

# AQUATOX Training Workshop (Day 2)

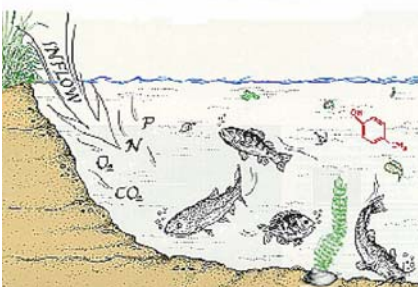
Philadelphia, PA  
October 24-26, 2006



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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

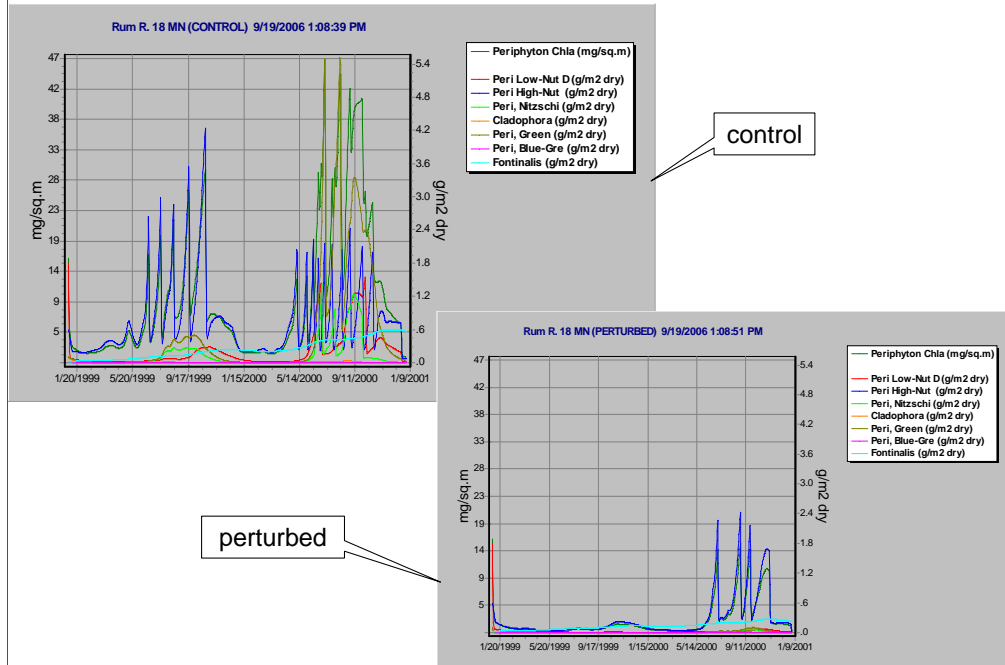
If development along the Rum River doubled TSS, what would be the impacts? Use **Rum18 calibration.aps**

If summer houses with septic tanks doubled TP in the Crow Wing River, what would be the impacts? Use **CrowWing72 calibration.aps**

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

The Rum River is a wild and scenic waterway with smallmouth bass and walleye fishing within commuting distance to St. Paul. The Crow Wing River is a broad, shallow river that is popular for float trips.

# Double TSS in Rum River

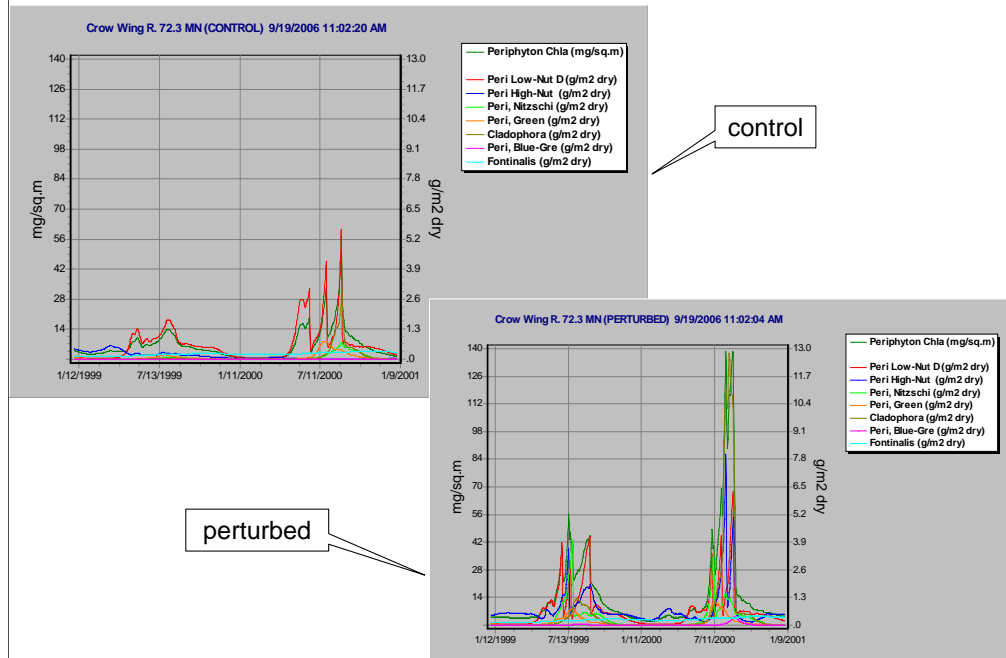


How has the Secchi depth changed?

How has the fishing changed?

Any other impacts?

## Double TP in Crow Wing River



What is impact on nuisance algae?

What is impact on phytoplankton?

How has the fishing changed?

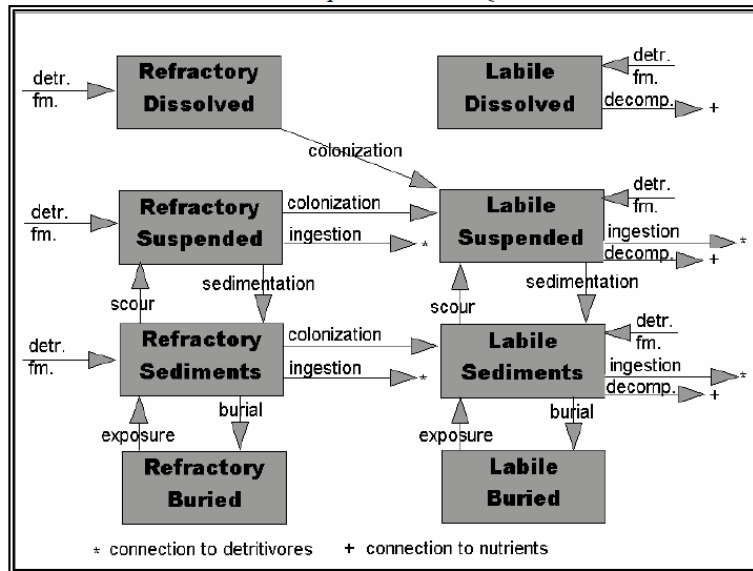
Any other impacts?

## **Remineralization**

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

# Detritus Compartments in AQUATOX

Figure 54  
Detritus Compartments in AQUATOX



## Remineralization Discussion:

Detritus is formed in several ways: through mortality, gamete loss, sinking of phytoplankton, excretion and defecation.

A fraction of mortality, including breakage of leaves from macrophytes, is assumed to go to refractory detritus; a much larger fraction goes to labile detritus.

Labile detritus decomposes quickly; refractory much more slowly.

## **Variable Stoichiometry**

- Ratios of elements in organic matter are editable on an organism by organism basis as well as for detrital state variables.
- 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.

The ability to define nutrient ratios for individual species and detritus was first added to AQUATOX Release 2.1.

## Default Nutrient to Organic Matter Ratios

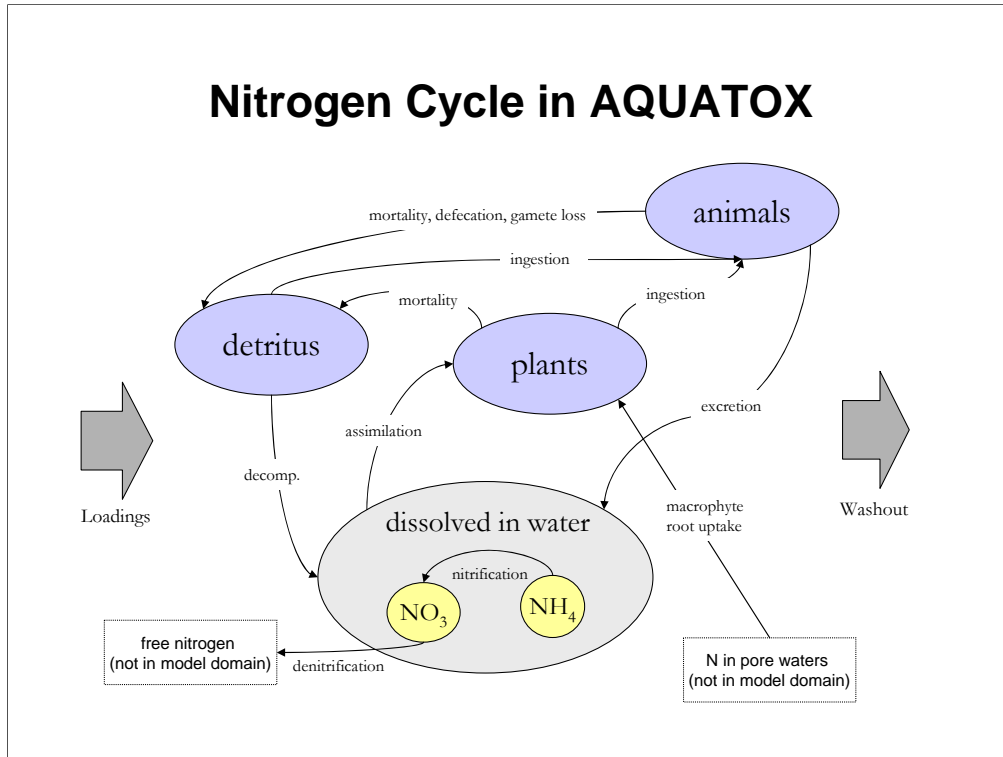
Compartment	Frac. N (dry)	Frac. P (dry)	Reference
Refrac. detritus	0.002	0.0002	Sterner & Elser 2002
Labile detritus	0.059	0.007	same as phytoplankton
Phytoplankton	0.059	0.007	Sterner & Elser 2002
Bl-greens	0.059	0.007	same as phytoplankton for now
Periphyton	0.04	0.0044	Sterner & Elser 2002
Macrophytes	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

- The actual values are not particularly important in this slide, the slide is just being shown for a couple reasons:
  - It shows that AQUATOX comes with default values.
  - It indicates the type of data that can be entered into AQUATOX if available, specifically the N to Organic Matter and P to Organic Matter ratios.

Sterner, R. W., and N. B. George. 2000. Carbon, Nitrogen, and Phosphorus Stoichiometry of Cyprinid Fishes. *Ecology* 81: 127-140.

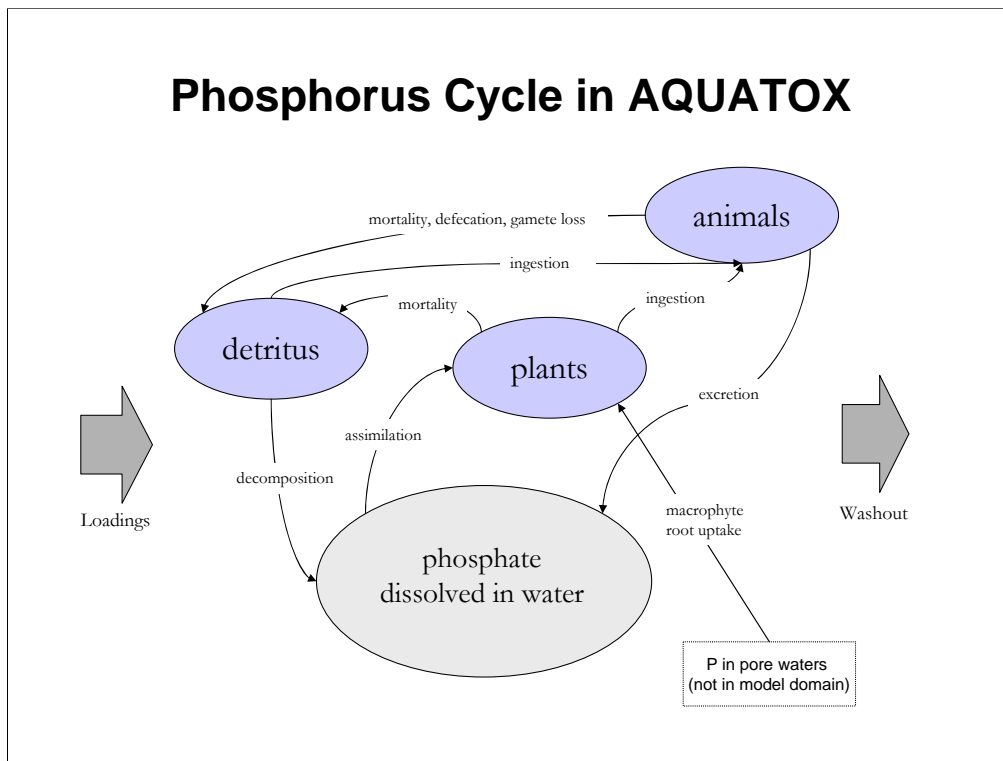
Sterner, R. W., and J. J. Elser. 2002. *Ecological Stoichiometry: The Biology of Elements from Molecules to the Biosphere*. Princeton University Press, Princeton NJ.





- The nutrient cycle is shown in this slide, the phosphorus cycle is identical to the nitrogen cycle with the exception of the various phases of nitrogen and the nitrification / denitrification processes.
- While this graph looks complex, there is really a fairly straightforward cyclical nature to the movement of nutrients within AQUATOX. Nutrients are taken up into higher organisms through ingestion and assimilation, nutrients are released back into the water column through mortality, defecation, and gamete loss.
- Nutrients from animals and plants break down into various forms of detritus and then are returned to the water column through detrital decomposition.
- Un-ionized ammonia ( $\text{NH}_3$ ) is not modeled as a separate state variable but is estimated as a fraction of ammonia.
- The un-ionized form of ammonia is toxic to invertebrates and fish. Therefore, it is often singled out as a water quality criterion. Un-ionized ammonia is in equilibrium with the ammonium ion,  $\text{NH}_4^+$ , and the proportion is determined by pH and temperature.

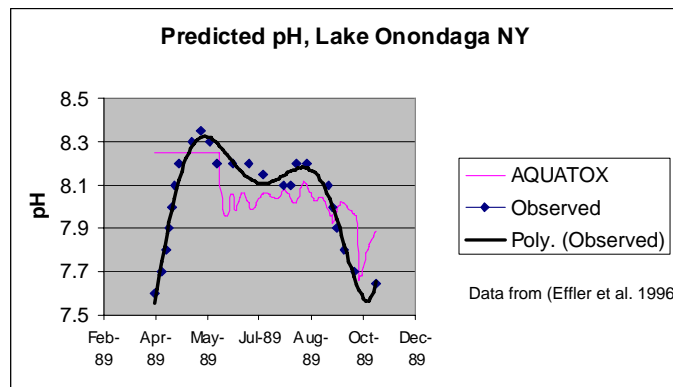
## Phosphorus Cycle in AQUATOX



The phosphorus cycle is almost identical, but it does not include multiple chemical forms in water.

## Dynamic pH also added to variable stoichiometry version:

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



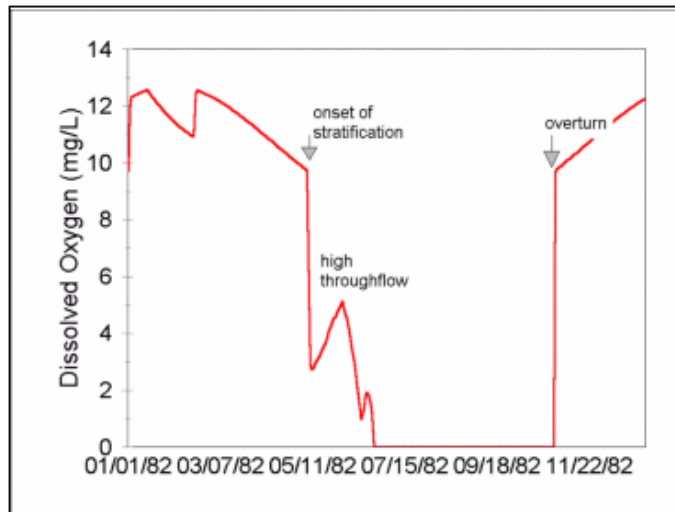
- Many models follow the example of Stumm and Morgan (1996) and solve simultaneous equations for pH, alkalinity, and the complete carbonate-bicarbonate equilibrium system.
- There are several reasons to go with a simpler pH formulation rather than the more complex formulation:
  - often detailed data are not available;
  - the iterative solution of the simultaneous chemical equations entails an additional computational burden;
  - precision of complex chemical models is unnecessary for ecosystem models.
- Only additional parameter required for AQUATOX to model pH in this manner is total alkalinity.
- This construct is applicable to pH 4.0 – 8.25.

Marmorek, D.R., R.M. MacQueen, C.H.R. Wedeles, J. Korman, P.J. Blancher, and D.K. McNicol. 1996. Improving pH and Alkalinity Estimates for Regional-scale Acidification Models: Incorporation of Dissolved Organic Carbon. *Can. J. Fish. Aquat. Sci* **53**:1602-1608.

Small, M.J., and M.C. Sutton. 1986. A Regional pH-Alkalinity Relationship. *Water Research* **20**:335-343.

Stumm, Werner, and James J. Morgan. 1996. *Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters*. Third ed. John Wiley & Sons. New York.

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



Anoxia in the bottom waters can occur as a result of decomposition of detritus, as shown in this graph of the hypolimnion.

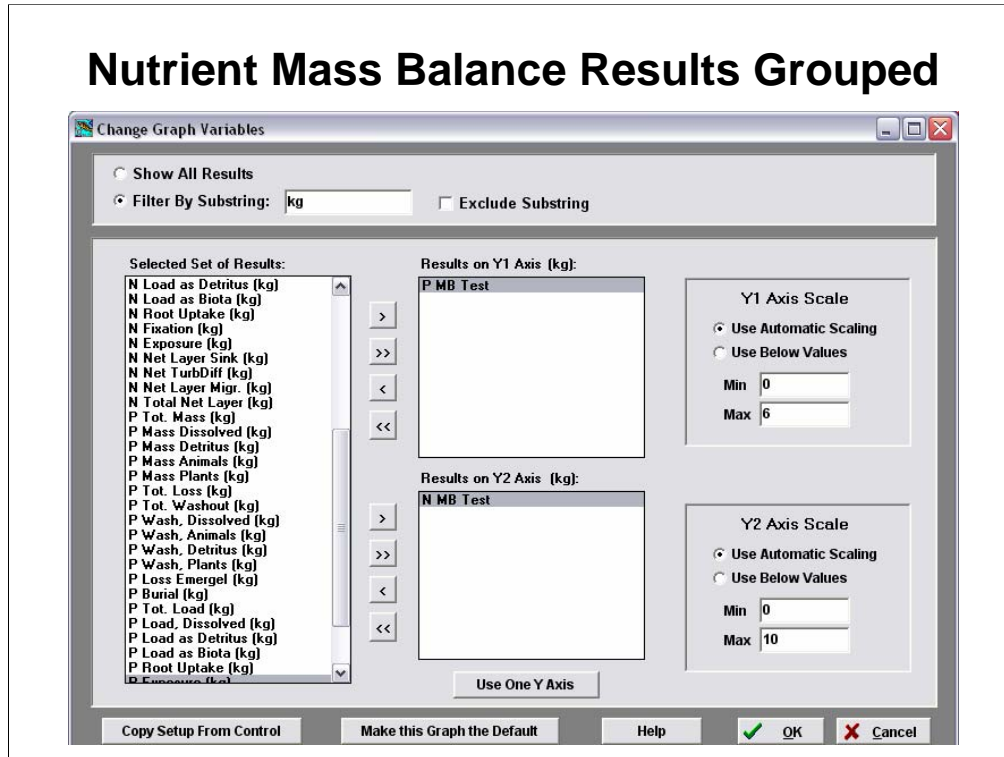
When anoxia occurs the model assumes that mobile zooplankton and fish migrate to the epilimnion.

## Demonstration: Stoichiometry and Mass Balance of Nutrients in Blue Earth River

- Additional output variables allow the user to track fate of nutrients
  - Nutrient Mass by Category
  - Nutrient Loadings by Category
  - Nutrient Loss by Category
  - Mass balance test =  
Total Mass + Loss – Load  
(*Should stay constant*)

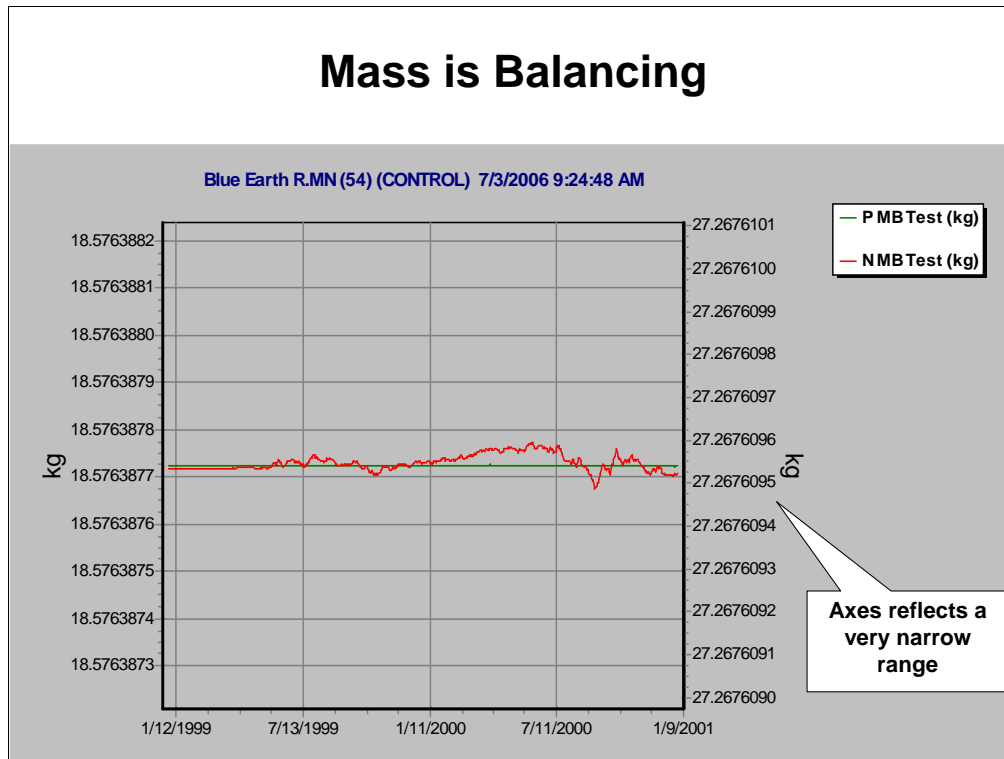
If you'd like to follow along within AQUATOX, load **BlueEarth54 Calibration.aps** that should still have results intact. We will now look at some of these results through the output screen.

