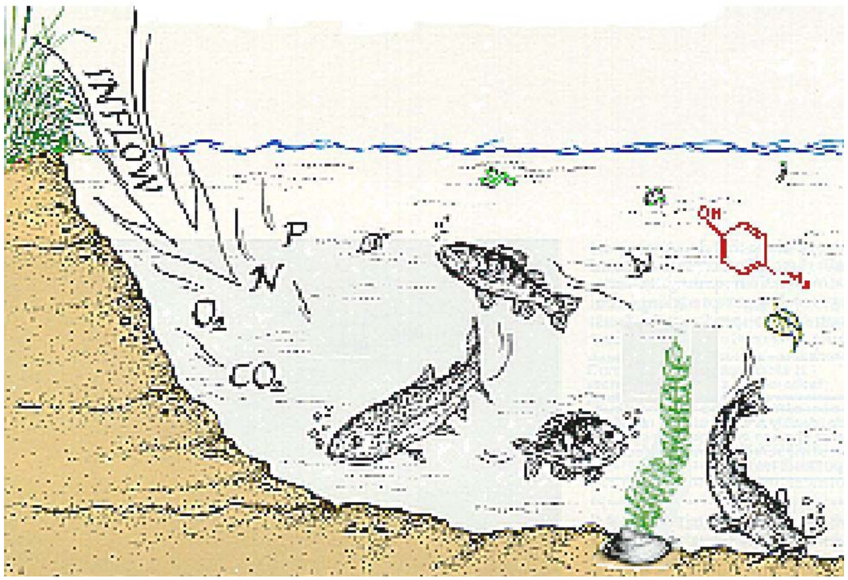
AQUATOX Training Workshop

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

Richard A. Park, Eco Modeling, Diamondhead MS
dickpark@CableOne.net
Jonathan S. Clough, Warren Pinnacle Consulting, Warren VT
jclough@warrenpinnacle.com
Marjorie Coombs Wellman, Office of Water, US EPA, Washington DC
wellman.marjorie@epamail.epa.gov

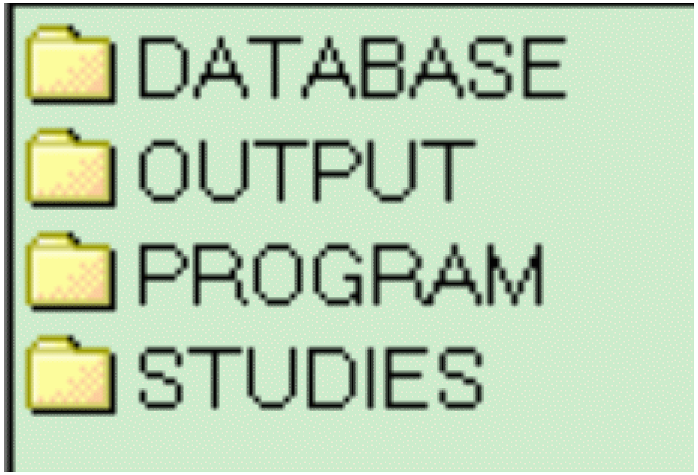


Introduction

- CD setup, installation
- Potential applications, regulatory endpoints
- Overview of AQUATOX
- Acceptance of AQUATOX
- What it does *not* do
- Structure, ecosystem primer
- State variables, processes, input requirements
- Capabilities

CD Setup: Files, Installation

- Data Folder
- Documents Folder
- Presentation Folder
- References Folder
- Reprints Folder
- AQUATOX Installation
    - » Which Installs to…



Potential Applications for AQUATOX

- Many waters are impaired biologically as well as chemically
- Managers need to know:
  - Most important stressor?
  - Implications of possible pollution control and/or restoration measures?
    - Differences in biotic communities
    - Improved water quality
  - Unintended consequences?
  - Recovery time?
  - Uncertainty around predictions?
- Science vs policy decisions

Regulatory Endpoints Modeled

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

Potential Applications
nutrients

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

Potential Applications of AQUATOX
toxic substances

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

Potential Applications
aquatic life support

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

Overview: What is AQUATOX?

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

Acceptance of AQUATOX

- Has gone through 2 EPA-sponsored peer reviews (following quotes from 2008 review):
  - “model enhancements have made AQUATOX one of the most exciting tools in aquatic ecosystem management”
  - “this is the first model that provides a reasonable interface for scientists to explore ecosystem level effects from multiple stressors over time”
  - “the integration of ICE data into AQUATOX makes this model one of the most comprehensive aquatic ecotoxicology programs available”
  - it “would make a wonderful textbook for an ecotoxicology class”
- Is gradually appearing in open literature

Comparison of Dynamic Risk Assessment Models

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

Comparison of Bioaccumulation Models: Biotic State Variables

Table 3.2. Comparison of Bioaccumulation State Variables

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

Imhoff et al. 2005

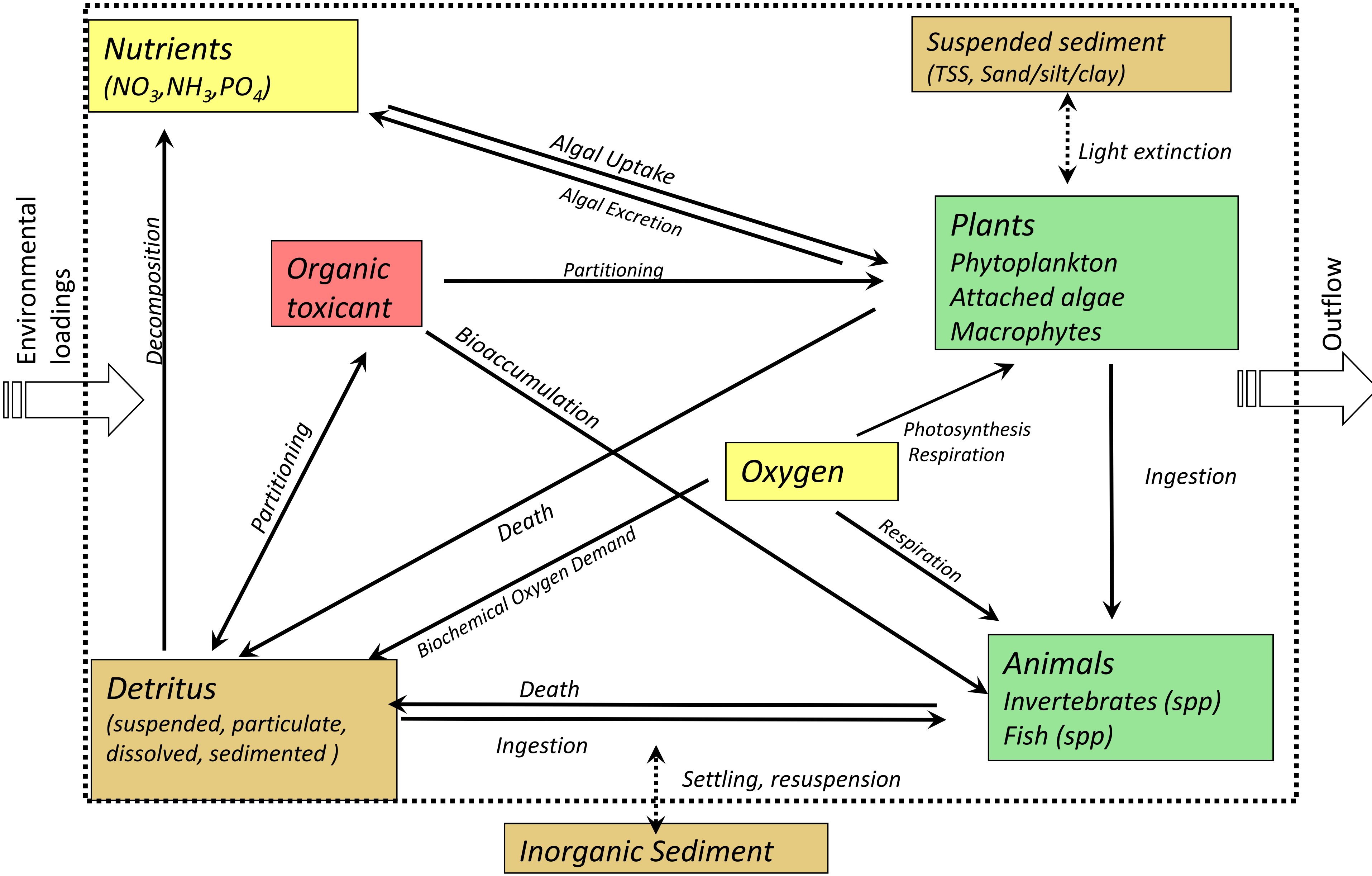
What AQUATOX does *not* do

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

AQUATOX Structure

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

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



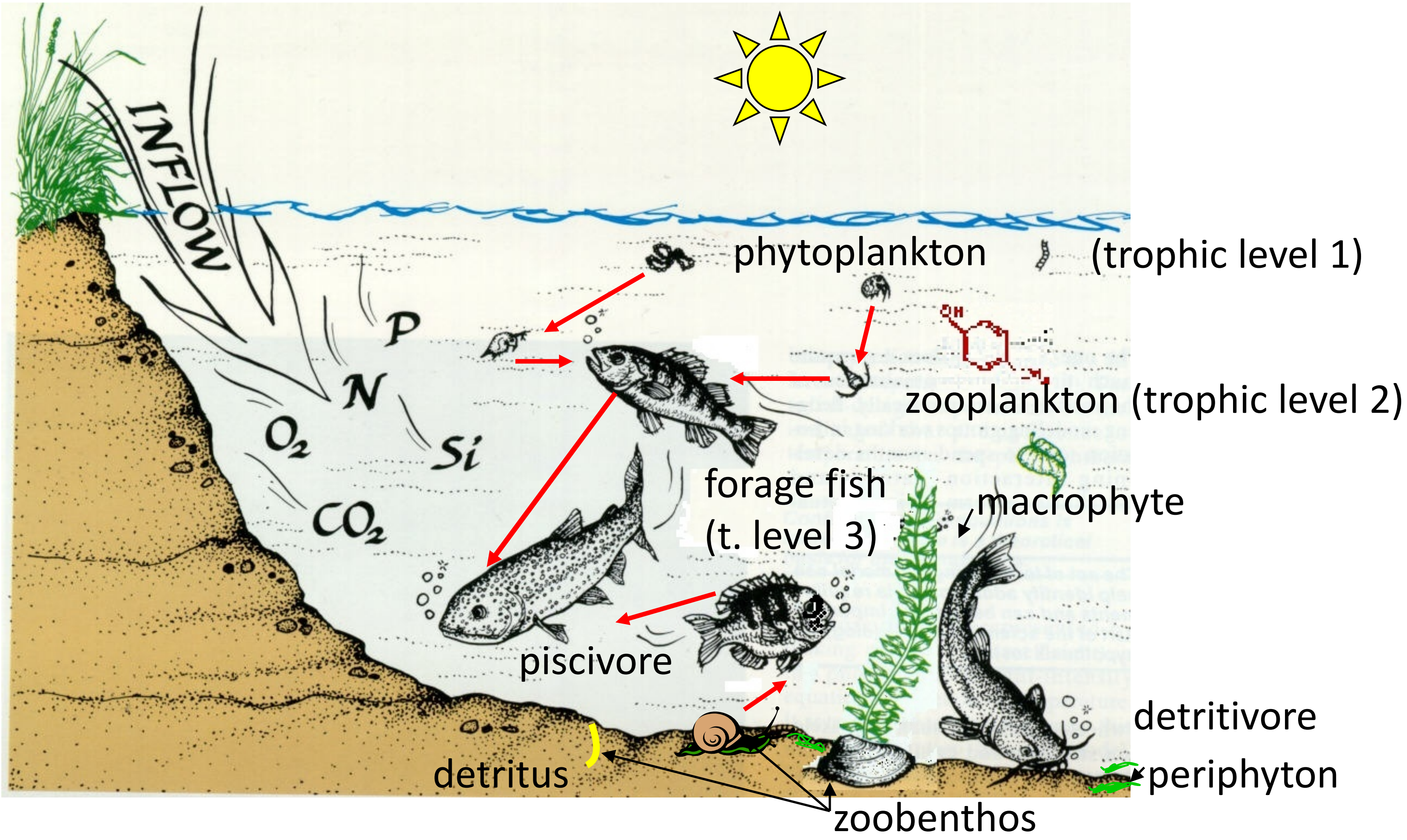
Processes Simulated

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

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

- Environmental effects
  - direct & indirect

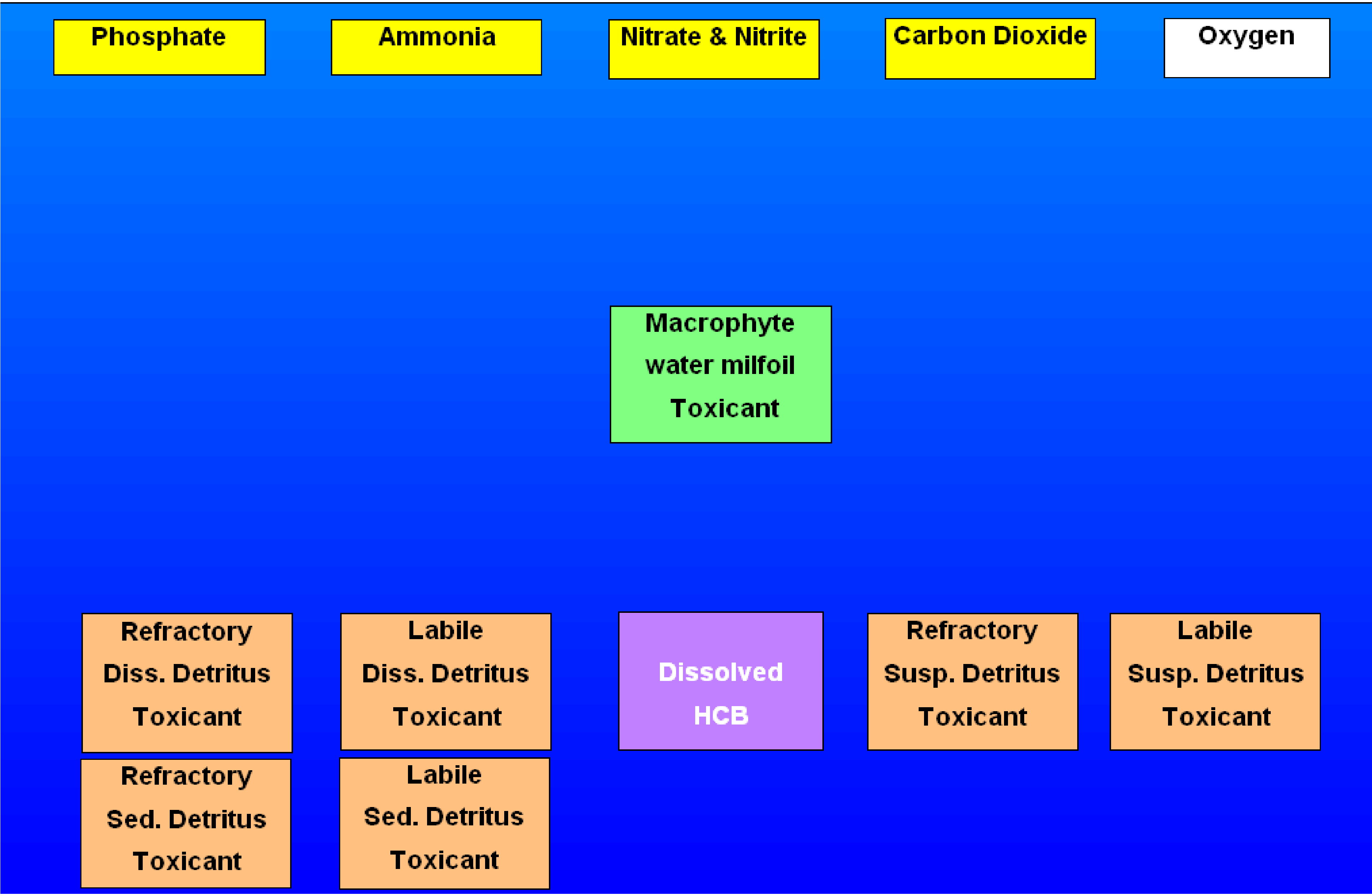
Ecosystem components



State Variables in Coralville, Iowa, Study

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

State Variables in Experimental Tank



Global vs. Site-Specific Input Requirements

Many model inputs are required on a site-by-site basis:

nutrient loadings
organics, sediment loadings
water volume setup
animal, plant initial conditions (often defaults with “spin-up”)
site characteristics
chemical loadings
temperature, pH

Many parameters may be assumed to be global parameters, i.e. no adjustment is required from site-to-site:

most animal, plant parameters
“remineralization” parameters
chemical parameters
chemical toxicity parameters

AQUATOX Capabilities

(Release 3 in red)

- Ponds, lakes, reservoirs, streams, rivers, estuaries
- Riffle, run, and pool habitats for streams
- Completely mixed, thermal stratification, or salinity stratification
- Linked segments, tributary inputs
- Multiple sediment layers with pore waters
- Sediment Diagenesis Model
- Diel oxygen and low oxygen effects, ammonia toxicity
- Interspecies Correlation Estimation (ICE) toxicity database
- Variable stoichiometry, nutrient mass balance, TN & TP
- Dynamic pH
- Biota represented by guilds, key species
- Constant or variable loads
- Latin hypercube uncertainty, nominal range sensitivity analysis
- Wizard & help files, multiple windows, task bar
- Links to HSPF and SWAT in BASINS

Release 3.1

- 64-bit-compatible software installer
- Updated Interspecies Correlation Estimation toxicity regressions
- Improved uncertainty & sensitivity output
- Additional outputs for diagenesis & bioaccumulation
- Improved database export & search capabilities
- More flexible linkage to HSPF watershed model
- Addition of sediment-diagenesis “steady-state” mode to significantly increase model speed
- Modification of denitrification code in goal of simplifying calibration and alignment with other models;
- Enabled importation of equilibrium CO2 concentrations to enable linkage to CO2SYS and similar models;
- New BOD to organic matter conversion relying on percent-refractory detritus input

Download available at EPA AQUATOX page

Lab 1: A Tour Through the AQUATOX Screens

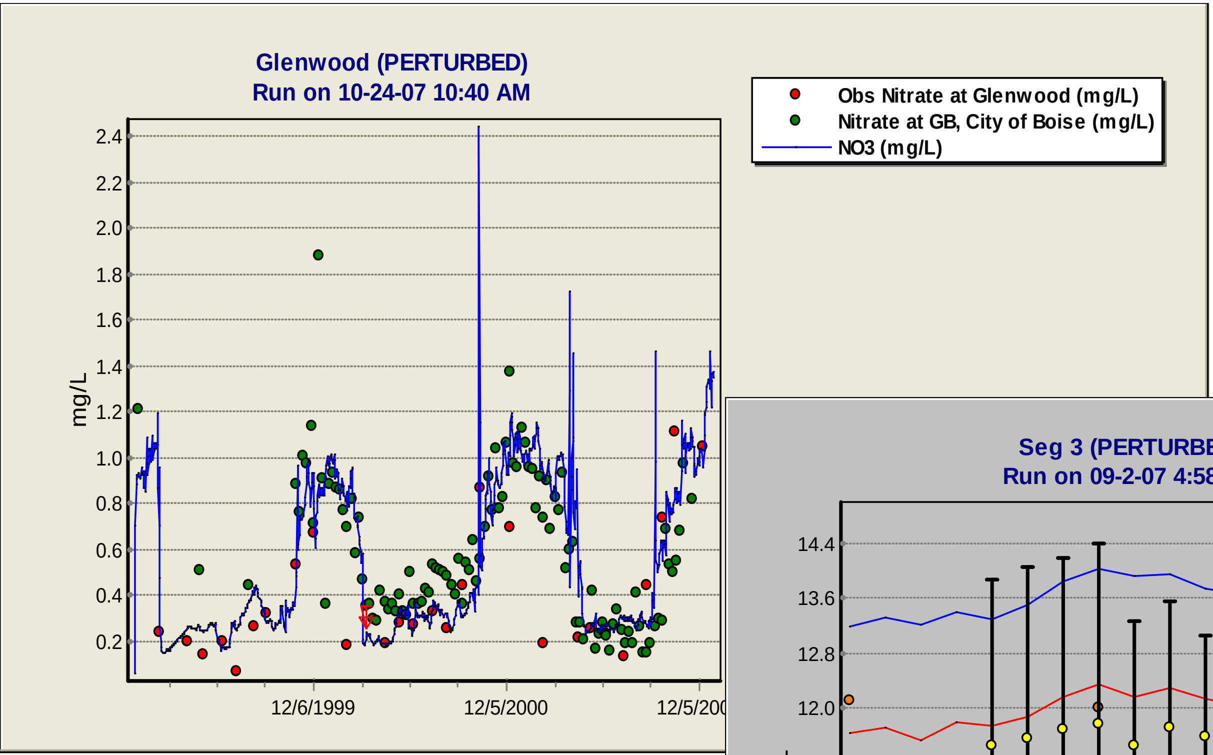
- ❑ Main Screen
- ❑ Toolbar
- ❑ Simulation Window
- ❑ Initial Conditions
- ❑ Chemical Screen
- ❑ Site Screen
- ❑ Stream Data
- ❑ Remineralization Data
- ❑ Setup Screen
- ❑ Rates Screen
- ❑ Libraries
- ❑ Uncertainty Screen
- ❑ Output Setup
- ❑ Control Setup Screen
- ❑ Help File
- ❑ Wizard
- ❑ Run Buttons
- ❑ Export of Results
- ❑ State Variable List (Chemicals, Nutrients, Organics, Plants, Animals, etc.)

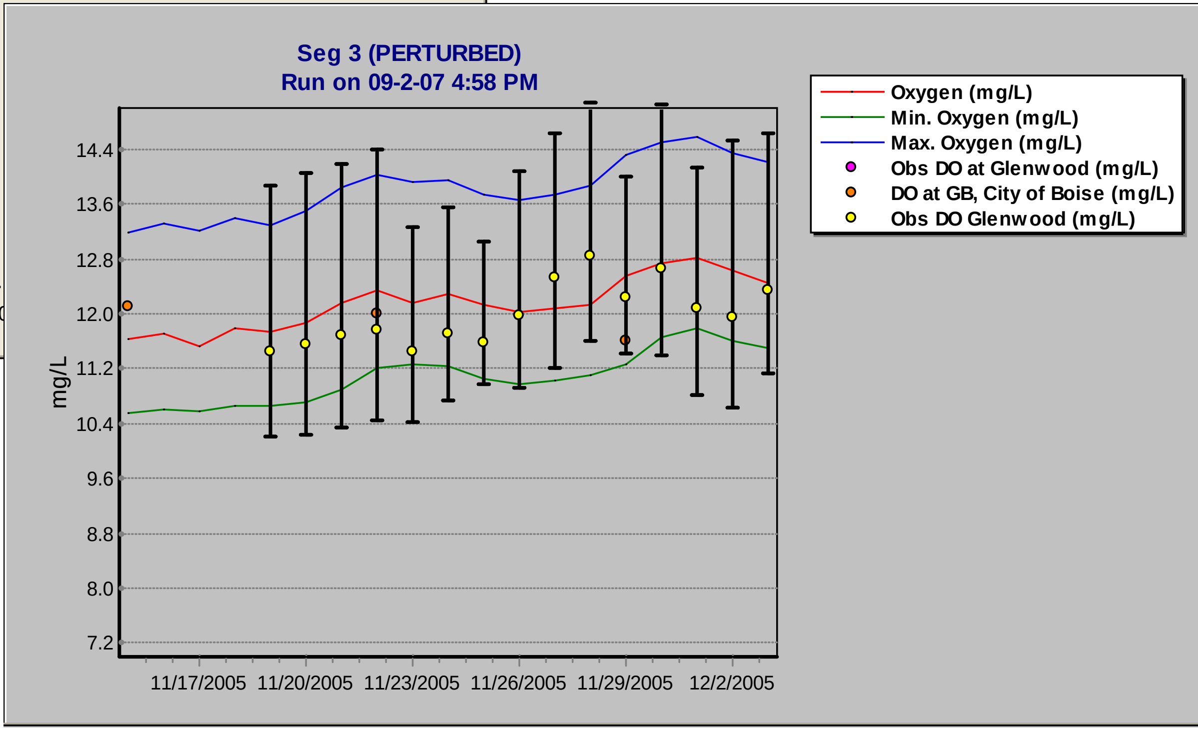
What are the Analytical Capabilities?

