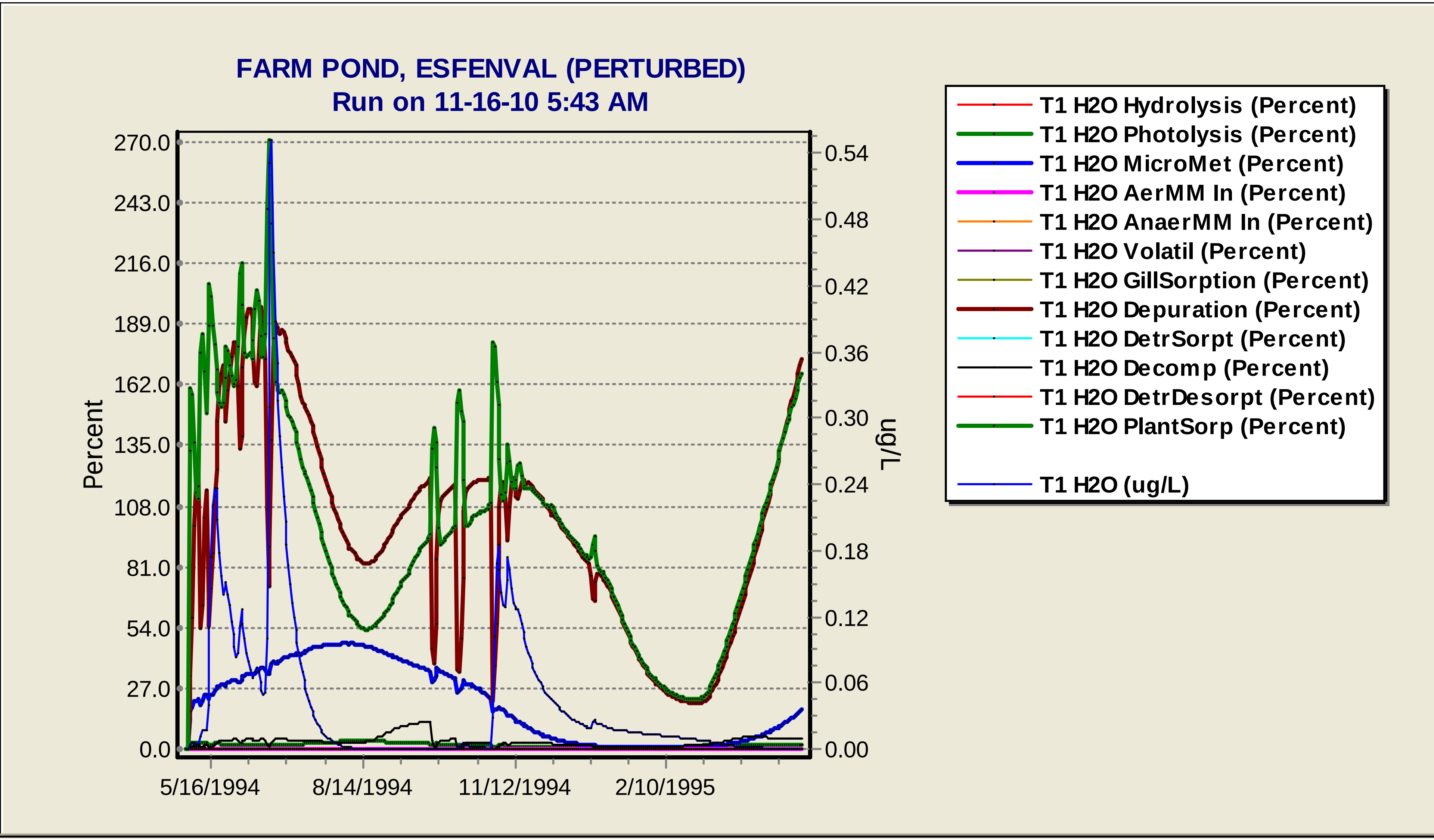


Fate of Chlorpyrifos in the Duluth MN Pond was Predicted Successfully

Multiple Dosing Levels



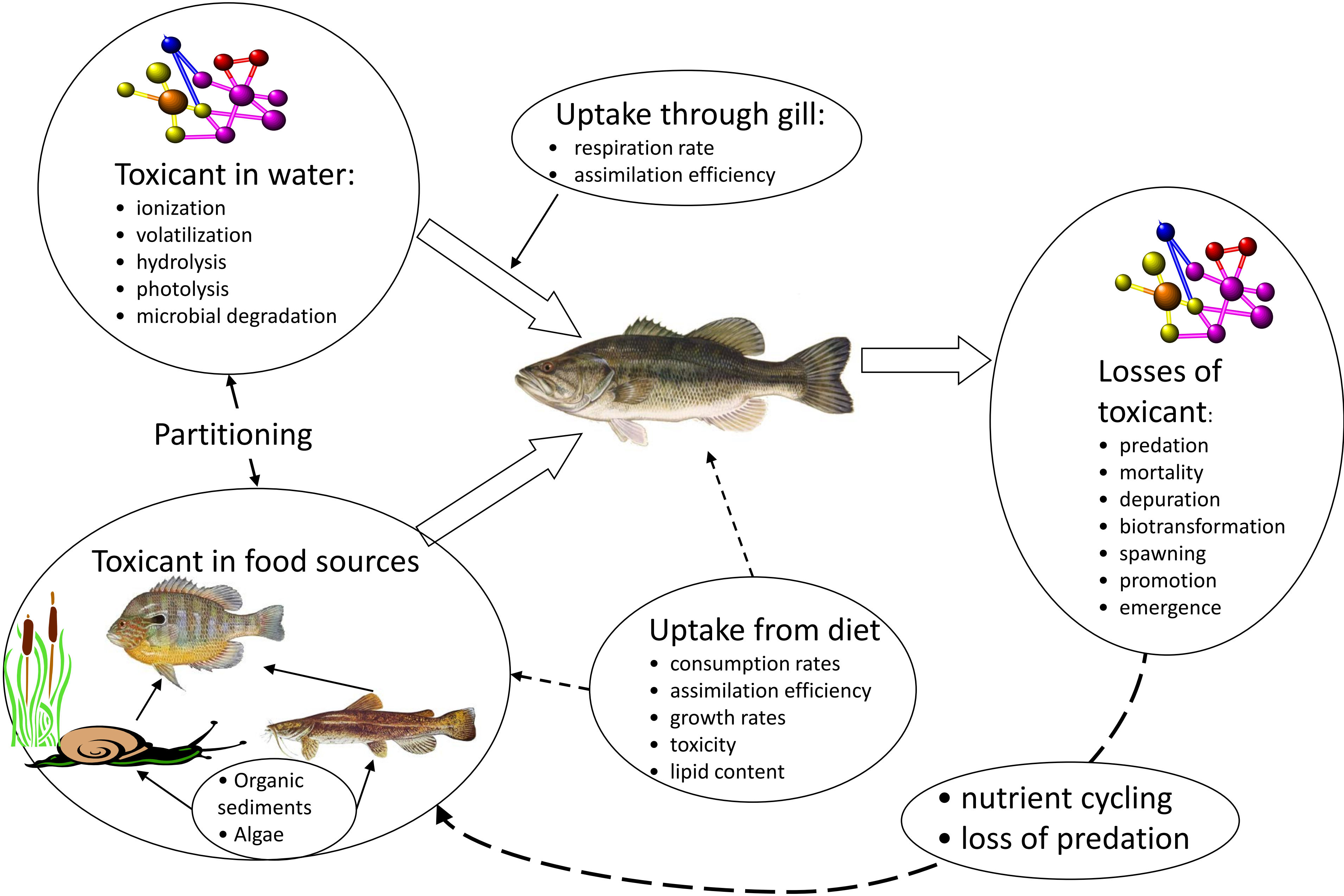
Esfenvalerate in farm pond is taken up and depurated by phytoplankton and lost by microbial degradation