## Nutrient Mass Balance Results Grouped



Using the change variables button and filtering on “kg” the nutrient mass balance results are all grouped together. Units are all in terms of kilograms of nitrate and kilograms of phosphate. As a demonstration, I will select the nitrogen mass balance test and phosphate mass balance test for interest. I will select Automatic Scaling if it’s not already selected.

# Mass is Balancing



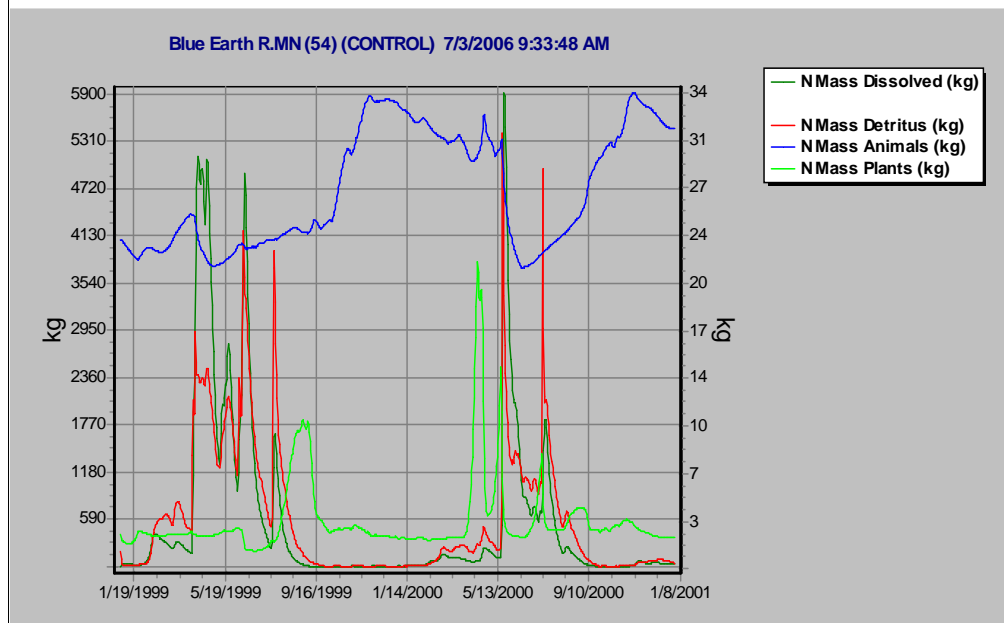
There are very small changes in mass because of machine error.

If you export these mass balance results they are accurate to  $4e-8$  kg or 40ug of nitrate over the two year simulation.

This machine error is not the same as the error produced by the differential equations solver for which you can set the relative error within the setup screen.

Occasionally when there are no nutrients left in the system the mass will not balance perfectly. This is a result of interactions within the food-chain that require uptake of nutrients from water to balance mass.

## Where are the Nutrients within the System?



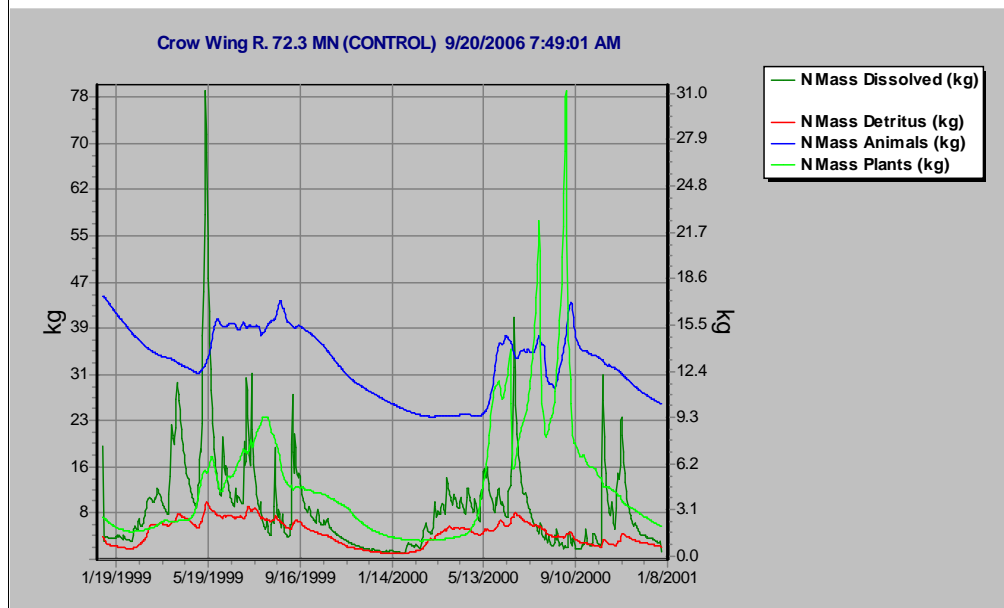
To examine where the nutrient mass is within the system at any given time, I will go to the Change Variables screen again and select N Mass Dissolved for Y axis 1 and N Mass Detritus, Animals, and Plants for Y axis 2.

(Filter “N Mass”)

Note the different units on the Y axes. There is a significant inflow of nitrogen into the system during May and lasting through July. Within Biota you can see that there are algal blooms that trap some of this nitrogen. Detritus matches dissolved inflow closely as the detritus category includes dissolved organic matter flows into the system. Finally, the nitrogen within animals remains fairly consistent throughout the simulation.



## Contrast Blue Earth with the Crow Wing River



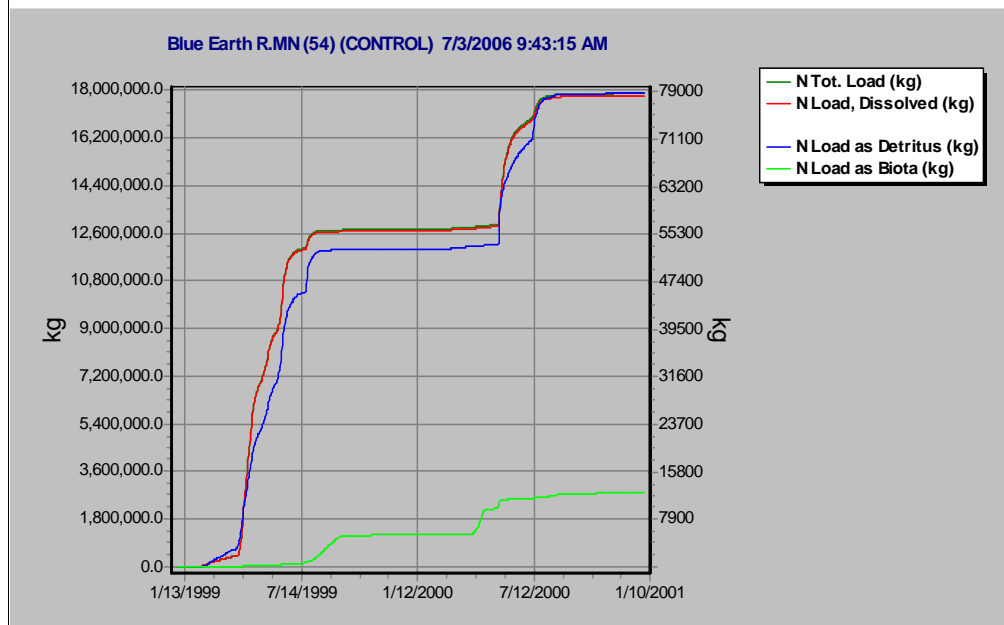
To look at a different system, I will now load in **CrowWing72 Calibration.aps** and select N Mass Dissolved for Y axis 1 and N Mass Detritus, Animals, and Plants for Y axis 2.

This time there is far less nitrogen washing through the system and far less nitrogen in the water column. Roughly two orders of magnitude less. N sequestered in detritus is also significantly lower.

Note, it's important to compare two sites of the same size when making such a comparison as the units are in a total mass basis.

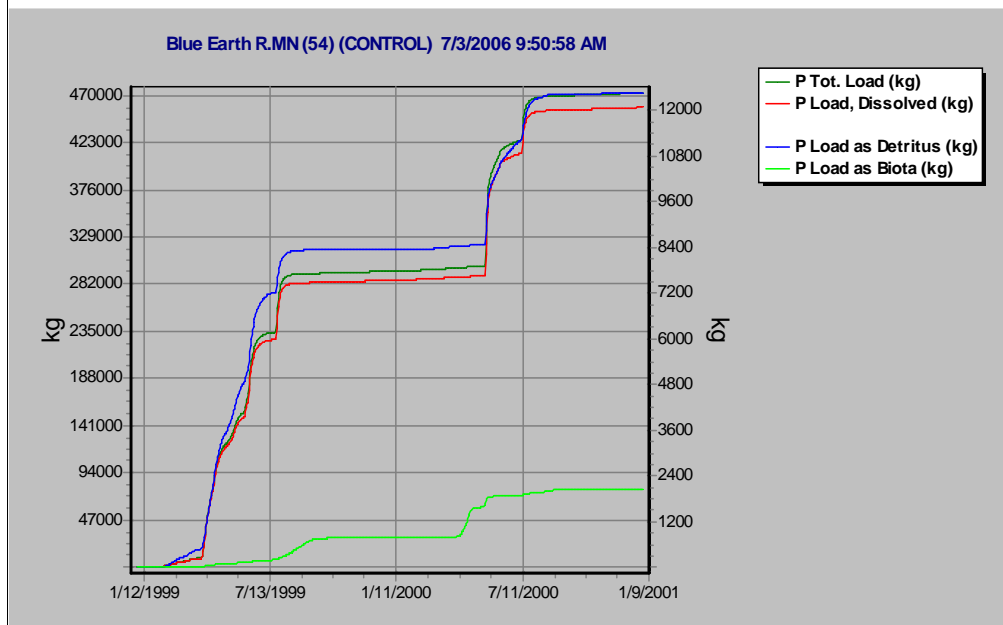
As an additional demonstration, I will also examine inflow loadings of nutrients with the graphic interface.

# Nitrogen Loadings, Blue Earth River



Most of the nitrogen loading in Blue Earth River is dissolved, although that is tracked closely by detrital loadings (note difference in scale), much of which is also dissolved. Loadings are calculated as cumulative; 1999 was a wet year so that there was a much larger cumulative loading.

# Phosphorus Loadings, Blue Earth River



Most of the phosphorus loading in Blue Earth River is dissolved, although that is tracked closely by detrital loadings (note difference in scale), much of which is also dissolved. Loadings are calculated as cumulative; 1999 was a wet year so that there was a much larger cumulative loading.

# **AQUATOX as a Part of BASINS**

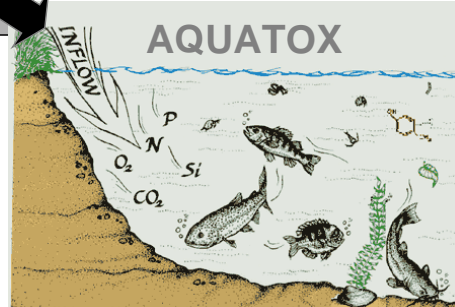
Integration of tools

## Purpose



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

- Provide time series loading data and GIS information to AQUATOX
- Create AQUATOX simulation using physical characteristics of BASINS watershed

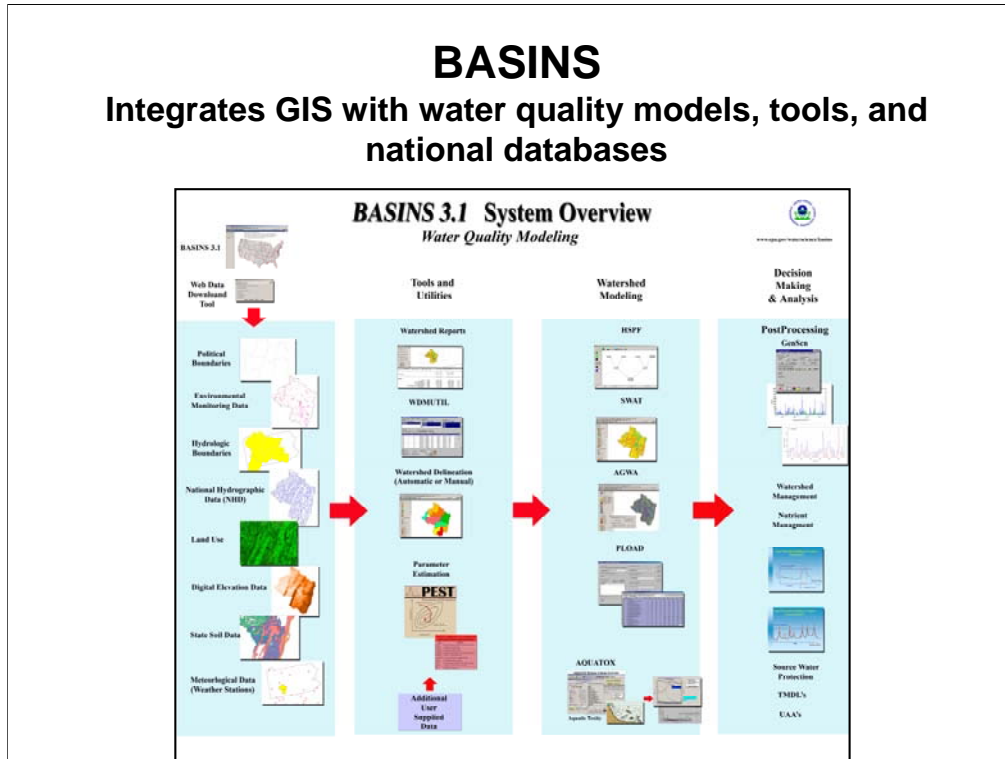


BASINS is a multipurpose environmental analysis system for use by regional, state, and local agencies in performing watershed and water quality based studies. BASINS makes it possible to quickly assess large amounts of point source and nonpoint source data in a format that is easy to use and understand. BASINS combines GIS technology, environmental data, watershed and water quality models and other tools. More information can be found on the BASINS web site at <http://www.epa.gov/waterscience/basins/basinsv3.htm>

BASINS 3.1 is able to link with AQUATOX. The GIS – based data and watershed models provide input data (pollutant loads, flow, and water body or channel characteristics to AQUATOX.

# BASINS

Integrates GIS with water quality models, tools, and national databases

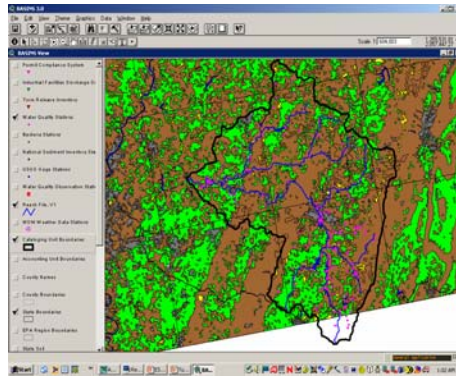


## Components

- National databases
- Assessment Tools & Utilities
- Watershed & Water Quality Models
- Post-processing & Analysis Tools

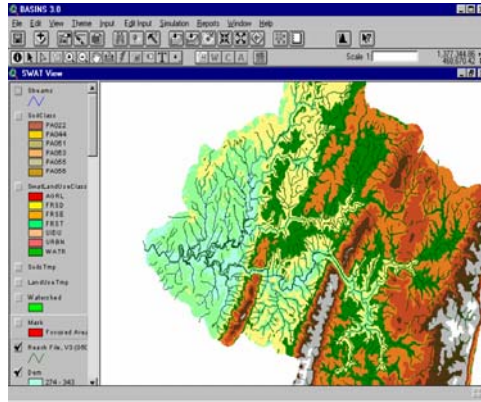
# BASINS GIS Data

- Stream networks
- Hydrologic units
- Landuse
- Soils
- Elevation
- Roads, cities
- WQ, facilities data
- Etc....
- Web data download tool



## Watershed & Water Quality Tools and Models

- Screening level
  - PLOAD
- Detailed
  - HSPF
  - SWAT
  - AGWA



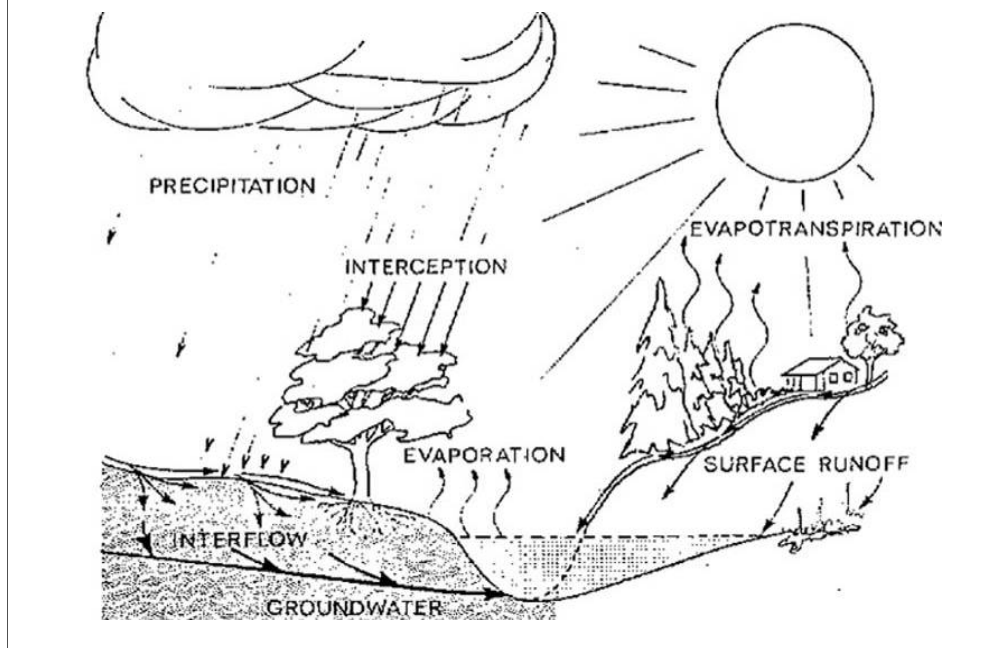
**PLOAD** is a relatively simple model that estimates NPS loads of pollutants on an **annual average basis, for any user-specified pollutant**. NPS loads may be calculated using either export coefficients or Schueler's Simple Method. The effects of BMPs, which serve to reduce NPS loads, and point source loads, may also be included in the computations.

**AGWA** stands for **Automated Geospatial Watershed Assessment**. AGWA is essentially a separate front end for SWAT and a model called KINEROS. For SWAT, AGWA provides a somewhat more automated interface than the AVSWAT-based one that's part of BASINS. KINEROS is an event-based model which estimates both overland and channel flow, including hydrographs and associated sediment export.

Neither PLOAD or AGWA can be linked directly to AQUATOX, because their outputs are not input parameters for AQUATOX. But the time series of flow and pollutant loadings into a stream network that HSPF and SWAT produce can be automatically formatted for import into AQUATOX.



## Simplified Hydrologic Model

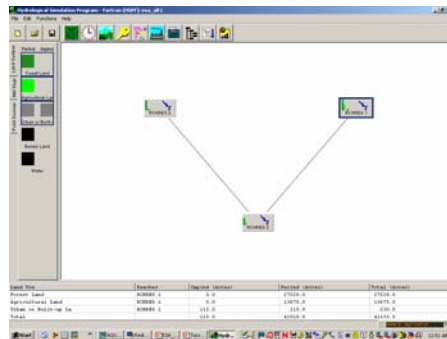


This is a very simplified representation of the hydrologic processes that SWAT and HSPF simulate.

# WinHSPF

## Hydrologic Simulation Program–FORTRAN

- Predicts loadings in mixed land use settings for bacteria, metals, **sediments, nutrients, algae as Chlorophyll a**
- Considers point source and nonpoint source loadings
- Natural and developed watersheds and water systems
- Continuous simulation, hourly meteorology
- Lumped parameters by landuse/watershed



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

The first watershed model in BASINS is HSPF. HSPF evolved from the old Stanford Watershed Model from the 1960s. The model's greatest strength is probably its versatility. It can be used to simulate runoff and transport of nutrients, general pollutants including pesticides and metals, and eroded sediments. HSPF is a lumped parameter model where the watershed is broken into multiple sub-basins that contain one impervious segment, and up to several pervious segments that each represent different land use types. "Lumped parameter" means that the physical processes simulated are assumed to be uniform within each sub-basin; exact location on the land is not tracked.

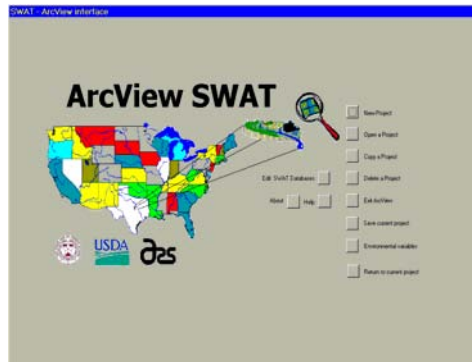
HSPF has a long history of nonpoint source modeling for TMDLs and many other purposes. It generally requires significant flow data from stream gages.

HSPF outputs are time series (generally hourly, but as frequently as 15 minutes) of flow and water quality (concentrations). HSPF does in-stream WQ simulation for some parameters, and AQUATOX will perform the simulations for other parameters.