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

Graphical Analysis

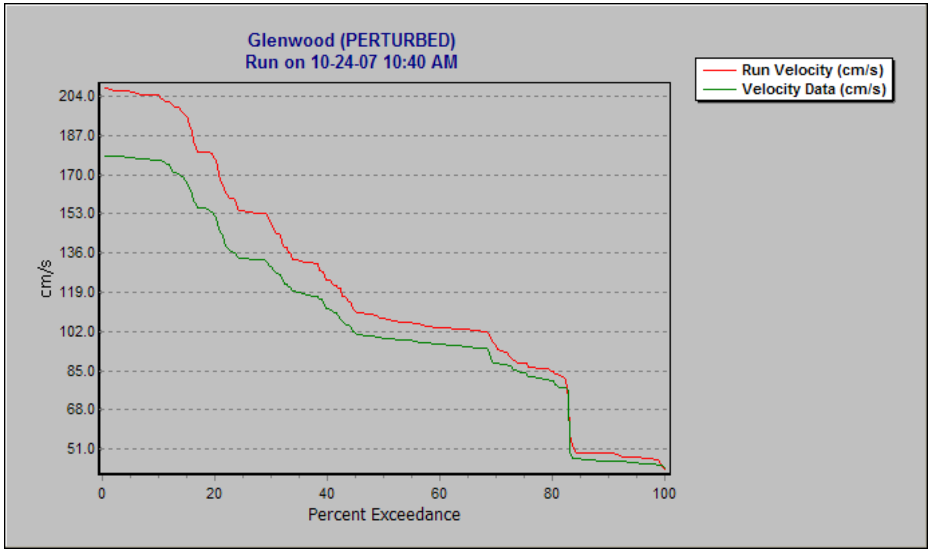
Compare observed data to model output

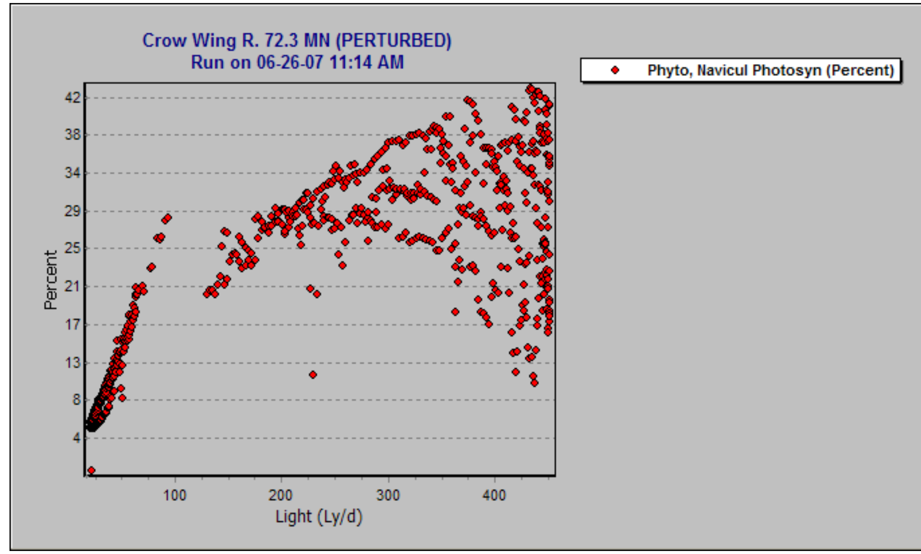




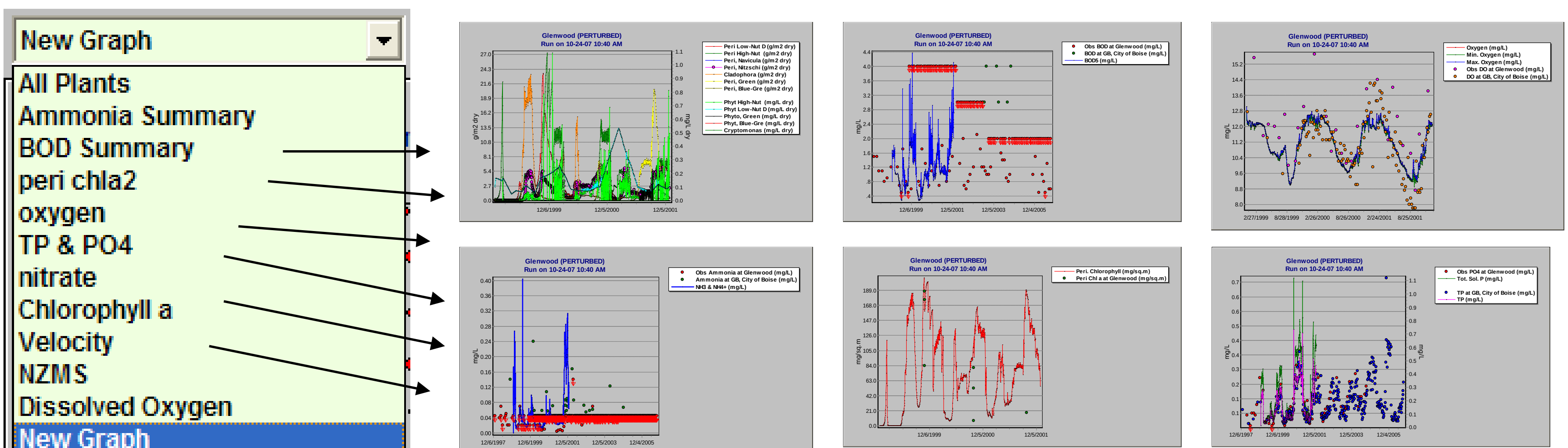
Graphical Analysis

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





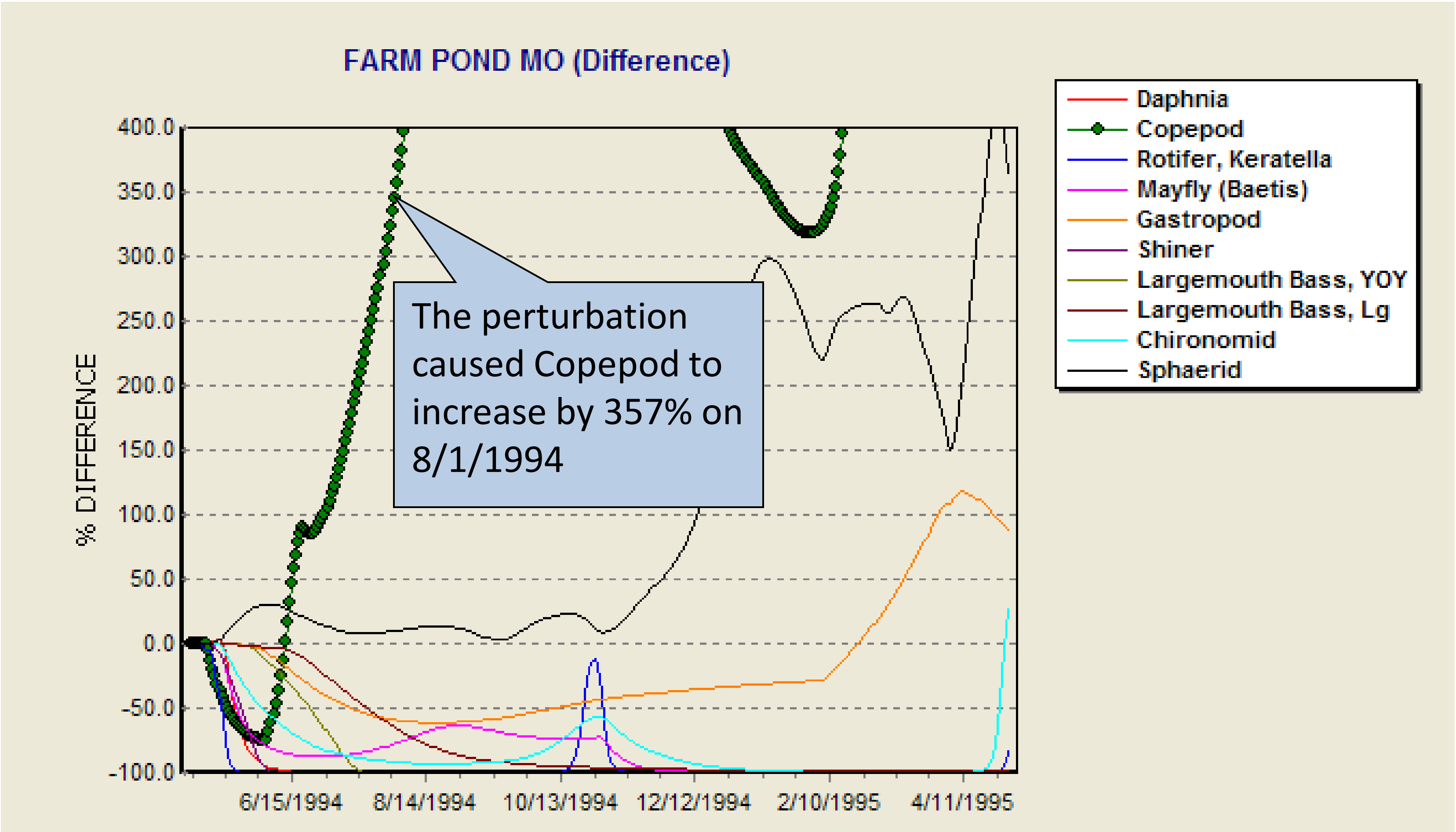
Graph Library saved within simulation



Comparing Scenarios: the "Difference" Graph

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

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



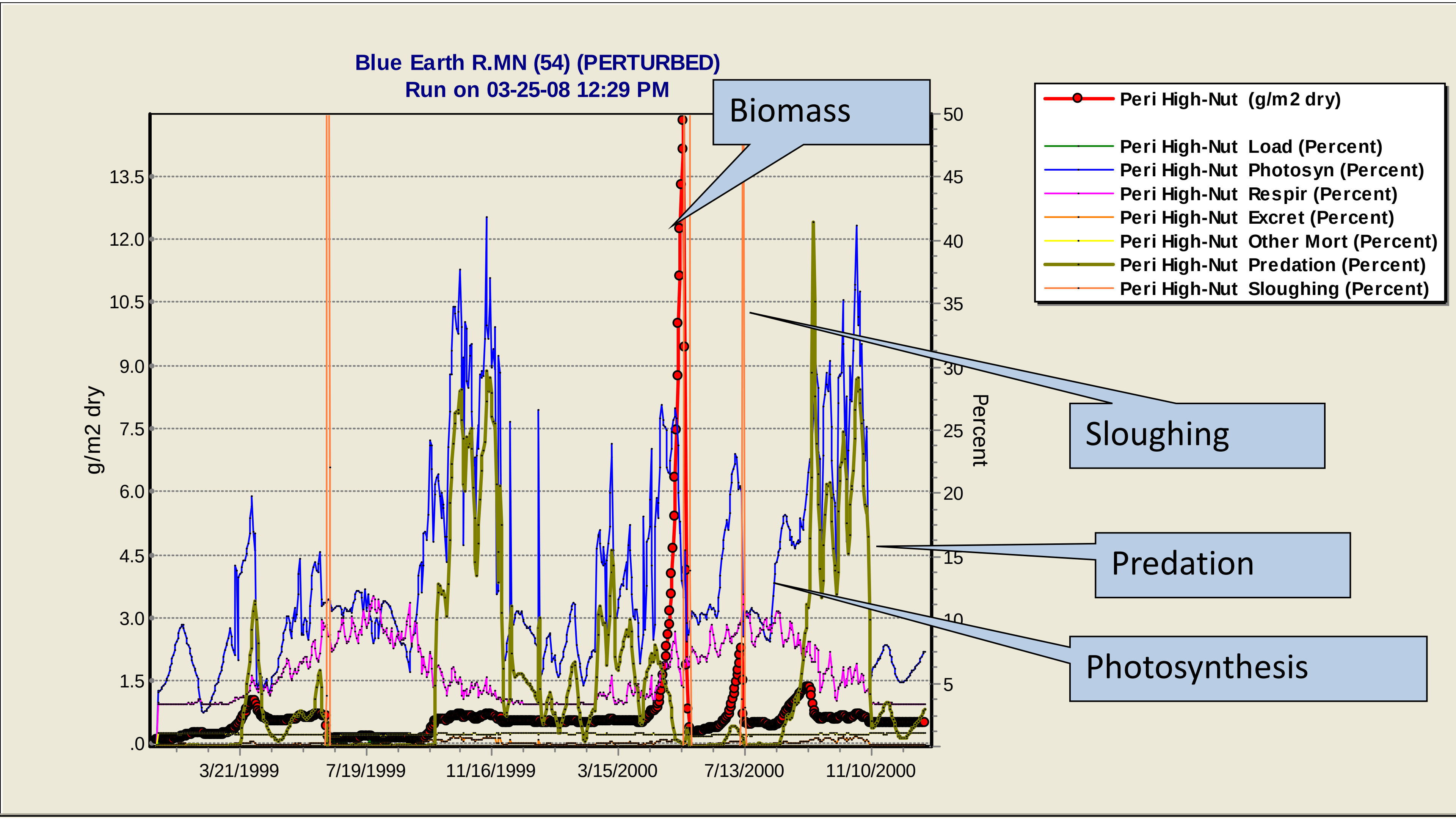
Process Rates

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

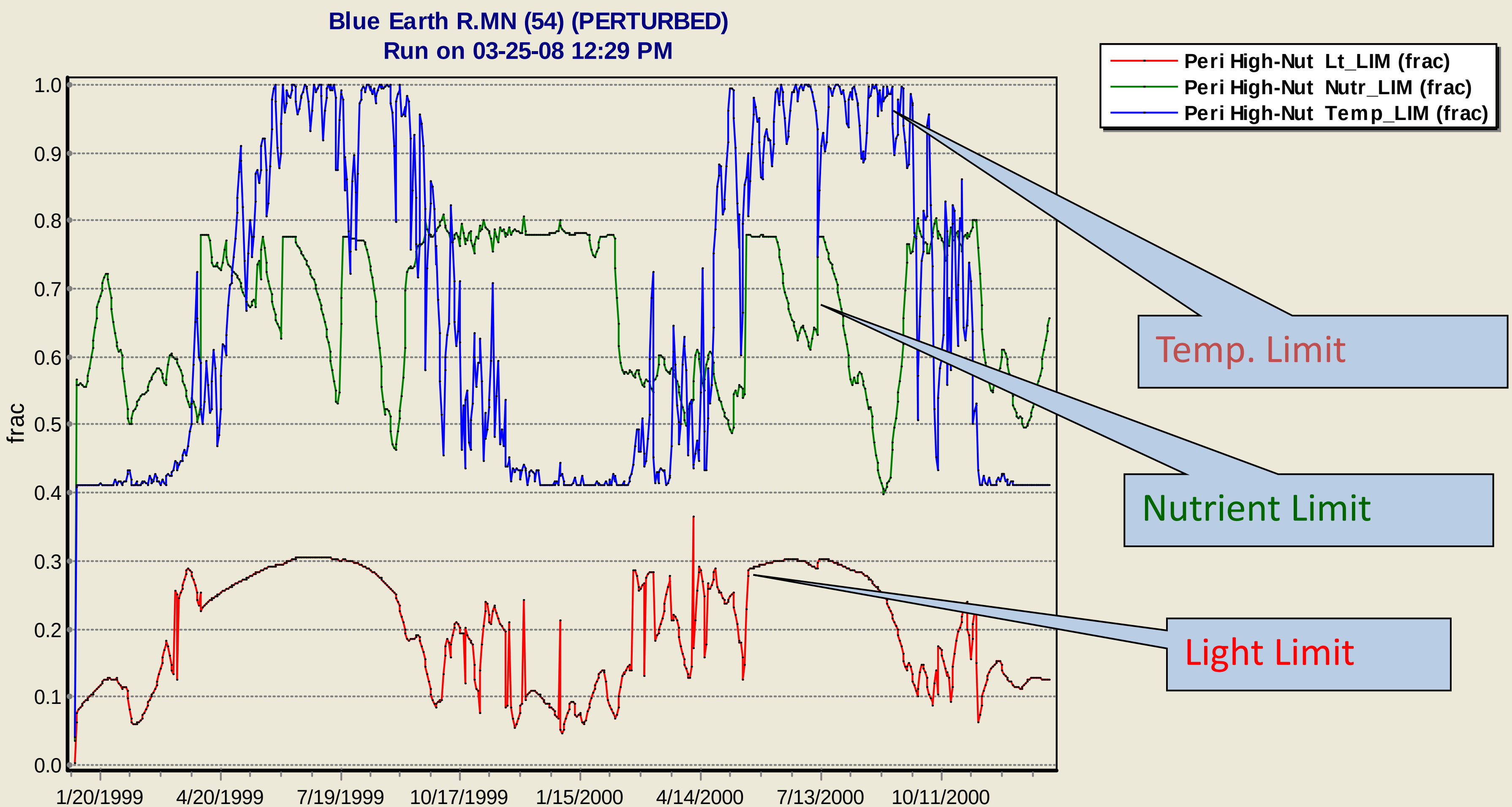
$$\frac{dBiomass_{Peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion$$
$$- Mortality - Predation + Sed_{Peri}$$

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

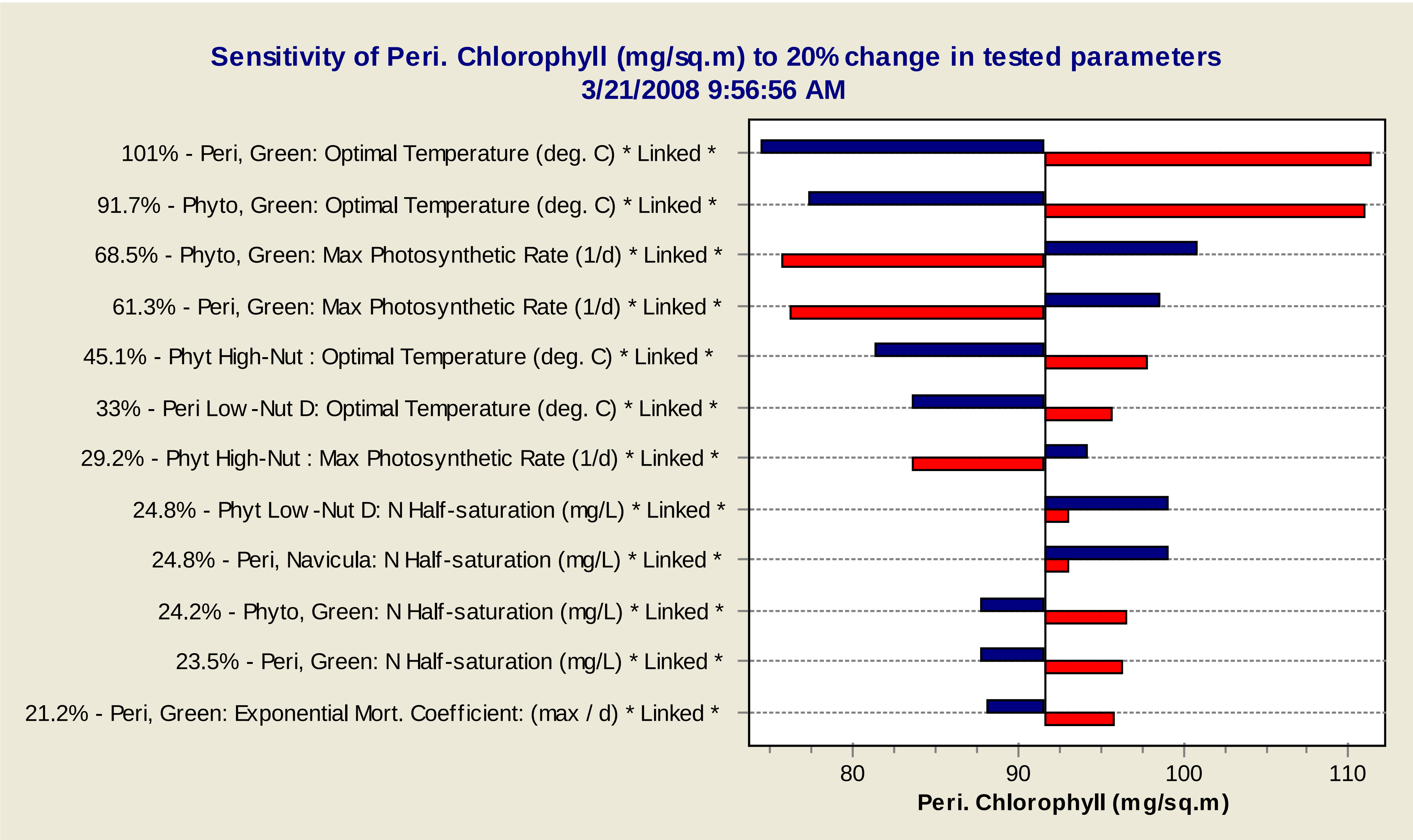
Rates Plot Example: Periphyton



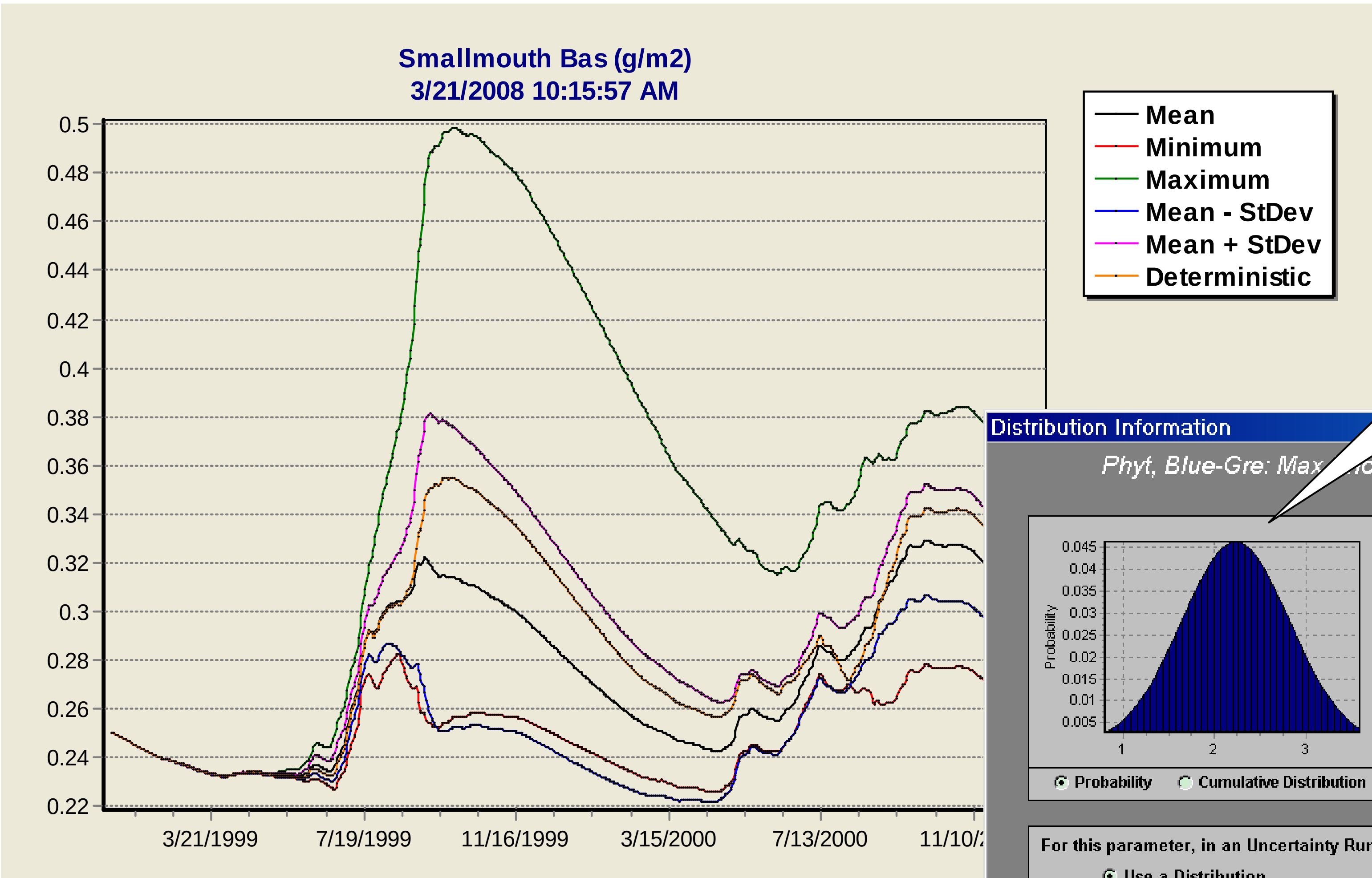
Limitations to Photosynthesis May also be Graphed



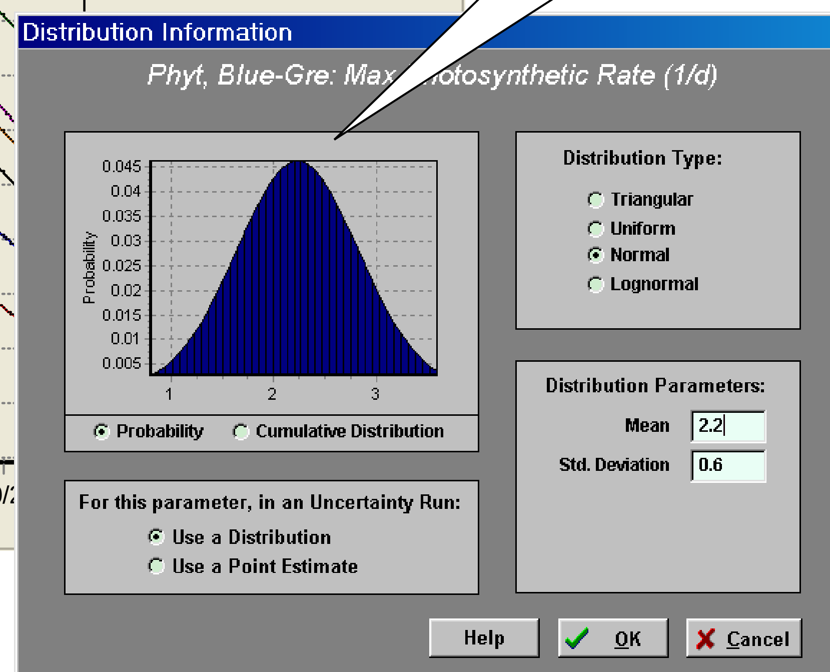
Integrated Nominal Range Sensitivity Analysis with Graphics