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

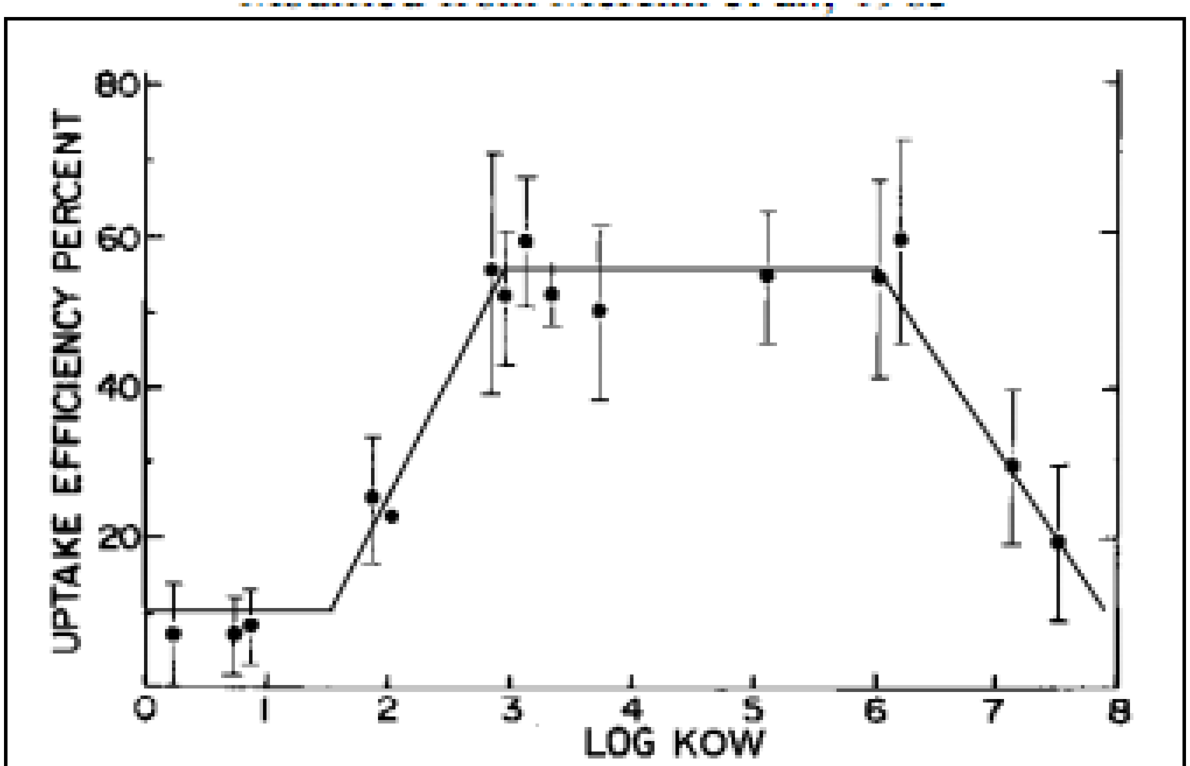
Bioaccumulation in AQUATOX



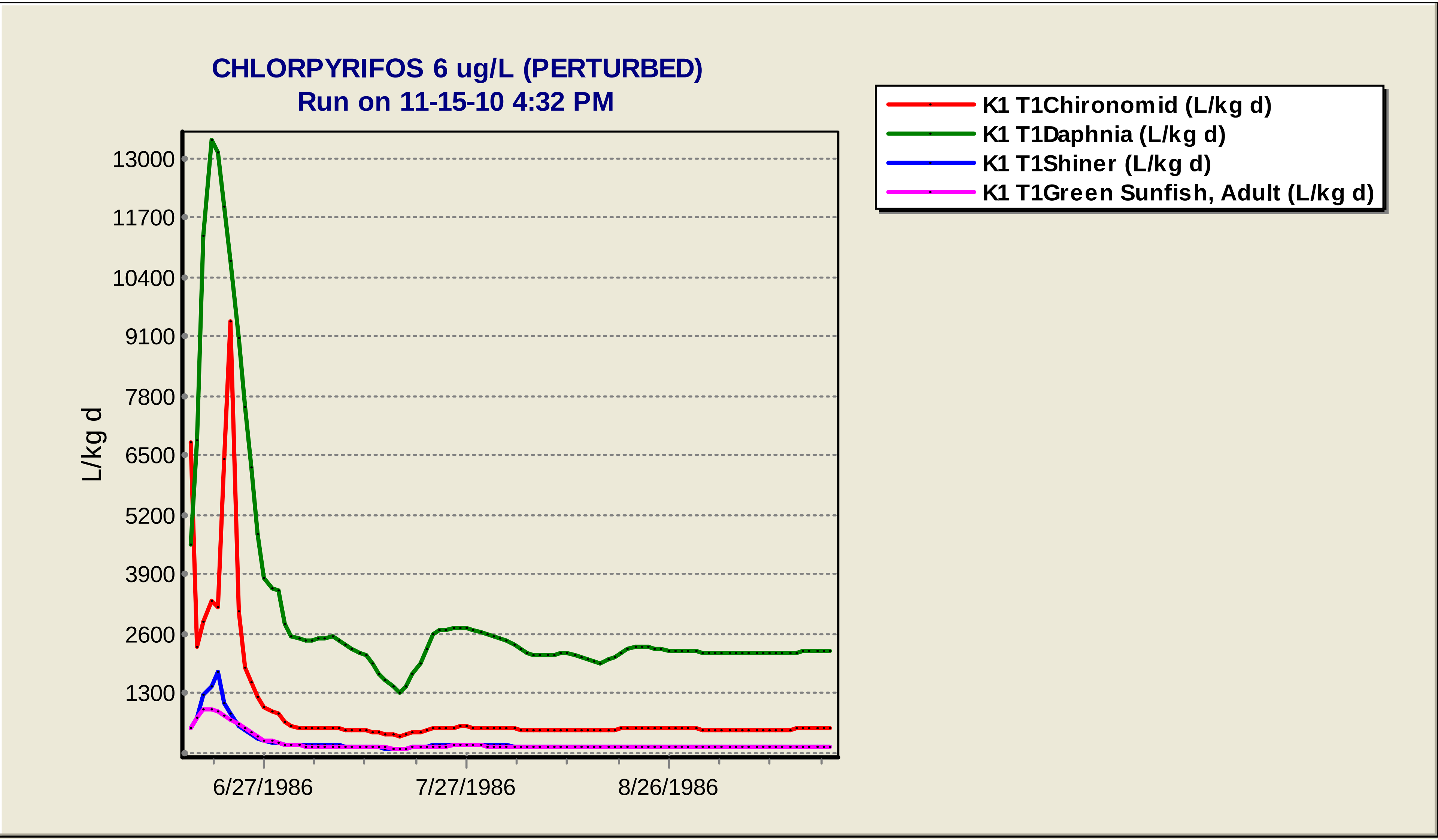
Gill Uptake is Function of Respiration and Efficiency of Toxicant Uptake