# SWAT

## Soil and Water Assessment Tool

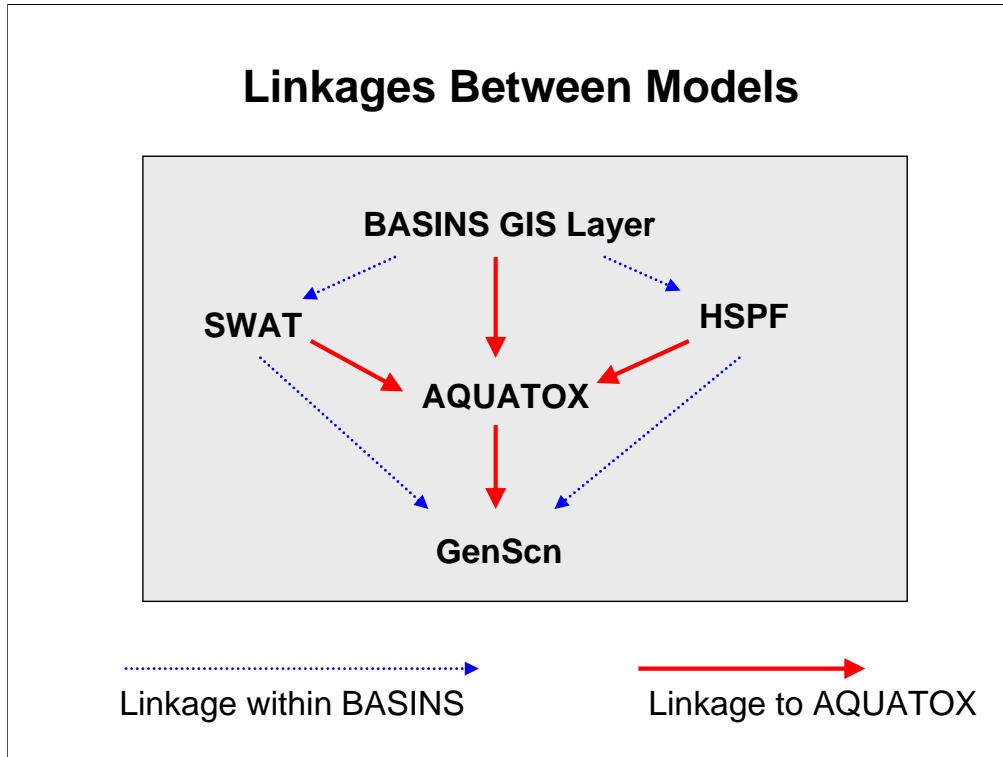
- Physically-based, watershed scale model
- Predicts impacts of land management practices on water, sediment, and agricultural chemical yields in large complex watersheds
- Models *water and sediment movement, nutrient cycling*, crop growth, metals, *pesticides*, etc.



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

The other main watershed model in BASINS is USDA's SWAT model.

SWAT is also a lumped parameter model, which like HSPF, process land use data for a delineated watershed to set up the model. Unlike HSPF, SWAT also considers soil data (STATSGO or SSURGO) and accounts for the relationships between soil types and land uses. SWAT is designed to simulate the fate and transport of nutrients and pesticides, particularly export from agricultural land. For pesticides and fertilizers, various management practices can be simulated: different timing and application rates, and tillage operations. SWAT is particularly suited to watersheds that do not have flow gages.



These are the specific data that are passed with the various AQUATOX/BASINS linkages:

- BASINS GIS to AQUATOX

- Channel geometry (length, depth, slope)

- HSPF to AQUATOX

- Geometry

- Time series: flow, water quality (nutrients, BOD, temperature, sand/silt/clay)

- SWAT to AQUATOX

- Geometry

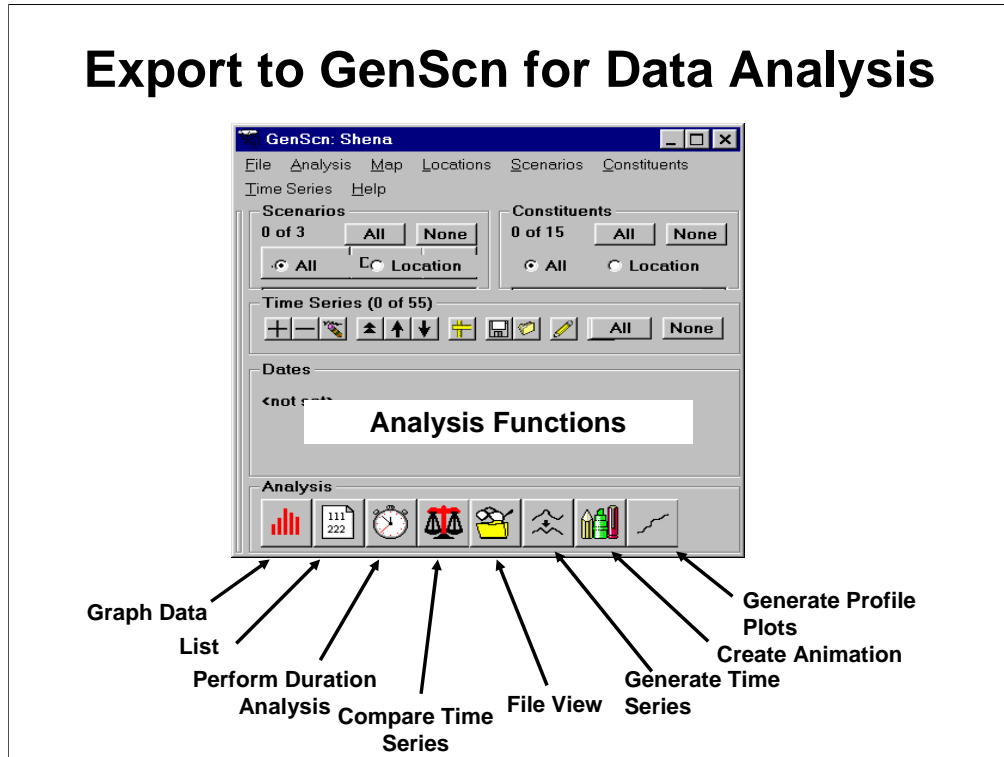
- Time series: flow, water quality (nutrients, BOD, pesticides, TSS)

- AQUATOX to GenScn

- All time series output

The linkage program takes the rather voluminous output from SWAT or HSPF and formats correctly it for AQUATOX, potentially a huge time savings for the user.

## Export to GenScn for Data Analysis

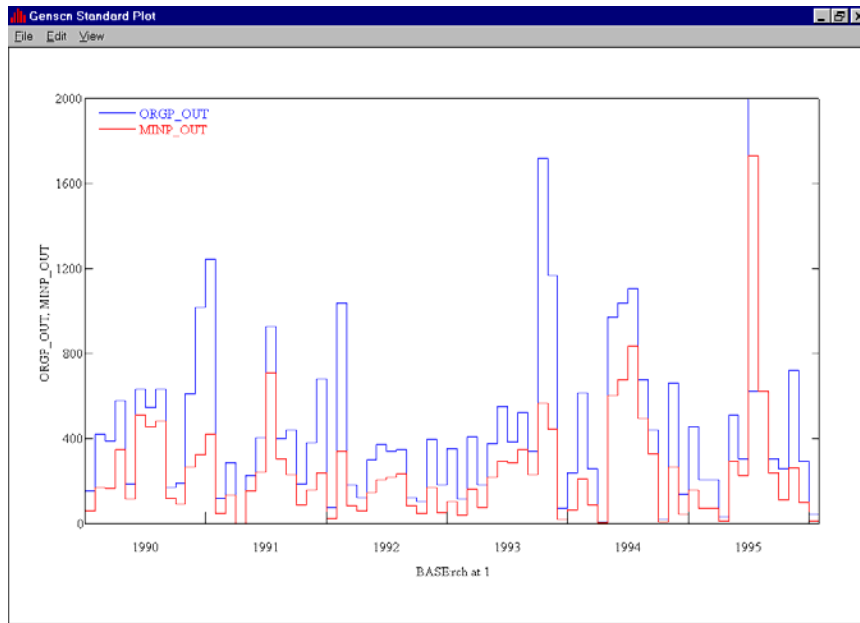


GenScn is a tool within BASINS for processing, analyzing and comparing time series data, which is very useful when dealing with the volumes of output data generated by dynamic models such as HSPF, SWAT, and AQUATOX. Even if you haven't run AQUATOX with data from HSPF or SWAT, the utilities in GenScn are very handy for analyzing model results.

We will be taking some of these functions and bringing them directly into the AQUATOX interface in Release 3.

# GenScn

## example comparison of time series



We have already seen how GenScn can be used to compare observed data against model predictions.

## Potential Applications

- What are the likely effects of land use changes on aquatic biota?
- Will changes in management lead to attainment of water quality standards?
- Current nutrient modeling projects are exploring how water quality criteria development process could be enhanced using AQUATOX linked with BASINS

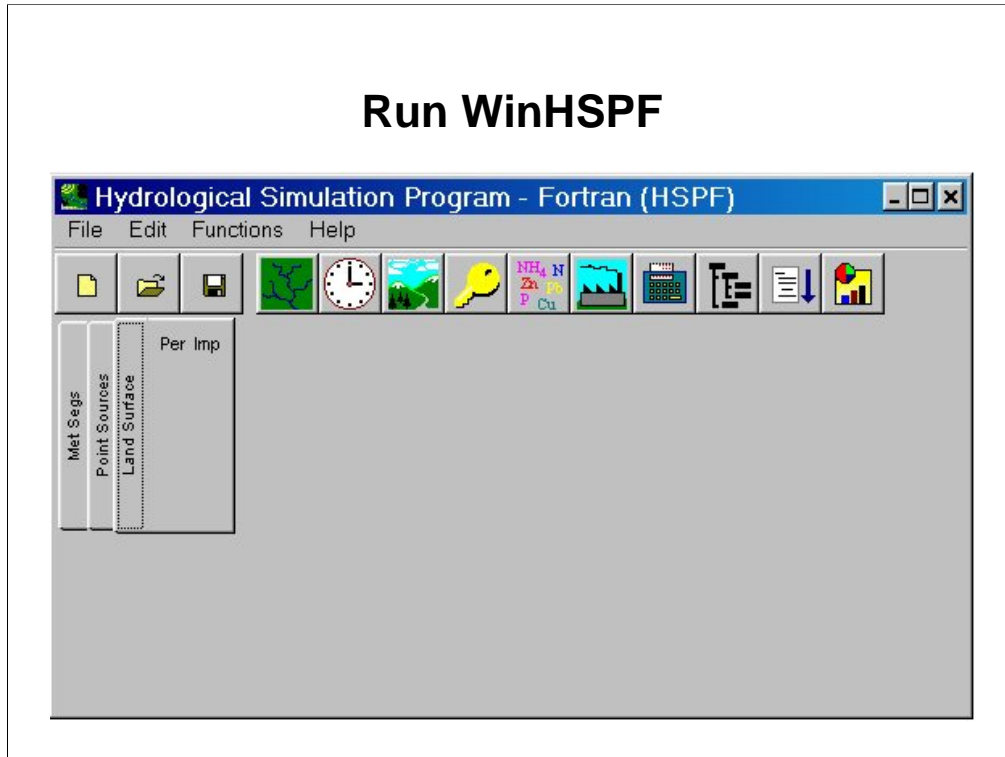
## **Lab 5: Linking AQUATOX to HSPF**

Objective: provide overview of steps in linking the two models

- Run WinHSPF
- Load REVATC.UCI
- Wait for Simulation to Load
- Tour of WinHSPF Interface
- Trigger Linkage
- Linkage Process



## Run WinHSPF



Find WinHSPF within your start menu. If this was installed as part of BASINS it may be in the BASINS directory.

Run WinHSPF and choose to open REVATC.UCI from your short-course CD. Note that BLUE.WDM must be included in the same directory as the UCI file.

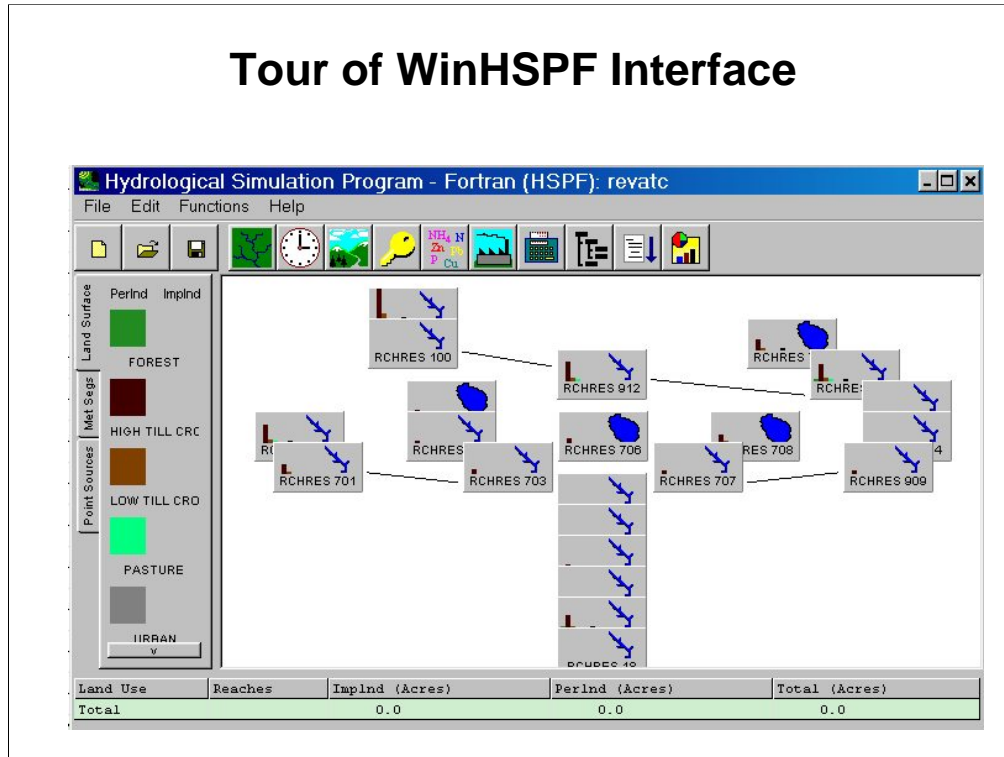
The UCI file is a text file that contains parameter values, all which are editable through the WINHSPF interface. The WDM file contains time-series input and output that WinHSPF utilizes.

## **Steps to Link AQUATOX to Hydrologic Model (e.g. HSPF)**

- Hydrologic model is calibrated;
- Appropriate pollutants for linkage to AQUATOX are selected within WinHSPF;
- WinHSPF software is told to produce specialized AQUATOX output files;
- The HSPF simulation is executed;
- AQUATOX is invoked from the WinHSPF interface, causing the linkage process to take place;
- WinHSPF is linked to existing AQUATOX simulation;
- AQUATOX simulation is run to examine effects of nutrients, sediments, flow regime as calculated by HSPF.

The HSPF linkage has been tested and utilized the most thoroughly so it is being shown as this example. Steps to link SWAT output are similar but not identical.

## Tour of WinHSPF Interface



The UCI file takes quite a while to load so we will look at some of the key portions of the WinHSPF interface. First of all, there are two important help files to utilize when working with WinHSPF. The WinHSPF.chm file will lead you through information about the WinHSPF GUI whereas the HSPF.chm contains data about the underlying FORTRAN model and all parameters, etc.

With respect to AQUATOX linkage, the two most important parts of the WinHSPF linkage are Functions, Output, where you can add an AQUATOX linkage and "Functions, AQUATOX" which triggers the linkage itself. While the file is loading we will explore these parts of the WinHSPF interface along with a few other features.

BASINS Support is available in many forms, by email the BASINS list-server is very useful: <http://www.epa.gov/ost/basins/listserv.htm>

## Time-Series Passed from WinHSPF to AQUATOX (*WinHSPF terminology in italics*)

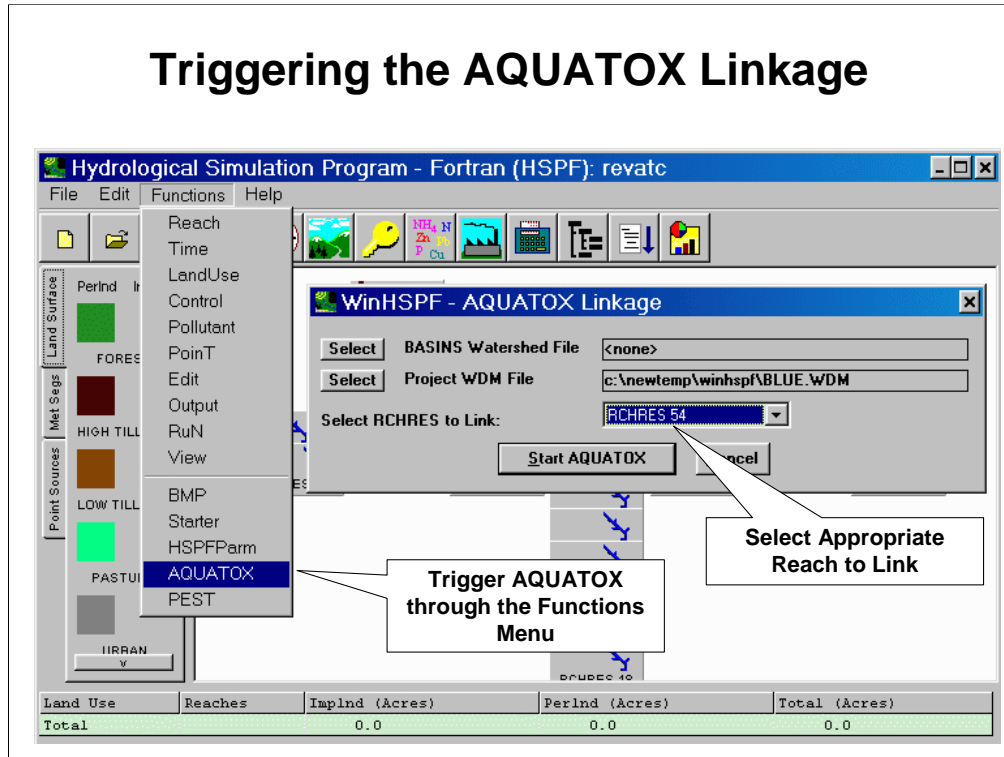
- *SARA*: Time series of surface area for the reach
- *AVDP*: Time series of average depth for the reach
- *SSD1, SSD2, SSD3*: Concentrations of suspended inorganic sediments, summed to represent TSS
- *VOL, IVOL, PSUP, VEVF*: Water volume information (time-series volume, inflow, precipitation, evaporation)
- *NO3, NO2, NH3, CO2, DO, PO4, PPO4, TORP*: Inflow loadings of nutrients, gasses
- *BOD, ORC*: Inflow loadings of suspended and dissolved detritus
- *TW*: Water Temperature of equivalent segment
- *TIQ1*: Toxicants, inflow loadings

The design of the BASINS linkage design was to have the AQUATOX reach be the equivalent as the HSPF reach and to

- pass inflow loads into that reach whenever AQUATOX will be doing the processing and
- pass concentrations / temperatures that are equivalent to the reach whenever AQUATOX is simply using the data as driving data and is not doing additional processing.

Reach 54 is a one mile “dummy reach” produced by the AQUA TERRA consultants when they ran their model. Because the AQUATOX linkage accepts loadings from an upstream reach only, if a segment is too long, point-sources and non-point-sources will be undercounted. To solve this problem a “dummy reach” was placed at the end of the segment that we are modeling

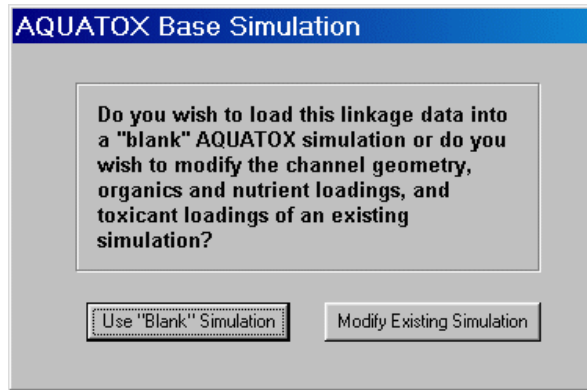
## Triggering the AQUATOX Linkage



The AQUATOX linkage is triggered after the simulation has been run in WinHSPF. Because this simulation takes 40 minutes on a very fast computer we're going to use the results. Like AQUATOX, when loading a UCI file, the results of the previous run are also loaded so we do not need to run the model for this lab.

As discussed in the tour, the output manager was used, *prior to the run*, to set up the model to produce AQUATOX output for the reach that you wish to link.

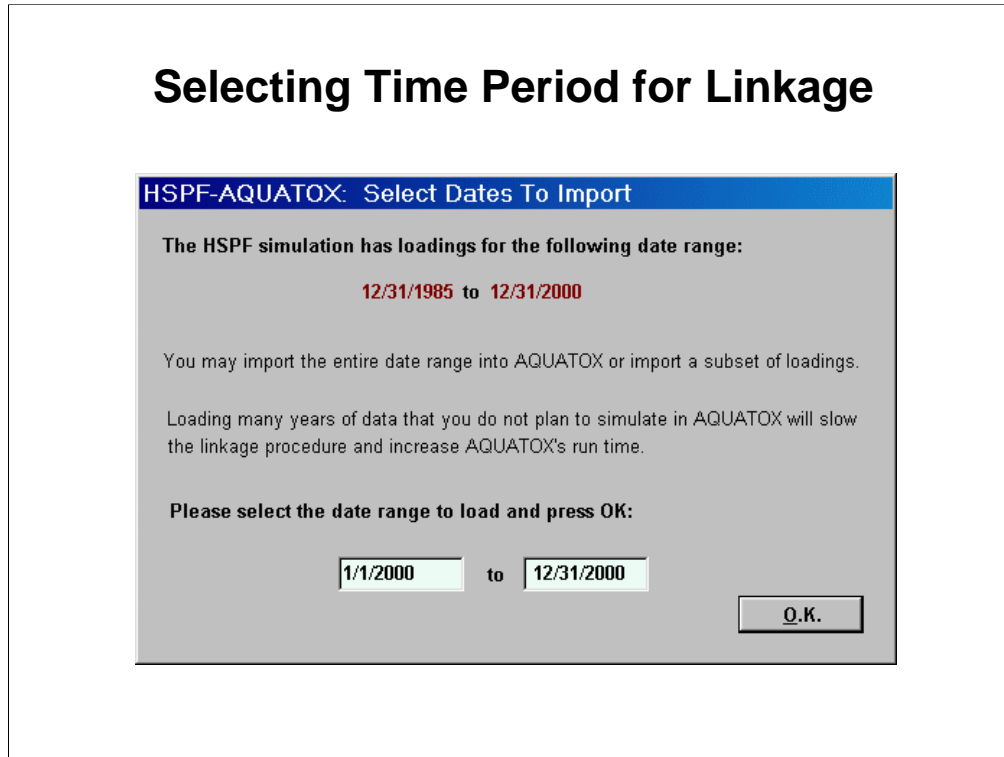
## Selecting AQUATOX Simulation



You will next see this dialog which asks you whether you wish to use a “blank” simulation or to modify an existing simulation. This dialog allows you to incorporate the TSS levels, nutrient levels, and volume conditions on an existing simulation, such as the stand-alone simulation that we created yesterday.

Select to “Modify Existing” and load **BE54\_1C.aps**

## Selecting Time Period for Linkage



The HSPF simulation ran for 15 years. However, we are only interested in the last year of data. So change the start date to 1/1/2000 for this linkage. If you choose the entire date-range and then only run the year 2000 the results will not be different. However, the model will have roughly 5500 entries for each time-series rather than 365. This will slow the linkage and increase the size of the AQUATOX simulation file and generally make it unwieldy to work with. So it makes sense to limit the time-series that are chosen.