Integrated Latin Hypercube Uncertainty Analysis with Graphics

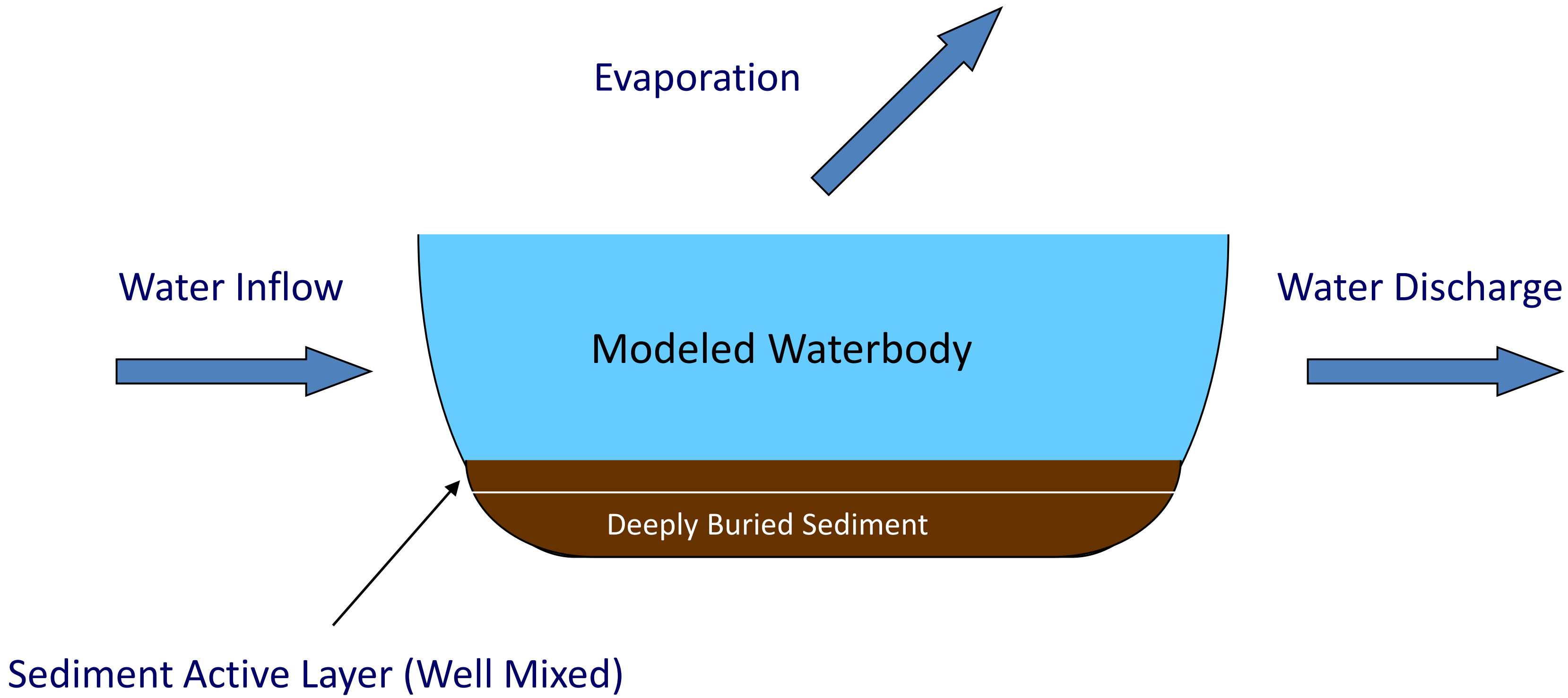


can represent all "point estimate" parameters as distributions

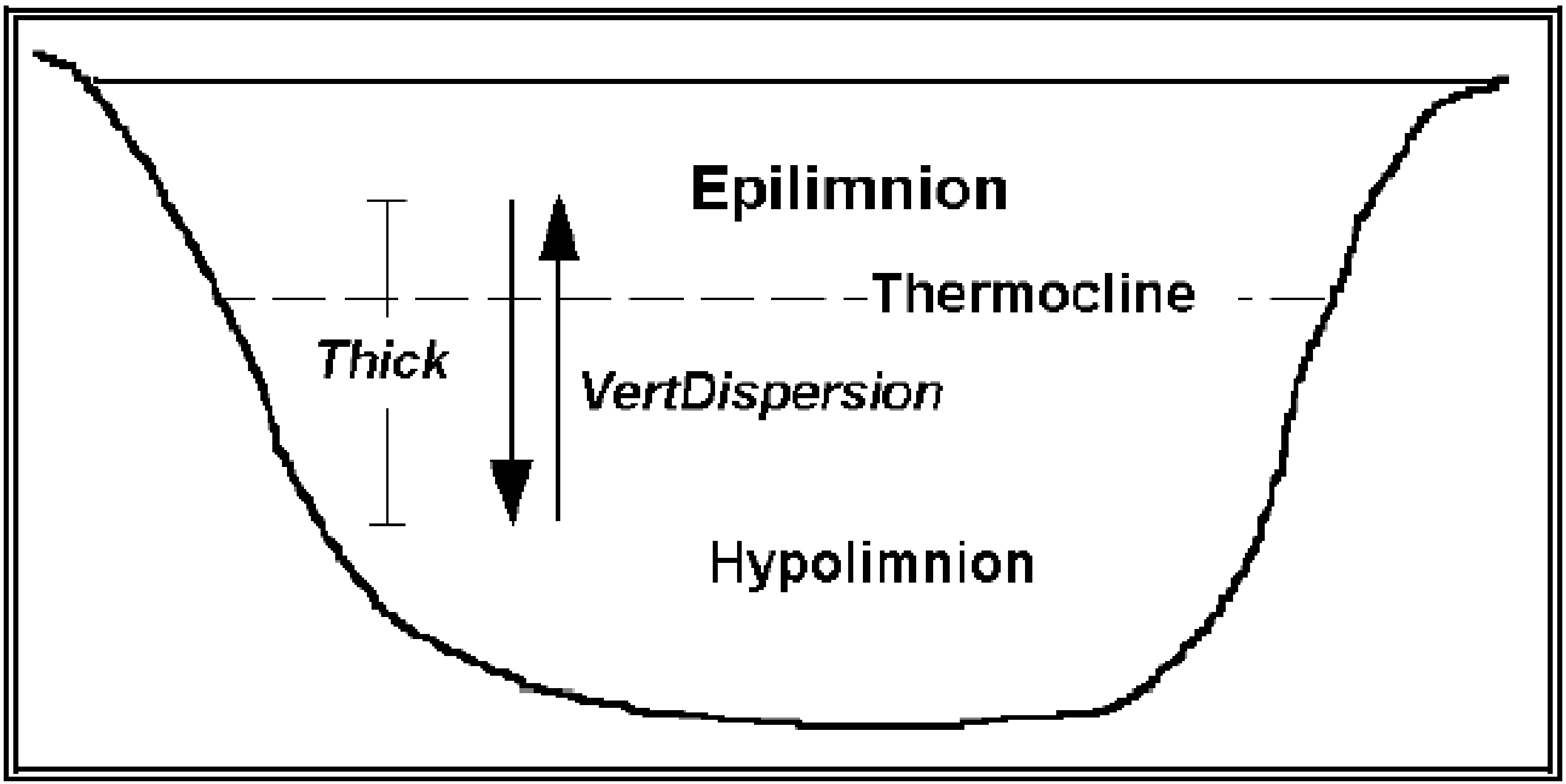


Physical Characteristics of a Site

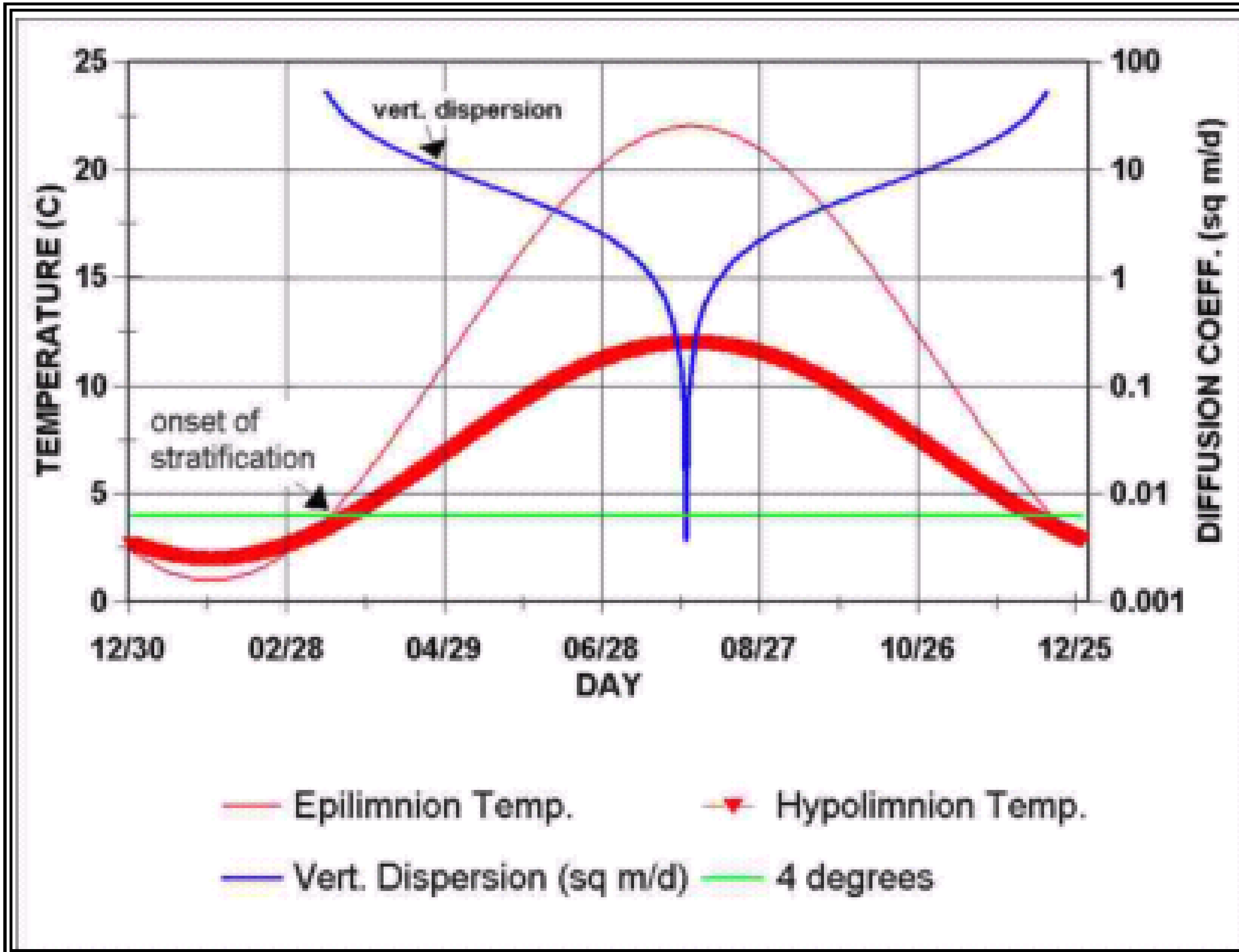
Water Balance and Sediment Structure



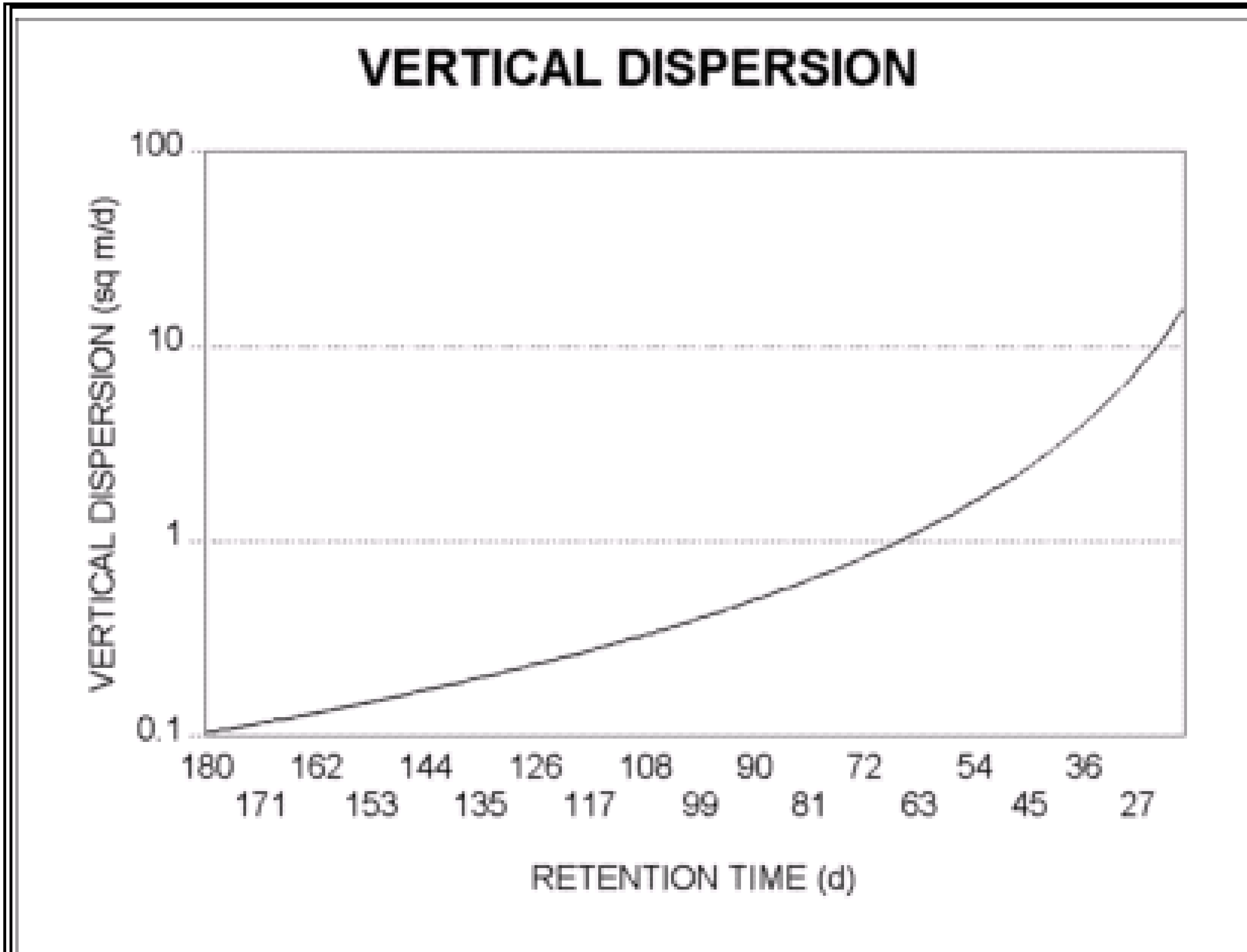
Thermal Stratification in a Lake



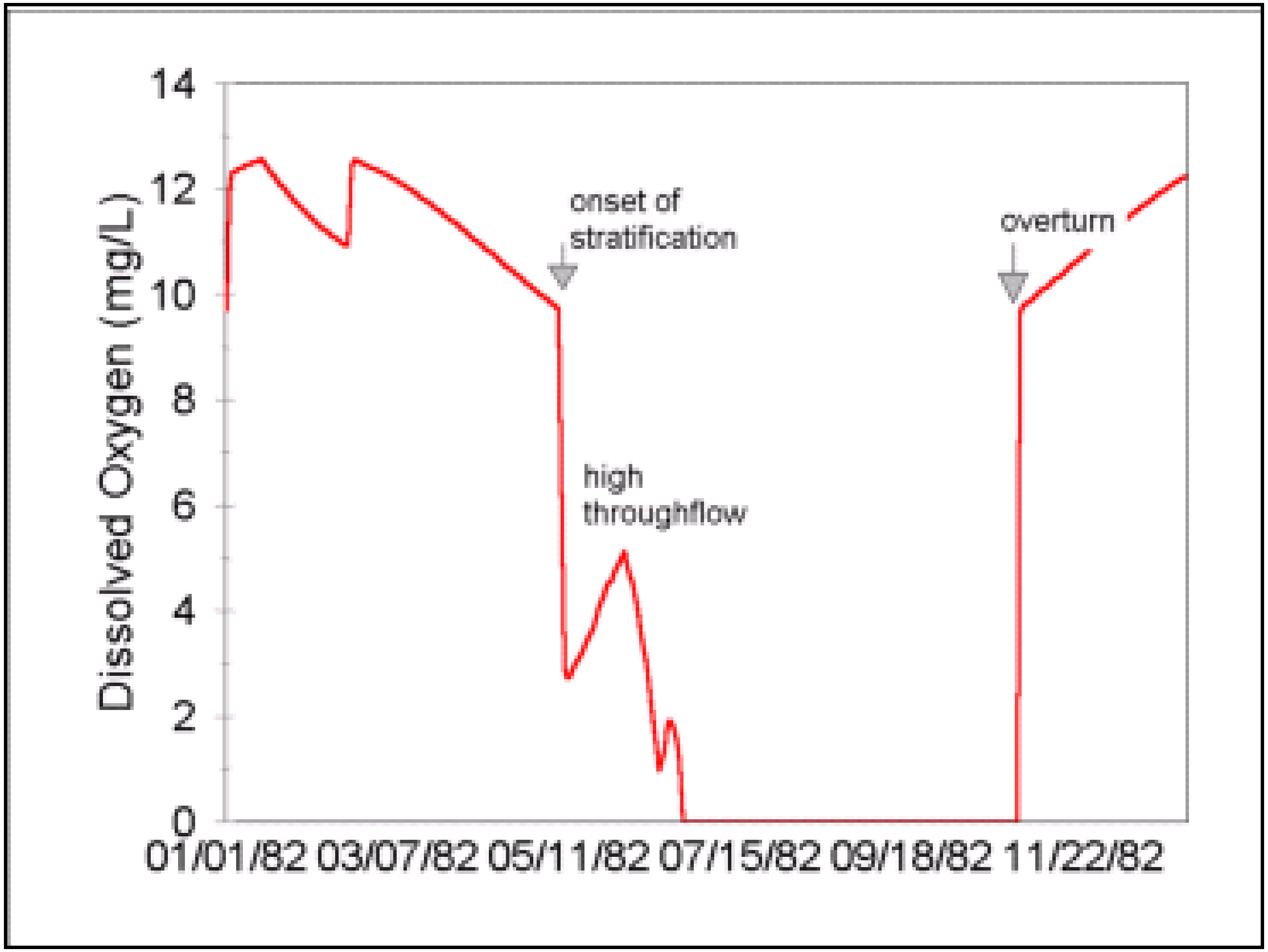
Stratification is a Function of Temperature Differences



Stratification also is a Function of Discharge



Predicted dissolved oxygen as function of stratification and mixing in deep reservoir



Reservoir management enhancements

Because reservoirs may be heavily managed, a user may specify:

- a constant or time-varying thermocline depth;
- options as to how to route inflow and outflow water
- the timing of stratification and overturn

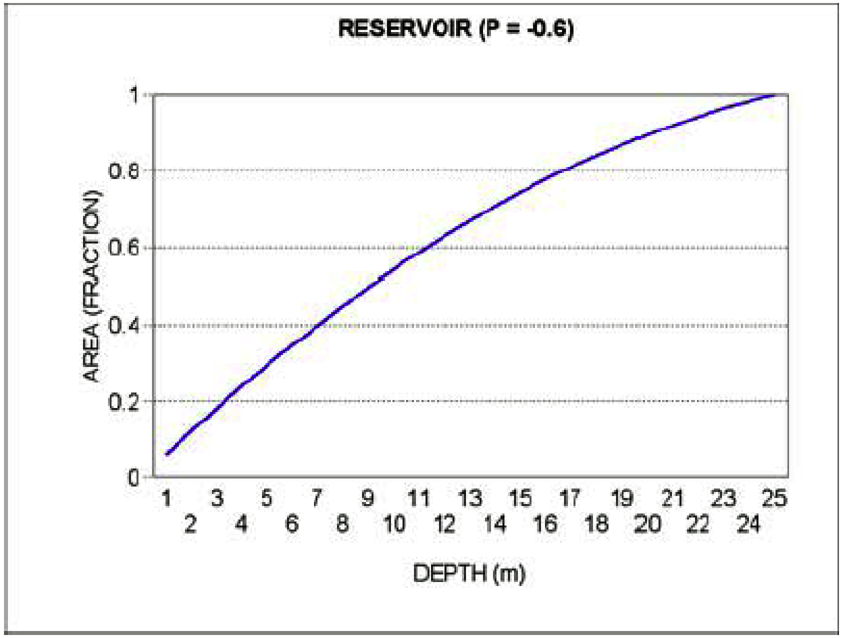
Bathymetric Approximations

The P parameter, differentiating different elliptic shapes, is calculated as a function of mean and maximum depth:

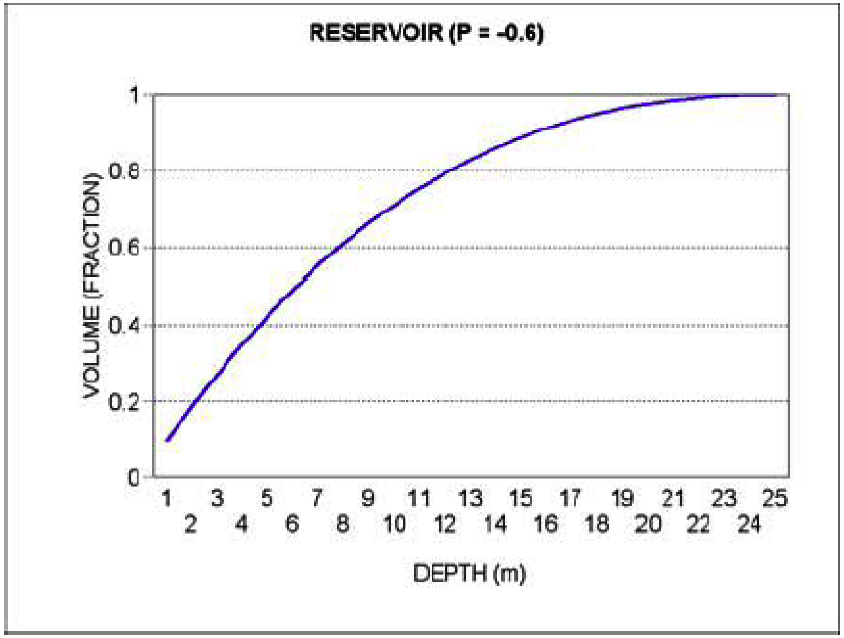
$$P = 6.0 \cdot \frac{ZMean}{ZMax} - 3.0$$

Based on these relationships, fractions of volumes and areas can be determined for any given depth:

Area as a Function of Depth



Volume as a Function of Depth

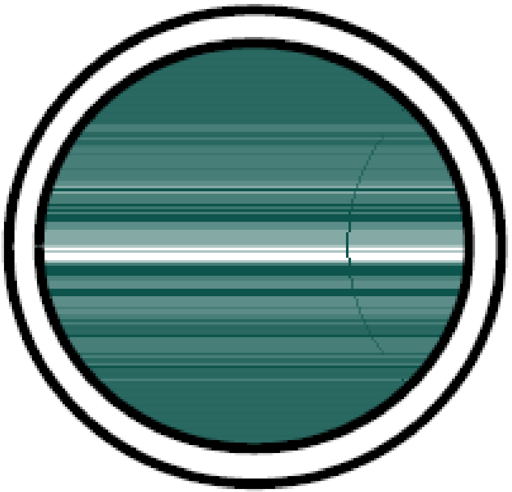


Littoral Fraction

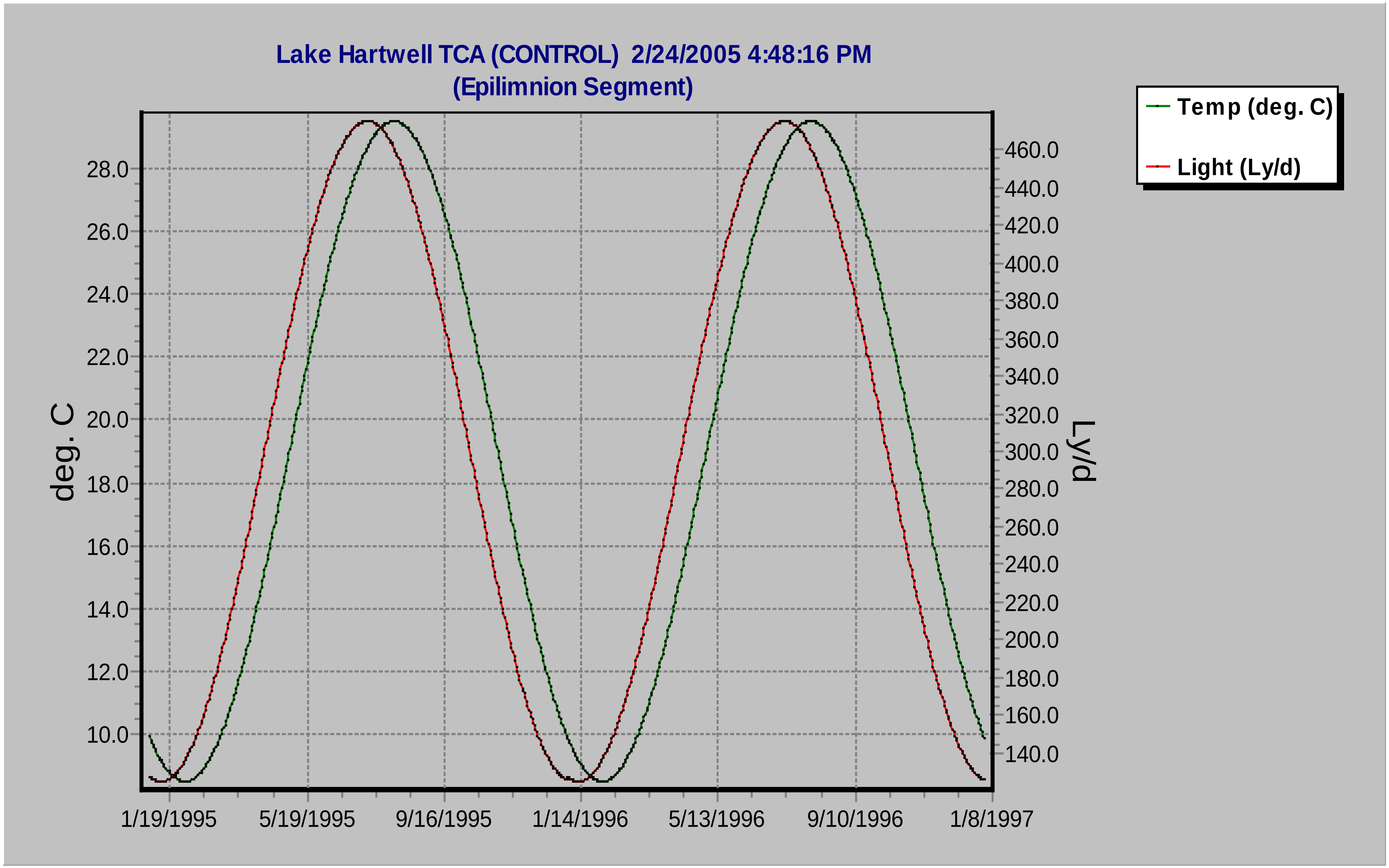
By setting Z to the depth of the euphotic zone, the fraction of the area available for colonization by macrophytes and periphyton can be computed:

$$FracLit = (1 - P) \cdot \frac{ZEuphotic}{ZMax} + P \cdot \left(\frac{ZEuphotic}{ZMax} \right)^2$$

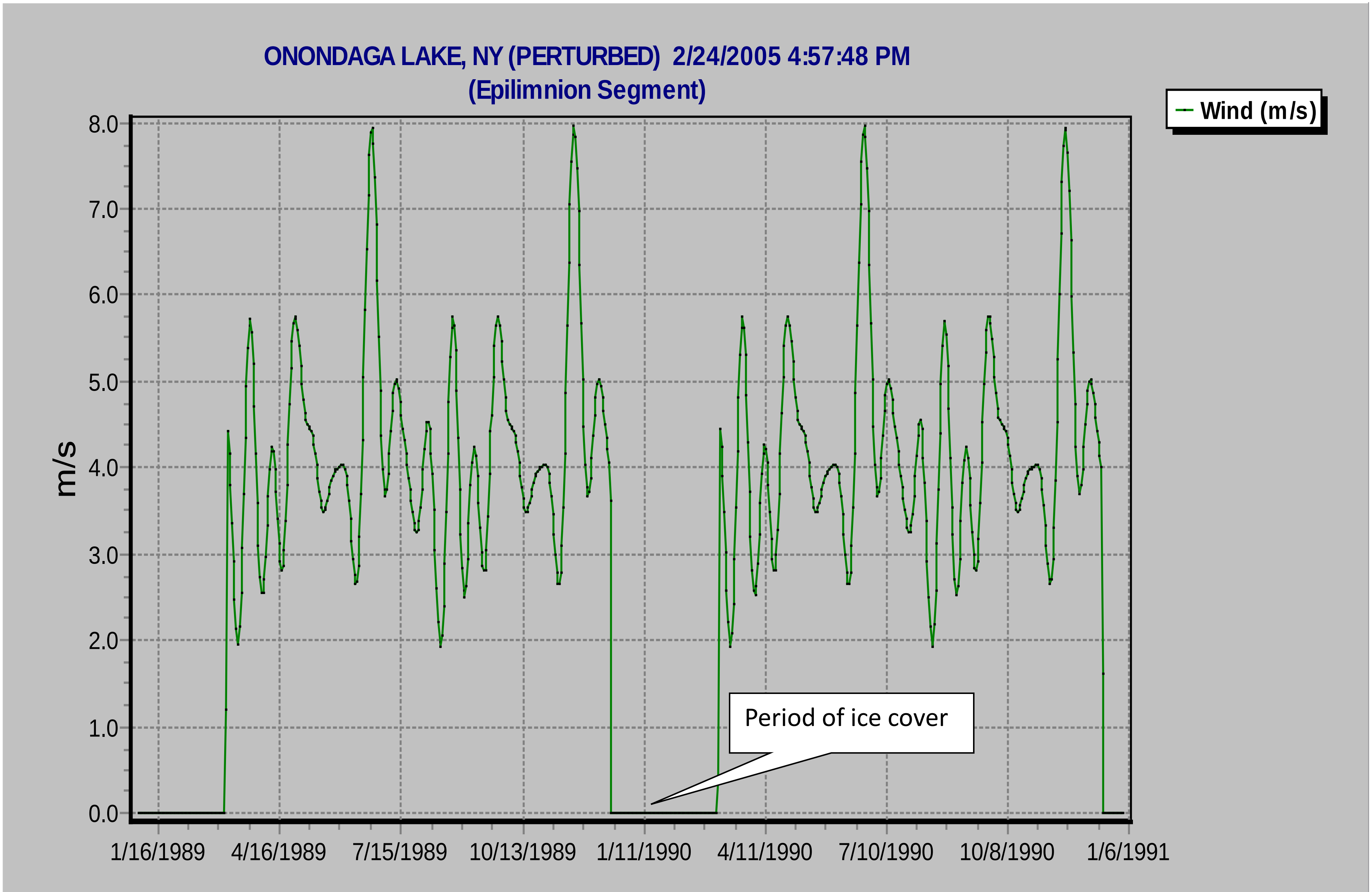
A relatively deep, flat-bottomed basin would have a small littoral area and a large sublittoral area:



Temperature and Light



Wind



ONONDAGA LAKE, NY (PERTURBED) 2/24/2005 4:57:48 PM
(Epilimnion Segment)
Wind (m/s)
m/s
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
1/16/1989
4/16/1989
7/15/1989
10/13/1989
1/11/1990
4/11/1990
7/10/1990
10/8/1990
1/6/1991
Period of ice cover

Modeling Plants with AQUATOX

- Equations
- Parameters
- Phytoplankton
- Periphyton
- Macrophytes
- Moss

Plant Derivatives

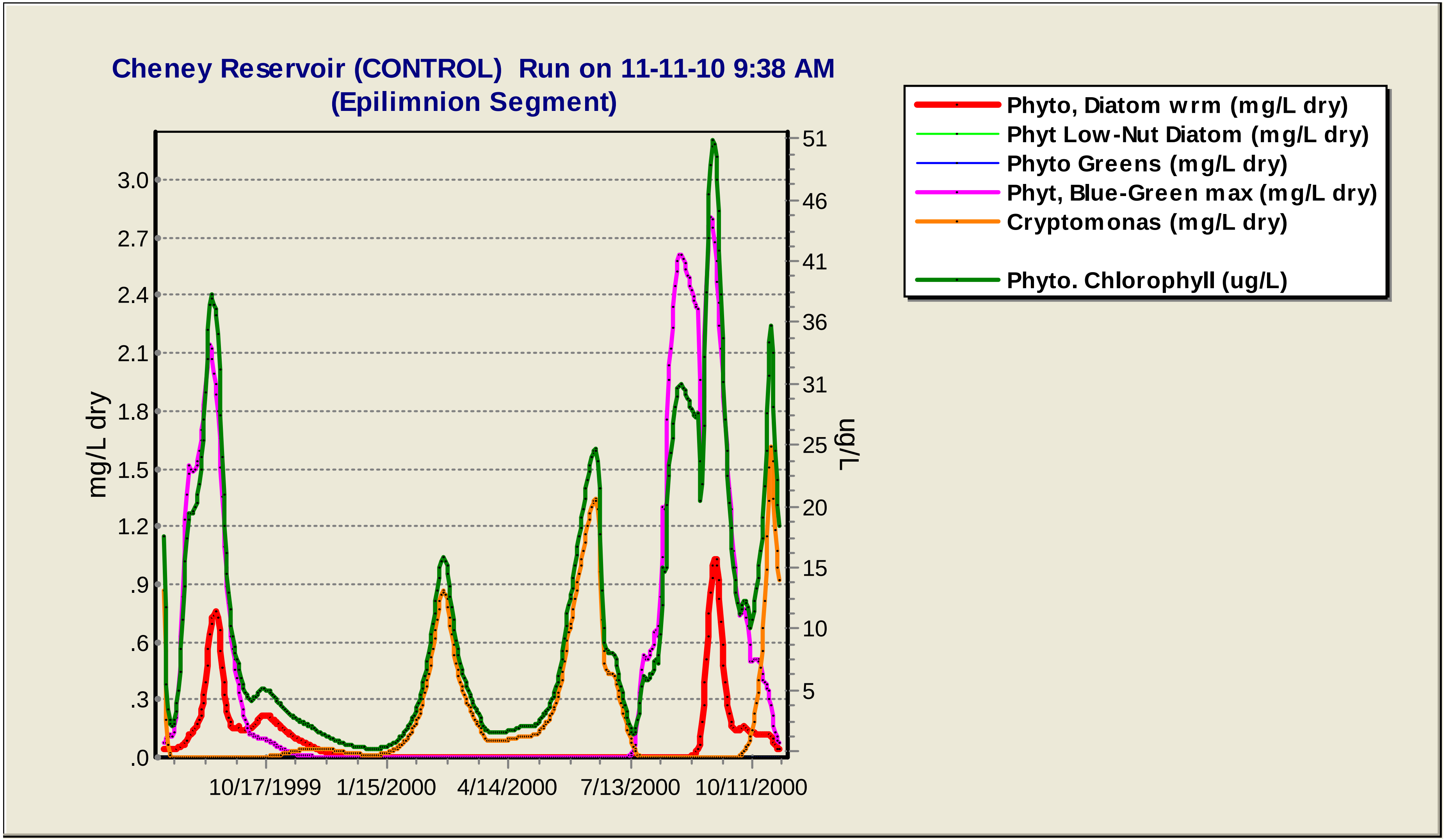
$$\frac{dBiomass_{phyto}}{dt} = Loading + Photosynthesis - Respiration - Excretion$$

$$- Mortality - Predation \pm \underbrace{Sinking - Washout \pm TurbDiff}_{\text{free floating plants}}$$

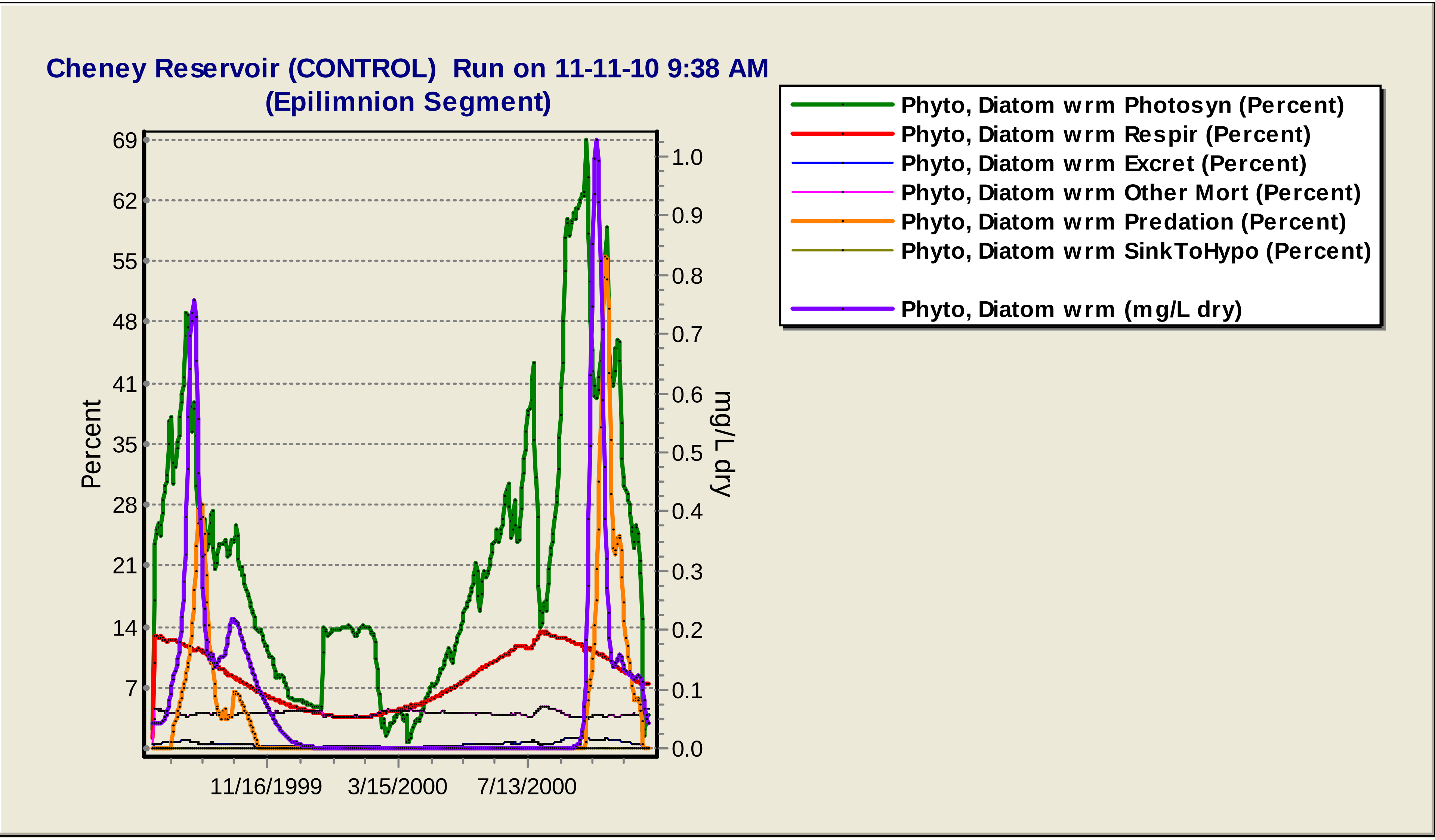
$$\frac{dBiomass_{peri}}{dt} = Loading + Photosynthesis - Respiration - Excretion$$

$$- Mortality - Predation - \underbrace{Slough}_{\text{bottom dwelling}}$$

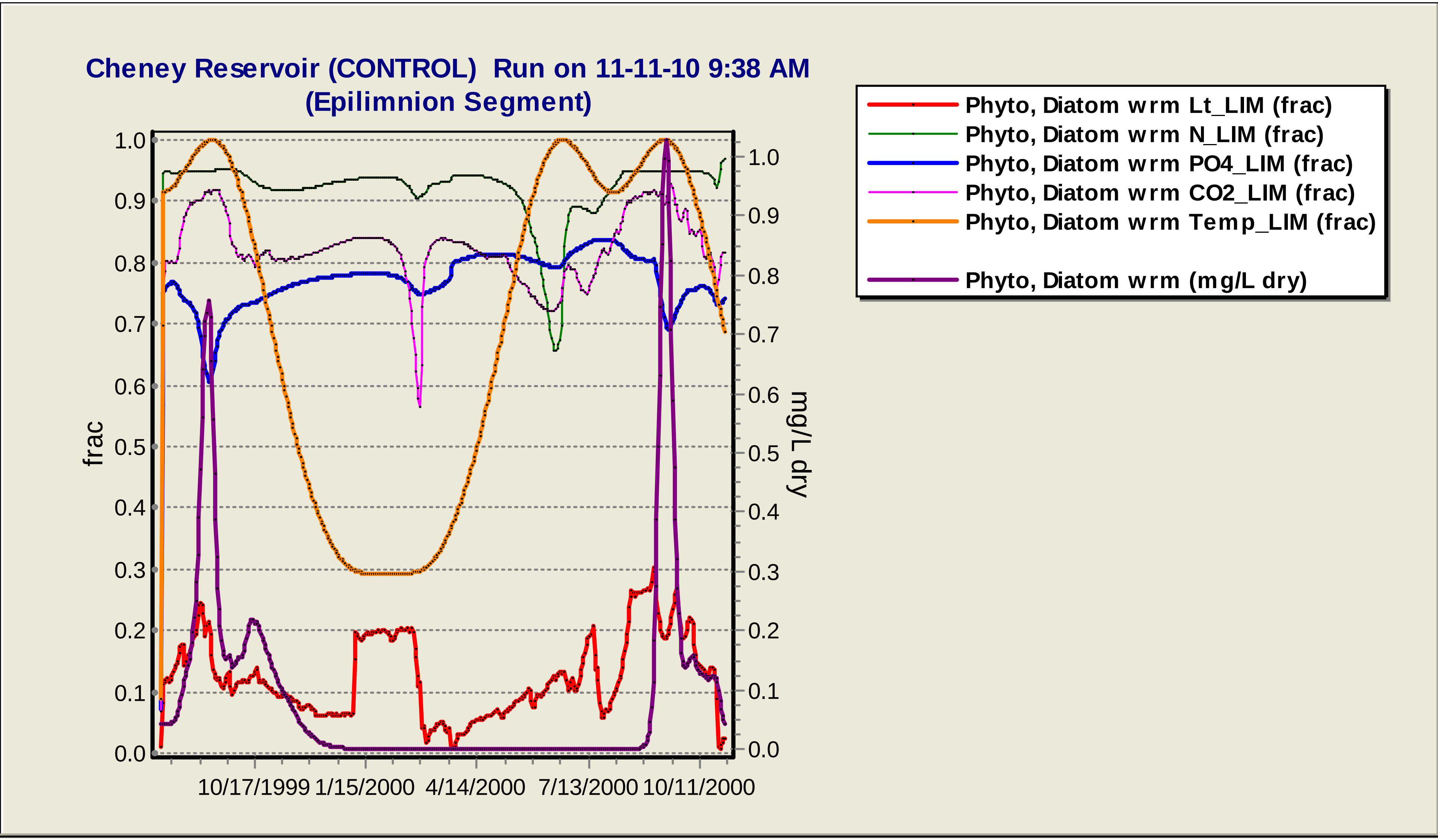
Phytoplankton Biomass Shows Succession chlorophyll *a* summarizes response



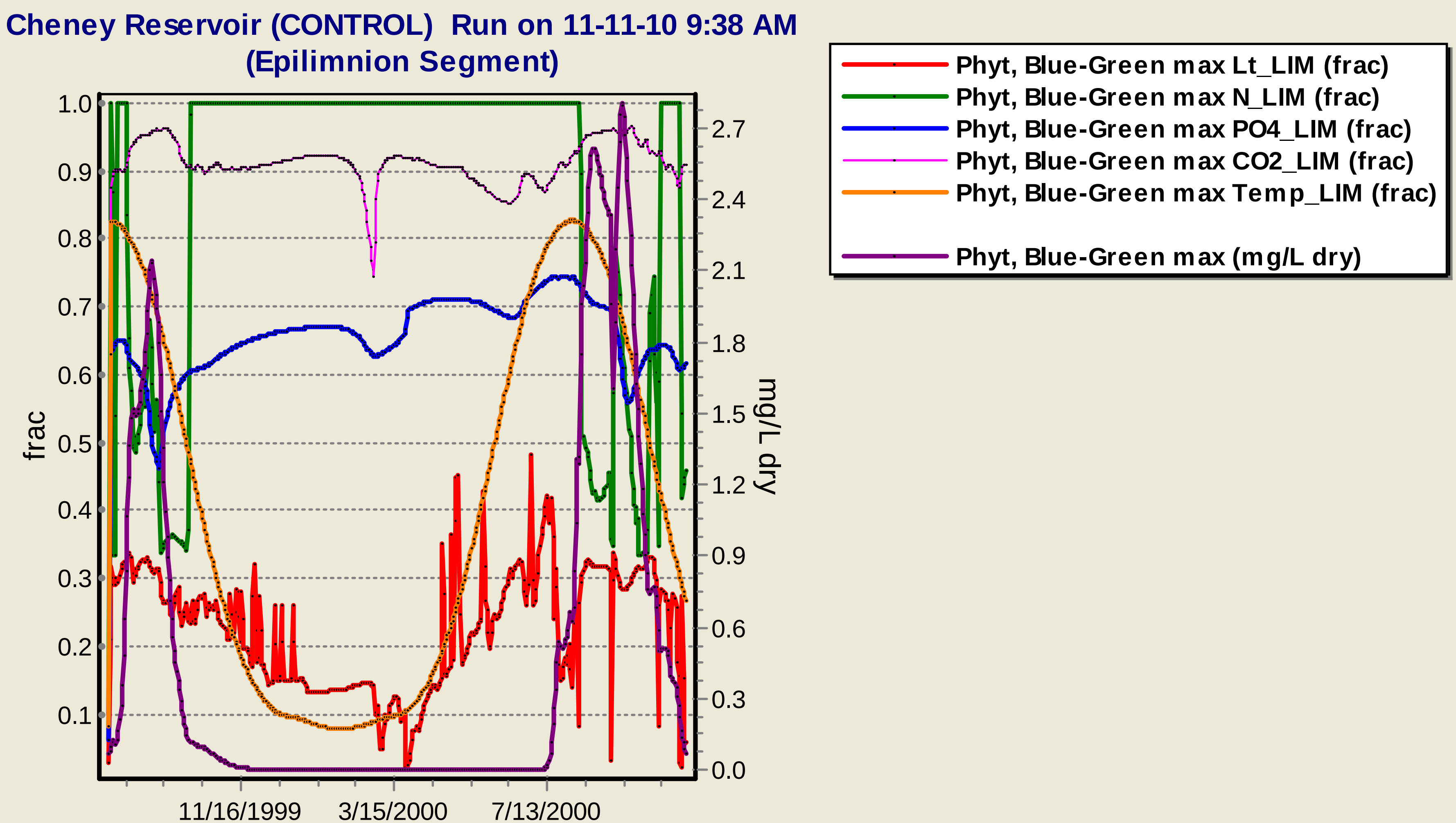
Rates can be saved and plotted for all processes



Time-varying limitations to photosynthesis also can be analyzed



Limitations on various groups can be compared



Calibration of Plants

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

Global vs. Site-Specific Plant Parameters

Most plant parameters may be assumed to be global as a plant species is not assumed to differ from one site to another.