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

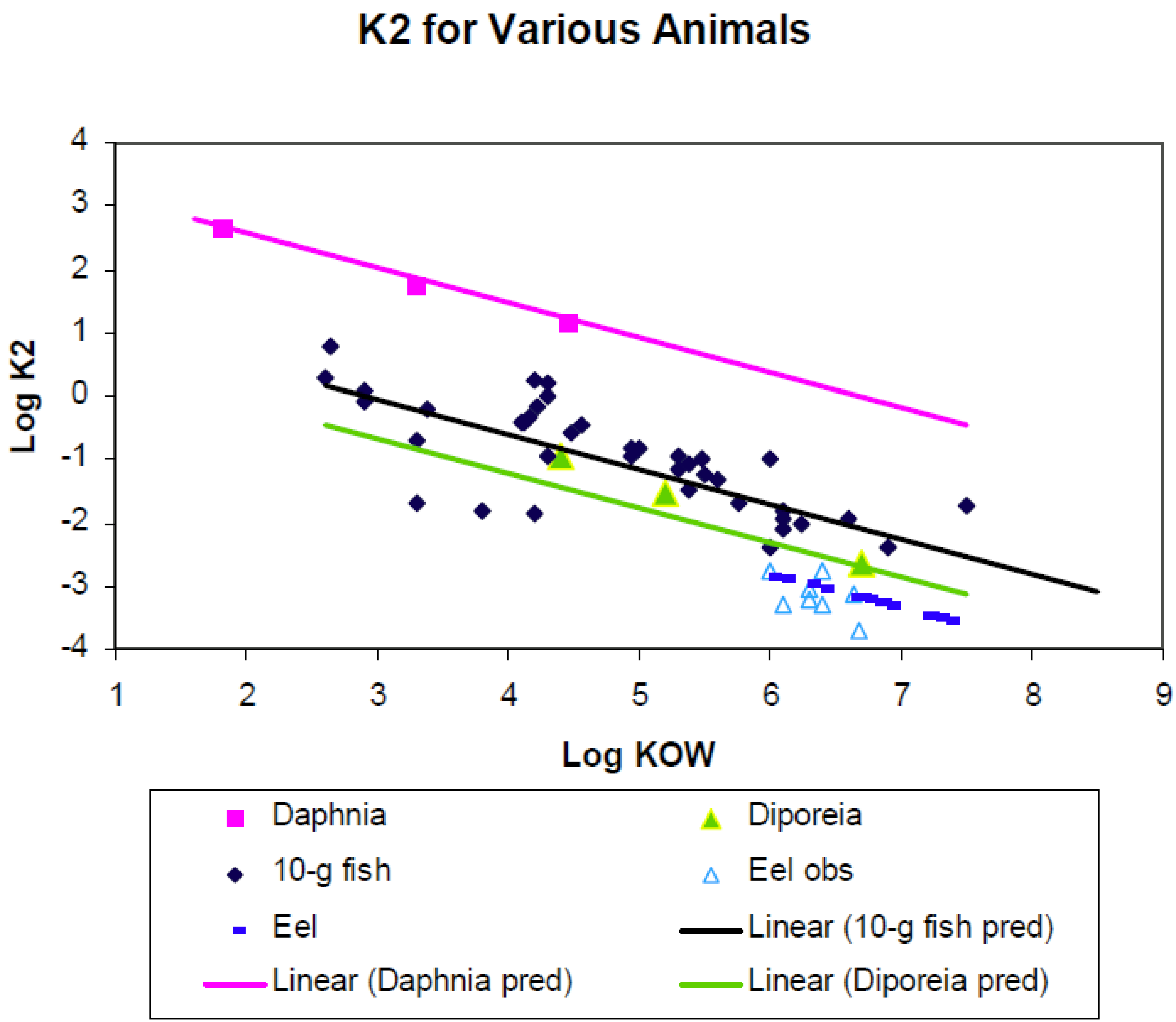
$$KUptake = \frac{WEffTox \cdot Respiration \cdot O2Biomass}{Oxygen \cdot WEffO2}$$