In most HSPF setups there will be a spin-up period required, or initial conditions will only be relevant to a particular date. Because of this, changing the time-period of an HSPF run is not as desirable as changing the linkage time-period using this dialog.

## Organic Matter Setup

**BASINS-AQUATOX Linkage: Please Characterize Organic Carbon Lo...**

AQUATOX will import BOD from the HSPF simulation. This must be characterized as Labile or Refractory organic matter. It is generally assumed that BOD is predominantly Labile in nature.

Refractory organic carbon loadings will then be added to the BOD loadings to get the weighted average for the labile to refractory ratio.

AQUATOX will assume that 10% of the BOD is Refractory (90% Labile) unless a different number using is specified using this screen.

**% of BOD that is Refractory**

Additionally, AQUATOX must characterize incoming loads of organic matter (BOD and Refractory Organic Carbon) as Dissolved or Particulate in nature.

AQUATOX will assume that the organic loadings are 10% particulate unless a different number is specified with this screen:

**% of Organic Loadings that are Particulate**

AQUATOX combines loadings of BOD (Biochemical Oxygen Demand) and ORC (refractory organic carbon) into the organic matter loadings for AQUATOX.

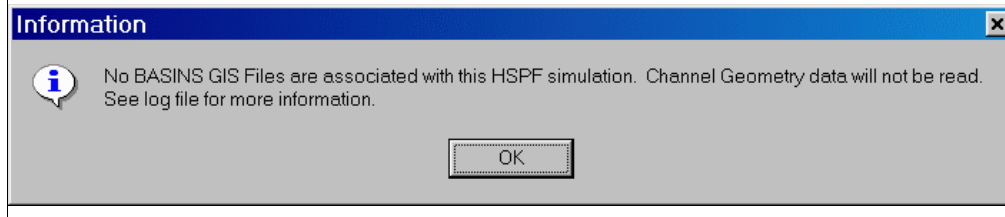
Because of this, the fraction of BOD that is refractory must be entered. The fraction of loadings that are refractory vs. labile are then calculated for all of the loadings, assuming that ORC is 100% refractory (by definition).

Additionally, the derived organic matter loadings must be broken into particulate vs. dissolved compartments. If you have no additional information about these loadings the default values shown here are appropriate in most cases.



## HSPF and BASINS

- HSPF may be run within the BASINS GIS framework or it may be run independently.
- If HSPF is run within the framework, additional channel geometry data from the GIS will be passed to AQUATOX.
- Otherwise, if it is run as a stand-alone model (as is the case with this lab), the following dialog box appears:



# Linkage is Complete

**Basins Linkage Information**

**You have linked an HSPF simulation to AQUATOX.**

The following categories of data were brought into AQUATOX if they were available:

- Simulation Start and End Time
- Dynamic Water Volume Data
- Nutrient Time-Series Loadings
- Plankton Time-Series Loadings
- Organic Chemical Time-Series Loadings
- Site Physical Characteristics

To see the detailed log of the model linkage, please click the button here →

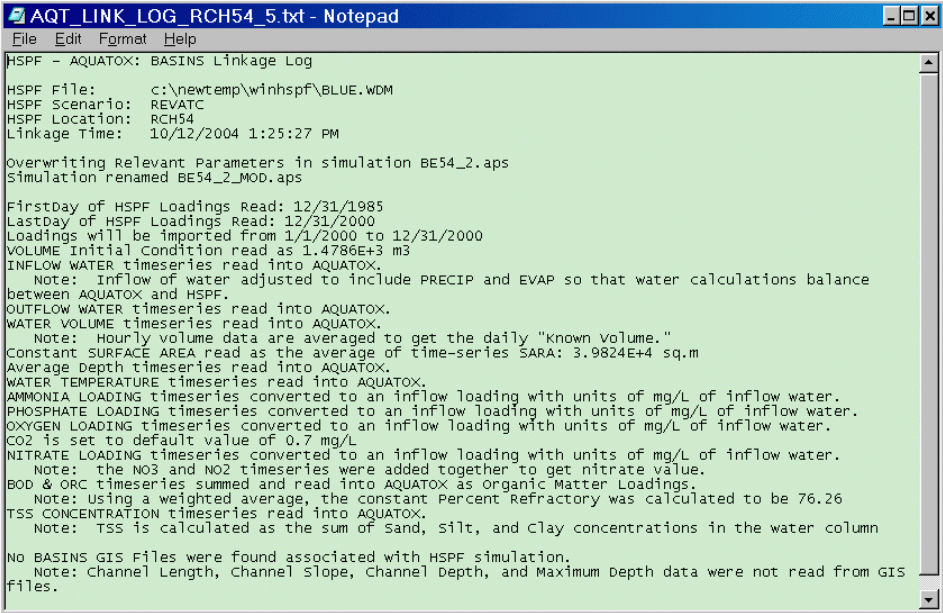
You may still wish to specify the following categories of data which are unavailable from the linkage:

- Nutrient Initial Conditions
- Organic Matter in the Sediment Bed
- Additional Plants and/or Animals
- Wind and Light Loadings
- Additional Organic Chemicals

**Additional Model Characteristics may be specified using the AQUATOX Simulation-Setup Wizard which is designed for user-friendly input of model parameters**

Now the linkage has completed its work, you should see the following screen. This screen produces a generic accounting for the type of data that has been passed from HSPF. To see exactly what has been passed you should view the log file.

## Log File Details Passage of Data



```
AQT_LINK_LOG_RCH54_5.txt - Notepad
File Edit Format Help
HSPF - AQUATOX: BASINS Linkage Log
HSPF File: c:\newtemp\winhspf\BLUE.WDM
HSPF Scenario: REVATC
HSPF Location: RCH54
Linkage Time: 10/12/2004 1:25:27 PM

Overwriting Relevant Parameters in simulation BE54_2.apr
simulation renamed BE54_2_MOD.apr

Firstday of HSPF Loadings Read: 12/31/1985
Lastday of HSPF Loadings Read: 12/31/2000
Loadings will be imported from 1/1/2000 to 12/31/2000
VOLUME Initial Condition read as 1.4786E+3 m3
INFLOW WATER timeseries read into AQUATOX.
Note: Inflow of water adjusted to include PRECIP and EVAP so that water calculations balance
between AQUATOX and HSPF.
OUTFLOW WATER timeseries read into AQUATOX.
WATER VOLUME timeseries read into AQUATOX.
Note: Hourly volume data are averaged to get the daily "known volume."
Constant SURFACE AREA read as the average of time-series SARA: 3.9824E+4 sq.m
Average Depth timeseries read into AQUATOX.
WATER TEMPERATURE timeseries read into AQUATOX.
AMMONIA LOADING timeseries converted to an inflow loading with units of mg/L of inflow water.
PHOSPHATE LOADING timeseries converted to an inflow loading with units of mg/L of inflow water.
OXYGEN LOADING timeseries converted to an inflow loading with units of mg/L of inflow water.
CO2 is set to default value of 0.7 mg/L
NITRATE LOADING timeseries converted to an inflow loading with units of mg/L of inflow water.
Note: the NO3 and NO2 timeseries were added together to get nitrate value.
BOD & ORC timeseries summed and read into AQUATOX as Organic Matter Loadings.
Note: Using a weighted average, the constant Percent Refractory was calculated to be 76.26
TSS CONCENTRATION timeseries read into AQUATOX.
Note: TSS is calculated as the sum of Sand, silt, and Clay concentrations in the water column

No BASINS GIS Files were found associated with HSPF simulation.
Note: Channel Length, channel slope, Channel Depth, and Maximum Depth data were not read from GIS
files.
```

The log file makes it clear exactly which parameters were changed within which file, which time-series were loaded, and the time of the linkage. Any errors that occurred within the linkage are also listed here. It is generally a good idea to look here just to see exactly how your simulation was modified.

You may now continue to work with the simulation either through the AQUATOX wizard or the main interface.

## Use of AQUATOX in development of water quality criteria

- Allows a mechanistic and comprehensive approach
  - Potential to develop criteria based on causal links between water quality and biota
  - Allows assessment of multiple stressors
- Allows assessment of technical feasibility of criteria attainment and of restoration potential
- We'll focus on nutrient criteria
  - What is the most important stressor driving algal response?
  - Go beyond chlorophyll a to evaluate quality, not just quantity, of algal responses (e.g., reduction of blue-green algae blooms)

The application of AQUATOX to the development of water quality criteria and the WQS process is in its early stages, but has great potential, particularly with regard to linking chemical and physical water quality and its ability to support designated aquatic life uses.

We will focus on nutrient criteria, and discuss it in the context of the Minnesota rivers modeling.

Use analytical power of AQUATOX to analyze what factors are driving algal response:

Suspended sediments & light? (we have already seen how sensitive the algae are to light regime)

Nutrients?

Organic loads

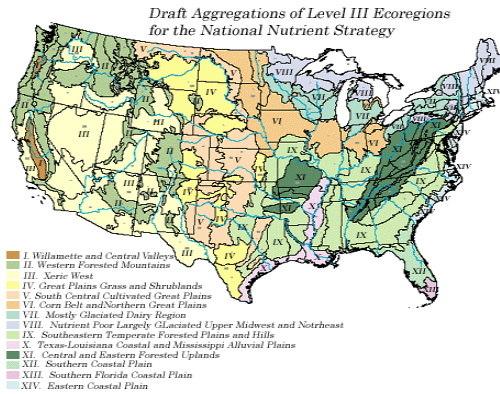
Flow regime

Herbicides?

Combination of factors

## Current EPA recommendations rely on the Reference Condition approach

- A nutrient benchmark
  - Is an indication of “normal” and “natural” N & P concentrations expected in each ecoregion for the stated water body type.
  - Not necessarily the target numeric criteria value.



This approach was based on lumping together existing monitoring data of nutrients, chlorophyll and water clarity from many waterbodies within an ecoregion, and developing reference conditions based on percentiles of those data. It did not keep the different parameters from individual waterbodies together in the analysis. Concerns have been raised by some parties as to whether the approach adequately captures cause-and-effect relationships, particularly when applying to individual sites.

In addition, designated uses and WQ management “goals” not necessarily synonymous with minimally impacted nutrient conditions.

## Section 304(a) Nutrient Criteria

- Are only guidance, not laws or regulations.
- States and Tribes have several options in adopting them, including:  
***“Develop nutrient criteria protective of designated uses using other scientifically defensible methods and appropriate water quality data.”***

The quote is from the Forward to the ecoregional nutrient criteria recommendation documents, signed by Geoff Grubbs, former director of OST.

## Nutrient criteria can be set using a variety of approaches & management goals

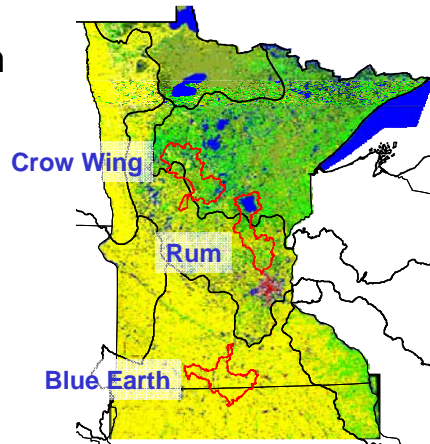
River	Nutrients	Algae & DO	Fish IBI	Approach
Crow Wing	Low	Low, benthic dominated. Low DO diel fluctuation	good (good habitat)	Protection
Rum	Moderate	Moderate, mix of benthic & sestonic. Moderate DO fluc.	good (good habitat)	Slight TP reduction
Crow	High	High, primarily sestonic, periodic blue-green dominance. High DO diel fluctuation	good-fair (good habitat)	Establish BOD goal that can be translated into TP and chlorophyll-a goals.
Blue Earth	High	High, primarily sestonic, blue-greens common. Very high DO diel fluctuation	poor (poor habitat)	TP & BOD reduction
Mississippi	Low-Moderate	Primarily sestonic, some blue-greens. Moderate DO diel fluctuation.	generally good (habitat variable)	Mass balance -- seek TP reductions to minimize mainstem and receiving water nutrient-related impacts.
Red	High	Low algal response in lower reaches because of high turbidity. Low DO fluc.	no data this study	Minimize impact on downstream uses and receiving waters

The table is from Heiskary, Steven, and Howard Markus. 2003. Establishing Relationships Among In-Stream Nutrient Concentrations, Phytoplankton Abundance and Composition, Fish IBI and Biochemical Oxygen Demand in Minnesota USA Rivers. St. Paul, MN: Minnesota Pollution Control Agency.

We will focus on the Blue Earth River, with its high algal blooms, of which the phytoplanktonic blue-greens are the largest and of most concern. Management goals for the Blue Earth also include reduction of BOD to reduce downstream impacts.

# Modeling Case Study: Minnesota

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



For this exercise, we made use of some chemical and biological data that MPCA had collected from medium sized rivers in Minnesota. These watersheds are in different ecoregions and have different mixes of land uses. This shows the locations of the watersheds for the three rivers we modeled, on top of 1992 NLCD (land cover database): the yellow color is row crop agriculture, and the green colors are forested land. The nutrient concentrations in these rivers span roughly an order of magnitude, increasing generally in a N-S direction from the Crow Wing to the Blue Earth, as the land becomes increasingly dominated by agriculture.



## Overview of MN modeling project

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

The intention of this demonstration is NOT to undercut the EPA recommendations, but rather to illustrate a technique to supplement and enhance it.

We are working on a project to investigate how AQUATOX, coupled with the watershed modeling capabilities in BASINS, can help in the development of WQC. It also looks at whether reasonable management practices and load reductions could be expected to lead to attainment of the criteria. The illustrations here were developed for the purposes of the workshop and are based on preliminary model simulations, and are subject to change. I hope also to illustrate how several of the tools in AQUATOX can be used.

With AQUATOX calibrated across a gradient of nutrient concentrations in similarly sized rivers, we have reasonable confidence in our ability to predict mean responses to hypothetical reductions in nutrient concentrations in the high nutrient system. This exercise focused on the Blue Earth river as an example of a water body in which nutrient reductions might be desired. We asked the question what sort of nutrient reductions might be needed to bring chlorophyll *a* in that river down to some predefined acceptable level, i.e. possible response variable criterion.

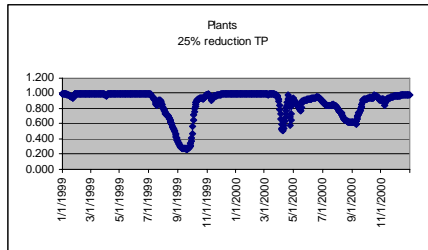
## **Step 1: Stressor Identification**

- Ran iterative 2-year runs using batch mode
  - Series of runs with different multiplicative loading factors for TP, NO<sub>3</sub>, NH<sub>3</sub>, TSS, BOD (individually, and with equal TP/TSS reductions)
- Screening analysis
  - Steinhaus community similarity index for sensitivity of algal communities
  - Phytoplankton graphs
- Focus on subset of stressors for more detailed analysis and target derivation

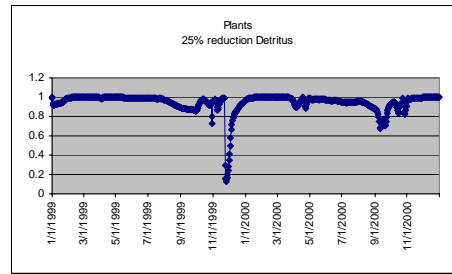
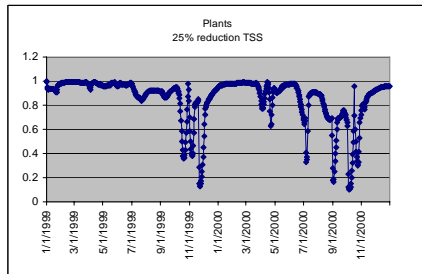
Because there were several stressors potentially affecting algal response in the Blue Earth, the first step we took was to see if we could eliminate some of them from consideration and simplify our analysis.

The batch mode came in very handy when setting up multiple runs for an exploratory analysis like this. I set them up to run overnight. I ran numerous iterations (25%, 50%, and 75% reduction for each factor) to screen out potential stressors that didn't seem to have much effect on the algae if they were reduced.

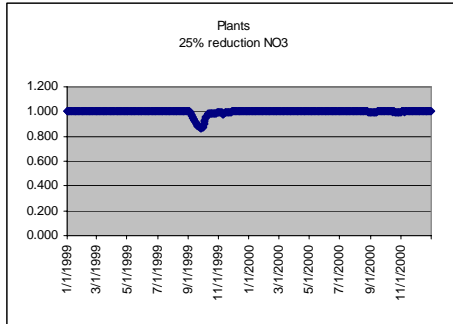
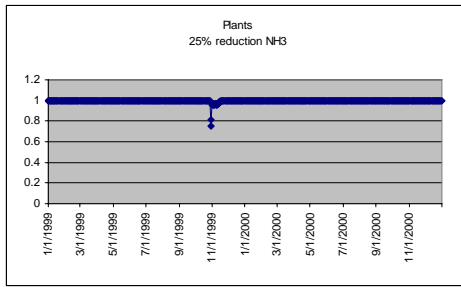
## Steinhaus Similarity Indices show changes in algal community



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



Steinhaus community similarity indices can be calculated easily by AQUATOX; the model calculates the similarity between the control and perturbed runs for plants, invertebrates, fish, and all animals. A Steinhaus index of 1.0 indicates that all species have identical biomass in both simulations (i.e., the perturbed and control simulations); an index of 0.0 indicates a complete dissimilarity between the two simulations. See Sec 4.4 of the Addendum to Release 2 Technical Documentation addendum for more information; we will also encounter it in Day 3.



Neither NH3 nor NO3 show much of an influence on in stream algal communities, at least by themselves

Given the lack of response to nitrogen reduction, we'll not focus on that any longer. It could, however, be very important for downstream communities (also a factor to be considered when setting water quality standards).

## WQC development method #1

- Ran selected scenarios (with TP and TSS reductions) for longer time
- Used long term (6-year) average as equivalent to target
- Focus on chl a and corresponding TP
  - Start with ecoregional chl a target of 7.85 ug/L
  - What reductions in TP will result in attaining long term chl a target?

We're presenting two hypothetical examples of nutrient criteria development. Both methods use AQUATOX to determine nutrient concentrations that would achieve an "acceptable" chl *a* concentration. **Method #1** presumes that the State (Minnesota) has accepted the 304(a) chlorophyll *a* concentration (but not necessarily the corresponding N and P values) as a criterion for stream and rivers in the relevant ecoregion. The value for the Blue Earth River is **7.85 ug/L**, which is assumed to apply to long-term (*i.e.* at least annual) mean concentrations in the River. The mean chlorophyll *a* concentration generated by the calibrated AQUATOX model of existing conditions in the Blue Earth River over a six-year simulation (1995 through 2000) is **18.3 ug/L**. Note that this reflects conditions over the entire year, not just the growing season or during blooms.

Because basing a criterion recommendation on only 2 years of data may not be reasonable, we loaded 6 years of HSPF output and fed it into AQUATOX. The ecoregional target value is presumed to be a long term average as well; so what we were looking for was a 6-year AQUATOX simulation which produced an average chl *a* concentration closer to the ecoregional target value.

We ran AQUATOX using simple, across-the-board multipliers in increments of 0.2, applied to the influent TP and TSS time series from the HSPF simulation. We used reductions of TSS as well as TP because most of the management measures that control P would also reduce TSS.

## Example Criteria Development Method 1

Start with reference condition chl\_a value (7.85 ug/L)

Parameter	# of streams	Reported min	Reported max	25 <sup>th</sup> Percentile (all seasons)	AQUATOX 6-yr average
TKN (mg/L)	136	0.57	4.42	0.65	
NO <sub>2</sub> + NO <sub>3</sub> (mg/L)	141	0.083	9.6	1.965	
TN (mg/L) calculated	NA	0.653	14.02	2.615	
TN (mg/L)- reported	32	1.65	10.06	3.26	
<b>TP (ug/L)</b>	187	11.25	1720	<b>118.13</b>	<b>268</b>
Turbidity (NTU)	32	4	160	15	
Turbidity (FTU)	74	0.975	178	7.69	
Turbidity (JCU)	56	4.23	116.5	10.15	
Chl a (ug/L)- fluorometric method	24	1.8	45.2	4.4	
<b>Chl a (ug/L)- spectrophotometric method</b>	25	3.76	90.6	<b>7.85</b>	<b>18.3</b>
Chl a (ug/L)- trichromatic method	3	9.38	31.0	9.38	

We used the model to explore the question of what sort of nutrient reductions would be required to achieve mean chlorophyll *a* in the Blue Earth river at or below hypothetical criteria concentrations. We did this analysis for two different hypothetical chl\_a numbers. The first was simply the 304(a) value, shown in red in this table.

The ecoregional recommendations are 118.13 ug/L for TP, and 7.85 ug/L chl a. The 6-year averages calculated by AQUATOX at baseline conditions were 268 ug/L and 18.3 ug/L, respectively.

## Effect of Input Load Multipliers on Blue Earth Mean Chlorophyll *a*

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

} 7.85 ug/L

We ran Blue Earth River AQUATOX model simulations with fractional multipliers applied to the influent TP loadings from the linked HSPF simulation. This table shows the resulting mean chlorophyll *a* concentrations from these runs.

These results suggest that >80 percent reduction in TP would be required to bring the mean chlorophyll *a* in the Blue Earth River down to 7.85 ug/L. By contrast, the 304a TP value (118.13 ug/L) corresponds with only a 56 percent reduction.

We used reductions of TSS as well as TP because most of the management measures that control P would also reduce TSS.

## **Method #1 Target**

- Results suggest more than 80% reduction of TP, if coupled with TSS reductions, necessary to attain the target chl a of 7.85 ug/L
- 304(a) recommendations suggest a 56% reduction of TP would be necessary

The 304(a) approach does not explicitly address the effects of TSS; we'll look at how TSS affects the algal response later.