Some plant parameters reflect site characteristics and may need to be calibrated for your site.

Critical Force for Periphyton -- reflects site's substrate
Carrying Capacity for Macrophytes -- reflects habitat
Optimum Temperature -- reflects cold-/warm-water species
Mortality Coefficients -- reflect quality of habitat

Plant Parameters

★ = important

Plant Data:

New

Plant: Phyto, Diatom (Search Names)

Scientific Name: Cyclotella (Search Scientific Names)

Plant Type: Phytoplankton

☐ Plant is Surface Floating

Toxicity Record: Diatoms (Edit All)

Taxonomic Type: Diatoms

Parameter	Value	Units	References
★ Saturating Light	22.5	Ly/d (Convert)	Collins & Wlosinski '83, p. 41
☑ **Use Adaptive Light**			
Max. Saturating Light	300	Ly/d (Convert)	Default
Min. Saturating Light	22.5	Ly/d (Convert)	min. for Cyclotella
★ P Half-saturation	0.017	mg / L	Collins & Wlosinski '83, p. 33, 0.055, 0.001
N Half-saturation	0.011	mg / L	Collins & Wlosinski '83, p. 36
Inorg. C Half-saturation	0.054	mg / L	C & W '83, p. 39 (greens)
Temp. Response Slope	1.8		
★ Optimum Temperature	20	°C	Collins & Wlosinski '83, p. 43 for range
Maximum Temperature	35	°C	
Min Adaptation Temp.	2	°C	
★ Max. Photosynthetic Rate	1.6	1 / d	mean, Collins & Wlosinski '83
Photorespiration Coefficient	0.026	1 / d	"
Resp Rate at 20 deg. C	0.08	g / g-d	Riley and von Aux, 1949, cited in C.& W.1983
★ Mortality Coefficient	0.003	g / g-d	calibrated
Exponential Mort. Coeff.	0.04	g / g-d	

Plant Parameters (cont.)

P : Organics	0.007	ratio	Sterner & Elser 2002
N : Organics	0.079	ratio	"
Light Extinction	0.144	1/m-g/m^3	
Wet to Dry	10	ratio	Kabam Appen C
Fraction that is lipid	0.023	(wet wt.)	Kabam Appen C

Phytoplankton Only:

★ Sedimentation Rate (KSed)	0.16	m / d	Collins & Wlosinski '83, p. 30
Temperature of Obs. KSed (estuary only)	0	°C	placeholder
Salinity of Obs. KSed	0	‰	placeholder
Exp. Sedimentation Coeff	0.693		2 x normal if photosyn. = 0

small for streams
>> for lakes

Periphyton and Macrophytes Only:

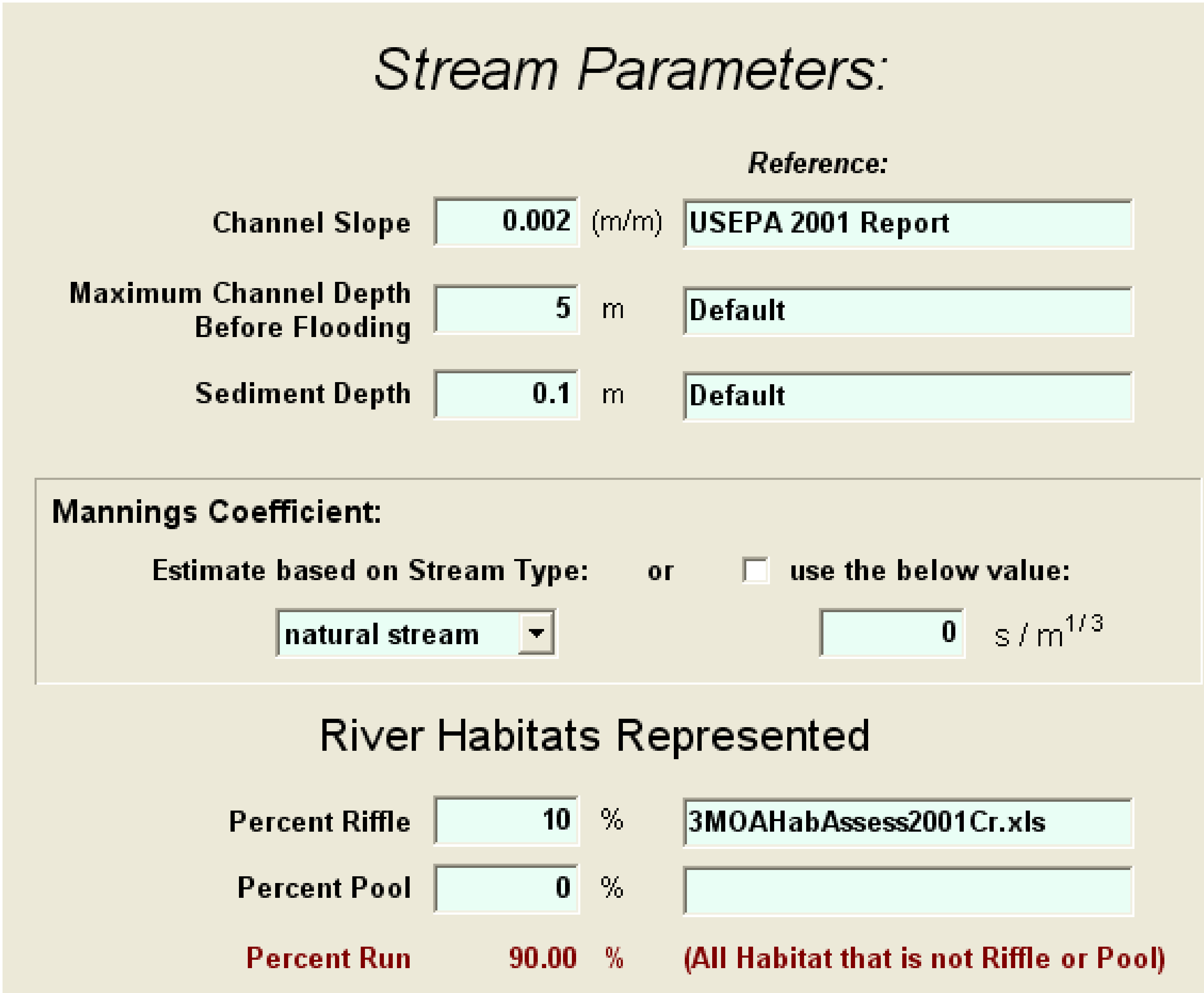
Carrying Capacity (macrophytes)	0	g / m^2	
VelMax (macrophytes)	0	cm / s	N.A.
Reduction in Still Water (periphyton)	0	fraction	
★ Critical Force (FCrit for periphyton only)	0	newtons	N.A.
★ Percent Lost in Slough Event (periphyton)	90	percent	90% lost in sloughing event as default

FCrit important for periphyton

If in Stream:

Percent in Riffle	0	%	
Percent in Pool	0	%	
Percent in Run	100.00	%	(All Biomass not in Riffle or Pool)

Habitats are characterized in the Site/Stream Parameters screen

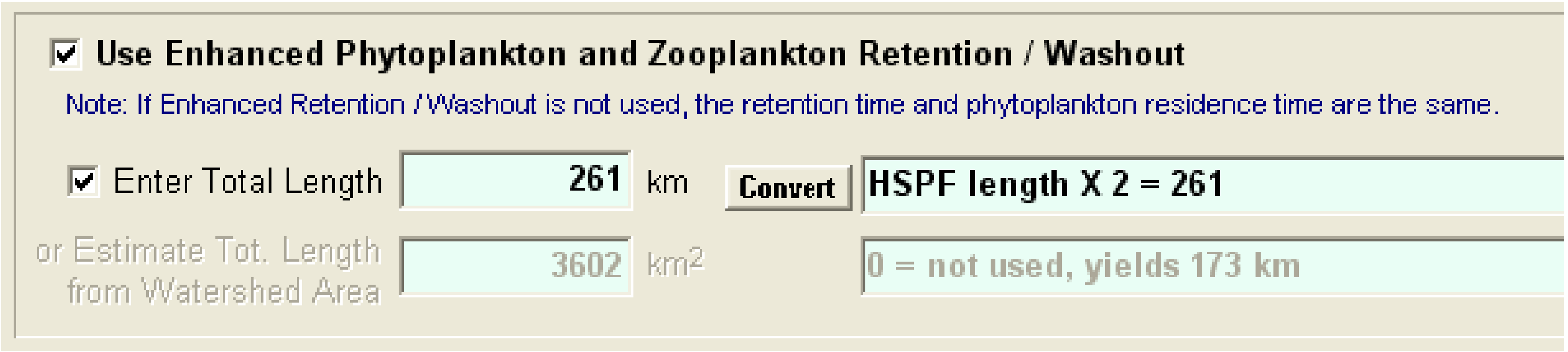


Difference Between Library Parameters and "Underlying Data"

- Libraries
  - are not attached to a simulation
  - are not saved when a simulation is saved
  - have no effect on simulation results
  - independent databases that may be loaded into a simulation or saved from a simulation for later reference
- Underlying Data
  - are attached to a simulation; are loaded and saved when a simulation is loaded and saved
  - will affect simulation results
  - are independent from Libraries, i.e. changing these parameters has no effect on Libraries

Modeling Phytoplankton

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



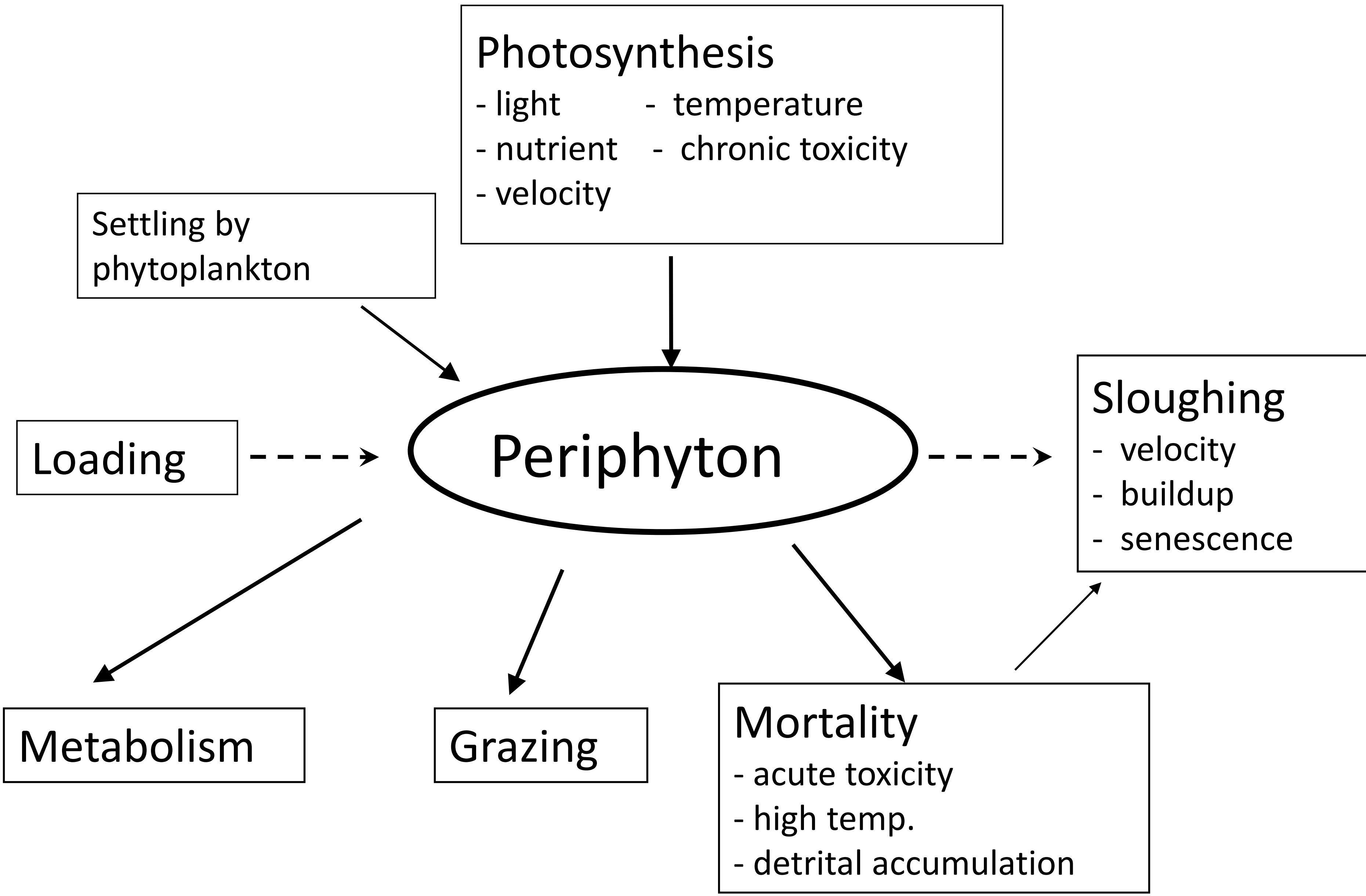
Modeling Cyanobacteria/Surface-Floating Plants

- Phytoplankton may be specified as “surface floating”
  - assumed to be located in the top 0.1 m
  - if limited by lack of nutrients or sufficient wind occurs they are assumed located within the top 3 m
- The averaging depth for “surface floating” plants is 3 m to correspond to monitoring data.
- Cyanobacteria are assumed to be “surface floating”
- Cyanobacteria are not severely limited by nitrogen due to facultative nitrogen fixation (if N less than ½ KN)

Modeling Periphyton

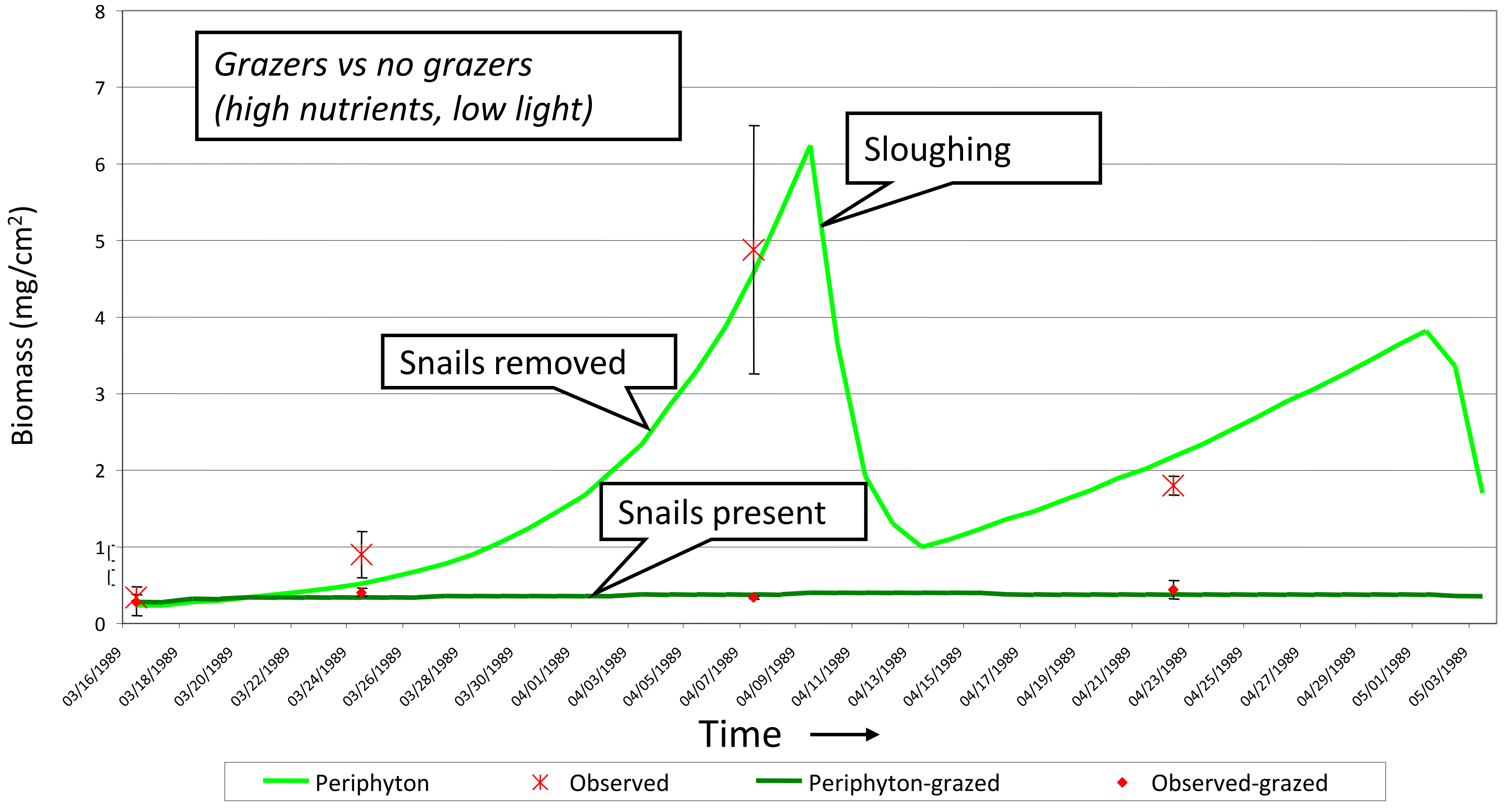
- Periphyton are not simulated by most water quality models
- Periphyton are difficult to model
  - include live material and detritus
  - stimulated by nutrients
  - snails & other animals graze it heavily
  - riparian vegetation reduces light to stream
  - build-up of mat causes stress & sloughing, *even at relatively low velocity*
- Many water body impairments due to periphyton

How AQUATOX Models Periphyton

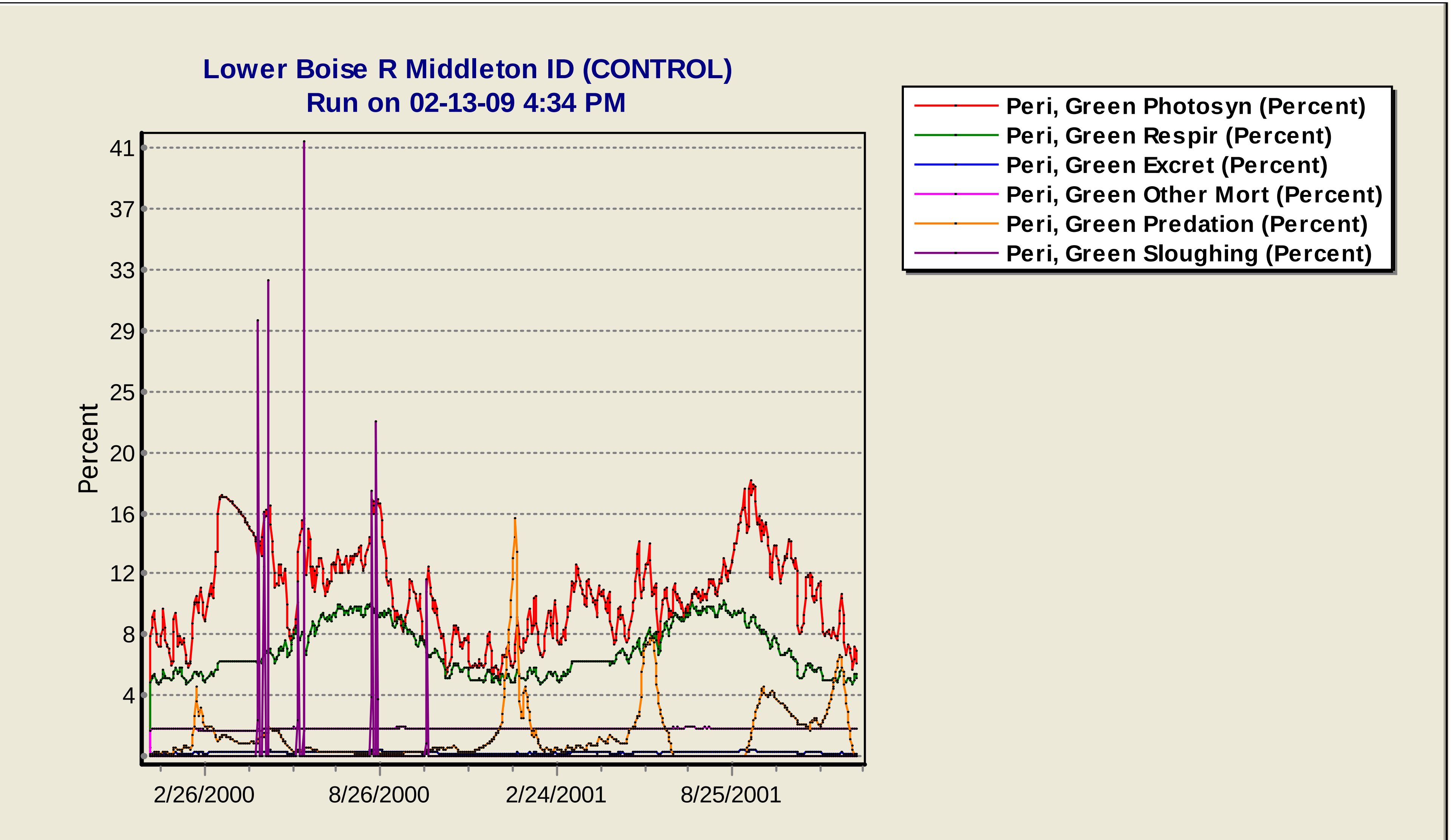


Several Independent Factors Affect Periphyton, Two Illustrated by Separate Simulations

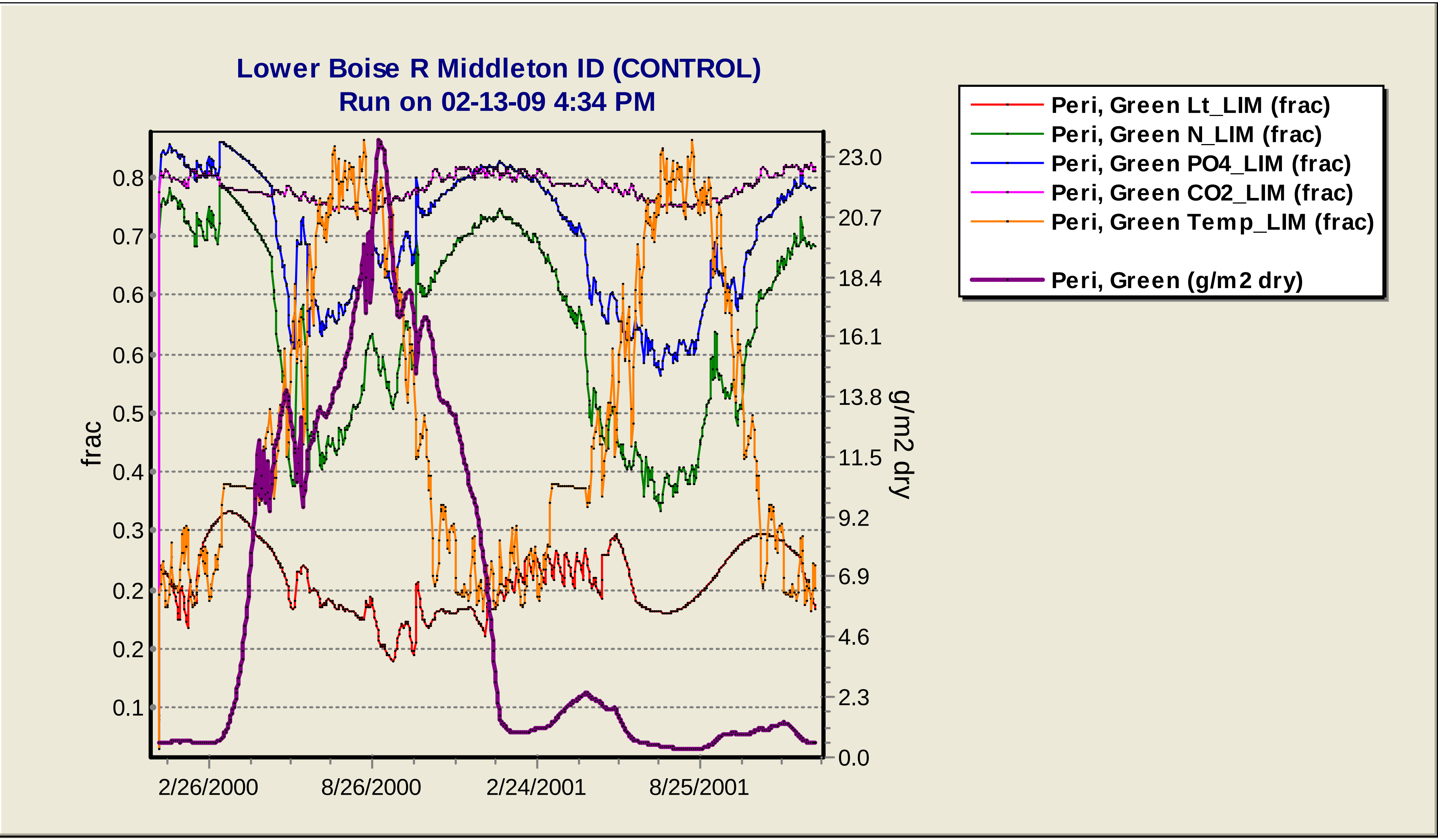
One important factor is grazing by snails another is sloughing



Sporadic Sloughing and Intense Grazing Characterize Periphyton



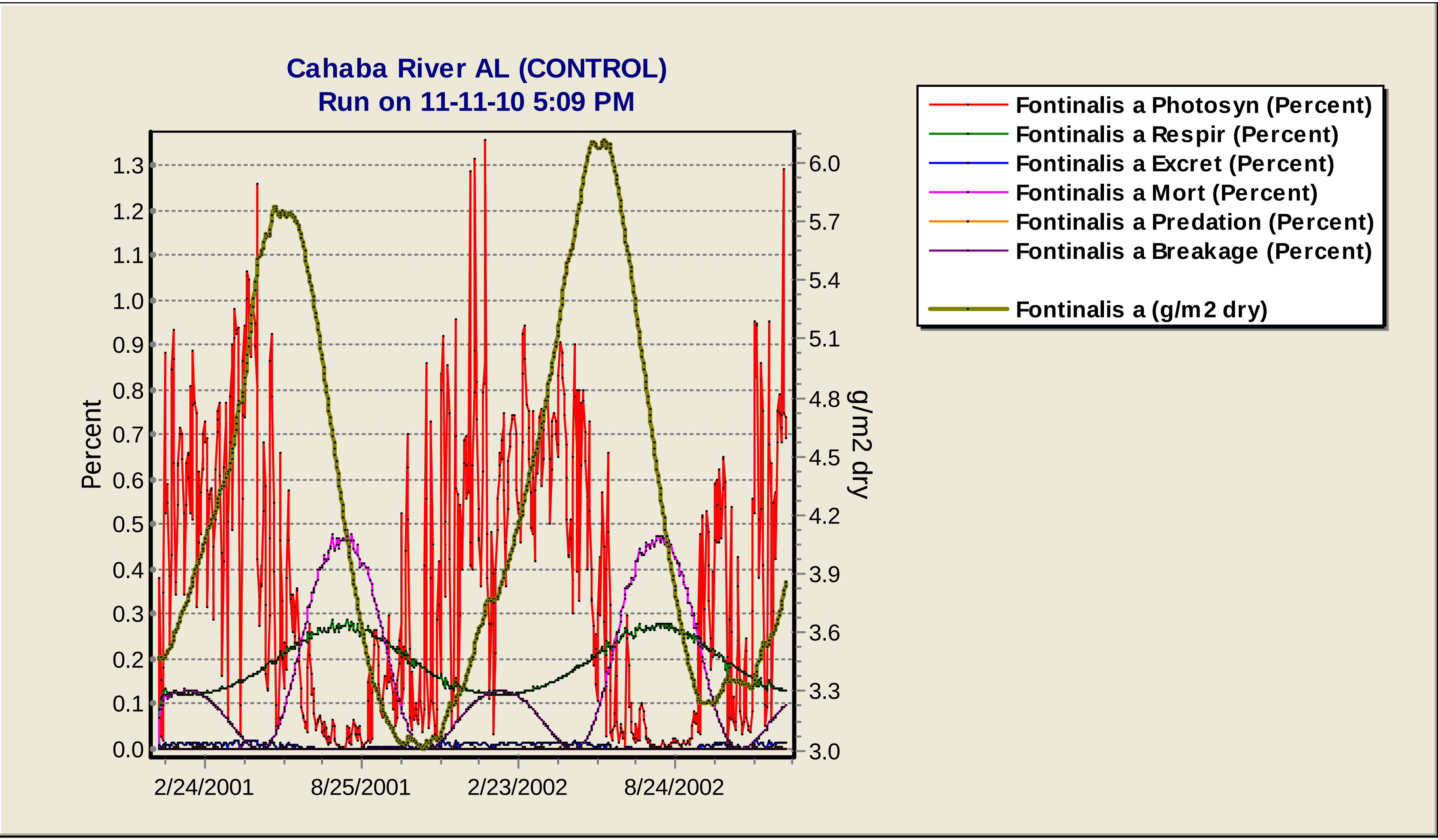
Nutrient limitation & self-shading are important, followed by winter temperature