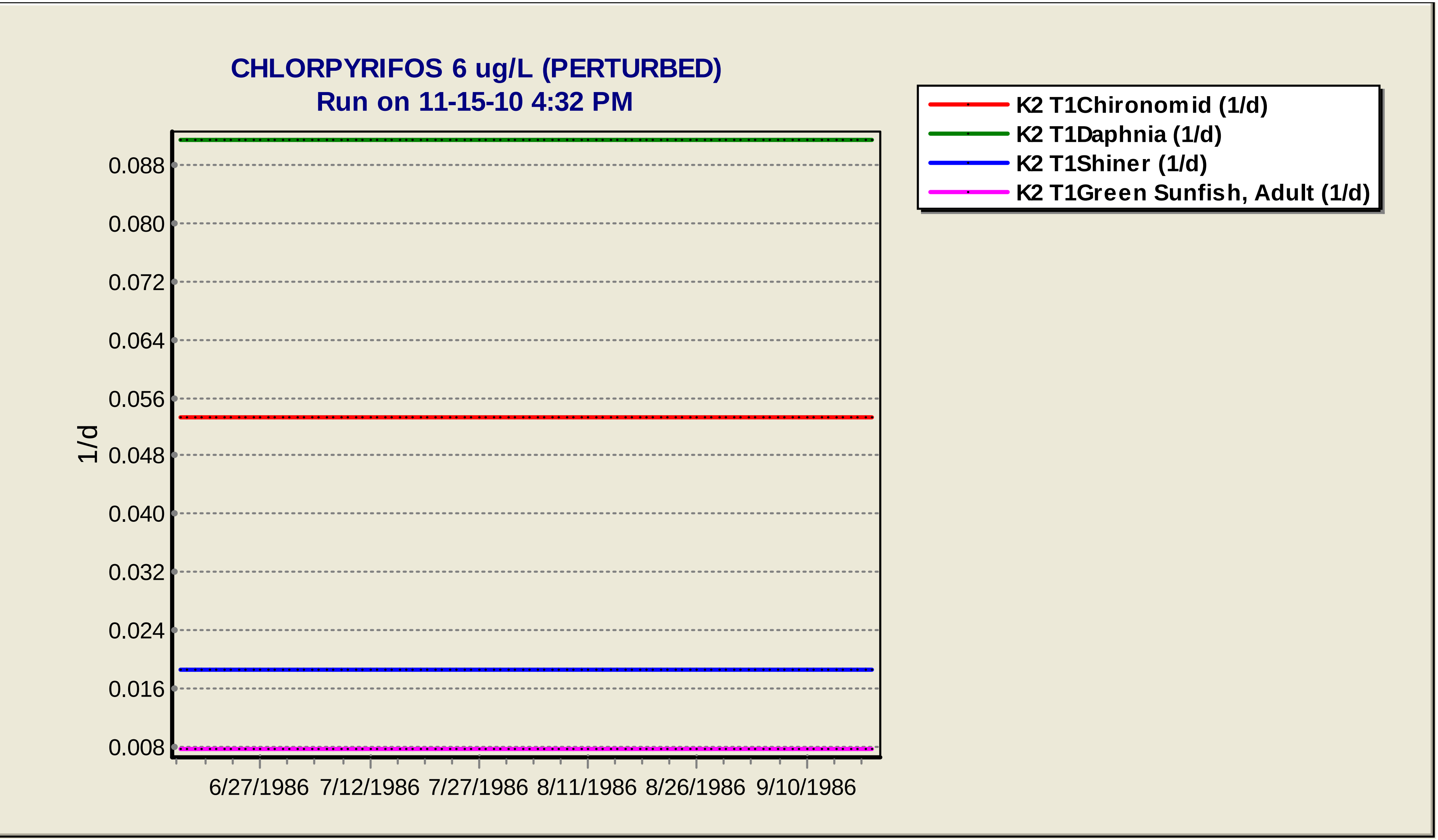
Chlorpyrifos Uptake Rates for Invertebrates and Fish in Pond