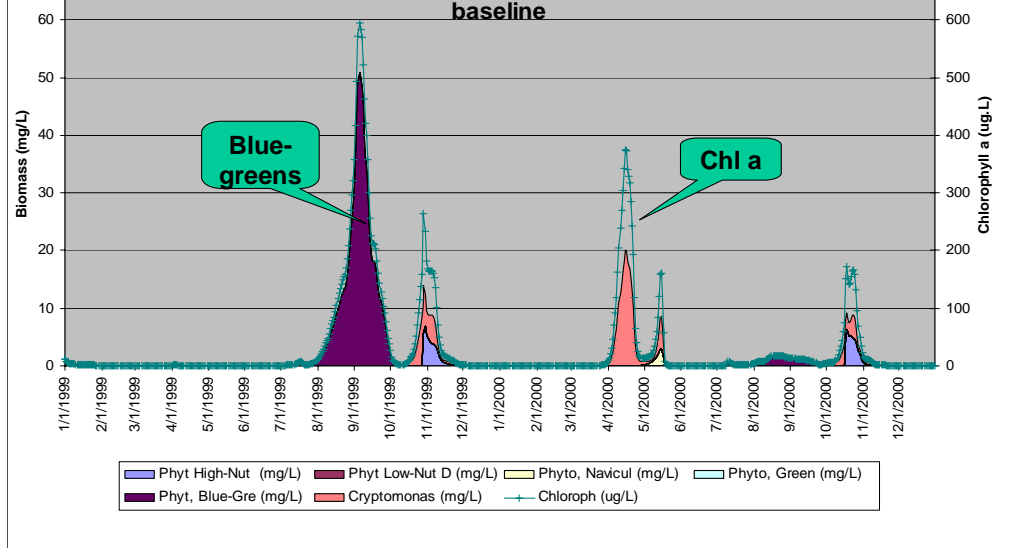
## WQC Method #2

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

If the State wishes to consider the composition of the algal community as well as the total chlorophyll *a* value, AQUATOX provides a way to do so.

Obviously, what percentage of blue-green is “acceptable” is subject to debate.

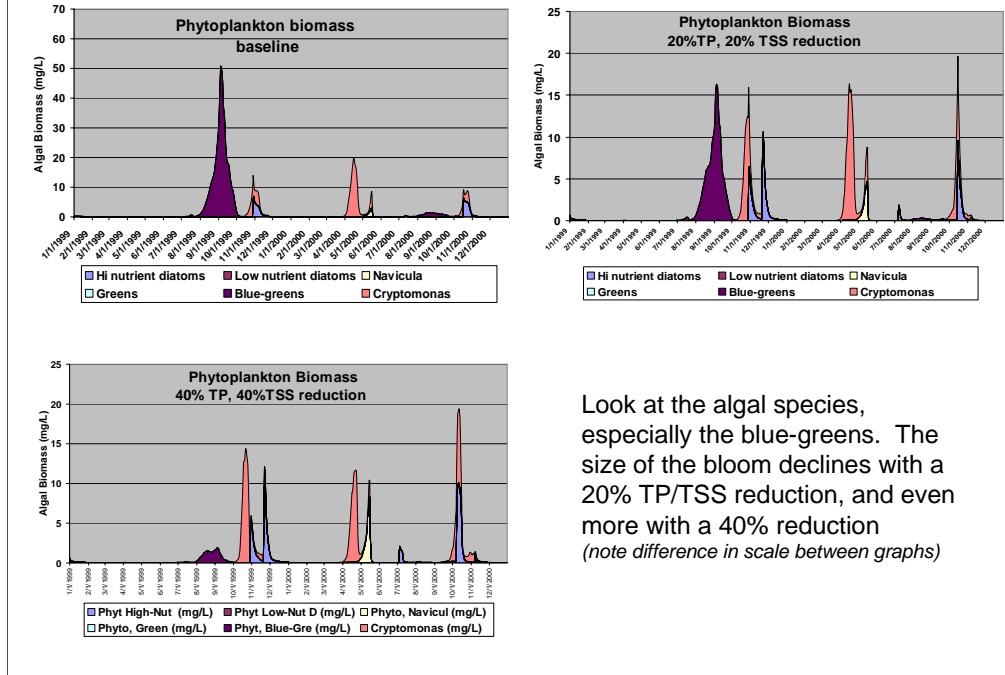
## Baseline conditions include large blooms, especially in 1st year



Very high chl a peaks (almost 600 ug/L) predicted in 1999. Largest bloom (in the fall) is dominated by blue-greens, and lasts almost 2 months; later bloom by cryptomonads, plus some hi-nutrient diatom.

Note that there is no spring bloom in 1999, probably due to light limitation or washout; it was a very high flow year.

## Compare Algal Species



Look at the algal species, especially the blue-greens. The size of the bloom declines with a 20% TP/TSS reduction, and even more with a 40% reduction (note difference in scale between graphs)

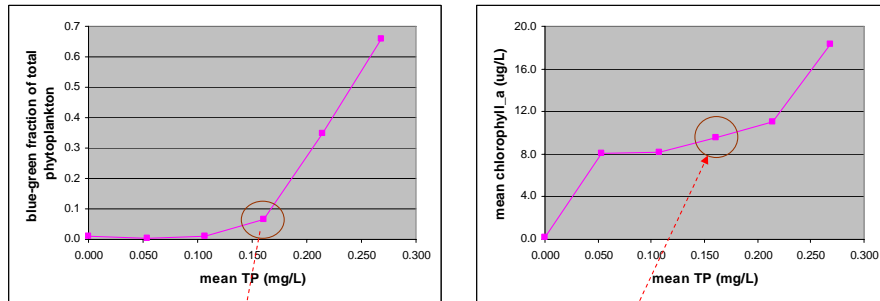
A reduction of blue greens, which are of significant concern in the Blue Earth, could be an alternative target for algal response. In this instance, a significant drop in blue-greens happens between 20 and 40% reduction of TP and TSS.

The blue-greens show the greatest response to the manipulations. Other algae spp respond, but to a lesser degree.

We used reductions of TSS as well as TP because most of the management measures that control P would also reduce TSS.

## Criteria Development

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



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

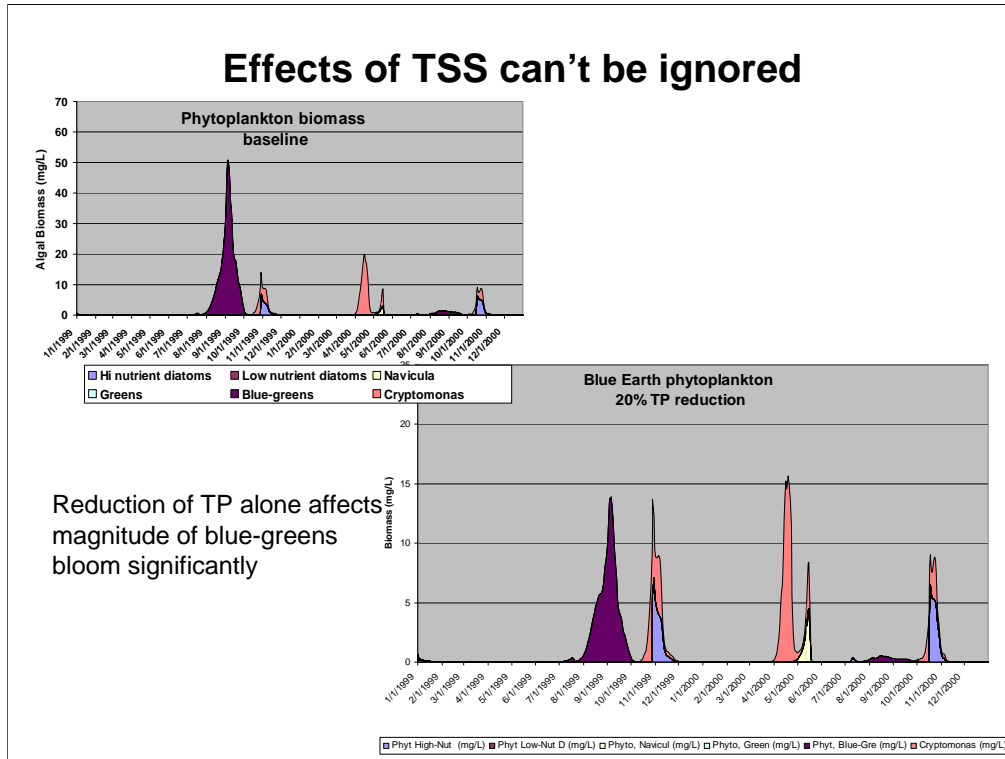
In the second example, we used the AQUATOX runs to estimate a chl *a* concentration that corresponds with the point where a shift between dominance of blue-greens and more desirable algal species occurs. The left figure shows blue-greens as a fraction of total water column phytoplankton, and the right shows mean chl *a* concentrations. Both are plotted as functions of mean TP, in increments of 20% reduction on the horizontal axis.

The left figure shows an inflection point at a approximately 0.161 mg/L, a 40 percent decrease in TP below existing concentrations. The inflection point occurs at a blue-green fraction of slightly less than 10% total phytoplankton; it also corresponds with mean chl *a* of 9.5 ug/L (on the right). The chl *a* value is slightly higher than the 304(a) number, and the TP value is substantially higher than the 304a value. So if the management goal focuses on the % blue-greens rather than chl *a* per se, and if “less than 10% blue-greens” is an acceptable target, 9.5 ug/L would be as our second hypothetical chlorophyll *a* criterion.

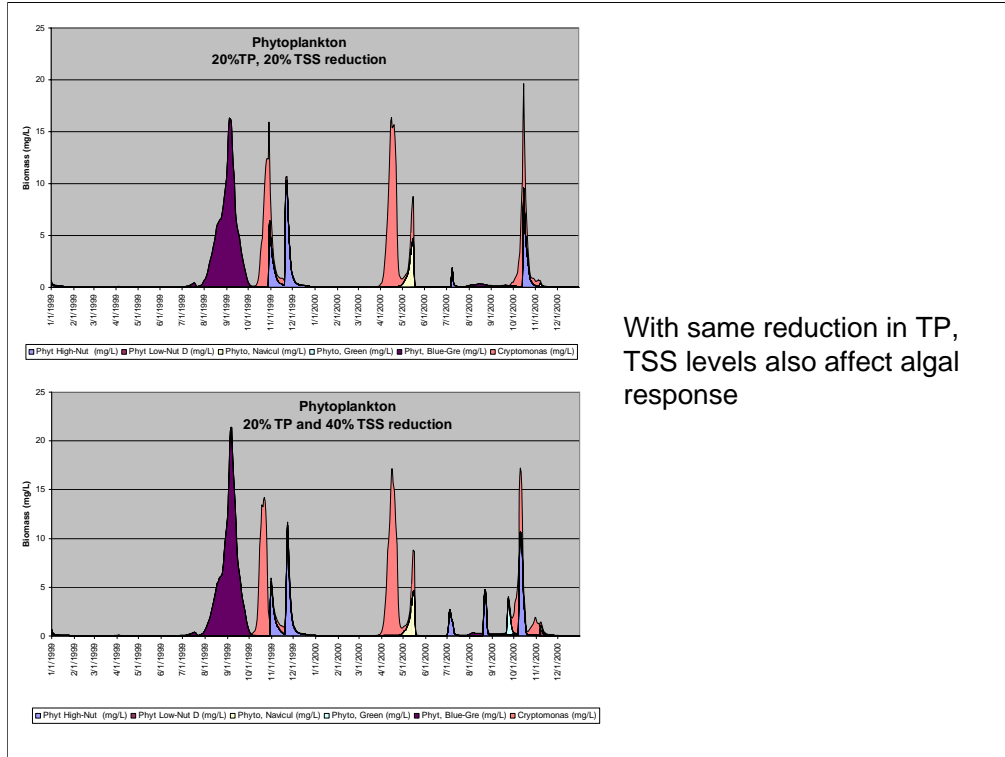
So we had two different hypothetical criteria values for chl\_a: the reference condition 304a number itself, and a slightly higher number corresponding with the inflection point in the left figure.

## **Method #2 Target**

- Results suggest that a 40% reduction of TP, if coupled with a corresponding reduction in TSS as well, would result in an algal community with a much reduced proportion of noxious blue green algae
- This is very preliminary, and one may wish to look at other aspects of algal response, such as...



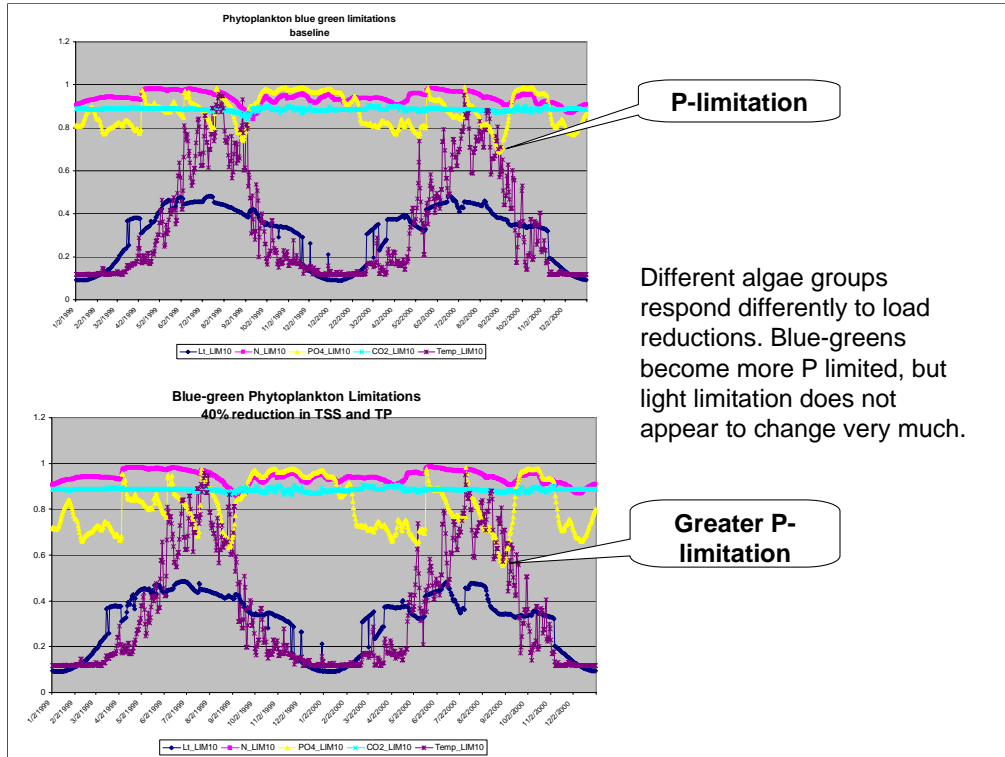
The previous slides included equal % reductions of TSS and TP. For the sake of illustration, let's accept that the reduced proportion of blue greens under a 20% TP reduction was an acceptable algal community. Let's look at the differences that TSS makes.



With same reduction in TP, TSS levels also affect algal response

With reductions in TSS as well as TP, we get more blue greens than with TP reduction alone, which may not be desirable. However, the increased light also allows high-nutrient dominated diatoms to show a series of small blooms.

The effects of TSS reduction may help to explain why in method #1 there was such a great reduction in TP required to get total chl a values down to the 304a criteria recommendation. Remember that most control measures would reduce TSS along with TP, so its effects can't be ignored.



By looking at the responses of the individual algae taxa to different reductions, it may be possible to tailor management actions to the desired community.



## Assessing Attainability of Hypothetical Criteria Through Use of BMPs

*Each scenario represents different combinations of BMPs:*

Scenario	% Buffers Installed	% Wetlands Restored	% Nutrient Mgt.	TP (mg/L)	Chl_a (ug/L)
Current conditions	0	0	0	0.268	18.6
BMP1	20	20	20	0.242	15.3
BMP2	30	20	20	0.224	14.4
BMP3	30	30	40	0.213	12.2
<b>304(a) Criteria</b>				<b>0.118</b>	<b>7.85</b>
<b>AQUATOX Method 1</b>				<b>~0.050</b>	<b>7.85</b>
<b>Method 2 Criteria</b>				<b>0.161</b>	<b>9.5</b>

With these two hypothetical response variable criteria as targets, we developed various mitigation scenarios that represent different combinations of BMPs and added them into the watershed model (BASINS/HSPF), then fed the HSPF results into AQUATOX simulations. This table shows baseline or existing condition results, and the results of three of the scenarios we modeled.

The bottom line is that despite substantial improvements in water quality, none of the modeled scenarios attained the 304(a) criteria for either TP or chl\_a. Nor did they attain any of the targets derived using AQUATOX. This demonstrates one of the main advantages that mechanistic modeling provides: the ability for States to assess the technical attainability of hypothetical criteria before they adopt them.

## Summary

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

So to summarize, we used mechanistic modeling to quantitatively link nutrient stressor and response variables in three Minnesota rivers. We identified TP and TSS as the most important stressors controlling instream phytoplankton concentrations, though not necessarily downstream conditions. Using these model results we derived an example of a hypothetical chl\_a criterion based on a biological metric that we came up purely with for illustrative purposes. And we used a linked watershed model to assess the attainability of this hypothetical criterion, as well the ecoregion 304a criteria, by adding BMPs at various densities into the watershed model and simulating their impact on water quality.

## Next Steps

- Finish Minnesota case study report
- Integration of AQUATOX analyses with biocriteria and aquatic life uses
  - Development of appropriate metrics
- Transferability of results
  - Analyses are site-specific, but results could be applied to groups of similar water bodies or watersheds
  - Criteria derived for a specific water body using a modeling approach could apply to similar waters
- Finish Lower Boise River project

The draft report on the Minnesota rivers project underwent a peer review and we are doing some additional analyses in response to their comments.

We are in the very early stages of integrating with biocriteria program, which has a lot of promise. For example, some state programs are in the process of developing biological metrics based on percentages of specific algae groups.

Although we simulated specific locations on specific reaches, results derived using this kind of an approach need not be considered applicable only to the modeled locations. One possibility might be to derive criteria based on simulations of a specific reach, and then apply those criteria to a group of water bodies that are judged to be sufficiently similar. For example, EPA's Office of Research and Development (ORD) has been using statistical approaches such as cluster analysis to come up with groups of watersheds throughout region 5 that are similar to each other in terms of their responses to nutrients. Mechanistic modeling could be seen as a logical step forward from this kind of work to real-world applicability.

## Nutrients in Cahaba River Alabama



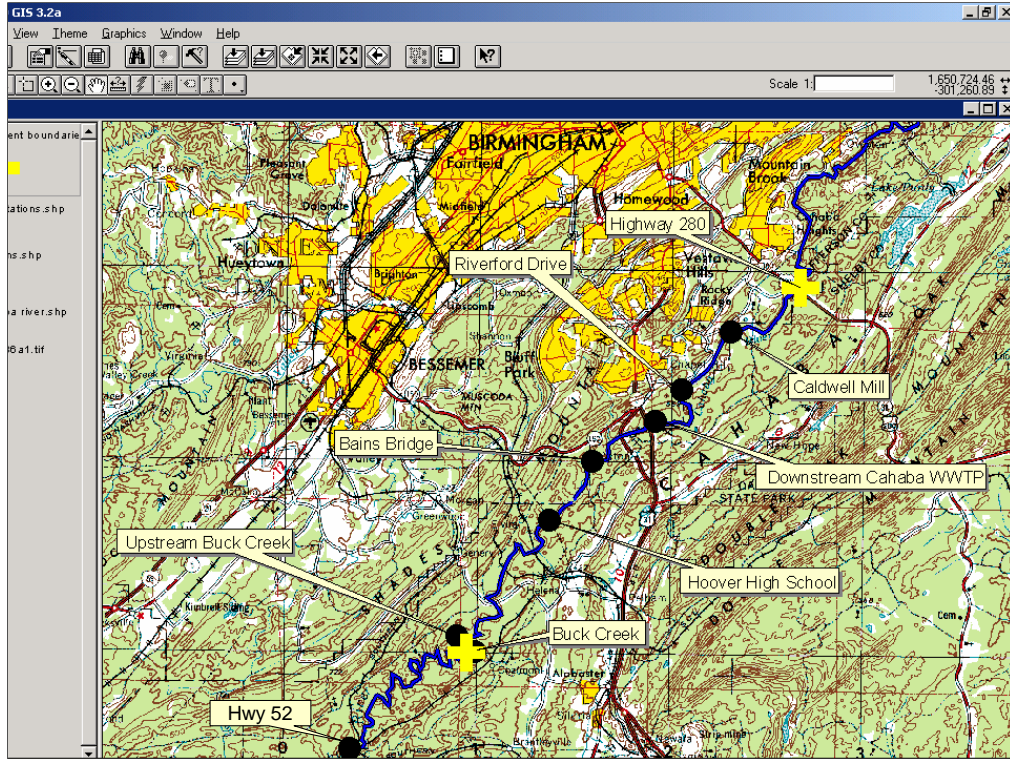
According to the Alabama Department of Environmental Regulation, the Cahaba River is impaired due to nutrients and siltation. In part the listing decision was driven by endangered species issues. Thus identifying the stressors driving the habitat impairment issues for several endangered fishes and mollusks was an important factor in selecting AQUATOX for this project.

Picture source <http://www.vis-info.com/Cahaba/toc.htm>

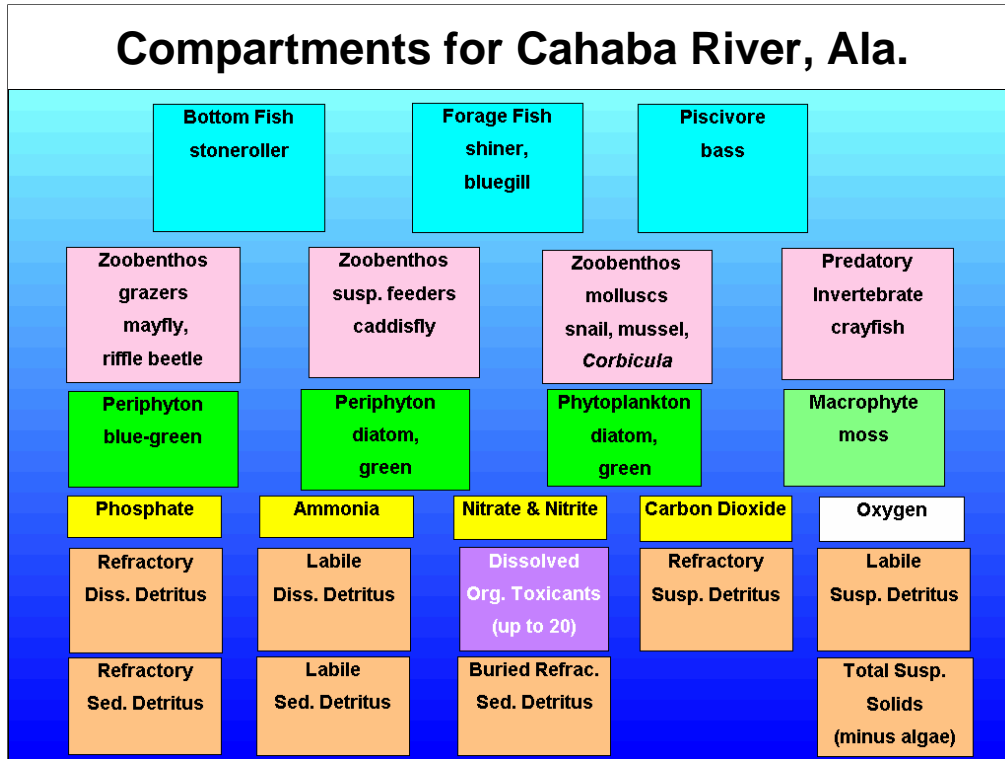
This example was prepared by Don Blancher, TAI Environmental Sciences, Inc. (presently of TEA, Inc.).