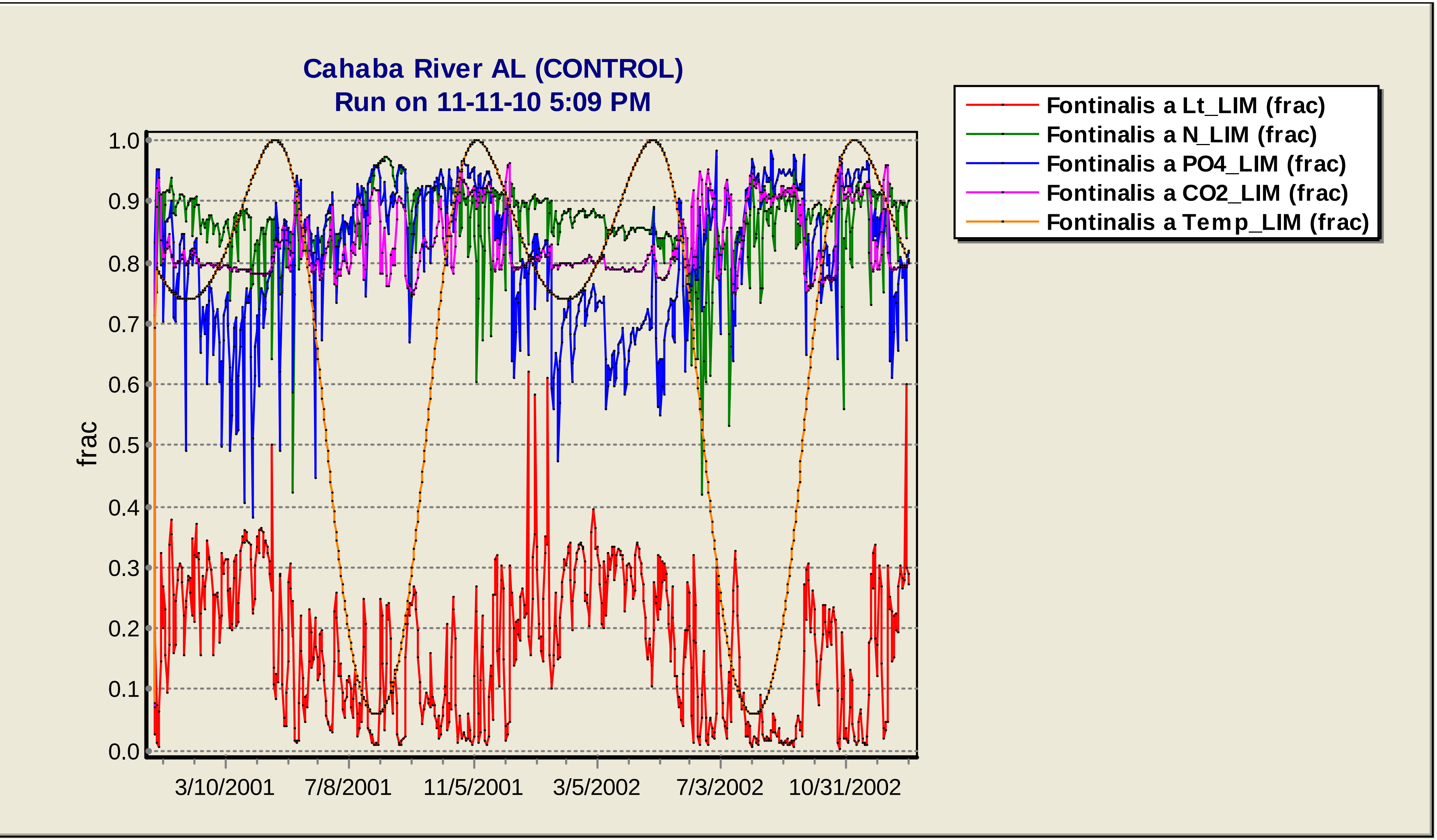
Modeling Macrophytes

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

Moss are stable component with little grazing or breakage, only summer die-back



Moss light limitation decreases when sloughing removes periphyton; summer temperature causes die-back



Lab 2: Setup of a New Study

- Rum River, MN, as template
- Rum River Background
- Use of the Wizard
- Site Characteristics
- Importing Loadings

Photo: MN Pollution Control Agency

Modeling Animals with AQUATOX

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

Animal Modeling Overview

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

Animal Derivatives

$$\frac{dBiomass}{dt} = Load + Consumption - Defecation - Respiration$$
$$- Excretion - Mortality - Predation - GameteLoss$$
$$- Washout \pm Migration - Promotion + Recruit - Entrainment$$

Note: *Promotion* includes emergence of aquatic insects

Animal Parameters

Animal Data:

Help

Animal: Mtn. whitefish adult

Scientific Name: Prosopium williamsoni

Size-Class Links | Trophic Interactions

Animal Type: Fish

Taxonomic Type or Guild: Game Fish

Toxicity Record: Trout | Edit All

Benthic Metric Designation:

Parameter	Value	Units	References:
Half Saturation Feeding	0.3	mg / L	Leidy & Jenkins '77 (cf. salmon)
★ Maximum Consumption	0.01	g / g·d	calc. from Hewett & Johnson '92, l. trout
★ Min Prey for Feeding	0.1	g/sq.m	bottom feeder
Sorting: degree to which there is selective feeding	1	unitless	Default -- no sediment effect
Suspended Sediments Affect Feeding: ☐			Default -- no sediment effect
Slope for Sed. Response	0	unitless	Default -- no sediment effect
Intercept for Sed. Resp.	0	unitless	Default -- no sediment effect
Temp. Response Slope	2.3		
★ Optimum Temperature	12	°C	Essig, 1998; see also Sauter et al. 2001
Maximum Temperature	23	°C	FishBase
Min Adaptation Temp.	0	°C	Sauter et al. 2001, based on spawning
★ Mean wet weight	300	g wet	
★ Endogenous Respiration	0.0015	1 / d	calc. from Hewett & Johnson '92 prms.
Specific Dynamic Action	0.172	(unitless)	cf. Hewett & Johnson '92

Animal Parameters (cont.)

Excretion : Respiration	0.05	ratio	default
N to Organics	0.1	frac. dry	Sterner and George 2000
P to Organics	0.031	frac. dry	Sterner and George 2000
Wet to Dry	5	ratio	default
Gametes : Biomass	0.09	ratio	
Gamete Mortality	0.9	1 / d	
★ Mortality Coefficient	0.001	1 / d	Handbook of Environ. Data (Jorgenesen, 1979)
Sensitivity to Sediment (lethal effects)	Zero Sensitivity		Default -- no sediment effect
Organism is Sensitive to Percent Embeddedness: ☐			
Percent Embeddedness Threshold	100	percent	No effect
Carrying Capacity	0.05	g/sq.m	calc. from Leidy & Jenkins 77
Frac. in Water Column	1	fraction	Default for this Animal Type
VelMax	400	cm / s	Default
Removal due to Fishing	0.0003	fraction / d	prof judgment (10%)

Animal Parameters (fish-specific allometric parameters)

Spawning Parameters:

Either ☑ Fish spawn automatically, based on temperature range

or Fish spawn on the following dates each year 12/30/1899 12/30/1899 12/30/1899

(Enter Dates M/d/yyyy) Year entered is irrelevant

Spawning Date Reference:

Either ☑ Fish can spawn an unlimited number of times each year

or Fish can only spawn 0 times each year

Allometric Parameters:

Consumption: Reference: **Fish Bioenergetics 3.0, trout**

☑ **Use Allometric Equation to Calculate Maximum Consumption:**

CA: **0.628** intercept for weight dependence

CB: **-0.3** slope for weight dependence

Respiration: Reference: **Fish Bioenergetics 3.0, trout**

☑ **Use Allometric Equations to Calculate Respiration:**

RA: **0.00264** intercept for species specific metabolism

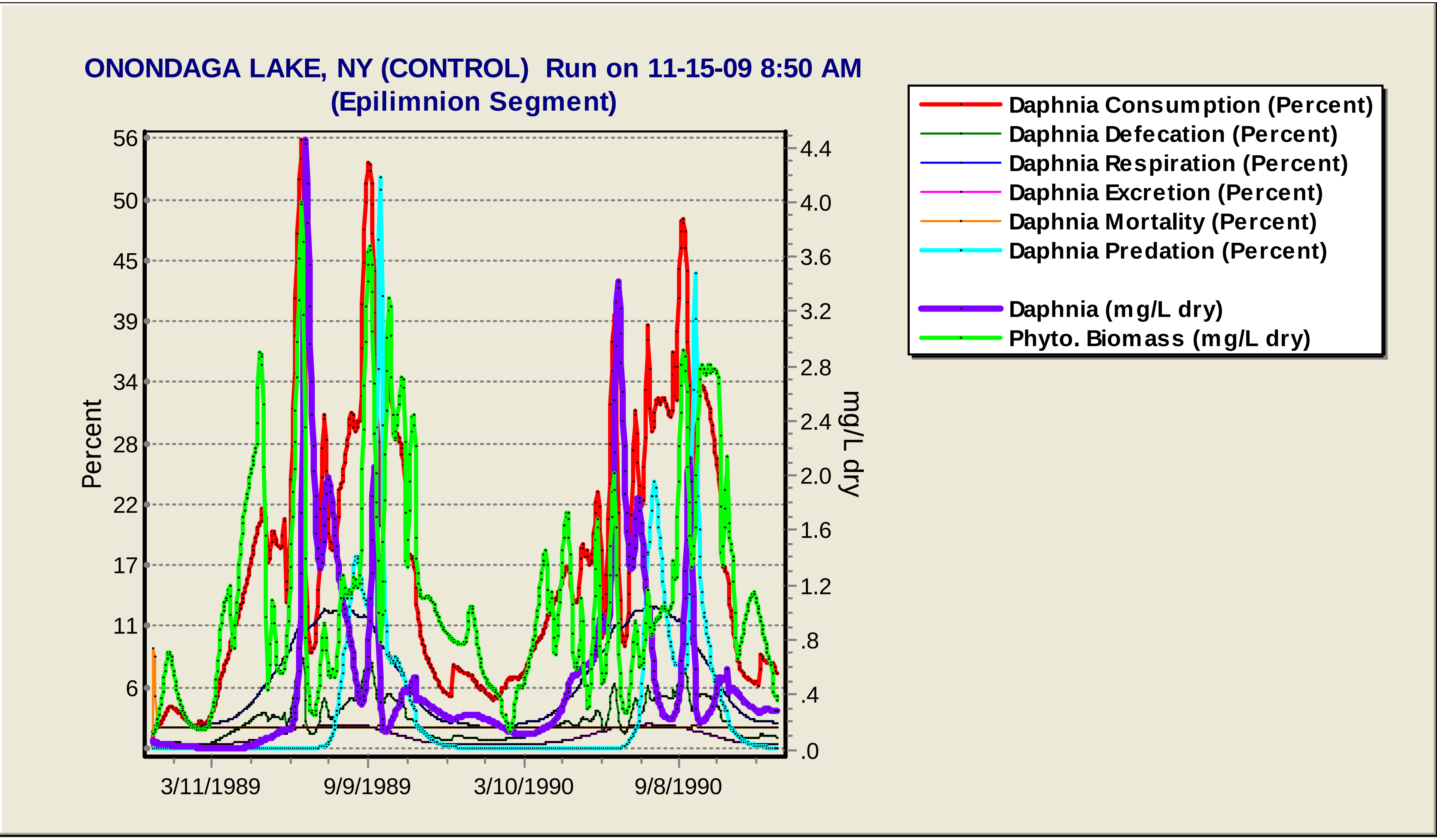
RB: **-0.217**

☑ Use "Set 1" of Respiration Equations:

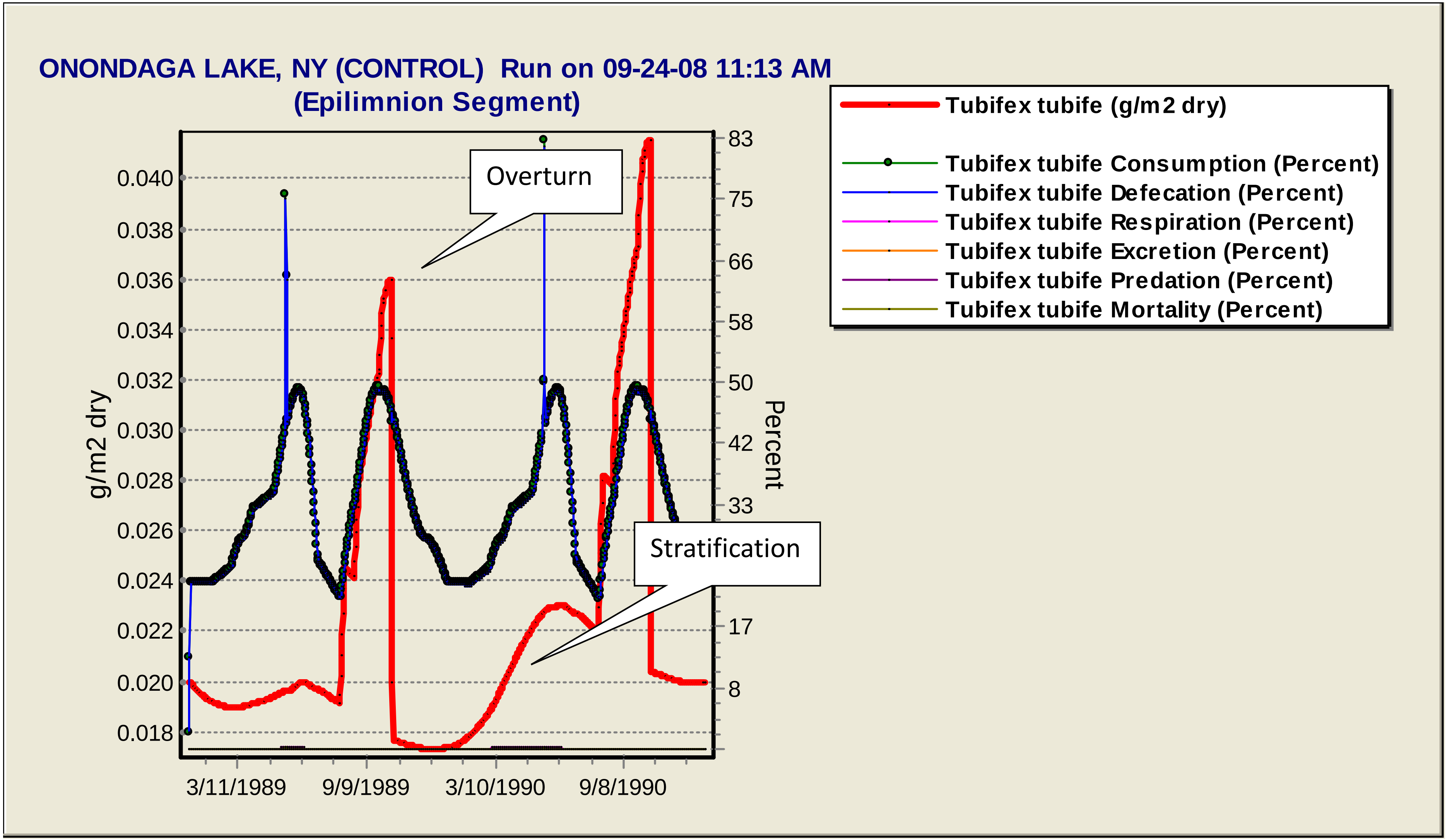
"Set 1" Parameters: weight dependence coefficient

RQ:	**0.06818**	**RTL:**	**25**	**ACT:**	**9.7**
RTO:	**0.0234**	**RK1:**	**1**	**BACT:**	**0.0405**
RTM:	**0**	**RK4:**	**0.13**		

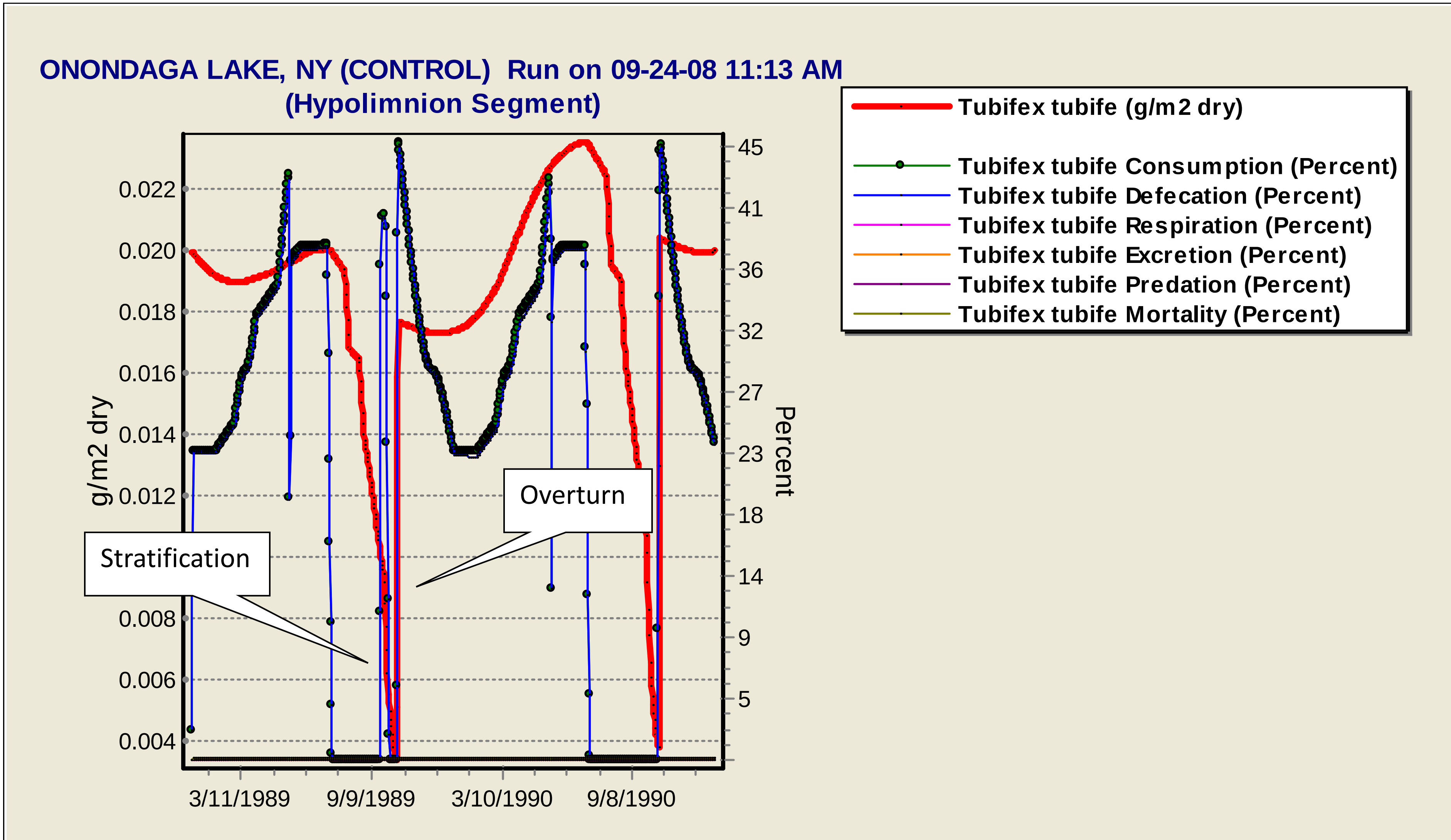
Zooplankton consumption is often tied to phytoplankton productivity



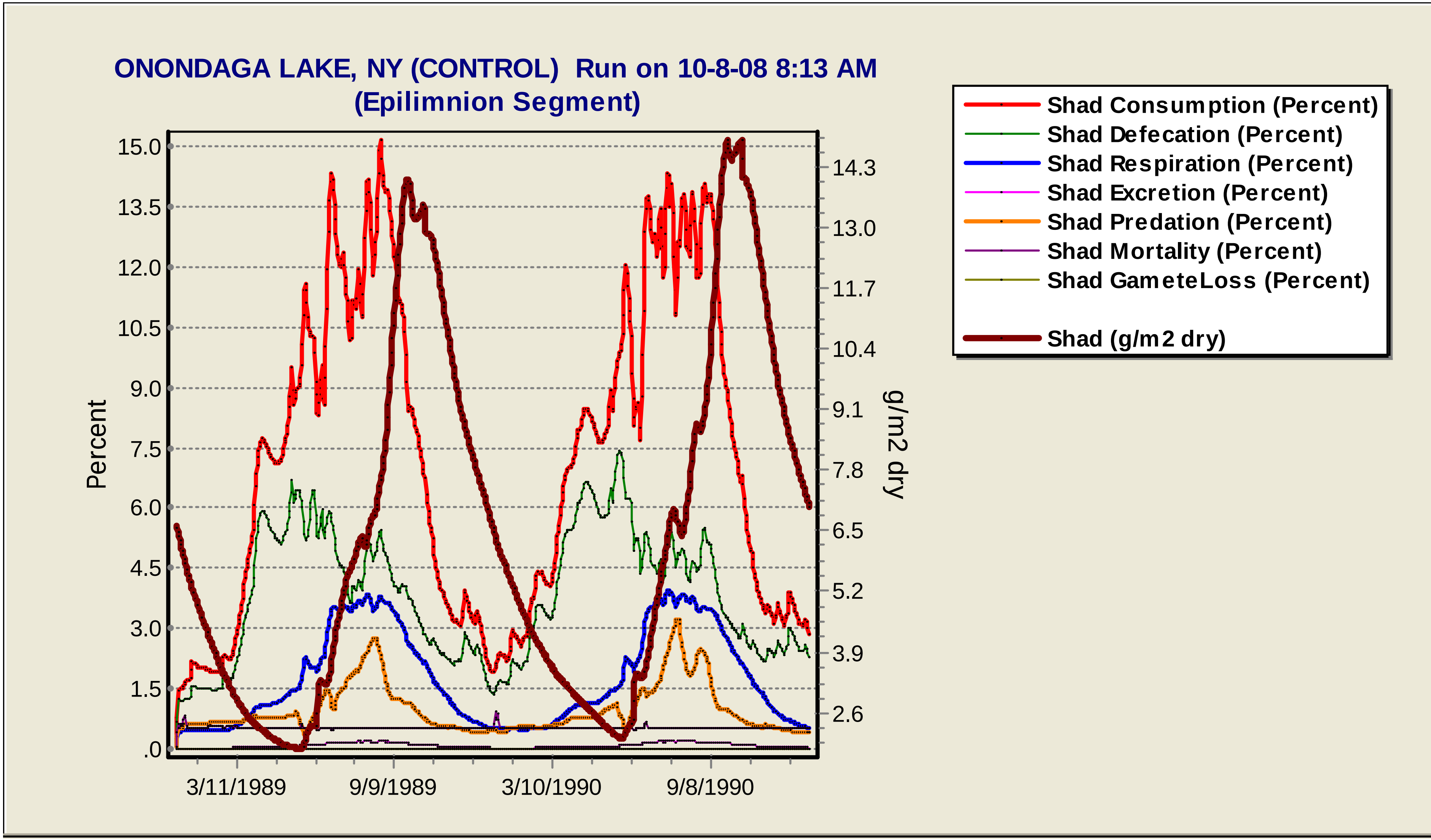
Benthic invertebrates are also tied to phytoplankton productivity through detritus



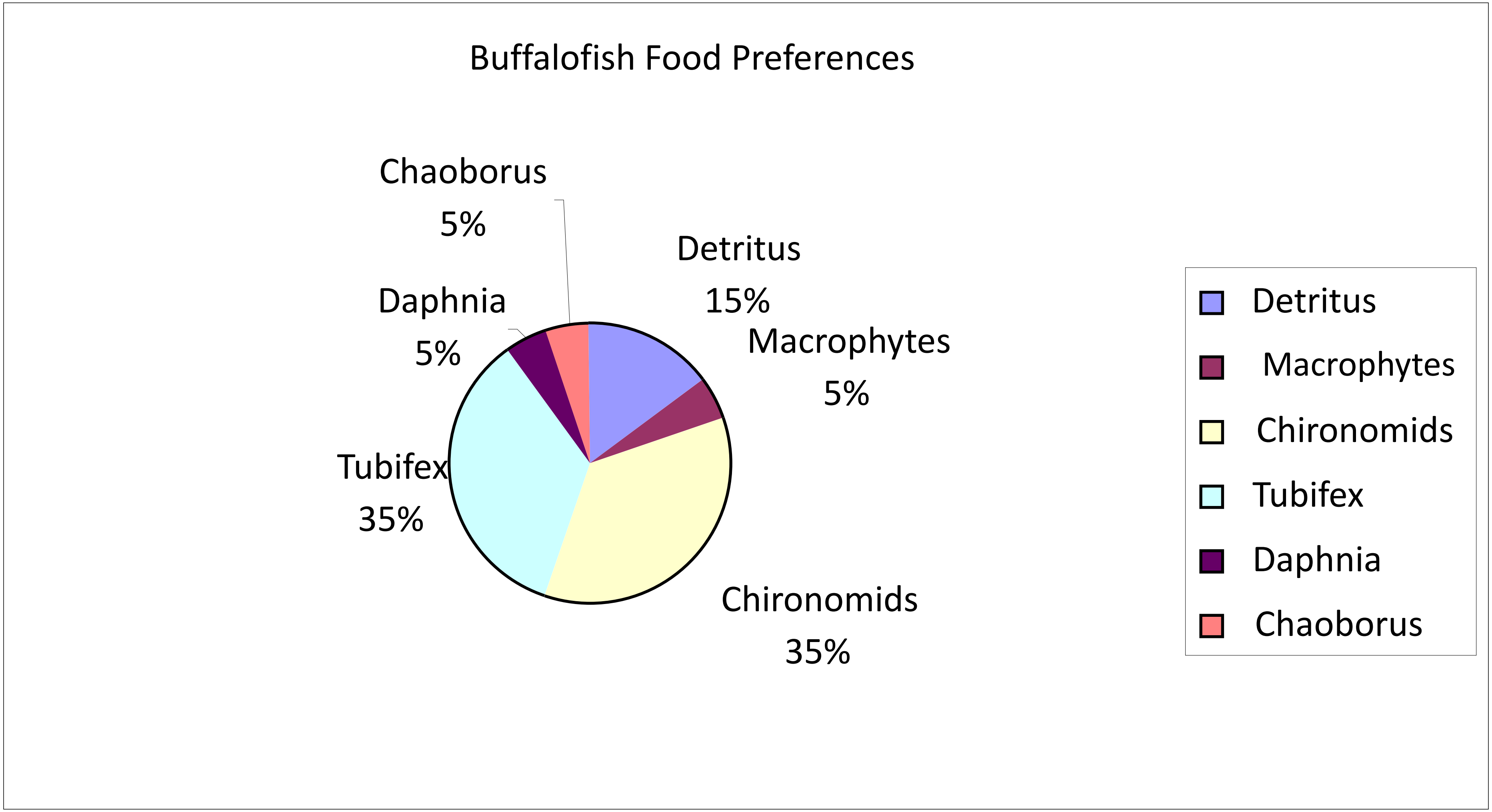
Tubifex in hypolimnion are tolerant of anoxia but stop feeding and slowly decline



Fish exhibit seasonal patterns based on food availability and temperature



Animals have food preferences, but can switch feeding based on availability



Foodweb Model specified as Trophic Matrix

Interactions are normalized to 100%

AQUATOX-- Trophic Interaction Matrix

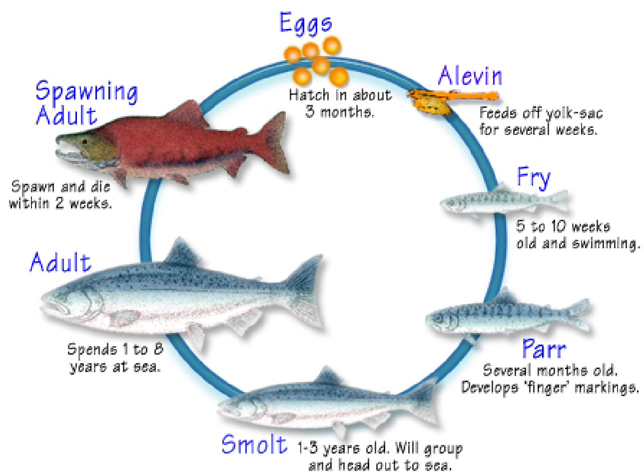
Preference percentages are initially normalized to 100% based on species in the simulation. Renormalize

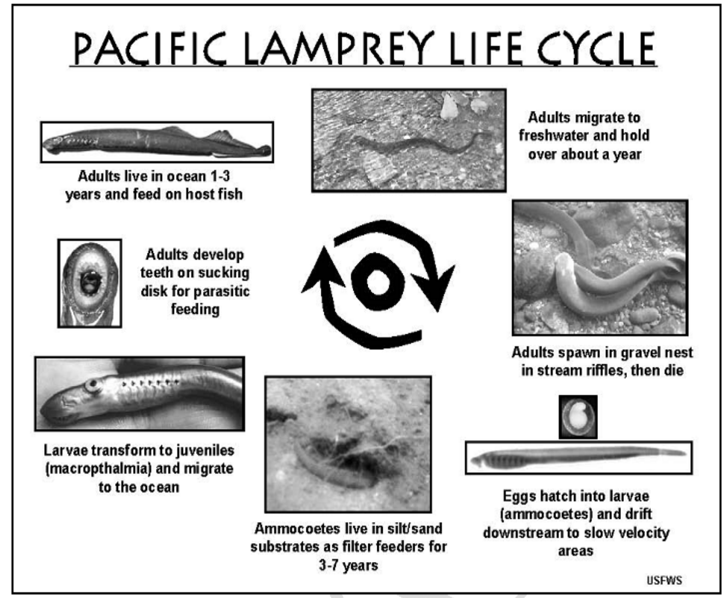
Show Preferences   Show Egestion Coefficients   Show Comments

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

Anadromous fish considerations

- Chinook Salmon and Pacific Lamprey Life Cycles





- Model Predictions:
  - Chemical bioaccumulation, onsite and off
    - Safe for consumption?
  - Nutrient effects on stream ecosystem
  - Toxicant effects on food web

Three Options for Anadromous Fish in AQUATOX

1. Migration into and out of system using loadings
   - Nutrient effects considered
   - Biomass coming and going must be specified
   - Toxicant loadings in returning fish must be specified
2. New Anadromous Fish model for Release 3.1
   - Size-class fish (juveniles and adults)
   - Off-site fish modeled in clean "holding tank"
   - Off-site location fairly simple (no toxic exposure)
3. Model all migration sites explicitly
   - Linked mode implementation, data requirements
   - Off-site toxicant uptake and loss explicitly modeled

Lab 3: Choice of Biota, Calibration of Glenwood Bridge, Lower Boise River, ID

- Check initial run with Rum River state variables
- Change Total Length for phytoplankton
- Change fish to reflect Boise R. species
- Minor calibration
- Discussion of model calibration goals