Depuration Rate Constants for Invertebrates and Fish – Default Option



Chlorpyrifos Depuration Rate Constants for Invertebrates and Fish in Pond



Alternative Chemical Uptake Model

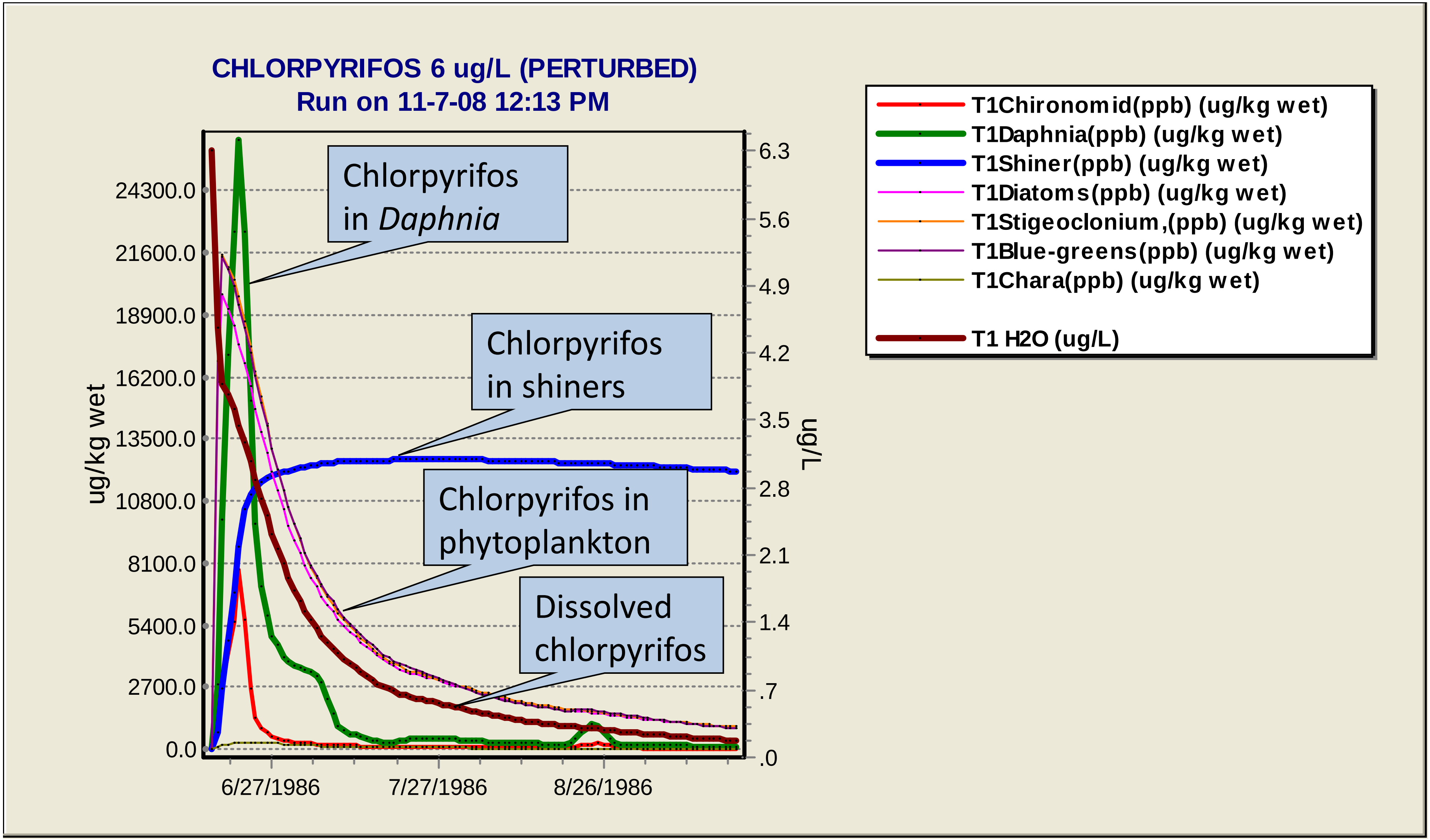
The user may enter two of the three factors defining uptake (BCF, K1, K2) and the third factor is calculated:

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

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

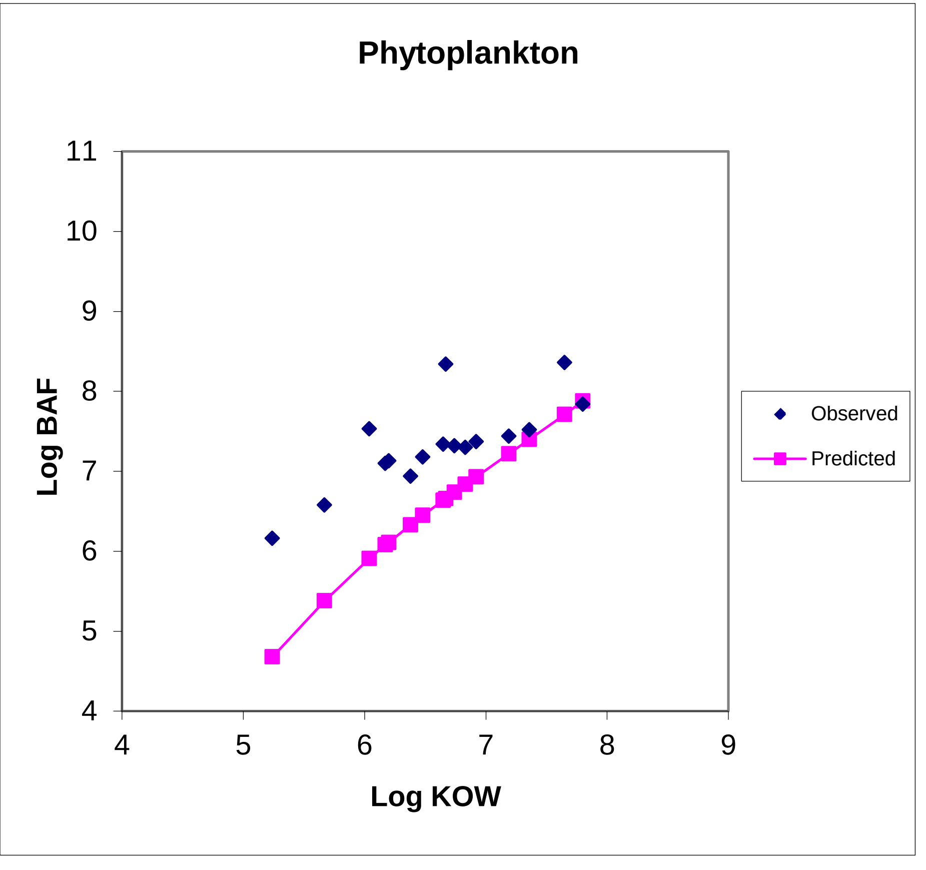
Dietary uptake of chemicals by animals is not affected by this alternative parameterization.