## Background

- Prior to 1975 Cahaba River experienced fish kills, low D.O., high ammonia, total residual chlorine, metals and pesticide loads
- In 1980's several studies noted the loss of several species of mussels and fish, most below the subject segment
- By early 1990's still had significant D.O. excursions (> 10% at Altadena station according to GSA) and significant levels of the herbicide atrazine
- Area has had a large amount of urban growth and development in watershed of subject segment, impacting River through non-point runoff of sediments
- Subject Segment from Highway 280 near Mountain Brook to Upstream of Buck Creek
- Draft 2000 303d List shows segment (Segment 2) as partially impaired
  - Nutrients
  - Sediments



The Cahaba River runs through a large portion of urban/suburban areas southeast and south of Birmingham and through the city of Hoover. The model was calibrated for the Caldwell mill station which represented conditions upstream of the major treatment plants located along the river. Downstream of this station, at least 7 treatment plants discharge into the Cahaba (directly and indirectly through Buck Creek) by the time the river reaches Shelby County Highway 52.



Periphyton were of major interest in looking at habitat impairment issues related to eutrophication of the Cahaba. Also, aquatic mosses were a major component of the primary producers and important to certain fish species (stonerollers). Another key factor was determining the importance of secondary production and the control of algae by grazers.

## Caldwell Mill - Cahaba RM 144.9



AQUATOX can model differing velocities and biotic preferences for runs, riffles, and pools.

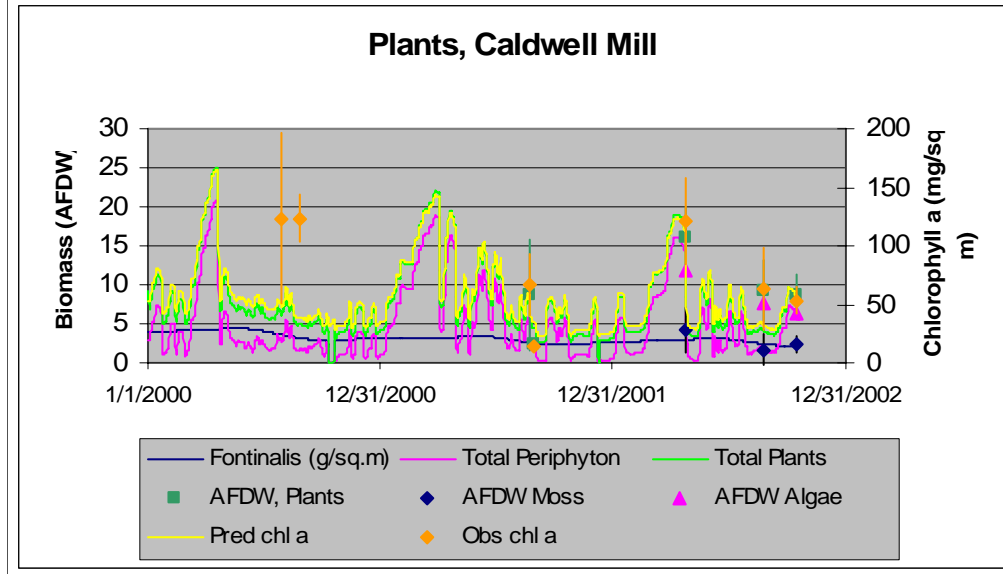


# Habitats are characterized in the Site/Stream Parameters screen

The screenshot shows a software window titled "Edit Stream Data" with a "Stream Parameters:" section. It includes input fields for Channel Slope (0.002 m/m), Maximum Channel Depth Before Flooding (5 m), and Sediment Depth (0.1 m). A "Mannings Coefficient:" section offers two options: "Estimate based on Stream Type" (set to "natural stream") or "use the below value" (set to 0 s/m<sup>1/3</sup>). The "River Habitats Represented" section shows Percent Riffle at 10%, Percent Pool at 0%, and Percent Run at 90.00% (All Habitat that is not Riffle or Pool). An "OK" button is at the bottom right.

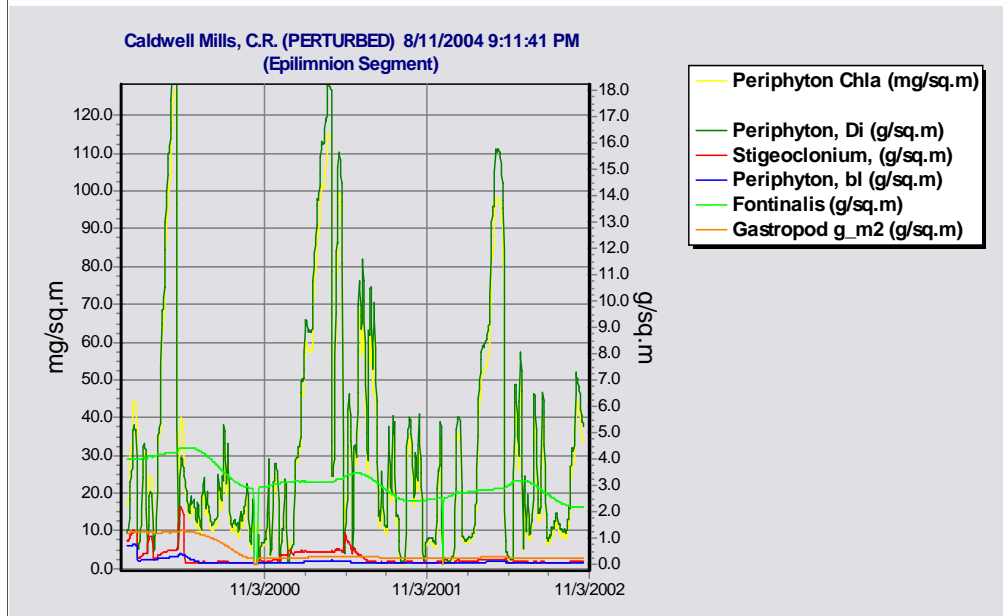
Parameter	Value	Reference
Channel Slope	0.002 (m/m)	USEPA 2001 Report
Maximum Channel Depth Before Flooding	5 m	Default
Sediment Depth	0.1 m	Default
Mannings Coefficient	0 s/m <sup>1/3</sup>	
Percent Riffle	10 %	3MOAHabAssess2001Cr.xls
Percent Pool	0 %	
Percent Run	90.00 %	(All Habitat that is not Riffle or Pool)

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



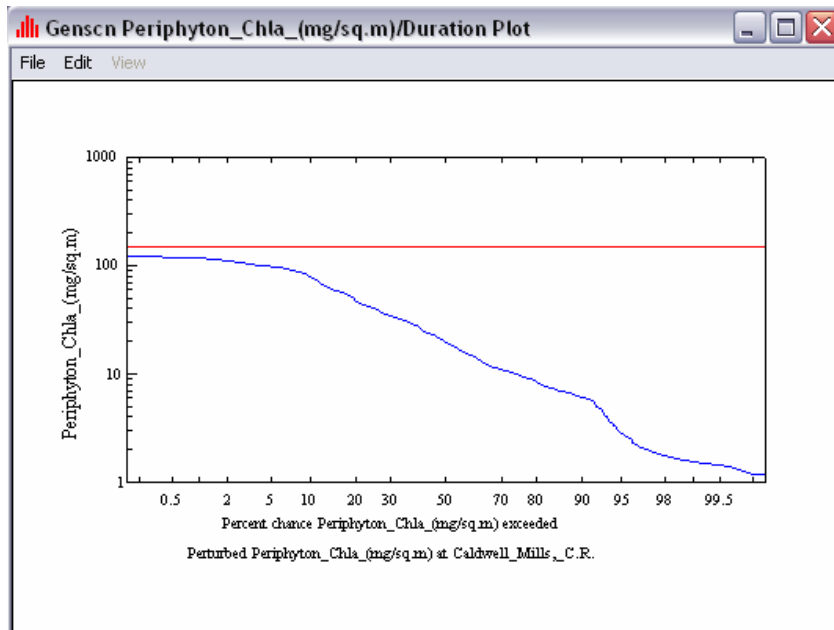
Visual inspections of fits of predictions to observed data are useful in evaluating how well patterns are represented, with allowance for the vagaries of widely spaced data points. Although not quantitative, they contribute considerably to the weight of evidence that the model is representing the periphyton dynamics realistically. The model was calibrated with data from Caldwell Mill. Beyond the transient conditions of the year 2000, the model seems to give a reasonable fit to the observed data, considering the spread in the observations as indicated by the error bars ( $\pm 1$  standard deviation).

## Diatoms dominate with minor greens in summer and moss



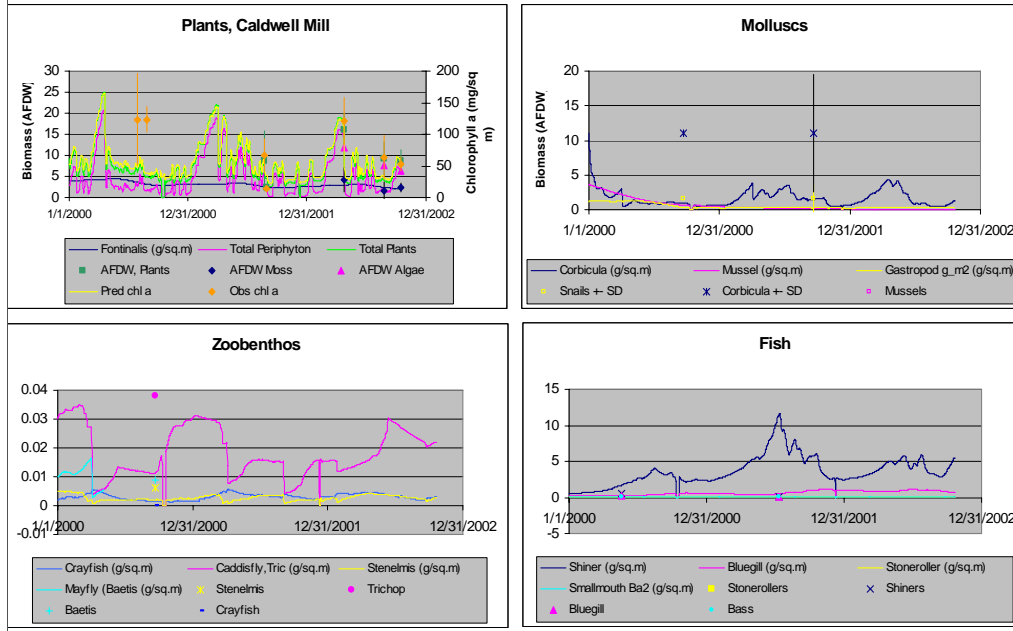
The periphyton exhibit considerable fluctuations. Examination of the detailed simulation of Caldwell Mill shows that diatoms dominate, although other simulations have seasonal succession of constituent groups, with diatoms in the spring, followed by greens and blue-greens in the summer. Under favorable conditions growth can be rapid, but scouring by storm events can be dramatic, and grazing by aquatic insects and snails can reduce the biomass quickly. The seasonal pattern is quite reasonable for a stream such as the Cahaba River, lending additional credence to the model results.

## Periphyton chlorophyll a did not exceed the 150 mg/sq m target value



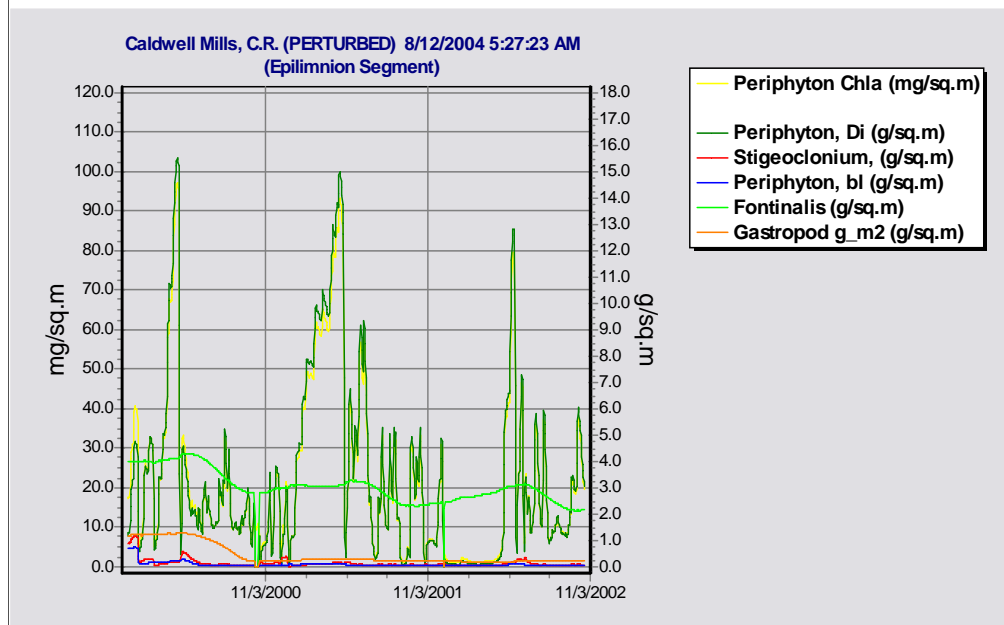
Data from AQUATOX was also analyzed using the BASINS tool GenScn to develop exceedance charts for looking at impairment from periphytic growth. A guidance value of 150 mg/m<sup>2</sup> periphyton chlorophyll a was used as the threshold of impairment for purposes of our analyses. These simulations indicated no exceedance.

## Animals also exhibited reasonable simulations for Caldwell Mill



Calibration of major secondary producers and fishes had reasonable ranges for the limited biomass measures observed for the station.

## Reduction of P to 11% decreases algae



By taking 11% of the phosphorus loading we see a slight reduction in diatoms and a greater reduction in greens.

## Set Control so Multiply Loadings are 1.0

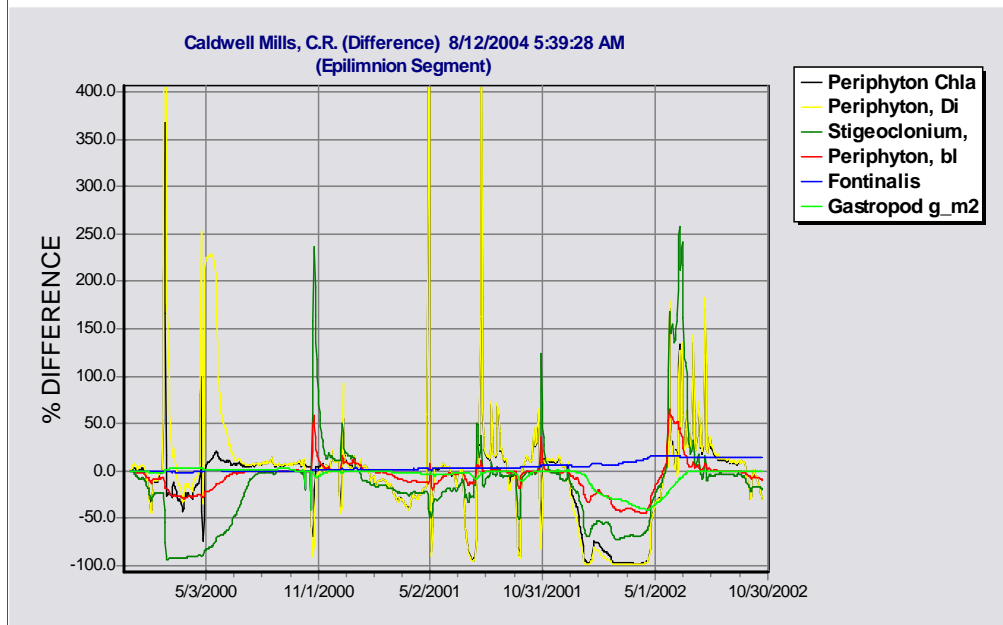
**Control Run Options**

<b>All Organic Toxicants:</b>		<b>Sand / Silt / Clay or TSS:</b>	
Zero-Out Initial Conditions	<input checked="" type="checkbox"/>	Zero-Out Initial Conditions	<input type="checkbox"/>
Omit Inflow Loadings	<input checked="" type="checkbox"/>	Omit Inflow Loadings (or all TSS)	<input type="checkbox"/>
Omit Point Source Loadings	<input checked="" type="checkbox"/>	Omit Point Source Loadings	<input type="checkbox"/>
Omit Direct Precipitation Loadings	<input checked="" type="checkbox"/>	Omit Direct Precipitation Loadings	<input type="checkbox"/>
Omit Non-Point Source Loadings	<input checked="" type="checkbox"/>	Omit Non-Point Source Loadings	<input type="checkbox"/>
Omit Toxicant in Organisms	<input checked="" type="checkbox"/>	Set Multiply-Loadings Factors to 1.0	<input type="checkbox"/>
Omit Buried Toxicants	<input checked="" type="checkbox"/>		
Set Multiply-Loadings Factors to 1.0	<input checked="" type="checkbox"/>		
<b>Nutrients: (Ammonia, Nitrate, and Phosphate)</b>		<b>Detritus:</b>	
Zero-Out Initial Conditions	<input type="checkbox"/>	Zero-Out Initial Conditions	<input type="checkbox"/>
Omit Inflow Loadings	<input type="checkbox"/>	Omit Inflow Loadings	<input type="checkbox"/>
Omit Point Source Loadings	<input type="checkbox"/>	Omit Point Source Loadings	<input type="checkbox"/>
Omit Direct Precipitation Loadings	<input type="checkbox"/>	Omit Direct Precipitation Loadings	<input type="checkbox"/>
Omit Non-Point Source Loadings	<input type="checkbox"/>	Omit Non-Point Source Loadings	<input type="checkbox"/>
Set Multiply-Loadings Factors to 1.0	<input checked="" type="checkbox"/>	Set Multiply-Loadings Factors to 1.0	<input checked="" type="checkbox"/>

Help  OK  Cancel

We can compare the perturbed simulation with reduced phosphorus to the control by setting the loadings multiplication factors to 1.0 in the control.

## Difference graph shows the decline better



A difference graph between the perturbed and control simulations demonstrates the decline of greens (*Stigeoclonium*) and diatoms with a reduction in phosphorus loadings to 11% of baseline. The sharp spikes are due to a slight shift in the timing of the blooms.



## Lab 6: Calibration of Cahaba River AL Study and Impacts of Invasive Snail

Calibrate Cahaba River AL study

- Start with MN parameters
- Modify to obtain good fit with minimal changes
  - calibrate  $FCrit$  (site-specific critical force for scour)
  - modify  $TOpt$  (optimum temperature) for warm water spp.

Analyze response to reduced nutrients

Analyze possible impacts of invasive snail

- Add *Potamopyrgus* (New Zealand mud snail)
- Run perturbed simulation
- Compare control and perturbed
  - flip between graphs, plot difference graph
  - what is impact on plants, animals, nutrients?

The objectives are to:

- demonstrate how general parameter set can be adapted to a Southern river
- demonstrate again how model can be used to analyze possible effects of nutrient reductions
- demonstrate use of model in forecasting impacts of invasive species

The Cahaba River AL data span a period of over two years with varying environmental conditions, so it would be desirable to take advantage of the full period in obtaining a site calibration. However, the flow dynamics force the integration to proceed with a short time step, prolonging the run time. Therefore, we will use pre-run simulations for the calibration, and you can experiment with them at a later time if you wish. Furthermore, we will start a couple simulations of nutrient reductions and addition of an invasive species before lunch and then examine the results when we return.

## Calibration of Cahaba River AL Study

- Open **Cahaba River AL MN prms.aps**
  - Control has results with MN parameters
  - Perturbed has results with  $FCrit$  increased
  - open **Cahaba River AL MN prms.xls** and observe fit
  - open **Cahaba River AL FCrit.xls** and observe fit
- Open **Cahaba River AL warm prms.aps**
  - Control has increased  $TOpt$  for most algae
  - open **Cahaba River AL warm prms.xls** to see fit

This exercise is designed to demonstrate how little is required to obtain a good stream ecosystem calibration in a completely different ecoregion using a standard parameter set (the “MN parameters”). The biggest change, and one that is likely for many sites, is to modify the  $FCrit$  critical force for scour parameter values for all periphyton. This is necessary because periphyton substrates differ from site to site. The Crow Wing and Rum Rivers in MN have cobbles and boulders and are more sensitive to higher current velocities than the bedrock outcrops in the Cahaba River; not only is the bedrock stable, it also provides abundant crevices and lee sides that are protected refuges for periphyton.

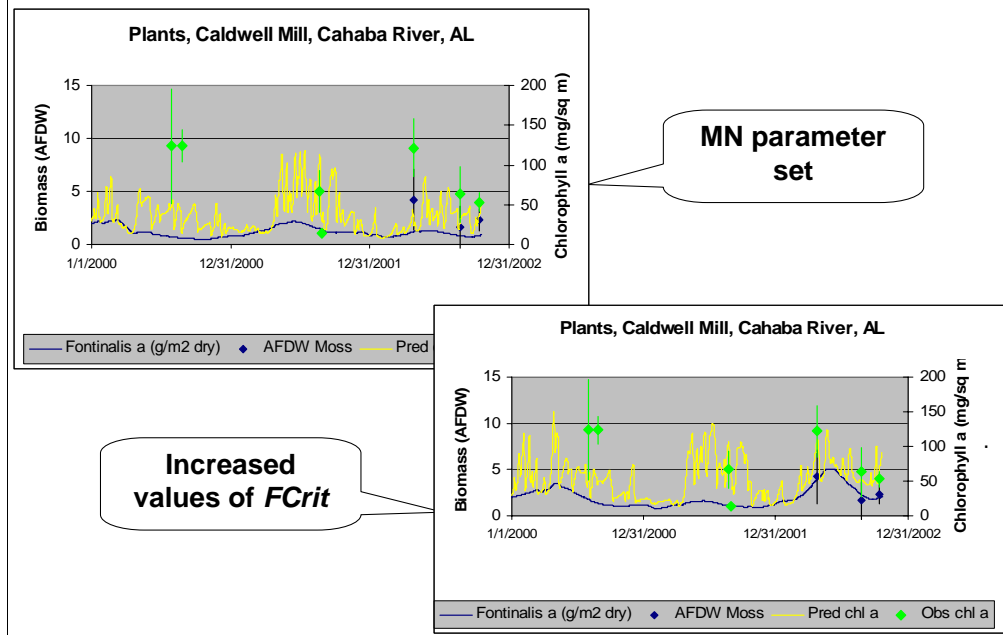
Of course, going from MN to AL one would expect differing temperature adaptations. It is necessary to change the  $TOpt$  or optimum temperature values for most algae or they would be intolerant of summer temperatures in AL.