Model Performance

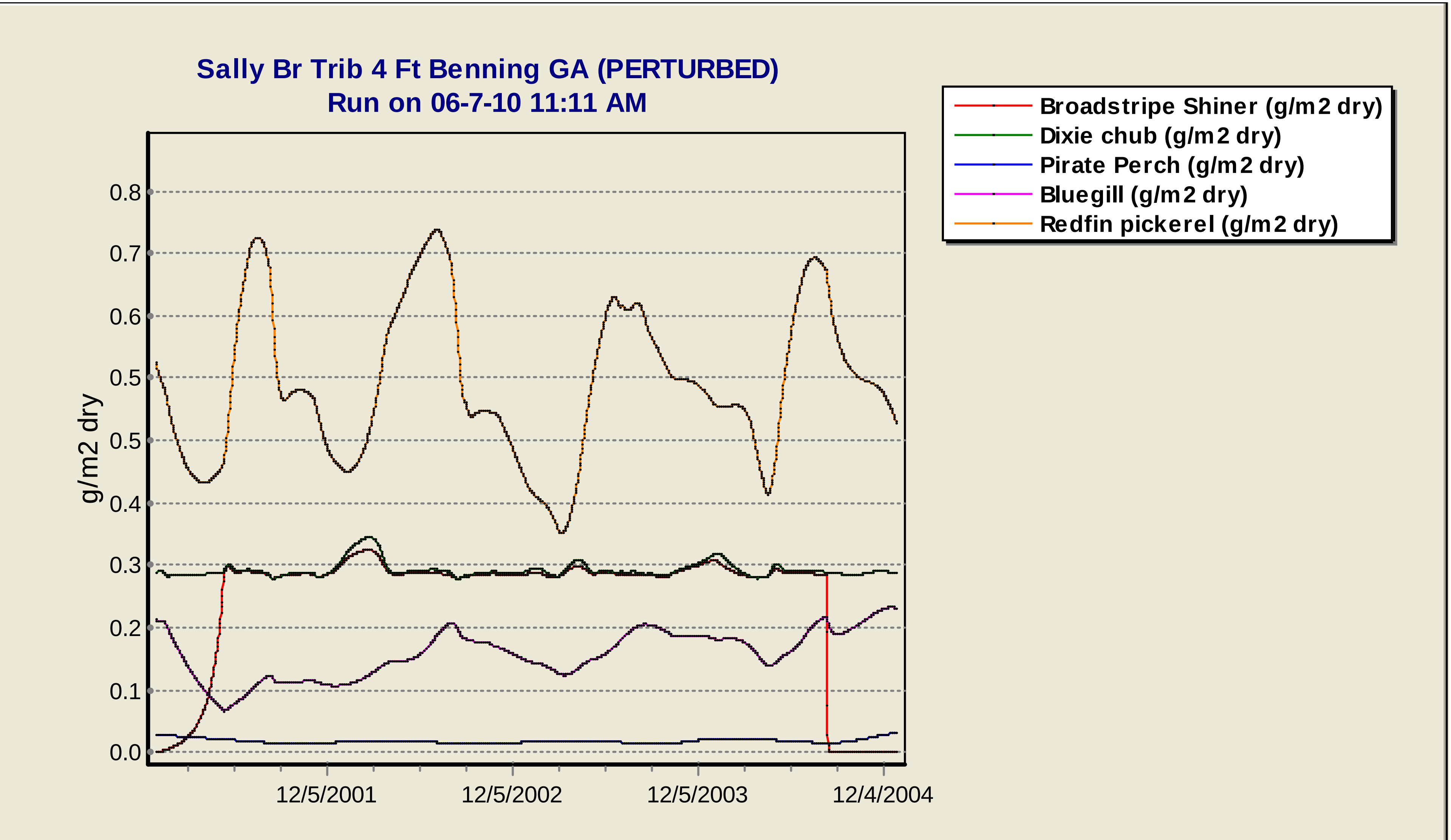
Sources of Parameter Values

Calibration Strategy for Minnesota Rivers

Weight-of-Evidence for Model Performance—Limited by Quantity and Quality of Data

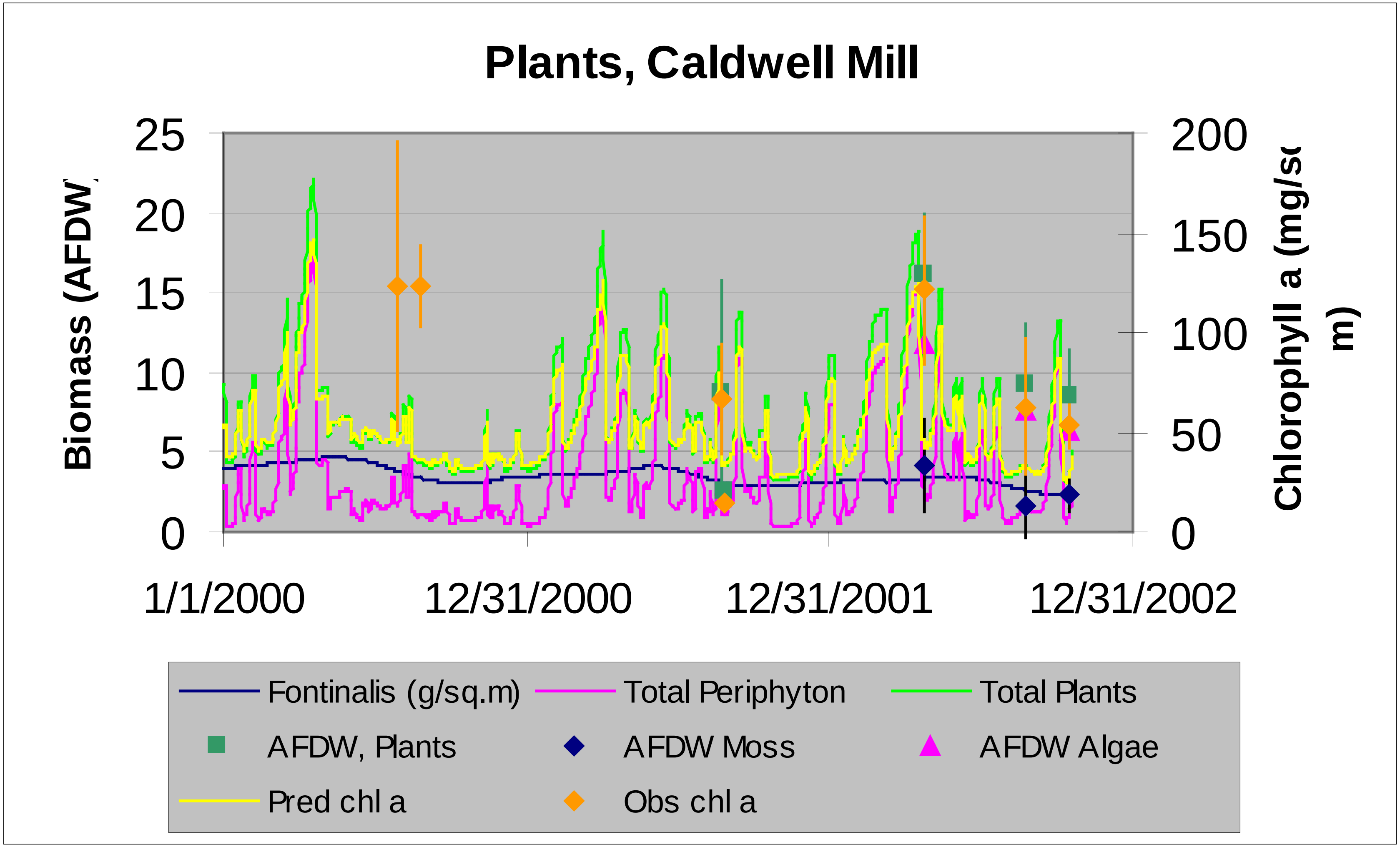
- Reasonable behavior based on general experience
- Visual inspection of data points and model plots
- Do model curves fall within error bands of data?
- Do point observations fall within model bounds obtained through uncertainty analysis?
- Regression of paired data and model results—is there concordance, bias?
- Comparison of mean data and mean model results
- Comparison of frequency distributions
  - Relative bias
  - F test
- Kolmogorov-Smirnov test of cumulative distributions

Reasonable ecosystem behavior test

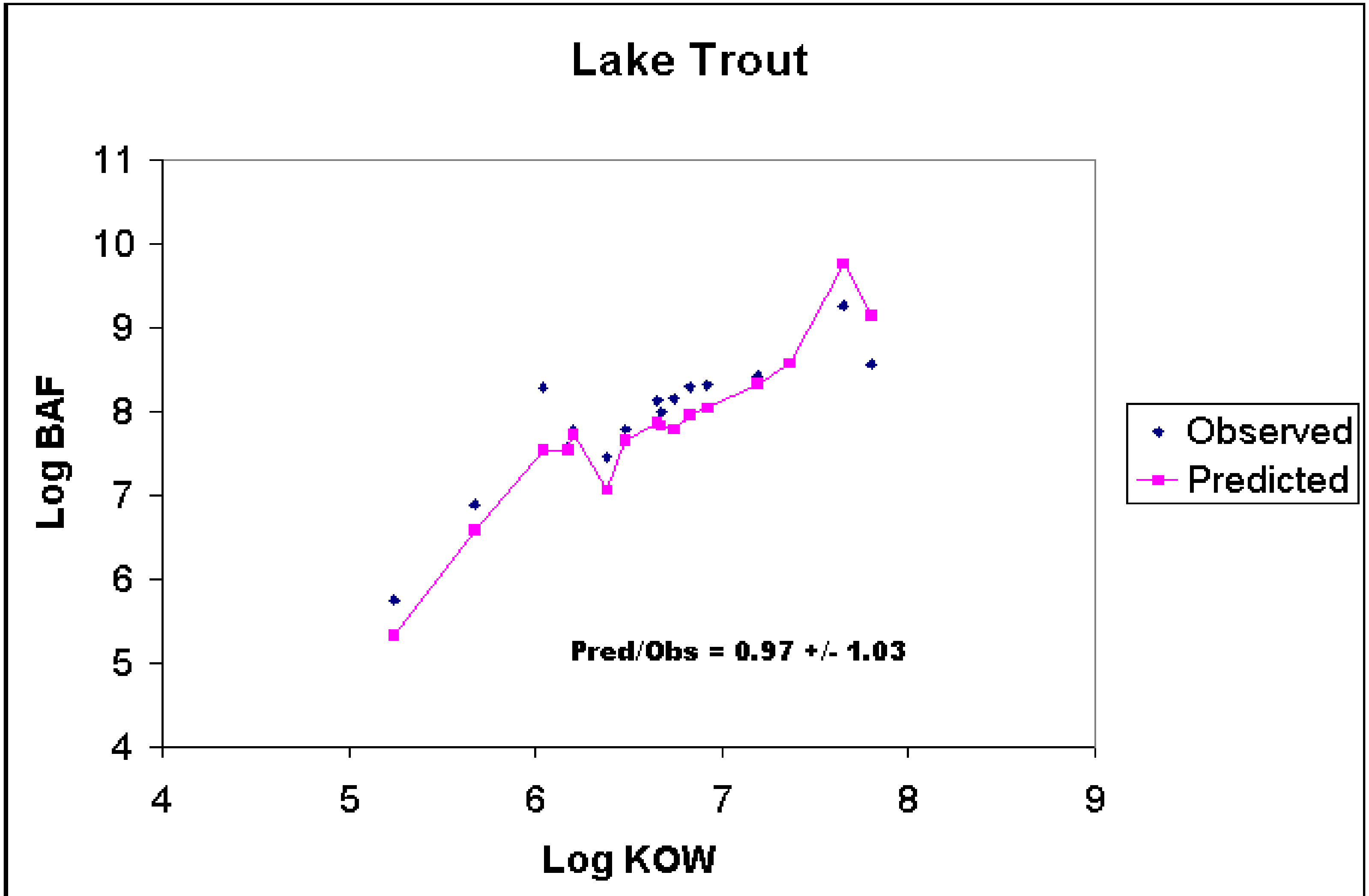


The model was calibrated for Caldwell Mill, Cahaba River, Ala.

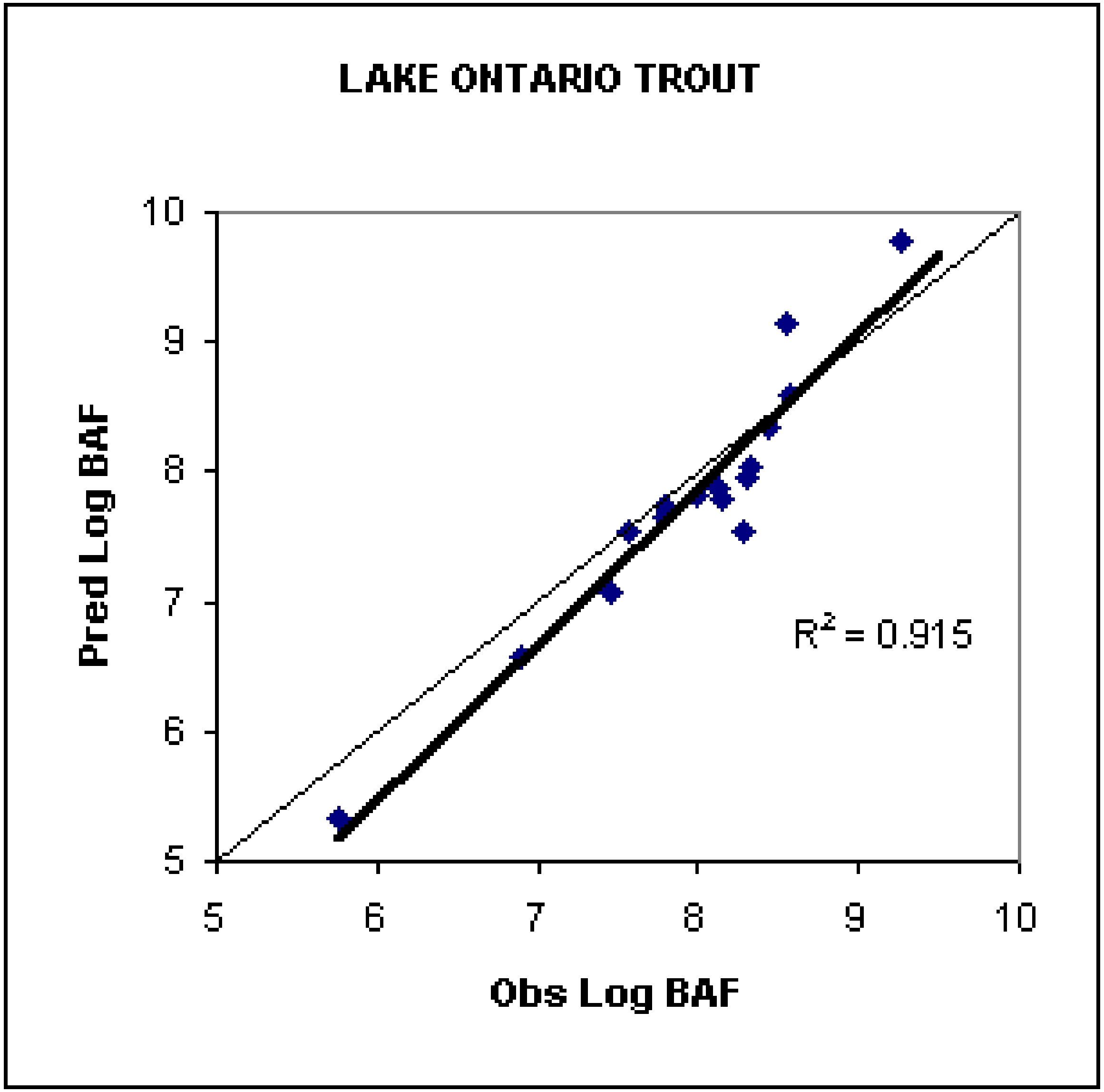
Once past the transient conditions of 2000, the fit was acceptable



AQUATOX validation with Lake Ontario PCB data



Regression of Lake Ontario observed and predicted PCB BAFs



Predicted/Observed Lake Ontario PCB BAFs

AQUATOX (Park, 1999)

	Phyto	Mysids	Trout
Mean	0.53	1.34	0.97
Std Dev	0.51	1.22	1.03

Gobas, 1993, model (results, Burkhard, 1998)

Mean	0.17	0.35	1.23
Std Dev	0.17	0.30	2.20

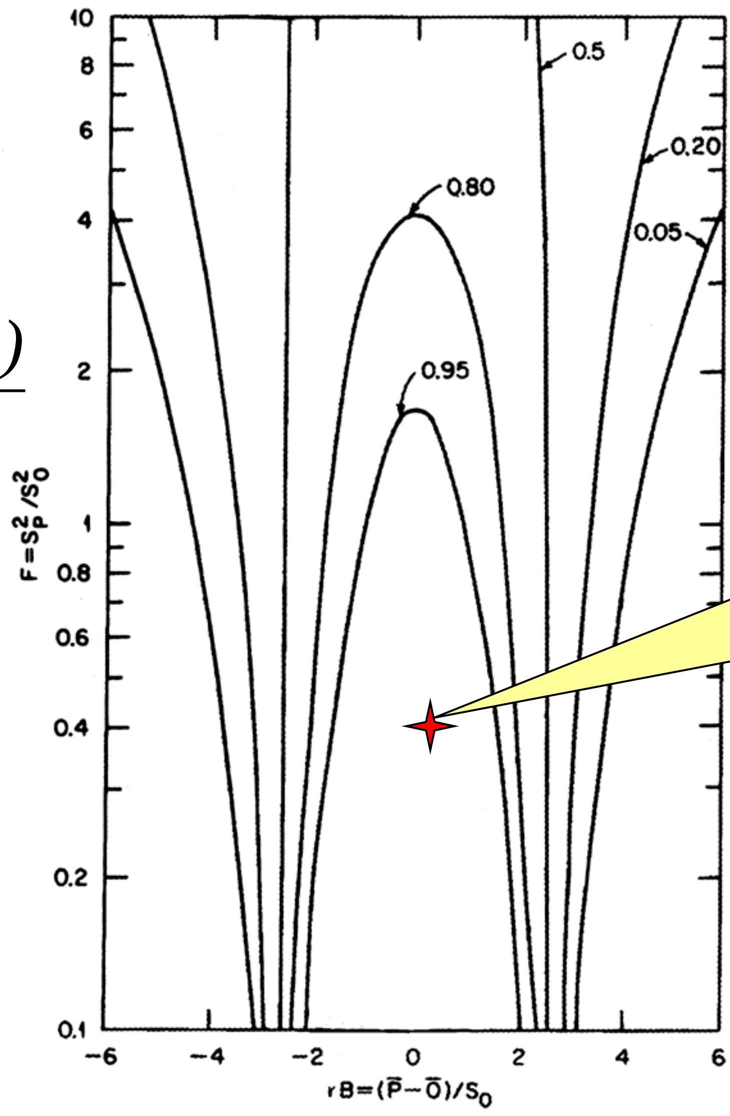
Thomann et al., 1992, model (results, Burkhard, 1998)

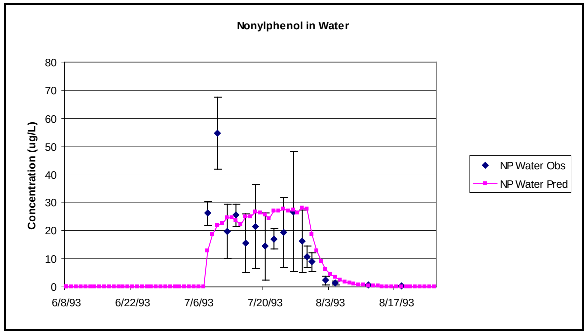
Mean	0.17	0.51	2.52
Std Dev	0.17	0.44	2.79

Statistical Comparison of Means and Variances

$$rB = \frac{(\overline{Pred} - \overline{Obs})}{S_{obs}}$$

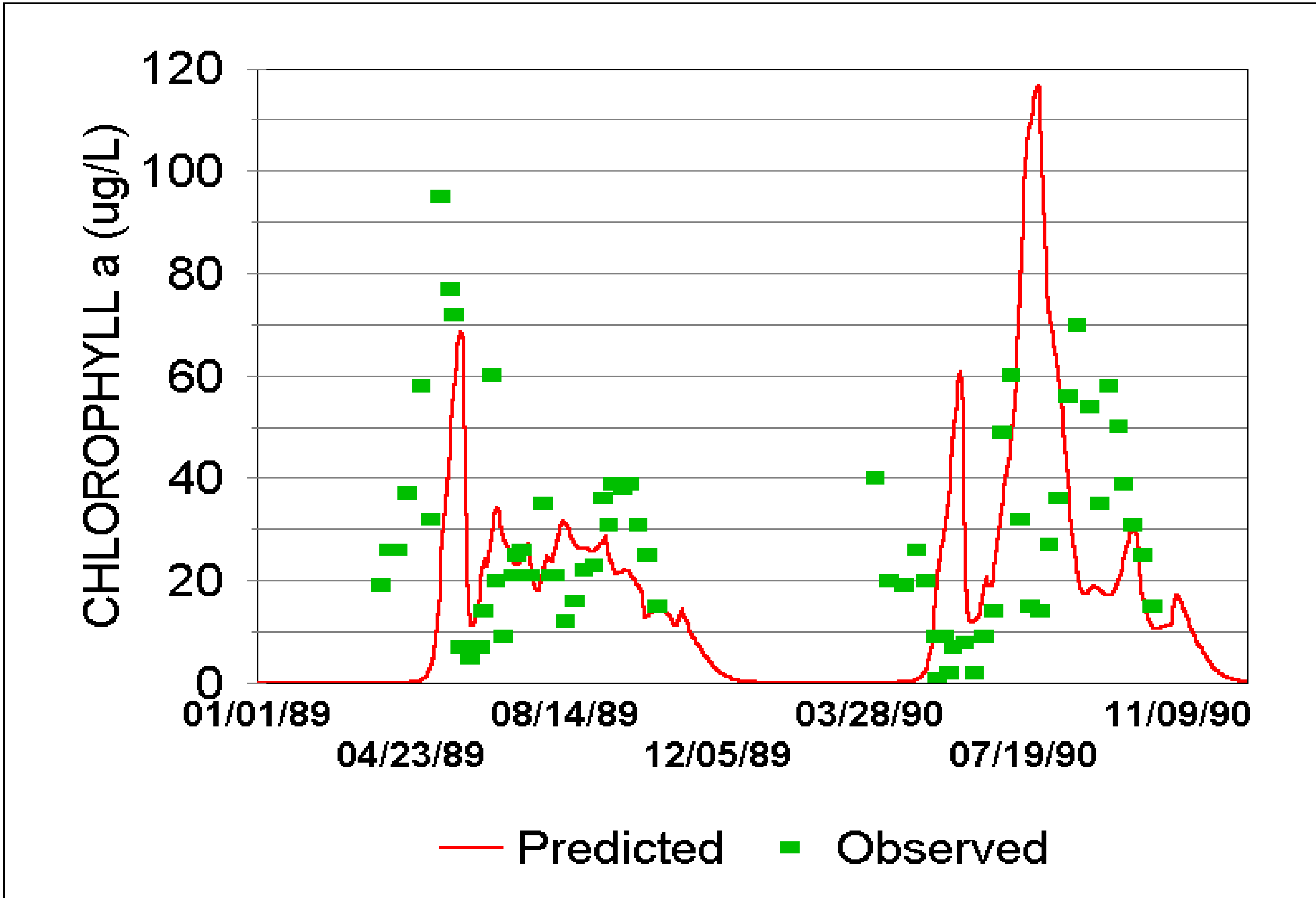
$$F = \frac{S^2_{pred}}{S^2_{obs}}$$



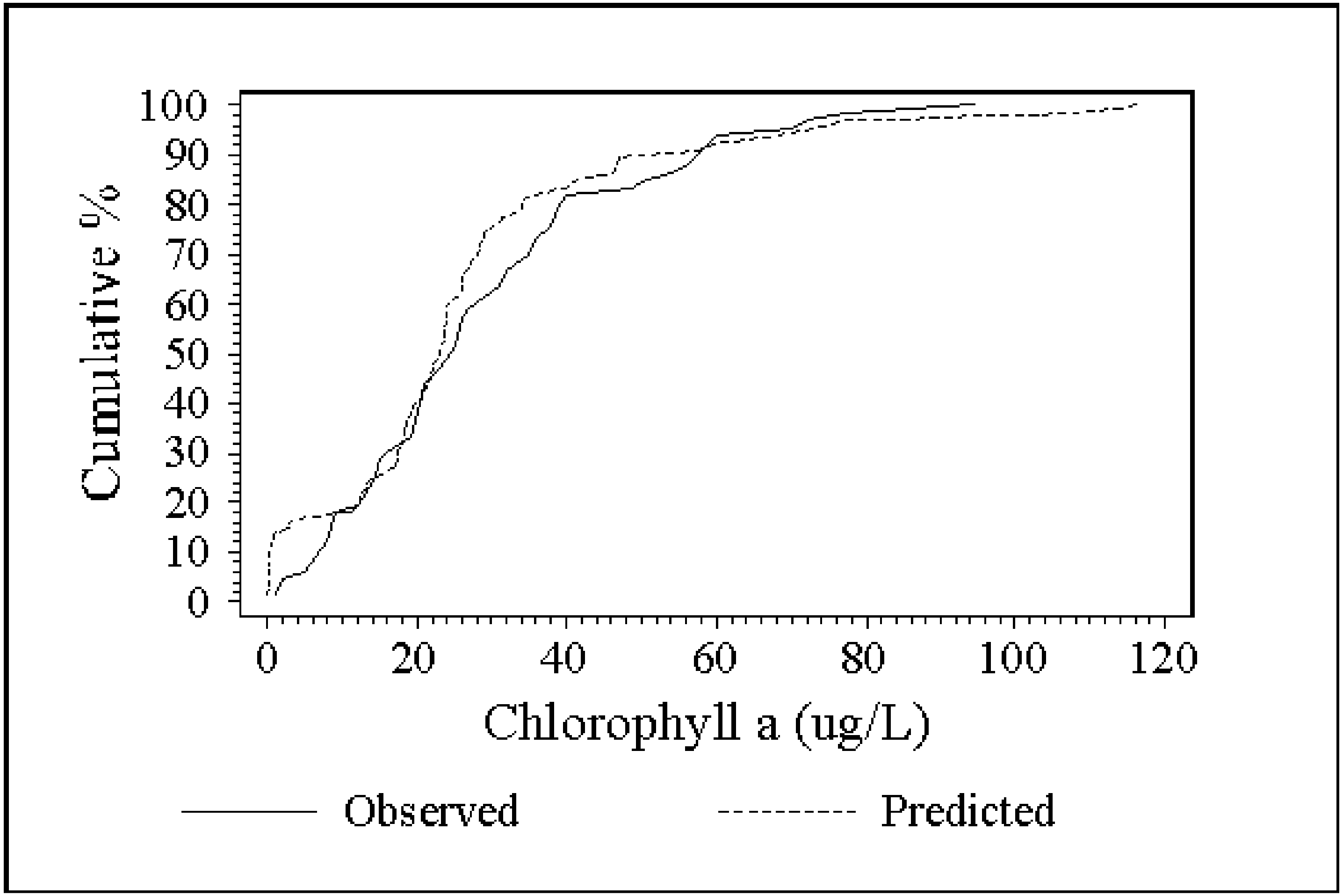


rB = 0.242, F = 0.400
pred & obs nonparametric statistical distributions are similar

Validation of AQUATOX with Lake Onondaga data—visual test

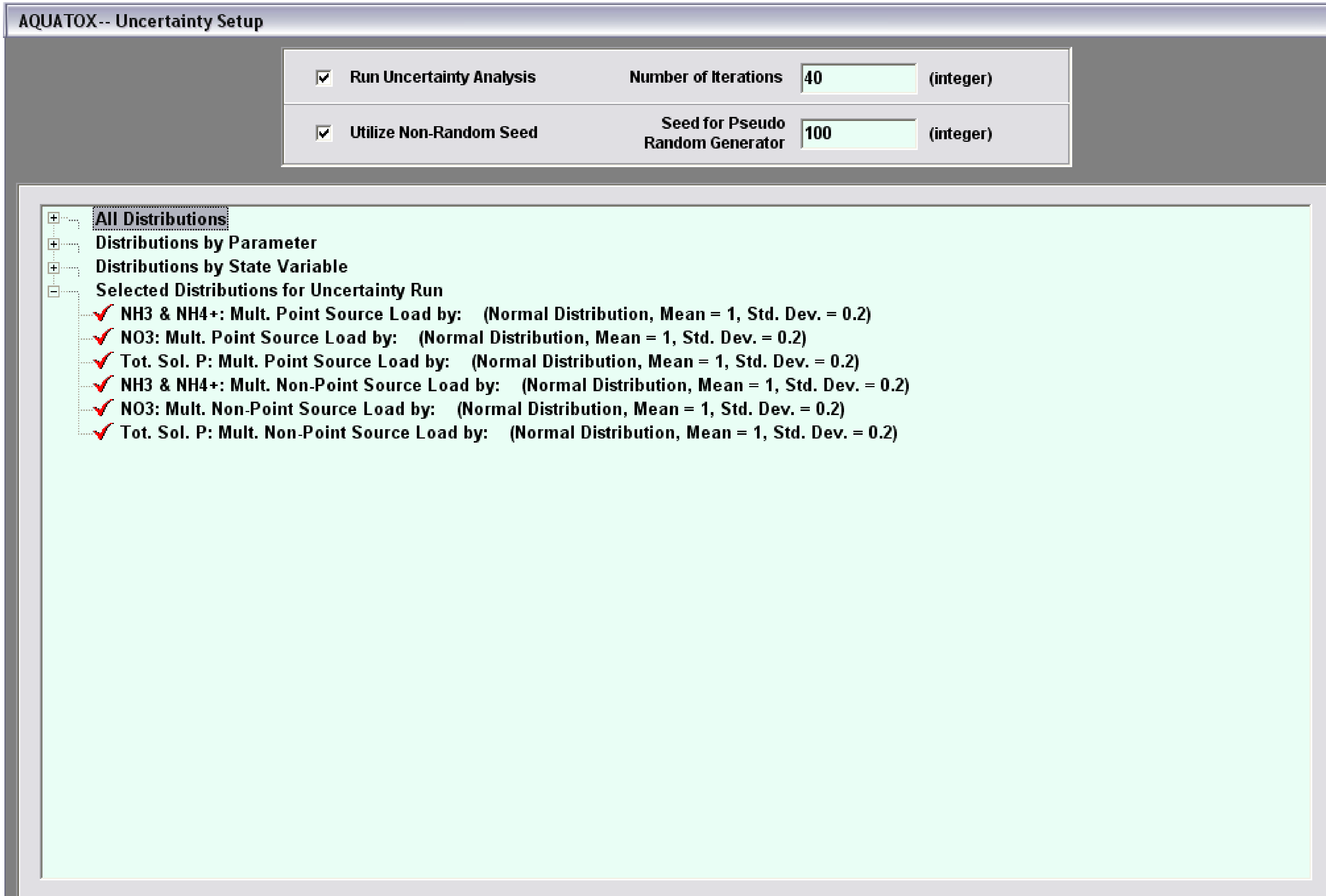


Validation with chlorophyll a in Lake Onondaga, NY

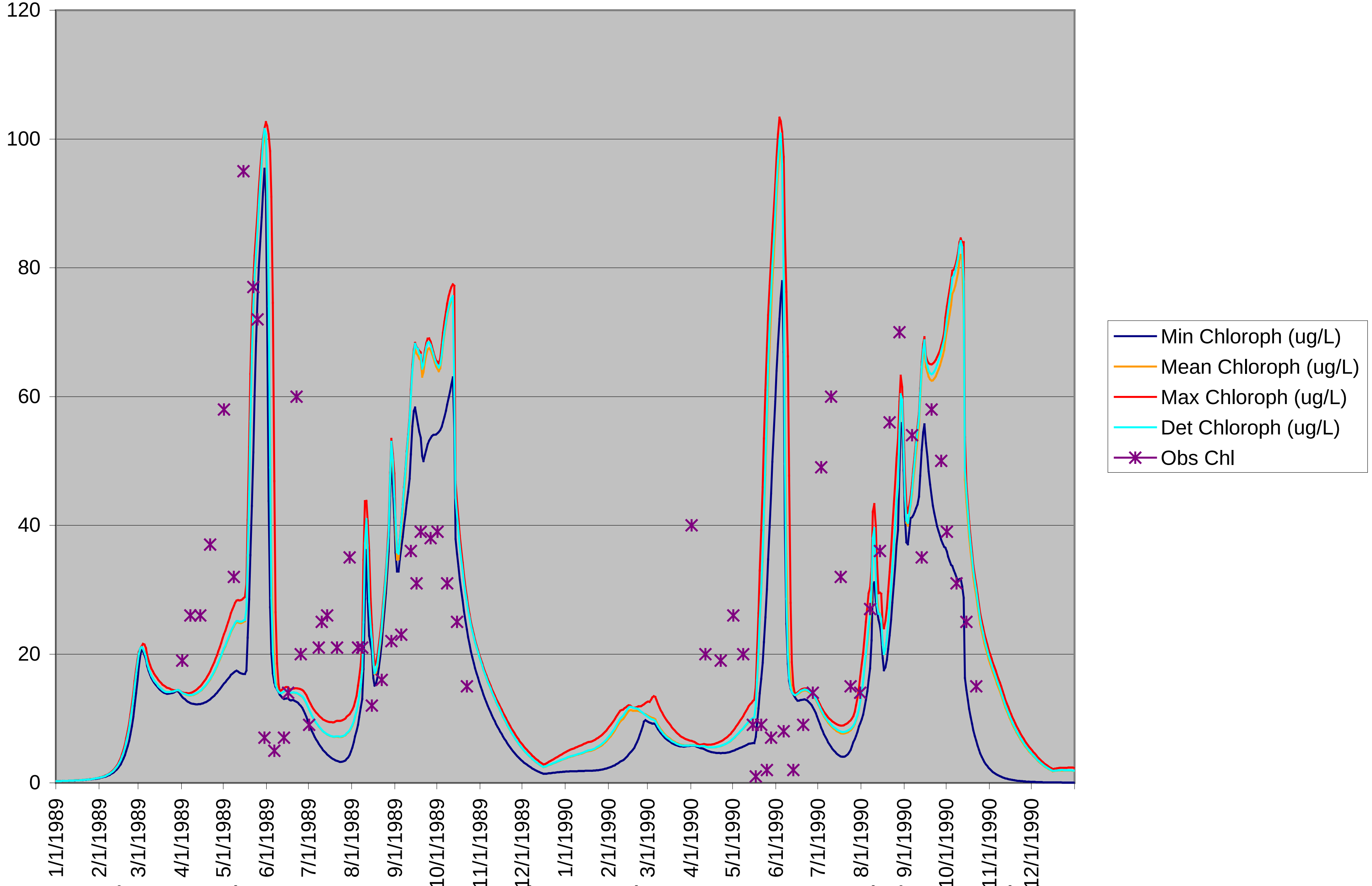


Kolmogorov-Smirnov p statistic = 0.319 (not sign. different)