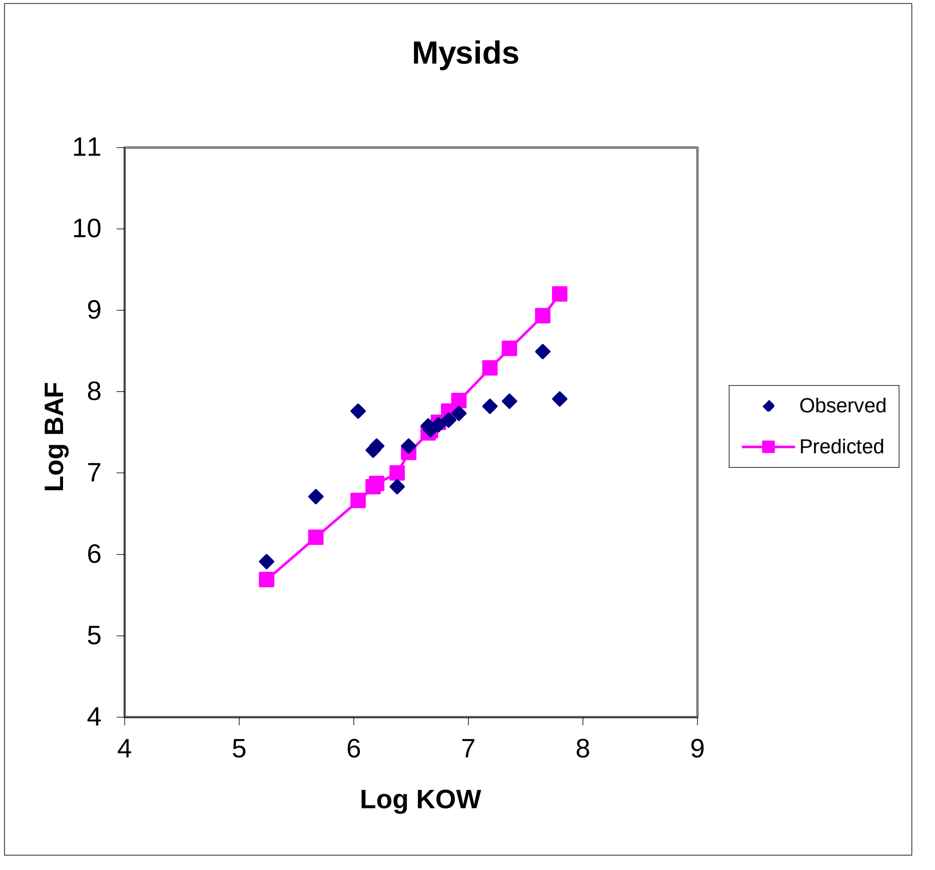
Model can trace how the toxicant is partitioned in the biota



Lake Ontario Bioaccumulation

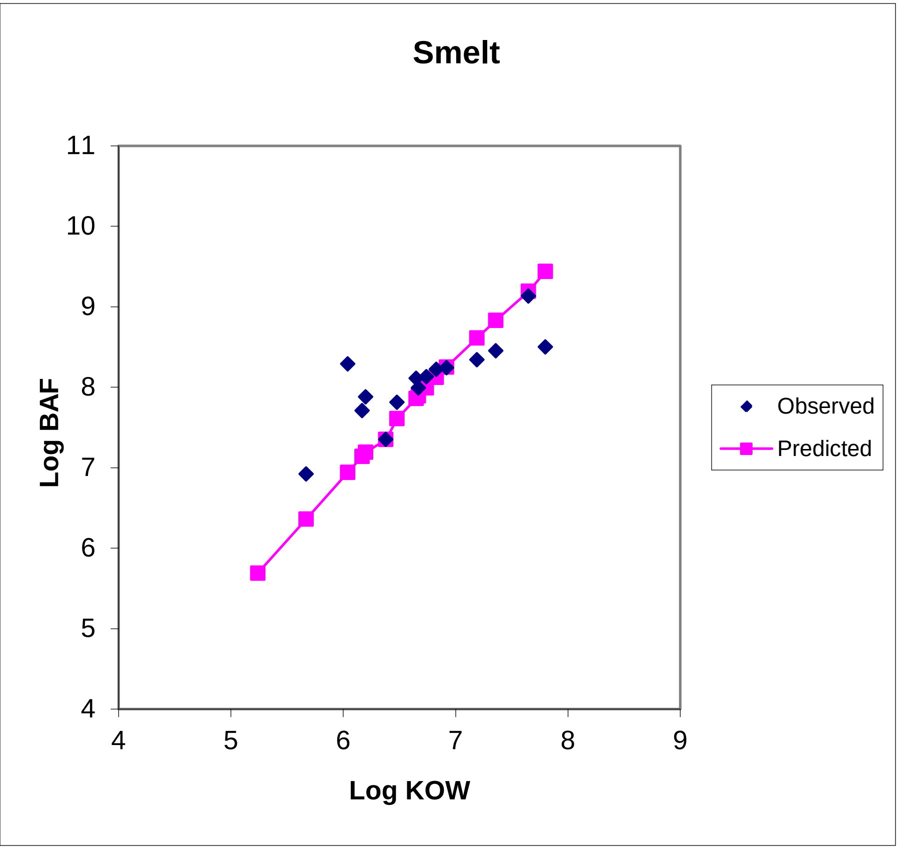
Observed and predicted lipid-normalized and freely dissolved BAFs for PCBs in Lake Ontario ecosystem components.