The differences between Control and Perturbed illustrate another advantage of this feature. Originally it was designed just to zero out a toxic chemical and to see the differences in the biota with and without the chemical. But by keeping one simulation the same (generally the Control) and incrementally changing parameter values and re-running the Perturbed, it is a powerful calibration tool.

*Note: all study files referenced above (\*.aps) are located in the AQUATOX/Studies directory.*

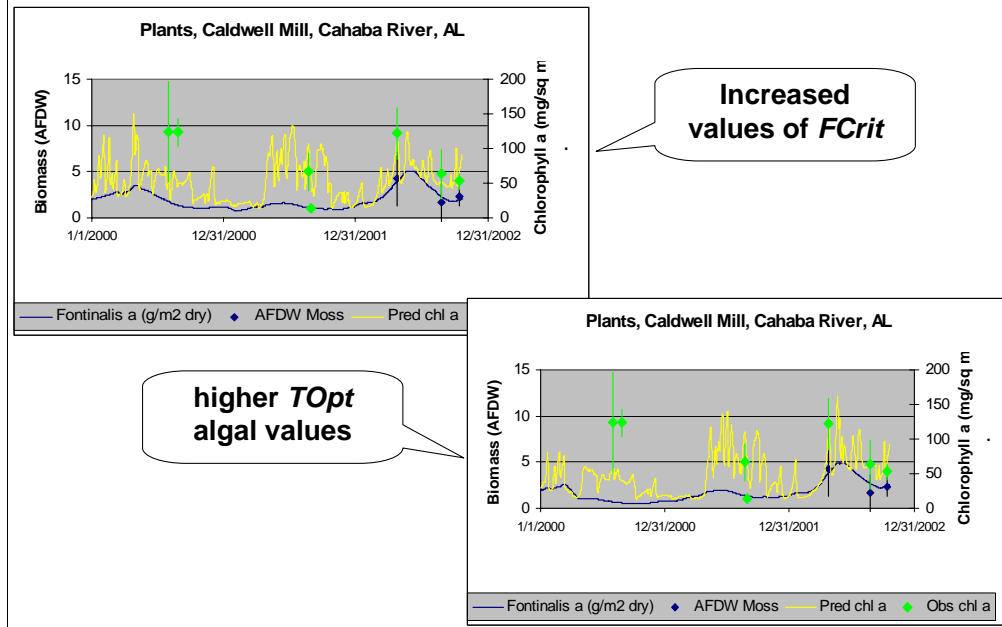
*All Excel files referenced above (\*.xls) are located in the AQUATOX/Data directory.*

## Changing scour parameter improves simulation of Cahaba River

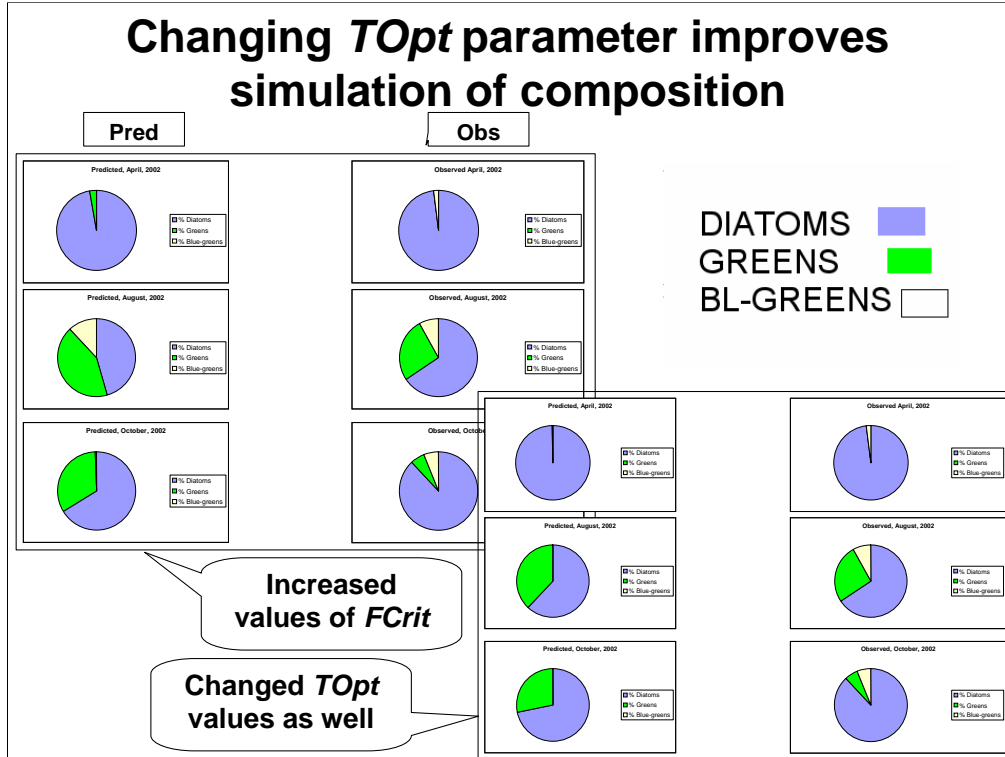


The scour parameter  $FCrit$  depends on site conditions, especially the nature of the substrate. The lowest  $FCrit$  values would be used where periphyton establish on stabilized sand waves; higher values would be used where the substrate is gravel and cobbles; the highest values would be used in places like the upper Cahaba River where the substrate is rough bedrock with cracks and extensive protected lee sides.

## Increasing optimum temperature values improves simulation slightly



The simulation does not fit the two observations in 2000. Discussion with the field biologists suggests that the early samples were not collected with an unbiased protocol. The instructors are divided as to whether the higher  $TO_{opt}$  provides a better fit—demonstrating the difficulty of visually evaluating a fit!



With  $FCrit$  and  $TOpt$  values increased from those in the MN parameter set, given the bedrock substrate and warmer temperatures, both the periphyton biomass and composition compare favorably with the observed values. As expected, the higher  $TOpt$  fits the observed dominance of diatoms in August; however, it is at the expense of the blue-greens.

To experiment with reductions in nutrients, set the TSP loading multiplier to some fraction; in the control setup check **Set Multiply-loadings Factors to 1.0** (so that if you re-run the control simulation there will be a difference from the perturbed); and run a perturbed simulation that is saved as “Cahaba River AL x%P.ap.s.”

## Reduction of Phosphate

- Open **Cahaba River AL.aps**
  - this is the same as above, but is a template for applications
  - decrease the P loading by a reduction factor
  - save as “Cahaba River AL x%P.aps”
  - run the perturbed simulation over the lunch hour

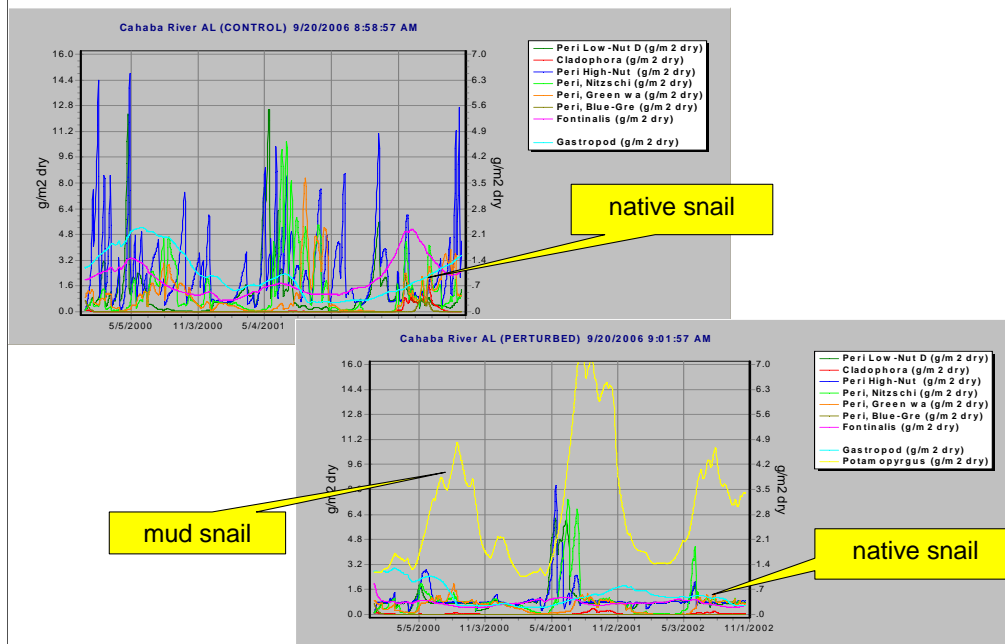
## Invasive Snail Species

- Open another copy of **Cahaba River AL.aps**
- Add the invasive snail *Potamopyrgus* as Snail2
  - set the initial condition to 1.2 and keep the “seed” value as 1e-5 (the default)
- Save as “Cahaba River AL invasive snail.aps”
- Run the perturbed simulation
- Inspect the perturbed, control, and difference graphs
  - how are the plants affected? the invertebrates? the fish? the nutrients?

*Potamopyrgus* is an invasive New Zealand species that is upsetting the ecology of streams in Yellowstone Park and elsewhere. We added *Potamopyrgus* to the simulation as an exercise in risk assessment of the potential impacts of an invasive species in the Cahaba River.

Hall, Robert O., Jr., Jennifer L. Tank, and Mark F. Dybdahl. 2003. Exotic Snails Dominate Nitrogen and Carbon Cycling in a Highly Productive Stream. *Frontiers in Ecology and the Environment* 1 (8):407-411.

## Dramatic decrease in algae and moss with introduction of New Zealand mud snail

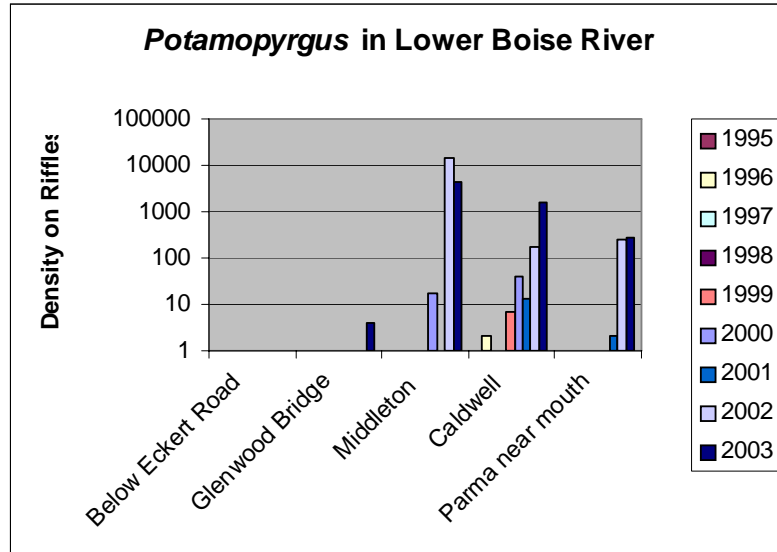


Keeping the axis scales the same to facilitate direct comparison of perturbed and control simulations, we see that algae, moss, and the native snail decline dramatically with the simulated introduction of *Potamopyrgus*.

*Tip:* you may wish to add *Potamopyrgus* to the Glenwood Bridge simulation on your own to forecast the introduction at this site on the Boise River.



**This is not an idle exercise: we are evaluating the impact of *Potamopyrgus* in the Lower Boise River project**



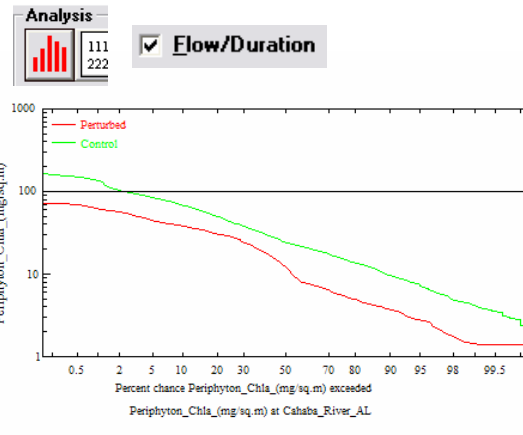
As an aside, in modeling nutrient-algal relationships in the lower Boise River the New Zealand mud snail has to be taken into consideration. Upstream is to the left and downstream to the right in the graph.

Data courtesy Dorene MacCoy, USGS.

*Tip:* you may wish to add *Potamopyrgus* to the Glenwood Bridge simulation on your own to forecast the introduction at this site on the Boise River.

## Analysis of Nutrients

- Open **Cahaba River AL x%.aps**
- Compare perturbed and control
- We will export to Genscn and plot duration for periphyton chl
- Is the decline acceptable?  
(in this example we use 11% TSP)



In this demonstration, we do not have observed data but rather we compare periphytic chl a in control and perturbed simulations by plotting duration, adding a line at 100 to represent a threshold for concern.

## Lake Onondaga, NY Validation

- “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
- Question: what would be the benefit of diverting WWTP effluent?

“Lake Onondaga is arguably the most polluted lake in the United States” according to Effler (1996) in the preface to his comprehensive book, which serves as the primary reference for the following information and data on the lake. The shore of this lake in central New York State was industrialized before 1800, and over the last hundred years at least thirty different chemicals were produced from nearby salt and limestone deposits. Unfortunately, the lake was a convenient dumping ground for waste products. Production of soda ash resulted in waste beds as much as 21 m deep and 8.1 km<sup>2</sup> in area along 30% of the lake shore; the wastes include NaCl and CaCl<sub>2</sub> that easily leach into the lake. The salinity of the lake was around 3‰ (parts per thousand) prior to closure of the soda ash plant in 1986; by 1990 the salinity had decreased to 1.3‰. Nevertheless, this salinity creates unusual density gradients and intense stratification of the lake. A chlor-alkali plant produced NaOH and Cl by electrolysis, using Hg as the cathode. From 1946 to 1970 as much as 75,000 kg of Hg were discharged into the lake. Aside from an advisory against eating fish from the lake, the high mercury levels may have adversely affected the functioning of the lake ecosystem.

The lake has been a receptacle for most of the domestic waste and urban runoff from Syracuse and the surrounding area. Prior to 1960 untreated and poorly treated sewage was discharged directly to the lake. In 1960 the Metropolitan Sewer District (METRO) primary treatment plant was completed; in 1979 it was upgraded to secondary treatment; and in 1981 tertiary treatment (removal of phosphorus) was instituted. By design, there is little reduction in ammonia in the sewage effluent. At present nearly 20% of the annual inflow into the lake is from METRO. Most troubling are the combined sewer overflows (CSOs) that carry storm water and raw sewage into tributary creeks about 50 times a year.

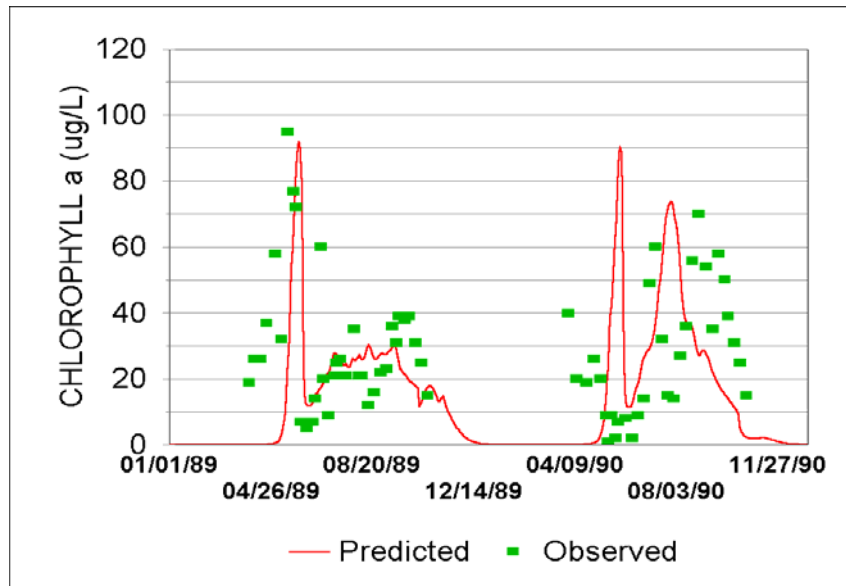
### **Model “fine tuning” in prior study**

- **Adjustment**
  - parameterization for resident groups
    - Cryptomonads, rotifers
  - workaround for inappropriate default
    - set to known thermocline depth
- **Result**
  - better prediction of chlorophyll a
    - blooms due to different algal groups
  - better prediction of DO, especially hypolimnion
- **See Validation Report**

A spring algal bloom was simulated by adding cryptomonads to the study. Rotifers were added as herbivores for the cryptomonads. A more unusual “tweak” was necessitated by the salinity of the lake. Salinity stratification causes a much shallower thermocline or mixing zone. The model computes the depth of the thermocline based on a regression relationship with lake length (wind fetch). The workaround was to set the lake length to a value that would force the depth of the observed shallower thermocline.

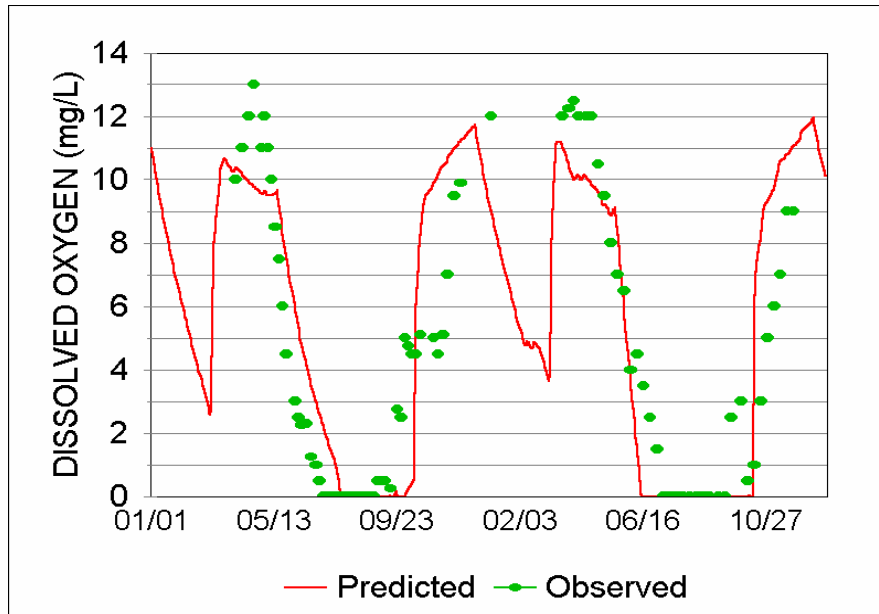
U.S. Environmental Protection Agency. 2000. AQUATOX for Windows: A Modular Fate and Effects Model for Aquatic Ecosystems-Volume 3: Model Validation Reports, Washington, DC.

## MODEL VALIDATION: AQUATOX provides reasonable simulation of chlorophyll a



The model was validated by running without any parameter changes. Your results will look a little different because of changes in the model since the validation. However, you will be able to run the simulation and paste the results into a template with observed data and graphs already set up.

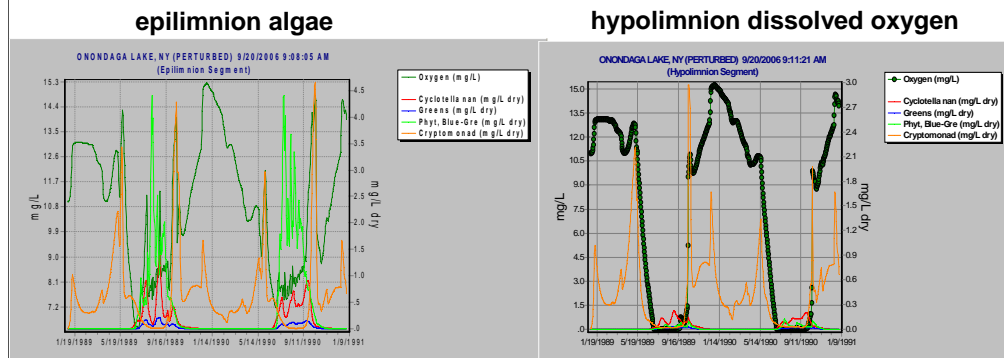
## MODEL VALIDATION: AQUATOX provides reasonable simulation of hypolimnetic DO



The bottom waters in Lake Onondaga go anoxic during the growing season, and AQUATOX captures that. The current model does a better job of capturing the high DO during the spring, as you will see when you run the model. Note the predicted dips in DO during the winter. Unfortunately, we don't have data during the periods of thin ice to verify these predictions.

## Lab 7: Calibration and Analysis of Alternatives for Lake Onondaga NY

- Open Onondaga 0.apss
  - Setup, Control: make sure unchecked
  - Run Perturbed
  - Output, Perturbed graph



Objectives of this lab:

- explore the concept of iterative calibration and how that might work
- apply the calibrated model to a “real world” problem—what would happen if the WWTP effluent were diverted?

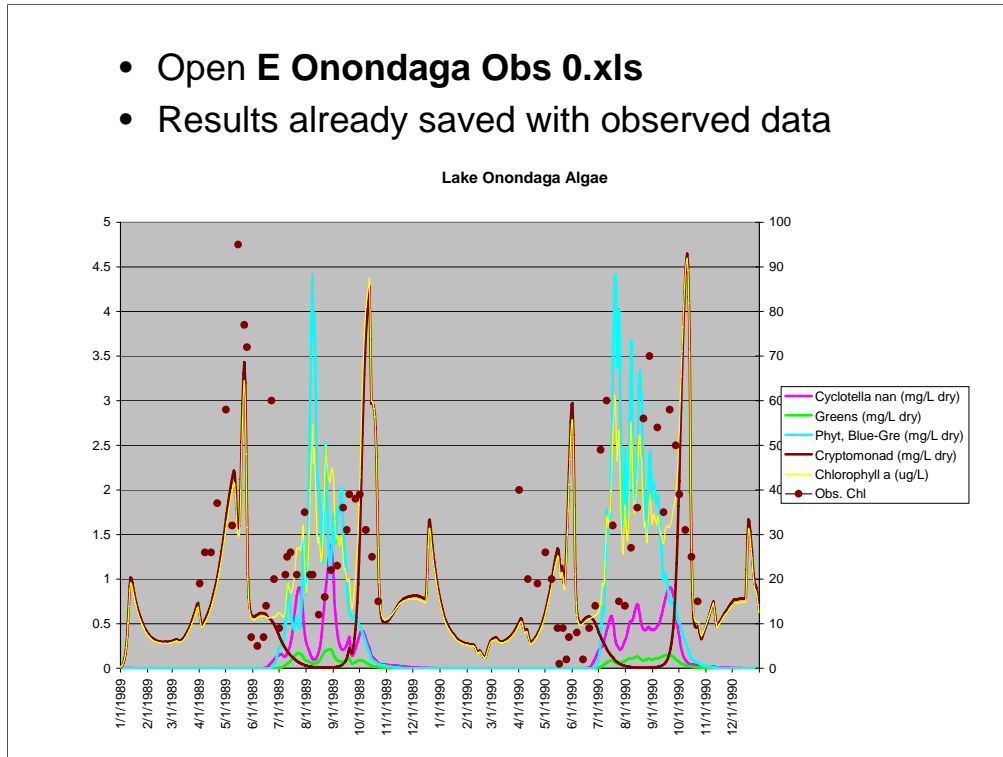
During Labs 2 and 3, we showed how you would apply AQUATOX to “your site” using site-specific characteristics. What would you do, however, if after that application process the model still does not fitting your observed data (for biotic composition, chlorophyll a, or other endpoint)?