We can run uncertainty analysis with distributions around nutrient loadings

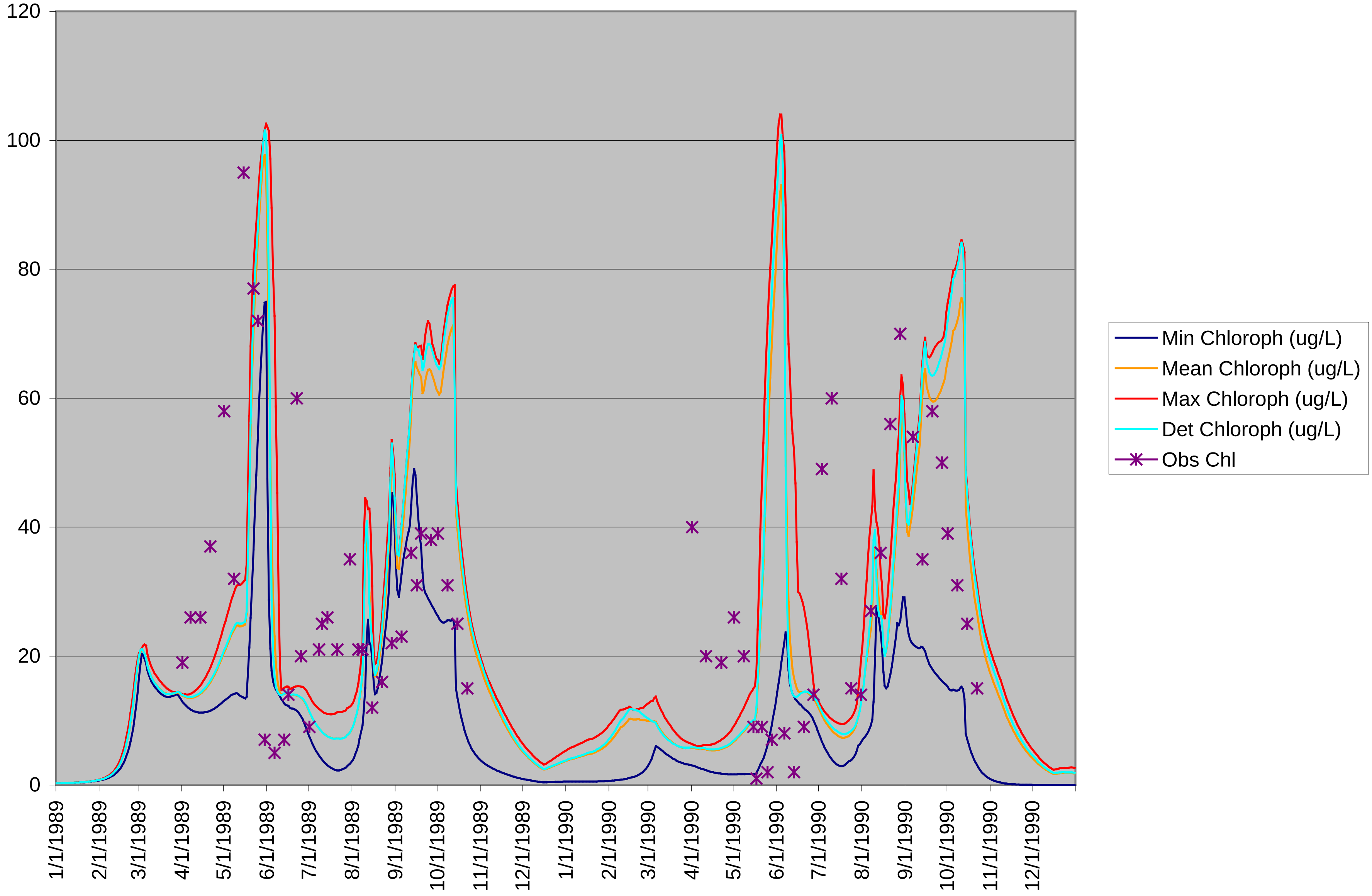


Plotting observed points with uncertainty bands for simulation suggests imperfect fit

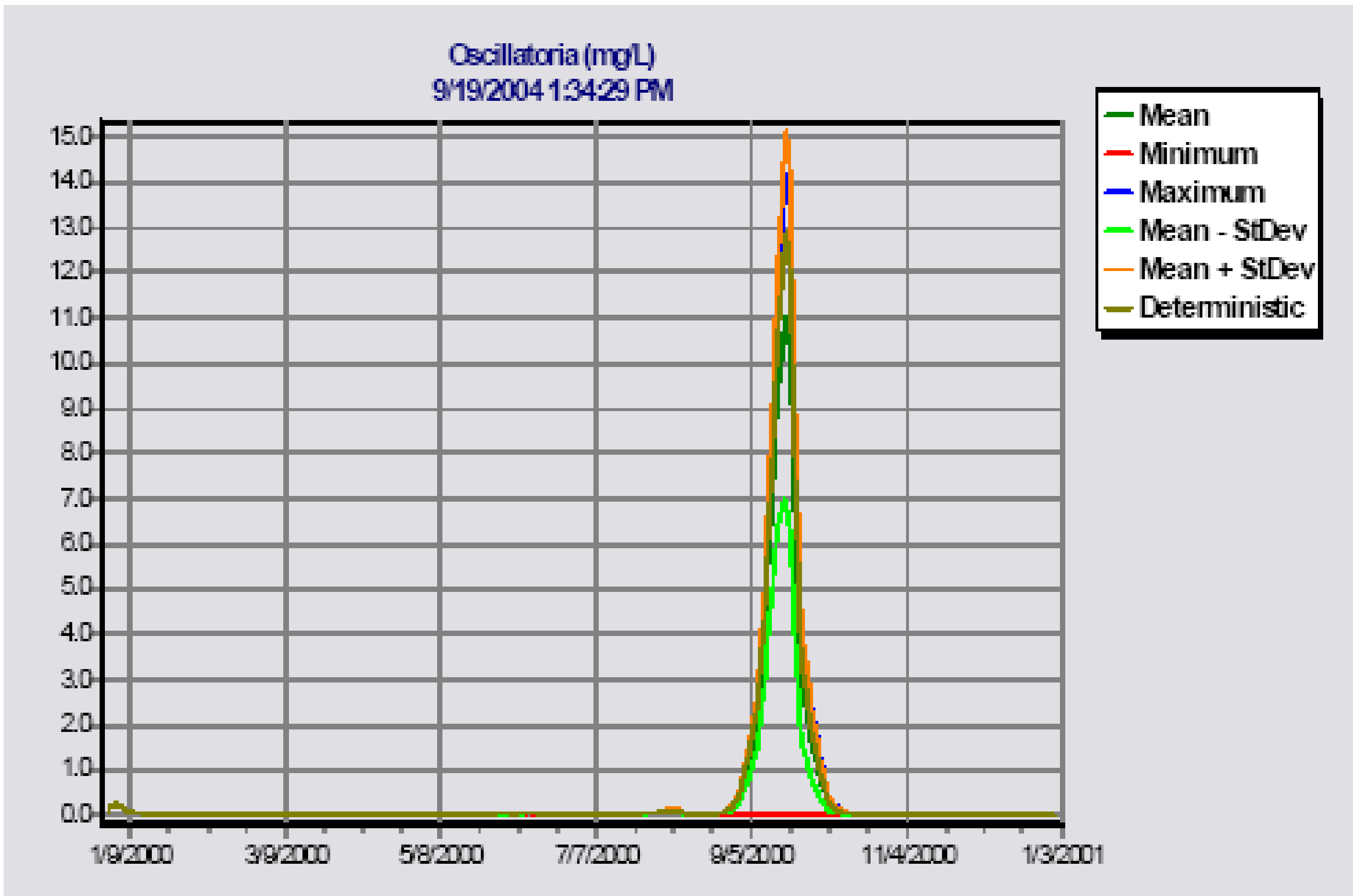


Lake Onondaga with more recent simulation than previous validation slide

With twice the standard deviations, more of the observed points fall within the envelope



Statistical sensitivity analysis of blue-green to saturated light parameter (74+-30)



AQUATOX

Data Sources for Parameter Values

One of the more challenging aspects of calibrating and applying AQUATOX to new waterbodies is finding appropriate values for the many biotic and chemical parameters contained in the model. The following are some of the data sources we have commonly used in the development of AQUATOX.

You will need Adobe Reader to view some of the files on this page. See EPA's PDF page to learn more.

Collins, Carol Desormeau, and Joseph H. Wlosinski. 1983. Coefficients for Use in the U.S. Army Corps of Engineers Reservoir Model, CE-QUAL-R1. Vicksburg, Miss.: Environmental Laboratory, U.S. Army Engineer Waterways Experiment Station.

- Part 1: Introduction and Phytoplankton parameters (PDF) (48 pp, 1.46MB)
- Part 2: Animal parameters (PDF) (44 pp, 1.29MB)
- Part 3: References (PDF) (33 pp, 1.01MB)

Leidy, G.R., and R.M. Jenkins. 1977. The Development of Fishery Compartments and Population Rate Coefficients for Use in Reservoir Ecosystem Modeling. Contract Rept. CR-Y-77-1, U.S. Army Engineer Waterways Experiment Station, Vicksburg Mississippi, 134 pp.

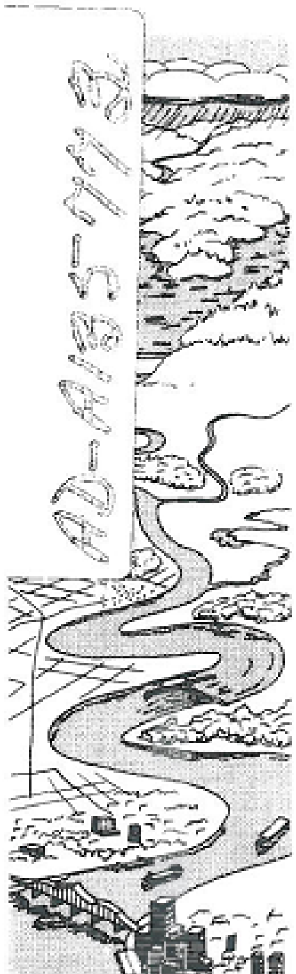
- Introductory material (PDF) (11 pp, 99MB)
- Parts 1- 3 (PDF) (63 pp, 1.12MB)
- Appendix A- F (PDF) (63 pp, 6.20MB)
- Appendix G-M (PDF) (37 pp, 2.35MB)
- Appendix N (PDF) (17 pp, 227KB)
- Appendix O - end (PDF) (45 pp, 502KB)

Leidy, G. R., and G. R. Ploskey. 1980. Simulation Modeling of Zooplankton and Benthos in Reservoirs: Documentation and Development of Model Constructs. Technical Report E-80-4 U.S. Army Engineer Waterways Experiment Station, Vicksburg, Miss.

- Introductory material, Parts 1-2 (PDF) (28 pp, 5.13MB)
- Part 3 (PDF) (79 pp, 20.3MB)
- Part 4 (PDF) (22 pp, 3.41MB)
- Part 5 (PDF) (34 pp, 5.09MB)
- Part 6 (PDF) (22 pp, 3.22MB)

Sources of parameters

US Army Corps of Engineers



ENVIRONMENTAL & WATER QUALITY
OPERATIONAL STUDIES

TECHNICAL REPORT E-83-15

COEFFICIENTS FOR USE IN THE U. S. ARMY CORPS OF ENGINEERS RESERVOIR MODEL, CE-QUAL-R1

by

Carol D. Collins and Joseph H. Wlosinski

Environmental Laboratory
U. S. Army Engineer Waterways Experiment Station
P. O. Box 631, Vicksburg, Miss. 39180

October 1983
Final Report

Approved For Public Release; Distribution Unlimited

Data Sources for Parameter Values

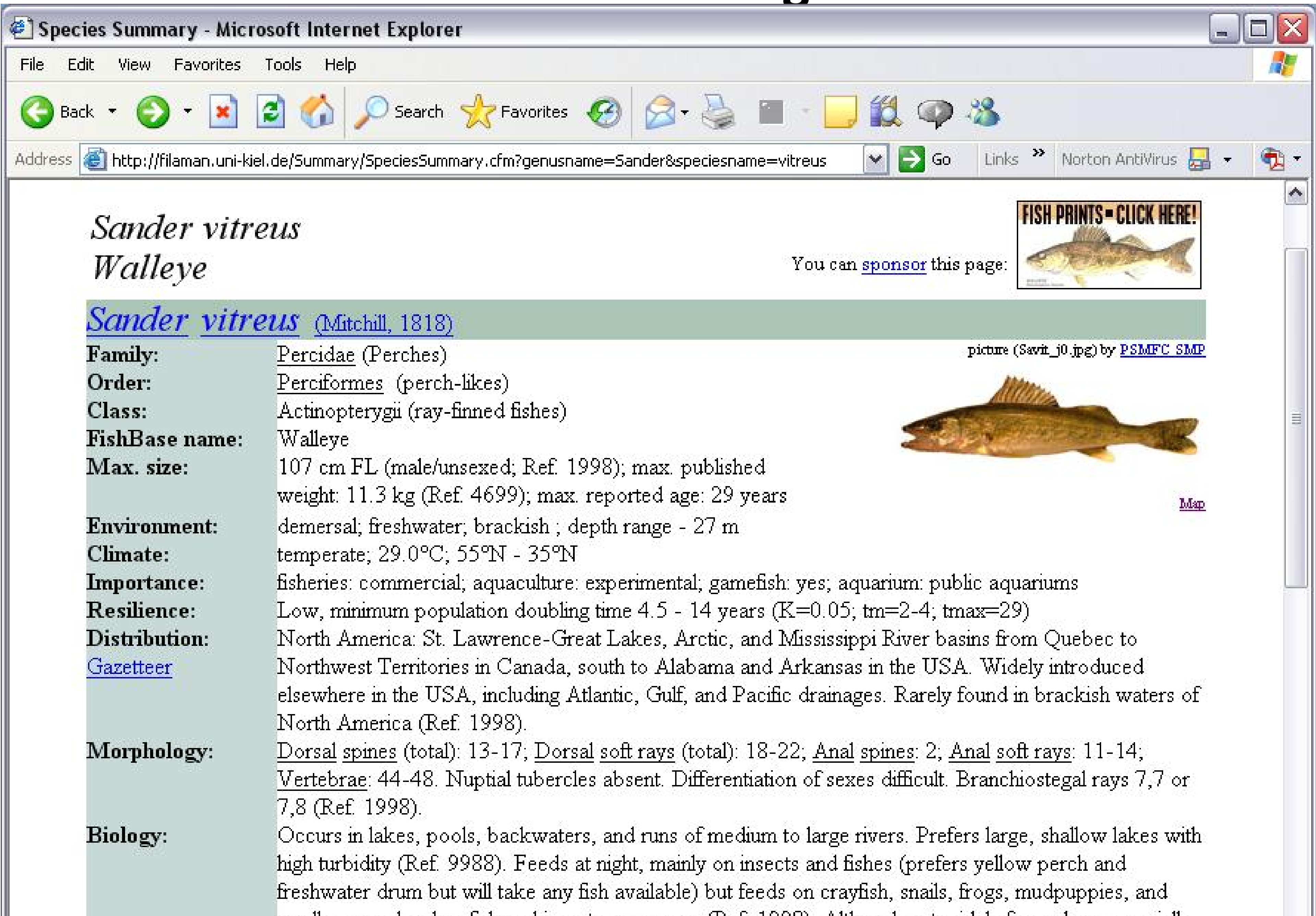
available for download from AQUATOX Web site
http://water.epa.gov/scitech/datait/models/aquatox/data.cfm

Table 7

Phytoplankton half-saturation coefficients for P limitation (mg/L)

SPECIES	PS2PO4	REFERENCE
Asterionella formosa	0.002	Holm and Armstrong 1981
Asterionella japonica	0.014	Thomas and Dodson 1968
Biddulphia sinensis	0.016	Quasim et al. 1973
Cerataulina bergonii	0.003	Finenko and Krupatikina 1974
Chaetoceros curvisetus	0.074-.105	Finenko and Krupatikina 1974
Chaetoceros socialis	0.001	Finenko and Krupatikina 1974
Chlorella pyrenoidosa	0.38-.475	Jeanjean 1969
Cyclotella nana	0.055	Fuhs et al. 1972
Cyclotella nana	0.001	Fogg 1973
Dinobryon cylindricum	0.076	Lehman (unpubl. data)
Dinobryon sociale var. americanum	0.047	Lehman (unpubl. data)
Euglena gracilis	1.52	Blum 1966
Freshwater phytoplankton	0.02-.075	Halmann and Stiller 1974
Microcystis aeruginosa	0.006	Holm and Armstrong 1981
Nitzschia actinastreoides	0.095	von Muller 1972
Pediastrum duplex	0.105	Lehman (unpubl. data)
Pithophora oedogonia	0.098	Spencer and Lembi 1981
Scenedesmus obliquus	0.002	Fogg 1973
Scenedesmus sp.	0.002-.05	Rhee 1973
Thalassiosira fluviatilis	0.163	Fogg 1973

Fishbase.org



Species Summary - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Search Favorites

Address http://filaman.uni-kiel.de/Summary/SpeciesSummary.cfm?genusname=Sander&speciesname=vitreus Go Links Norton AntiVirus

Sander vitreus
Walleye

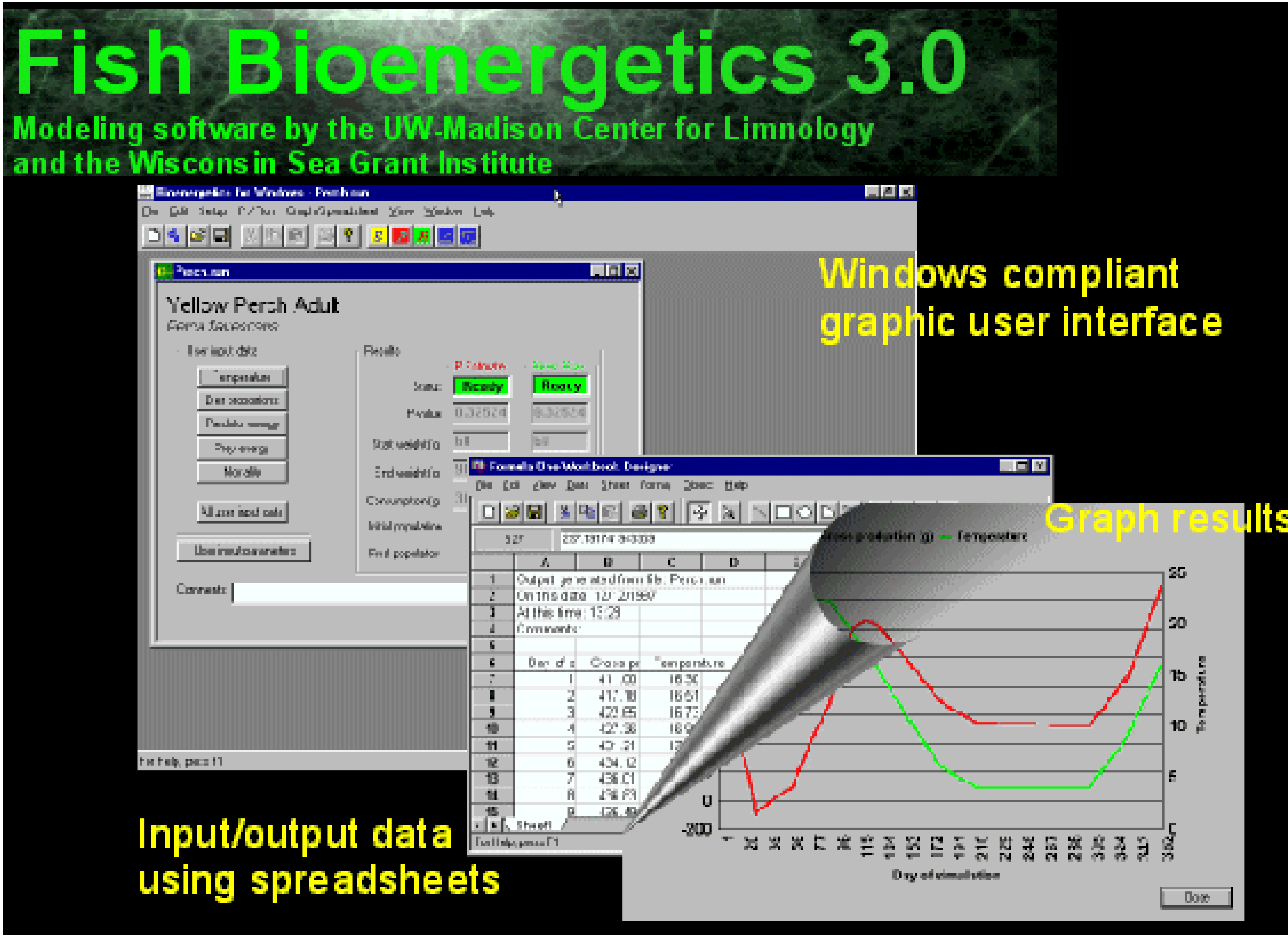
You can sponsor this page: FISH PRINTS = CLICK HERE!

Sander vitreus (Mitchill, 1818)

picture (Savit_j0.jpg) by PSMFC SMP

Map

Family:	Percidae (Perches)
Order:	Perciformes (perch-likes)
Class:	Actinopterygii (ray-finned fishes)
FishBase name:	Walleye
Max. size:	107 cm FL (male/unsexed; Ref. 1998); max. published weight: 11.3 kg (Ref. 4699); max. reported age: 29 years
Environment:	demersal; freshwater; brackish ; depth range - 27 m
Climate:	temperate; 29.0°C; 55°N - 35°N
Importance:	fisheries: commercial; aquaculture: experimental; gamefish: yes; aquarium: public aquariums
Resilience:	Low, minimum population doubling time 4.5 - 14 years (K=0.05; tm=2-4; tmax=29)
Distribution: Gazetteer	North America: St. Lawrence-Great Lakes, Arctic, and Mississippi River basins from Quebec to Northwest Territories in Canada, south to Alabama and Arkansas in the USA. Widely introduced elsewhere in the USA, including Atlantic, Gulf, and Pacific drainages. Rarely found in brackish waters of North America (Ref. 1998).
Morphology:	Dorsal spines (total): 13-17; Dorsal soft rays (total): 18-22; Anal spines: 2; Anal soft rays: 11-14; Vertebrae: 44-48. Nuptial tubercles absent. Differentiation of sexes difficult. Branchiostegal rays 7,7 or 7,8 (Ref. 1998).
Biology:	Occurs in lakes, pools, backwaters, and runs of medium to large rivers. Prefers large, shallow lakes with high turbidity (Ref. 9988). Feeds at night, mainly on insects and fishes (prefers yellow perch and freshwater drum but will take any fish available) but feeds on crayfish, snails, frogs, mudpuppies, and



Fish Bioenergetics 3.0
Modeling software by the UW-Madison Center for Limnology
and the Wisconsin Sea Grant Institute
Windows compliant
graphic user interface
Yellow Perch Adult
Graph results
Input/output data
using spreadsheets
Day of simulation

ECOTOX (EPA Toxicity Database)

U.S. Environmental Protection Agency

ECOTOX Database

Recent Additions | Contact Us | Print Version   Search: [ ] GO

EPA Home > ECOTOX

About ECOTOX / Help

Quick Database Query

Advanced Database Query

Frequently Asked Questions

Data Download

The ECOTOX (ECOTOXicology) database provides single chemical toxicity information for aquatic and terrestrial life. ECOTOX is a useful tool for examining impacts of chemicals on the environment. Peer-reviewed literature is the primary source of information encoded in the database. Pertinent information on the species, chemical, test methods, and results presented by the author(s) are abstracted and entered into the database. Another source of test results is independently compiled data files provided by various United States and International government agencies. Prior to using ECOTOX, you should visit the "About ECOTOX/Help" section of this Web Site. In addition, it is recommended that you consult the original scientific paper to ensure an understanding of the context of the data retrieved from the ECOTOX database.

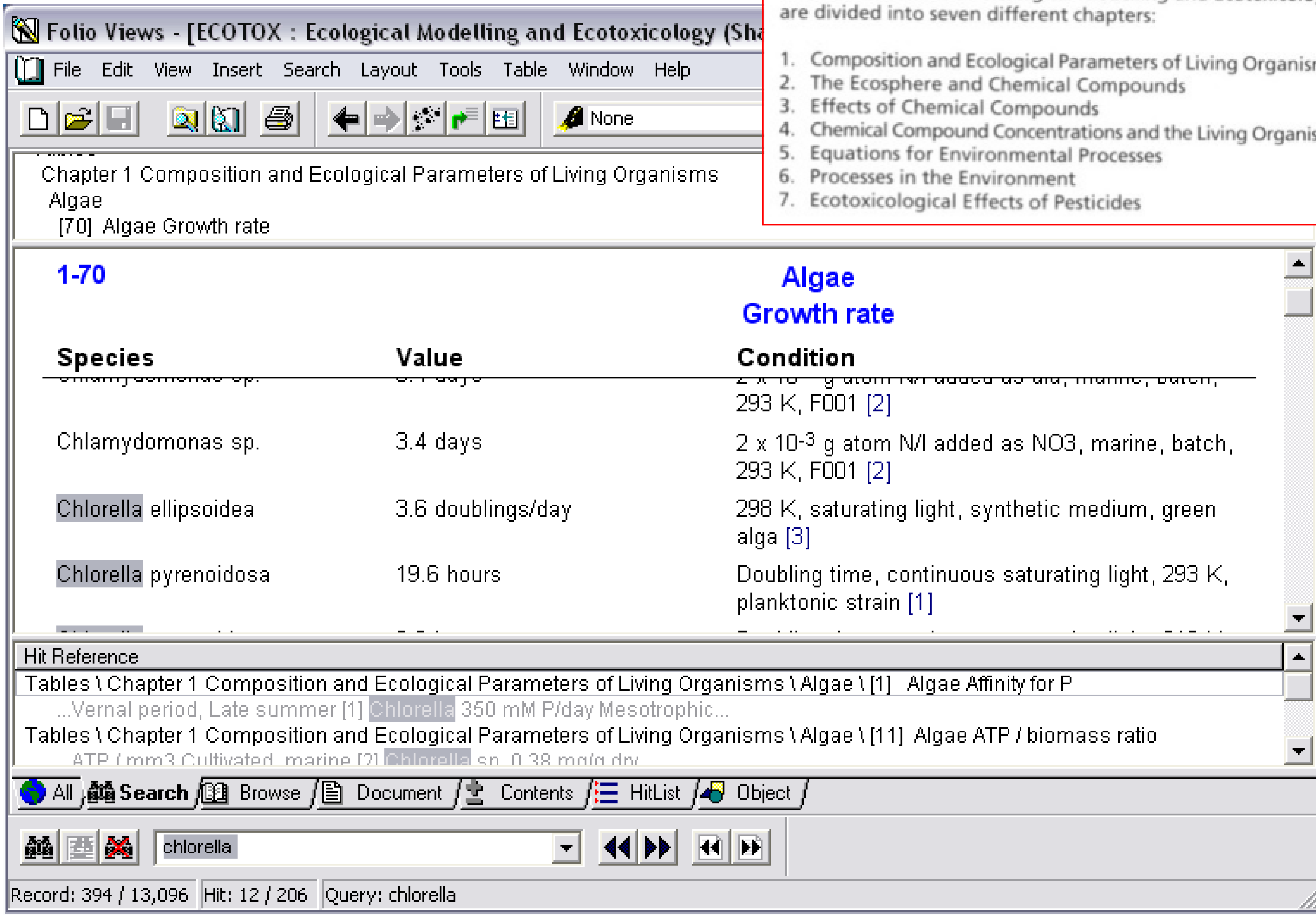
If you use a popup blocker program, ECOTOX reports, help and browse features will not display. Please add the ECOTOX web site to your popup browser exception list to ensure full usability.