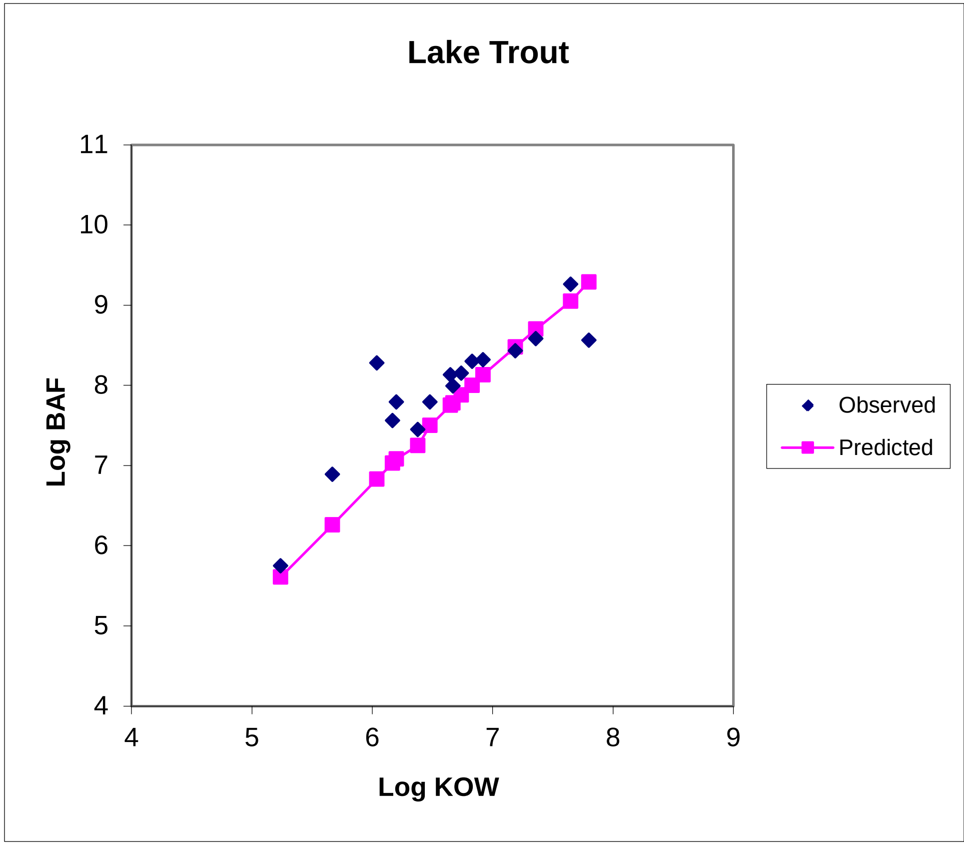




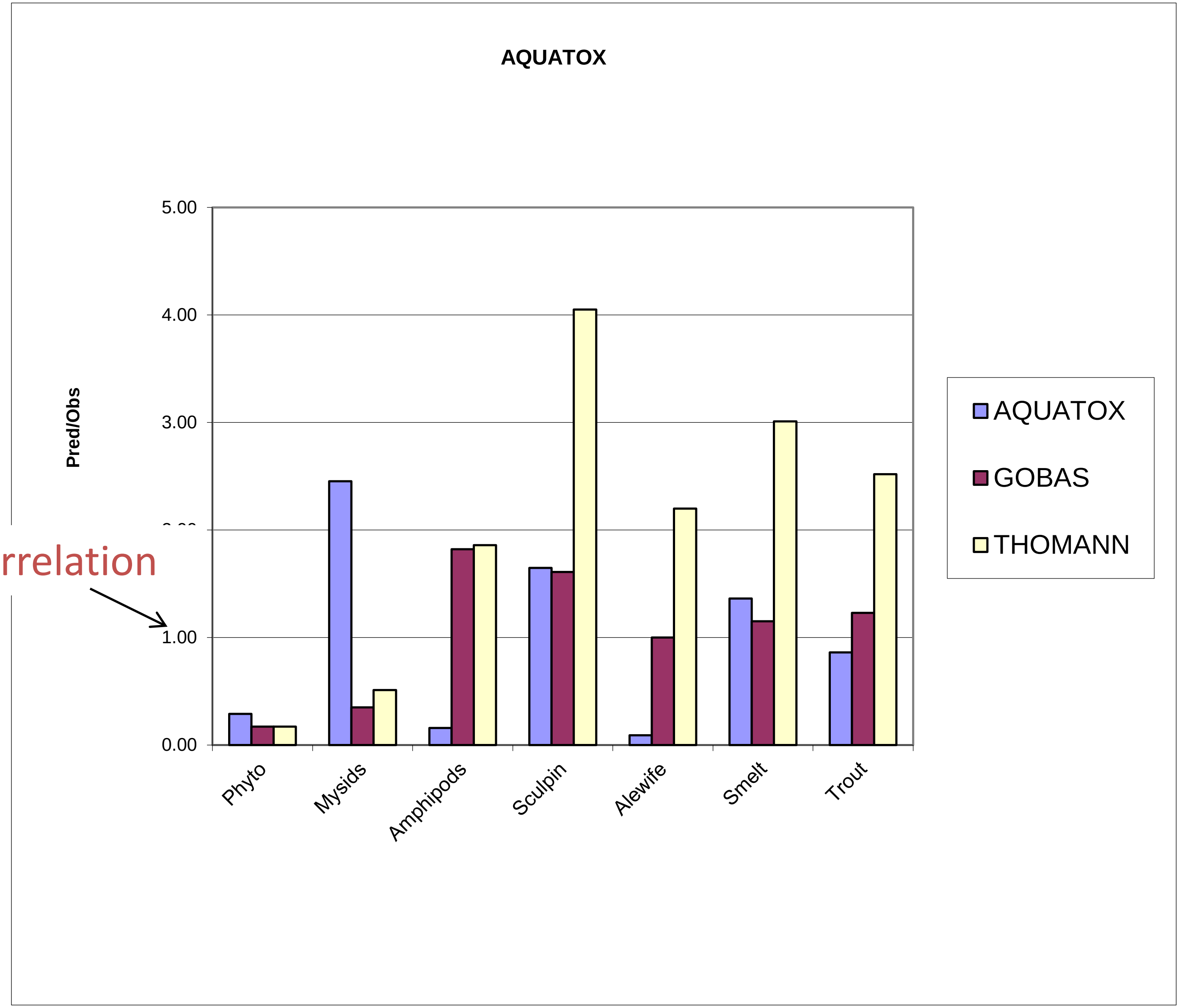
Lake Ontario Bioaccumulation

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





Lake Ontario BAF model comparison



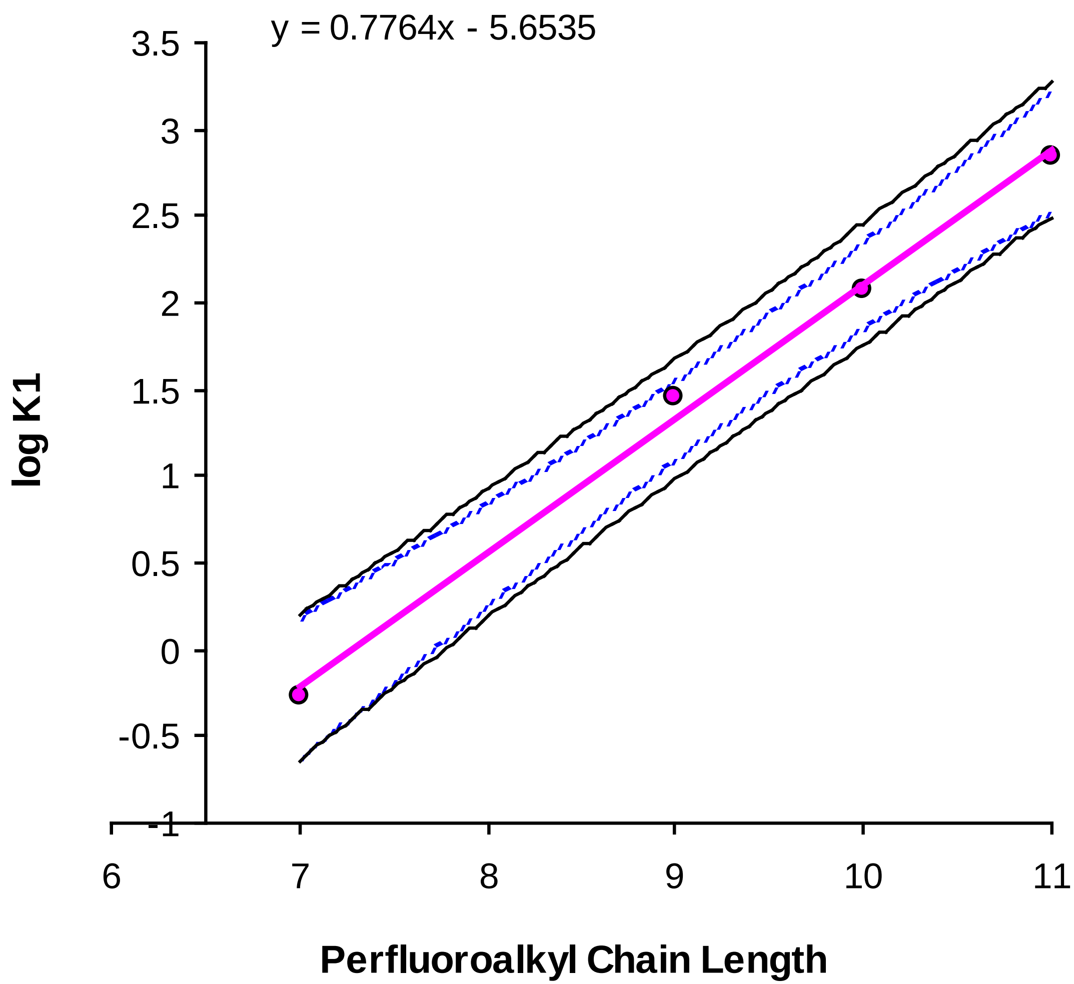
Perfect correlation