Office of Research and Development | National Health and Environmental Effects Research Laboratory | Mid-Continent Ecology Division

ECOTOX (Elsevier product)

The tables in *ECOTOX: Ecological Modelling and Ecotoxicology* are divided into seven different chapters:

1. Composition and Ecological Parameters of Living Organisms
2. The Ecosphere and Chemical Compounds
3. Effects of Chemical Compounds
4. Chemical Compound Concentrations and the Living Organism
5. Equations for Environmental Processes
6. Processes in the Environment
7. Ecotoxicological Effects of Pesticides

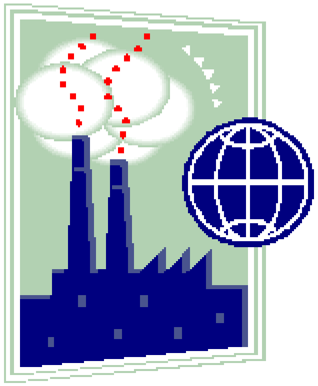


Search
Main ARS Site
Enter Keywords Go
This site only
Advanced Search
Products & Services
Publications
Public Databases and Programs
ARS Cotton Database
BARC Weather Stations
Pesticide Properties Database
Global Change Master Directory

Products & Services

PPDB

The ARS Pesticide Properties Database



Technical Contact: Don Wauchope
ARS, Southeast Watershed Res. Lab.
don@tifton.cpes.peachnet.edu

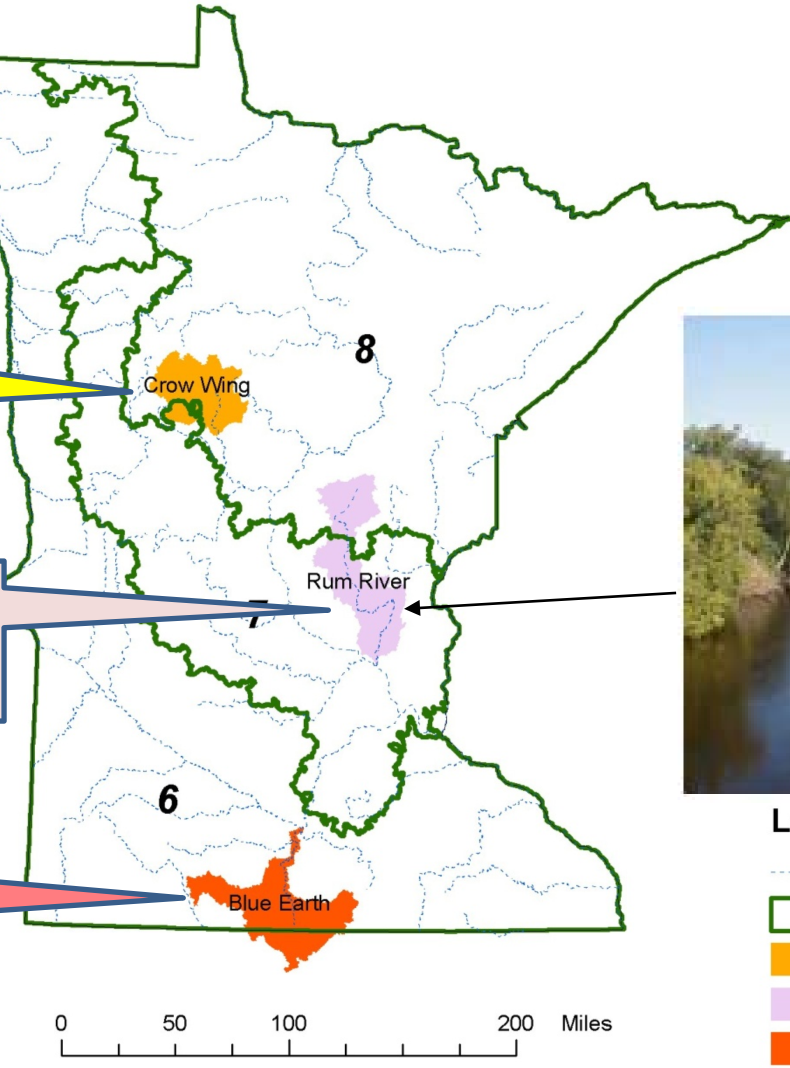
Page Modified: 01/25/2005

Minnesota Streams Calibration

Low nutrient
low turbidity

Moderate nutrient
moderate turbidity

High nutrient
high turbidity



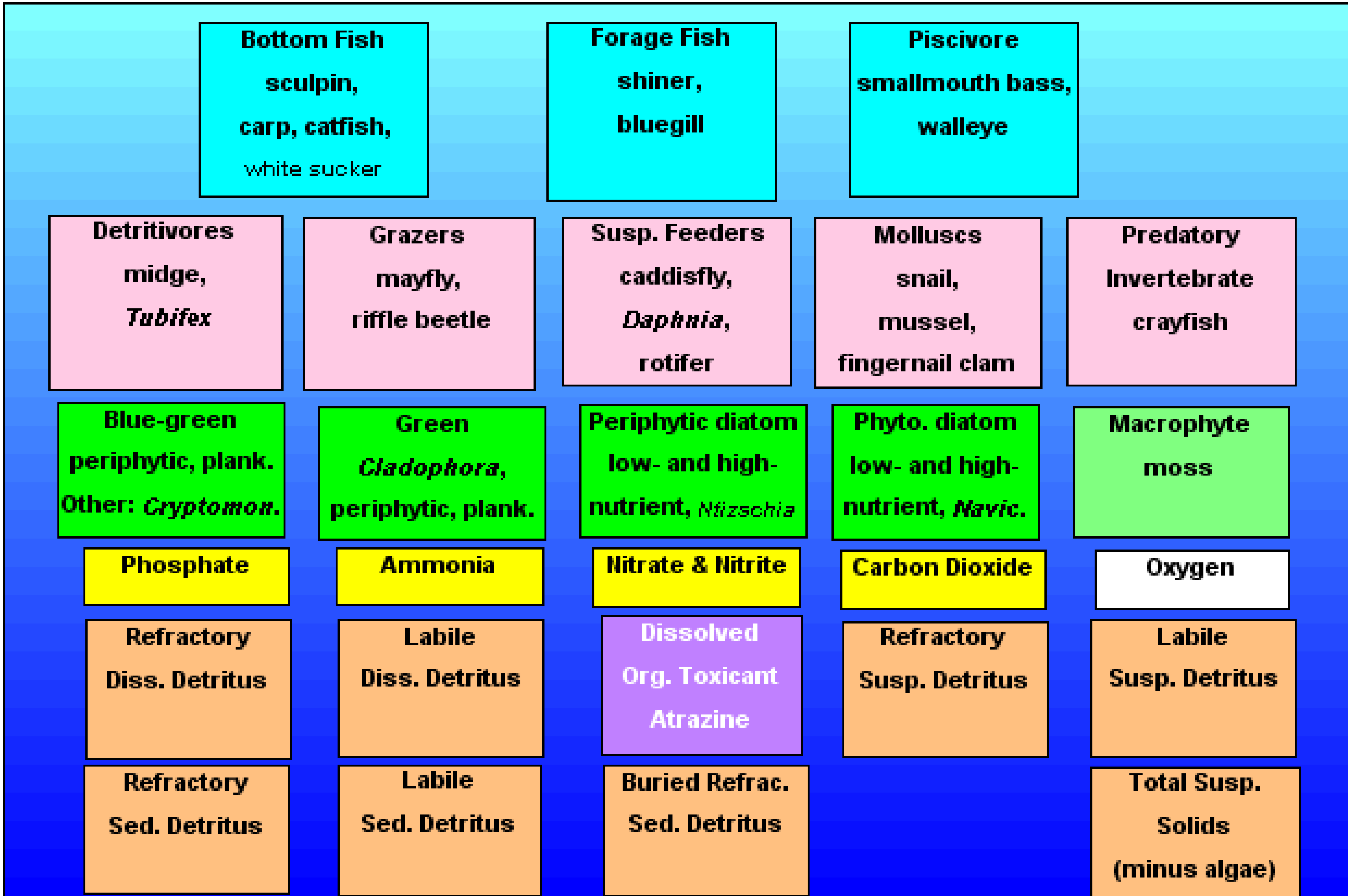
Calibration Strategy for Minnesota Rivers

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

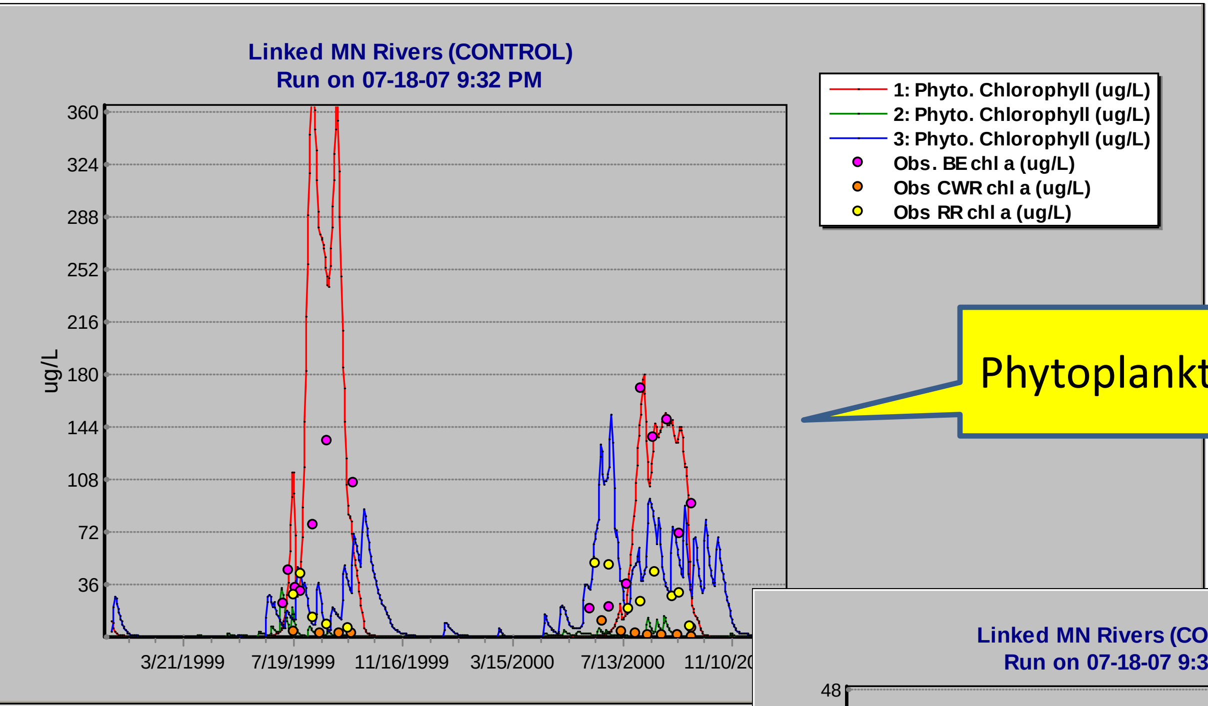
Rum River, Minnesota

(Heiskary & Markus, 2003)

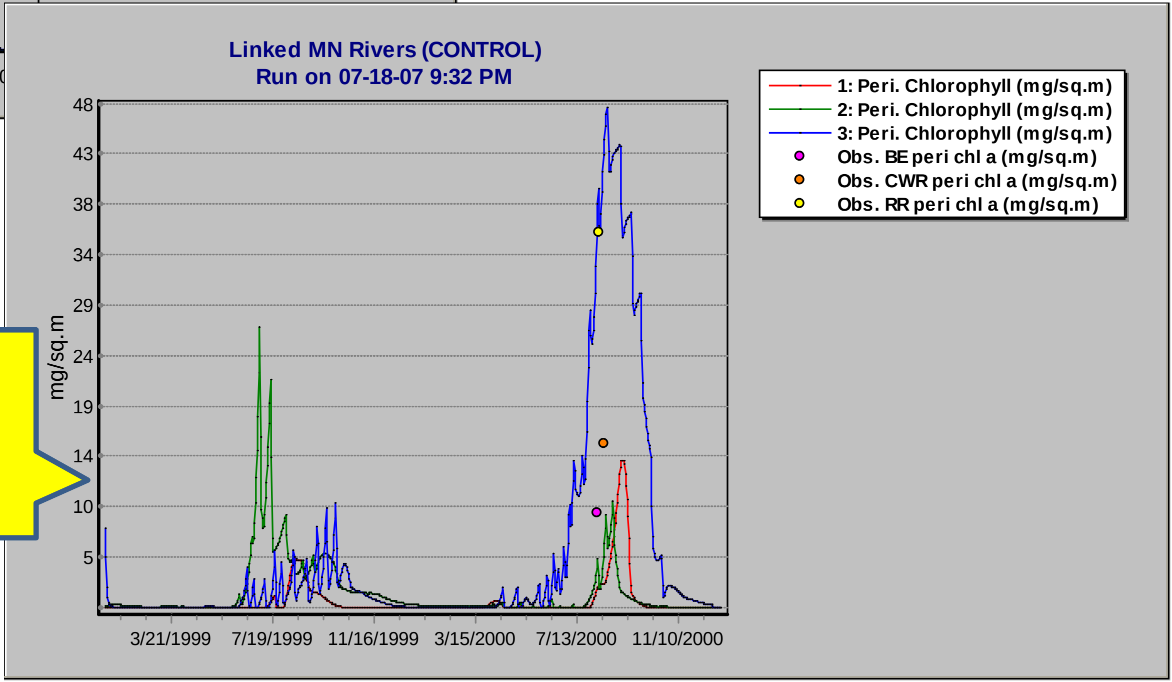
State variables in MN rivers simulations



Chlorophyll *a* Trends in MN Rivers

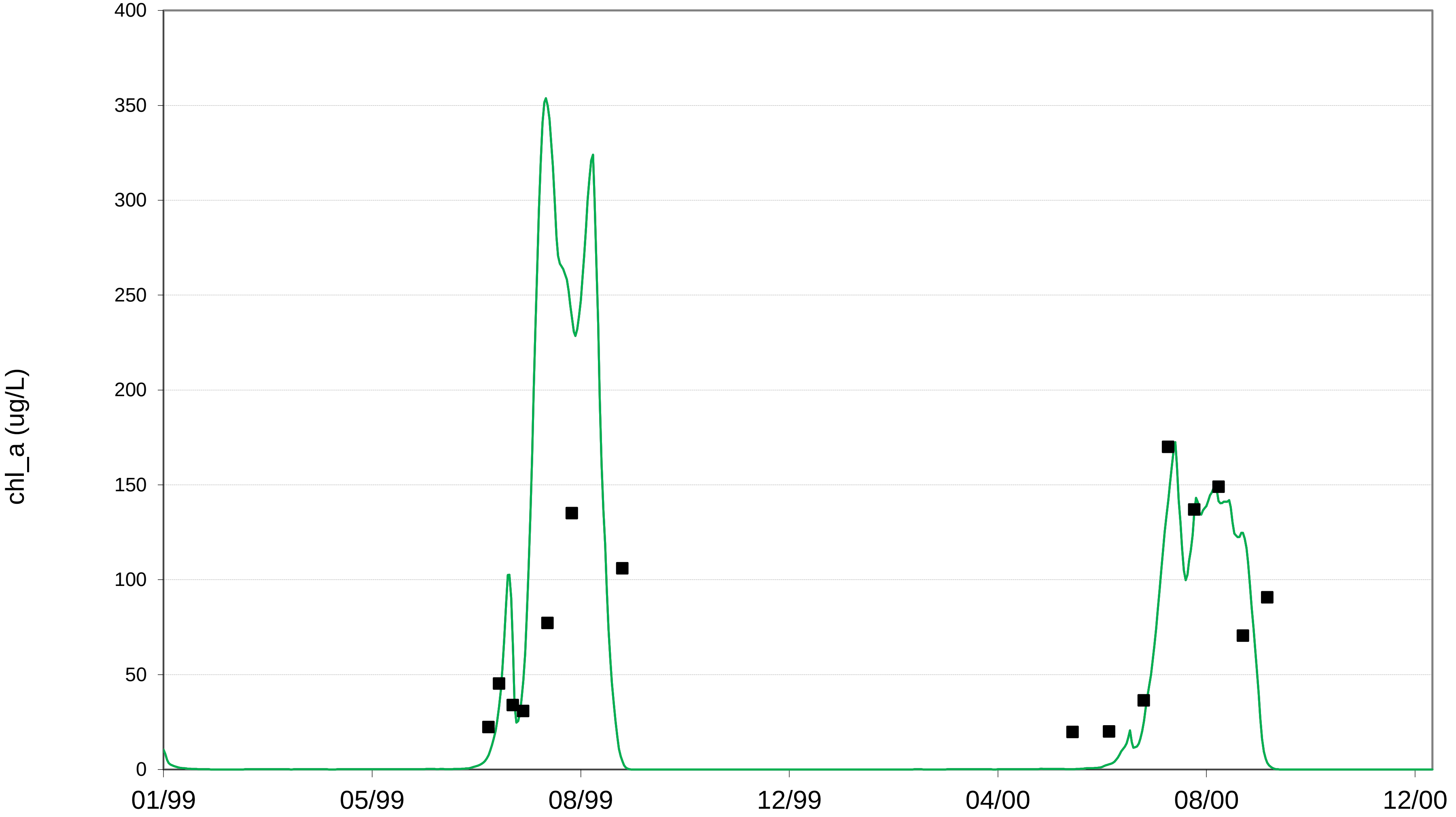


Phytoplankton follow nutrient trend

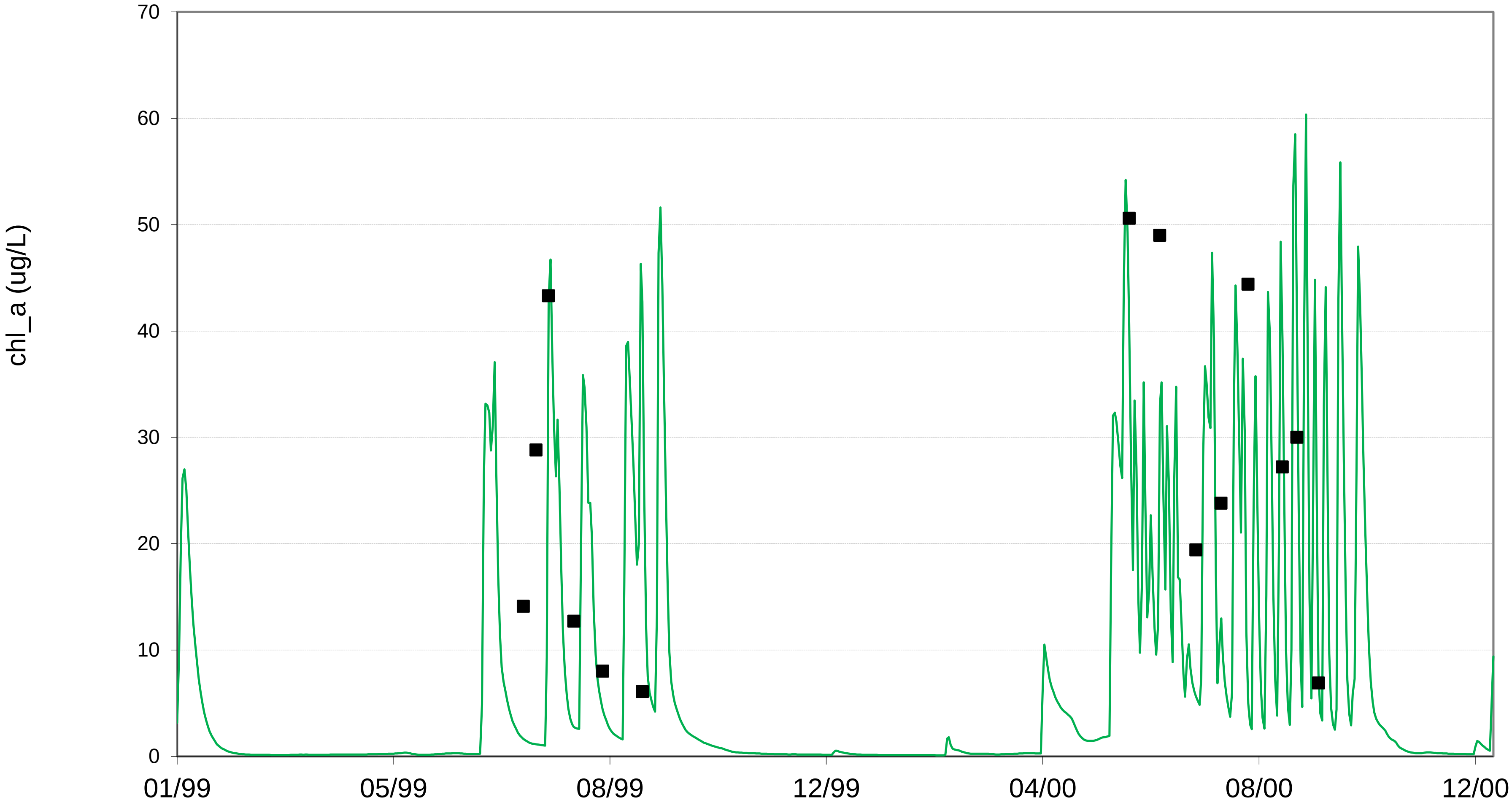


Periphyton reach maximum in Rum River with moderate nutrients and turbidity

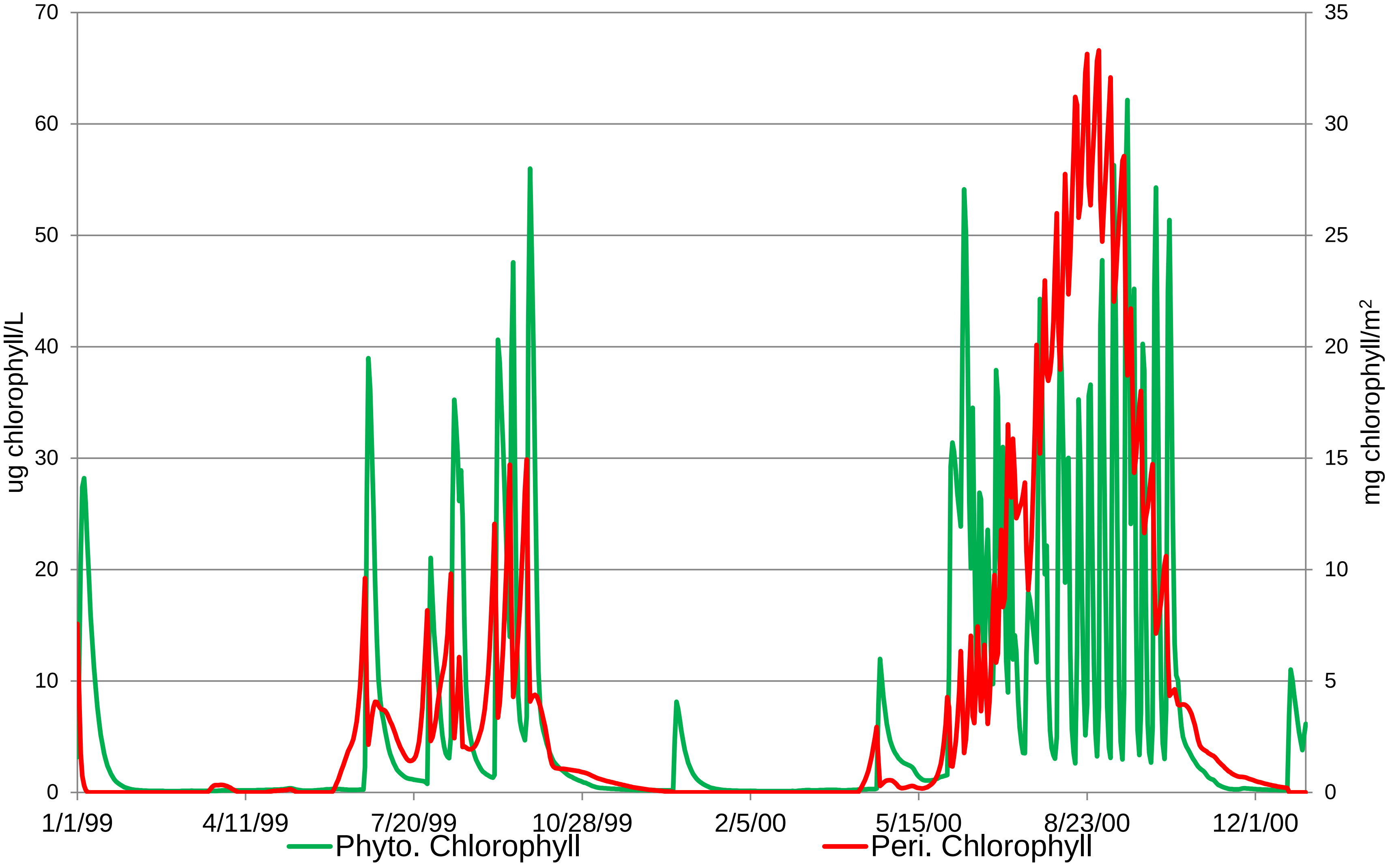
Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Blue Earth River at mile 54



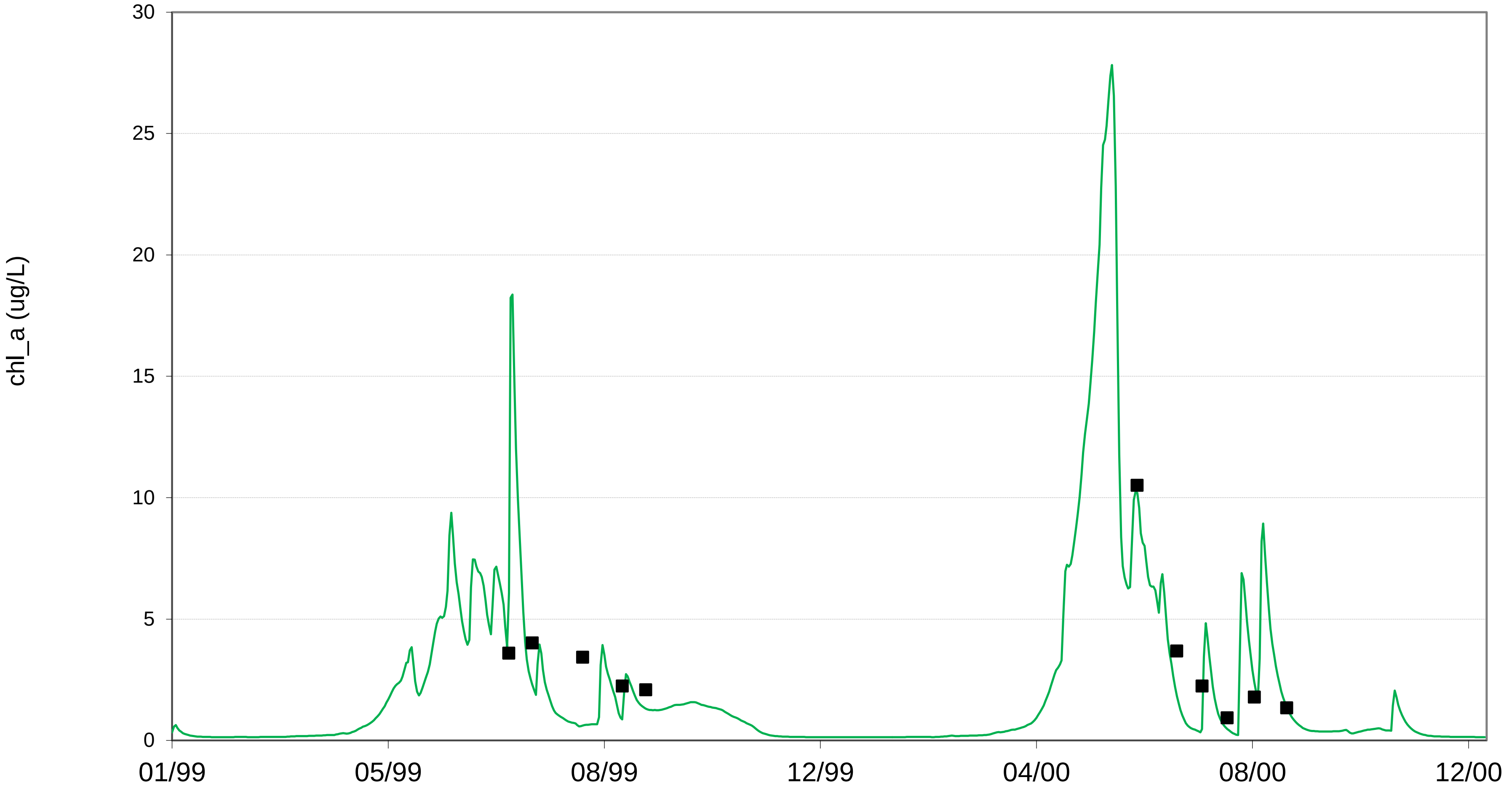
Observed (symbols) and calibrated AQUATOX simulations (lines) of chlorophyll *a* in Rum River at mile 18



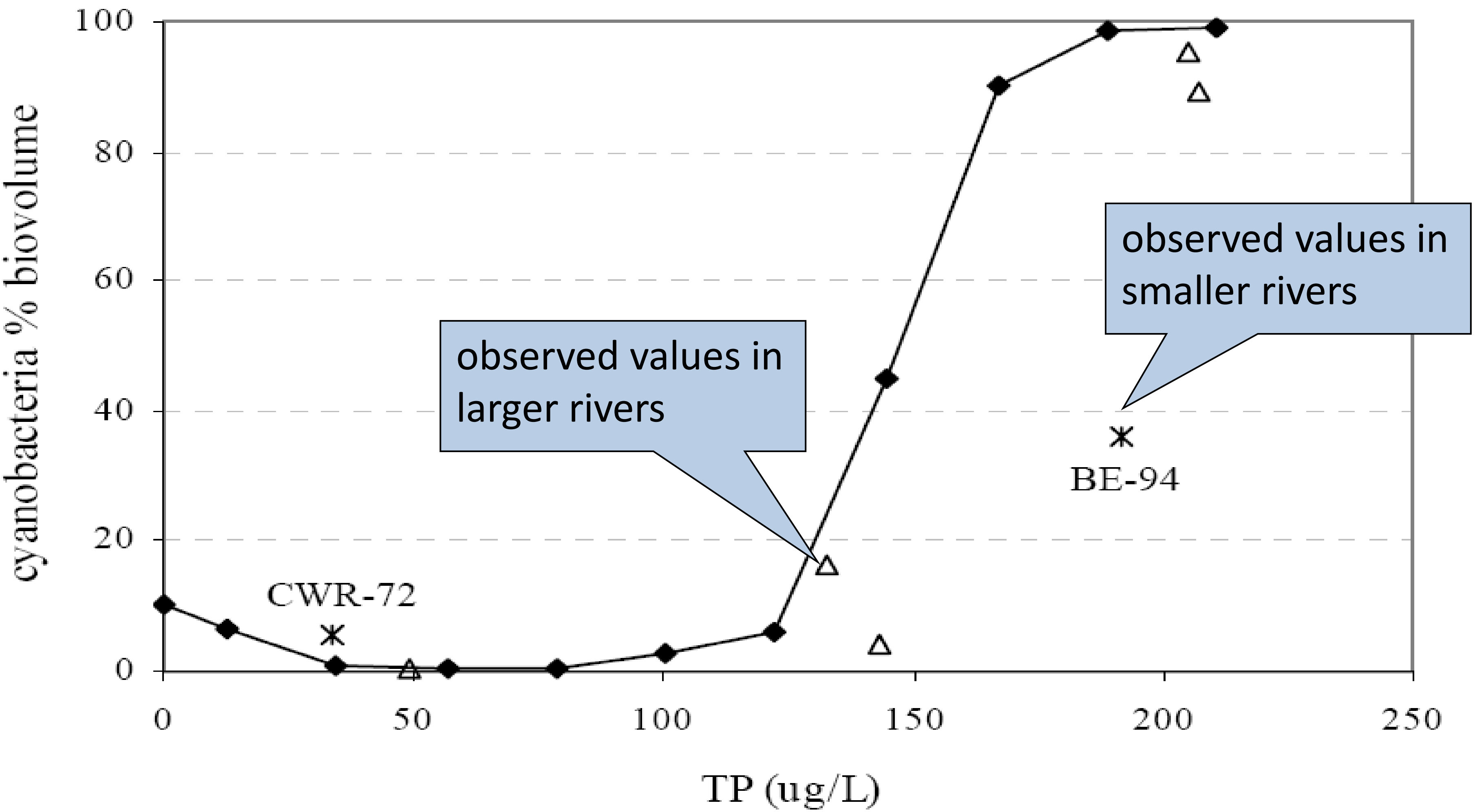
Sestonic algae are largely a result of sloughed periphyton in the Rum, a very shallow river



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



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



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