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

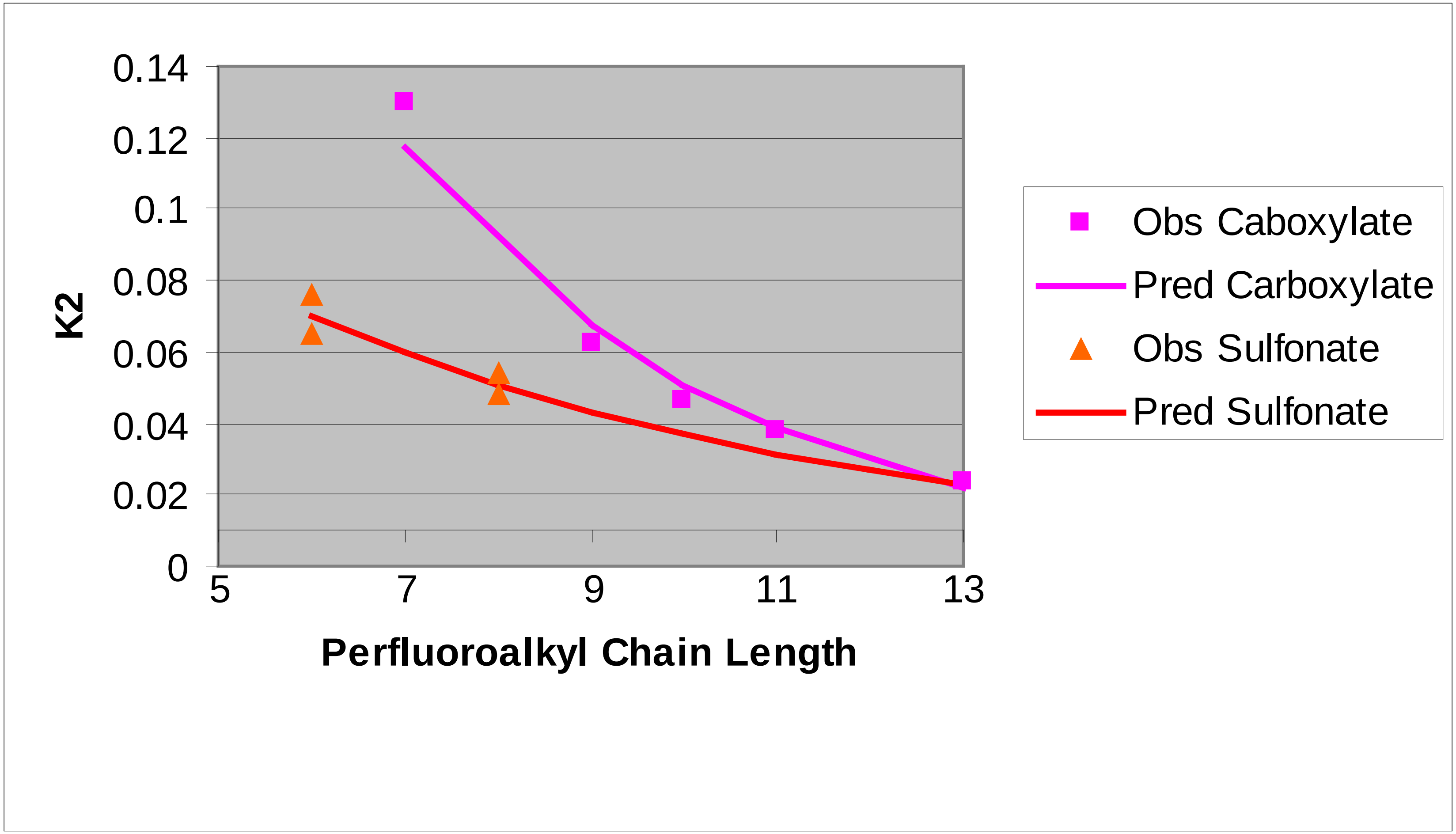
Uptake of carboxylates can be predicted by chain length

data from Martin et al., 2003



Depuration rate is also a function of chain length

data from Martin et al., 2003



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)