Calibration is the process of changing model parameters, within their range of uncertainty (reasonable ranges as defined by literature if possible) to give your model an acceptable fit to the observed data. Try to change as few variables as possible from their *a priori* best estimates.

Calibration is like trying to solve a puzzle. It requires creative thought and a real understanding for why the model is behaving like it is.

After you have completed calibration, if you have an independent data set to test your model against, you can then go through a model validation process. Finally, you can apply your model and forecast or play “what if” games about the effects of different environmental conditions.

- Open E Onondaga Obs 0.xls
- Results already saved with observed data



We will start by examining this “un-calibrated” parameterization for Onondaga Lake.

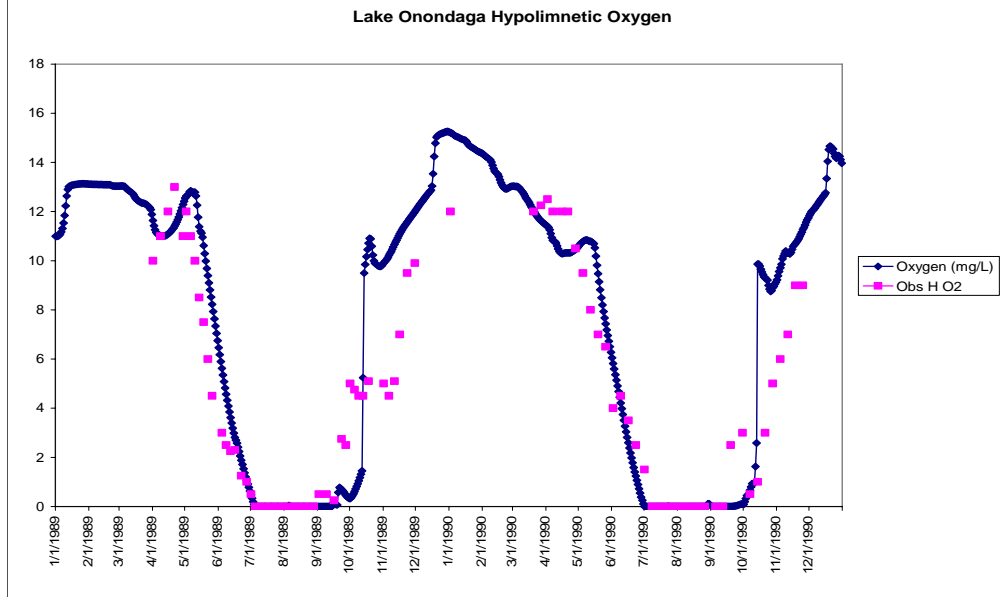
Observe algae, and chl a (epilimnion)

The fit is OK, but could be better. Also, we have some information on taxonomic distribution suggesting that additional calibration would be desirable.

We will continue to calibrate with two goals. First, we’d like to reduce the size of the fall cryptomonad bloom, which is not supported by the chlorophyll a data. Secondly, we’d like to increase the composition of greens. According to Effler (1996), aside from blue-greens, greens are “dominant” in summer.



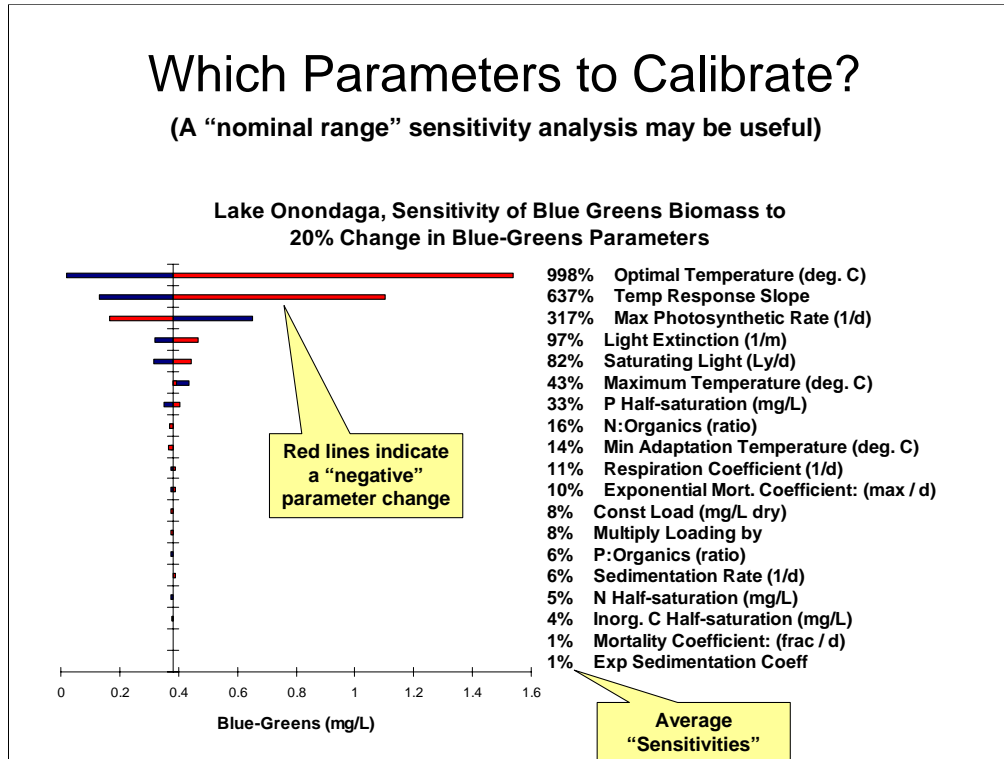
- Open **H Onondaga Obs 0.xls**
- Results already saved with observed data



View Hypolimnion: DO is important, especially the anoxia in summer; algae are residual

# Which Parameters to Calibrate?

(A “nominal range” sensitivity analysis may be useful)



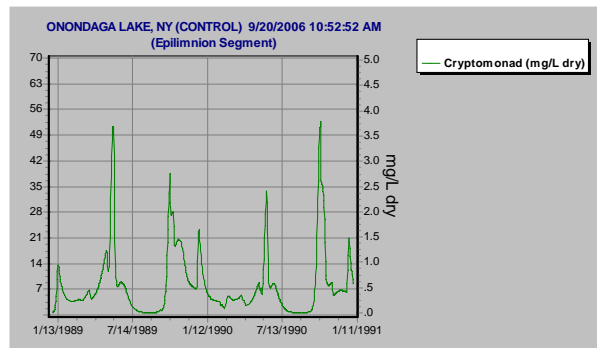
This is a tornado diagram that displays the sensitivity of a given output variable to a fixed percentage change to a set of model inputs. Automated sensitivity analyses will be included as part of Release 3. As this diagram was produced using Release 3 we are just using it as an example of the type of analysis you might use in a calibration. (We are not trying to modify blue-greens biomass in this case.)

The Average Sensitivities listed here give you the percentage change in the output you would expect given a 100% change in the model input. A 998% sensitivity therefore means if you changed an input by 10% you might get a 100% change in the model output.

In this case, the blue-greens biomass is averaged over the last year of the simulation.

Another source of information for which parameters to calibrate would be the Animal and Plant lectures (slides from day 1) in which we have put a star next to “key” parameters. You generally want to calibrate parameters for which the model has a reasonably high sensitivity and for which the scientific literature indicates at some uncertainty.

- Calibrate to reduce fall cryptomonad blooms
  - double-click *Cryptomonad* in Main screen
    - change Exponential Mortality Coefficient from 0.07 to 0.09 (29% change)
  - run Control (with control setup unchecked)
  - Output, Control Graph
    - fall blooms are reduced especially in year 1
    - compare control to perturbed to confirm this

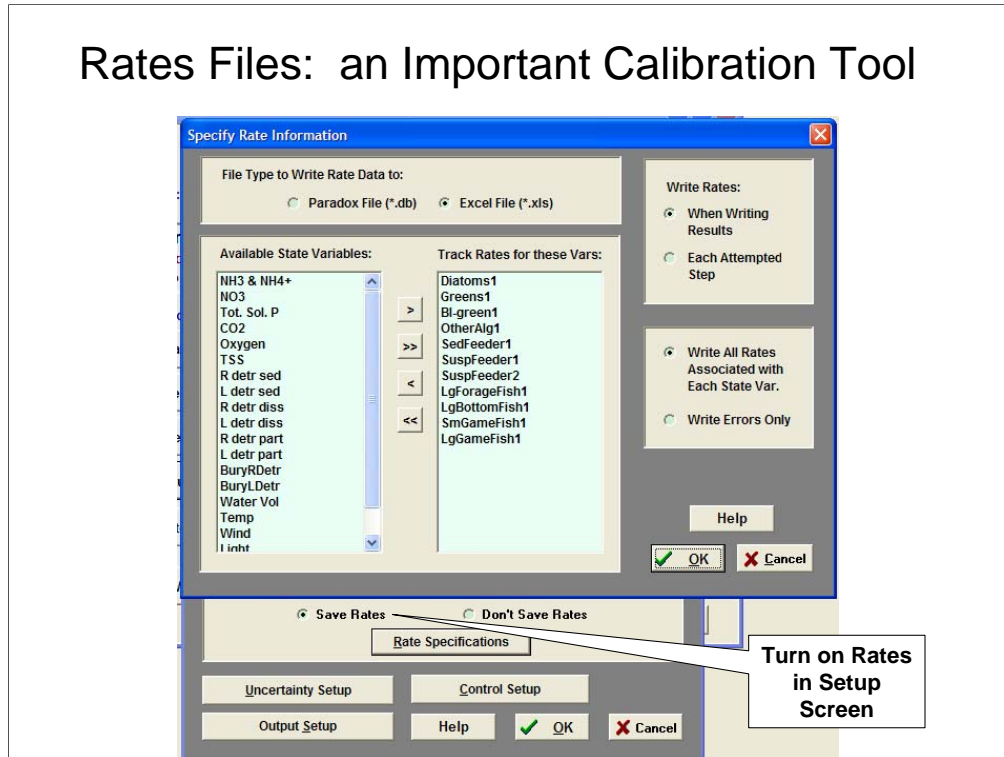


Because this change provided the intended result (to some extent) and because this is a reasonable value for the exponential mortality parameter (which is fairly uncertain), we will keep this change in the model calibration.

(Make a note in your “calibration log” as to the change and move on.)

Your simulation should now match **Onondaga 1.aps**

## Rates Files: an Important Calibration Tool



Rates files show why a state variable is increasing or decreasing. Each process that adds or reduces a state variable's concentration will be listed as a separate column within the Excel file produced. These processes may be found in the differential equations for each state variable modeled (see the technical documentation or the "Animal" and "Plant" lectures).

We will now turn on the rates for our intermediate calibration and examine the Excel file produced.

## Question: Why are Greens Limited during the Summer?

To start to look at this answer we will examine the rates file.

A	X	Z	AA	AB	AC	AD	AE	AF	AG
Date	Greens	Load2	Photosyn2	Respir2	Phot.Rsp.2	Non Tox M	Predation2	Washout2	Sediment2
7/1/1989	0.003627	0.00%	36.19%	10.60%	0.86%	3.00%	0.00%	0.62%	0.46%
7/2/1989	0.00442	0.00%	37.82%	10.86%	0.90%	3.06%	0.00%	0.56%	0.51%
7/3/1989	0.005693	0.00%	37.38%	10.44%	0.88%	2.92%	0.00%	0.54%	0.49%
7/4/1989	0.007427	0.00%	38.11%	10.36%	0.89%	2.88%	0.00%	0.48%	0.48%
7/5/1989	0.009777	0.00%	38.77%	10.32%	0.90%	2.85%	0.00%	0.45%	0.48%
7/6/1989	0.012924	0.00%	38.99%	10.30%	0.90%	2.84%	0.00%	0.70%	0.38%
7/7/1989	0.017171	0.00%	39.42%	10.28%	0.91%	2.82%	0.00%	0.47%	0.47%
7/8/1989	0.022758	0.00%	39.31%	10.32%	0.90%	2.82%	0.00%	0.53%	0.48%
7/9/1989	0.030275	0.00%	39.54%	10.30%	0.91%	2.81%	0.00%	0.50%	0.47%

Photosynthesis is less than 20% of PMax

	A	AL	AM	AN	AO	AP	AQ	AR
1	Date	Lt LIM2	N LIM2	PO4 LIM2	CO2 LIM2	Nutr LIM2	Temp LIM	Chem LIM
182	7/1/1989	0.20624	0.866071	0.976176	0.923067	0.866071	0.95292	1
183	7/2/1989	0.210933	0.866044	0.976322	0.923536	0.866044	0.951876	1
184	7/3/1989	0.216813	0.866202	0.976525	0.924735	0.866202	0.951876	1
185	7/4/1989	0.223169	0.866496	0.976783	0.92672	0.866496	0.95082	1
186	7/5/1989	0.228516	0.866839	0.977027	0.92844	0.866839	0.949752	1
187	7/6/1989	0.230703	0.866925	0.977235	0.929717	0.866925	0.948673	1
188	7/7/1989	0.234188	0.867169	0.977436	0.930119	0.867169	0.947582	1
189	7/8/1989	0.233272	0.867271	0.977572	0.926149	0.867271	0.946479	1
190	7/9/1989	0.235576	0.867482	0.977731	0.926242	0.867482	0.945364	1

Light Limitation is the culprit – shading from diatoms?

The rates file that you requested has automatically been placed in the OUTPUT directory of your AQUATOX installation. Rates for state variables are output in units of percentage of mass using the following equation:

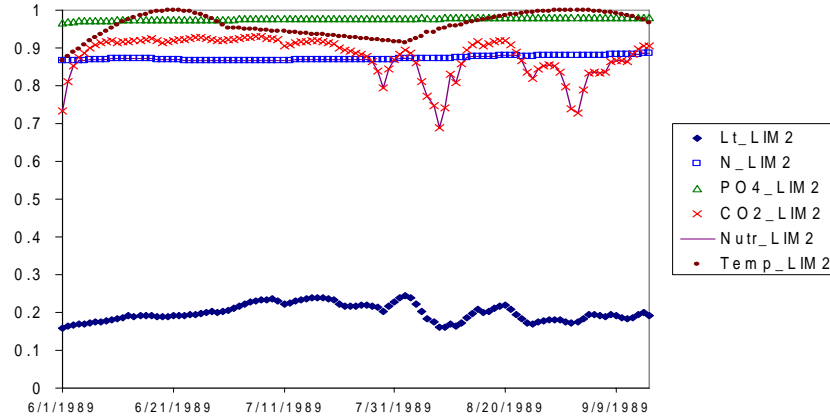
$$\text{Rate (fraction/day)} = \text{Rate (mass/day)} / \text{State (mass)}$$

**To facilitate the observation of rates, select cell B2 and then select “Window” “Freeze Panes” within Excel. Then navigate to view rates for greens during the summer.**

Because the photosynthesis rate is so important to plants, limitations are also produced for photosynthesis. These columns can be distinguished by the \_LIM at the end of them. They are interpreted as fraction limitation on photosynthesis. Note that Nutr\_LIM is the minimum of N\_LIM, PO4\_LIM and CO2\_LIM and is the overall nutrient limitation imposed on photosynthesis.

Viewing rates is important to get an intuitive sense for why a model is behaving the way that it is.

## Photosynthetic Limitations for Greens



**Light limitation is biggest limit to photosynthetic growth in Greens during the summer period. Blame light competition with Diatoms?**

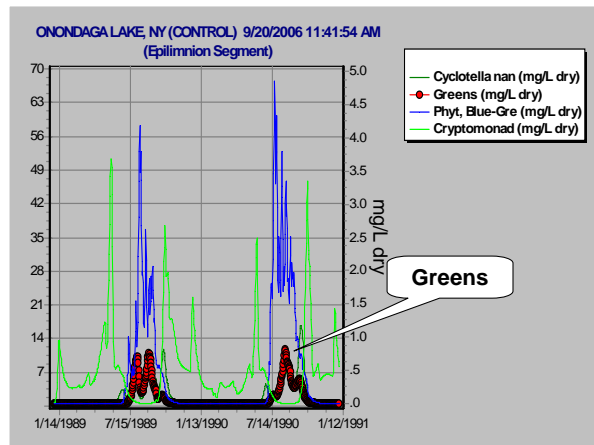
Graphs of photosynthetic limitations are often useful for understanding why growth is limited. In this case, light limitation predominates (dark blue diamonds at the bottom of the graph.)

The Nutr\_LIM line represents the minimum of the N\_LIM, PO<sub>4</sub>\_LIM and CO<sub>2</sub>\_LIM symbols.

Using this terminology, photosynthetic limitation is calculated as

$$\text{Nutr\_LIM} \cdot \text{Temp\_LIM} \cdot \text{Lt\_LIM}$$

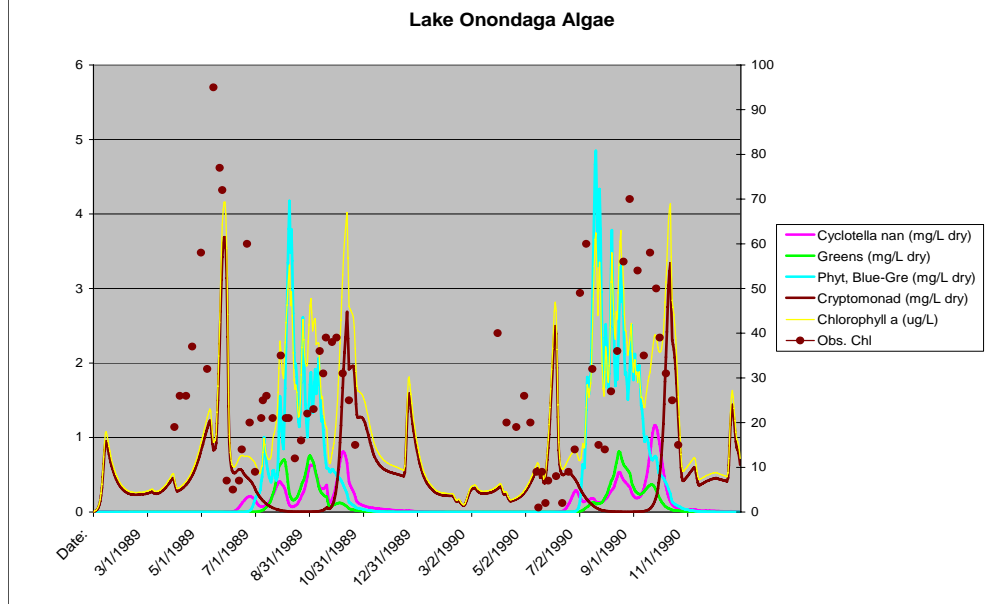
- Calibrate to obtain dominant greens
  - greens are dominant in summer (Effler, 1996)
    - simulation shows dominant diatoms
  - double-click *Cyclotella nana* in Main screen
    - change TOpt from 20 to 15
  - run Control
  - Output
    - Control Graph
    - greens now “dominant” in summer (at least with respect to diatoms)



Don't forget to ensure that the Control Setup dialog has no checked boxes before running this simulation as "Control."

This simulation saved as **Onondaga 2.aps**

## It is time to check “Final” calibration against observed data using Excel



To obtain output in Excel format and use template:

Export Control Results.

Select NH<sub>3</sub> & NH<sub>4</sub><sup>+</sup> through Inflow

Export Control Results to Excel 97 format

Cut and paste into **E Onondaga Obs 0.xls** (“A” tab)

inspect fits to observed data

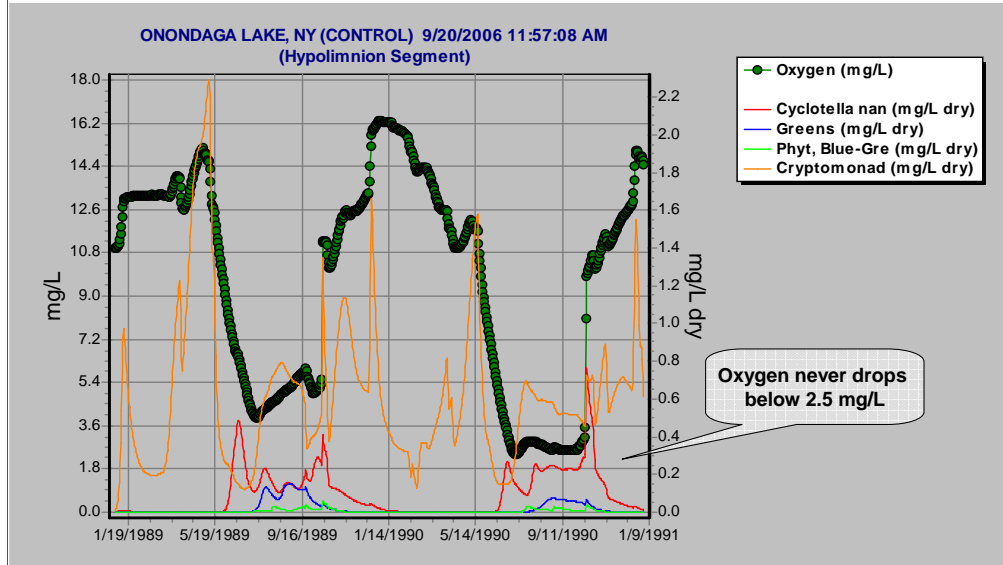
- The greens biomass is now much more prevalent in the summer;
- Cryptomonad blooms in the fall have been reduced;
- The overall fit to chlorophyll *a* is similar;
- For now, we will accept that we have met the goals of our calibration.

We could go through the same export to Excel procedure for hypolimnion files (but the fit isn't improved over original or significantly changed)

The capability to graph AQUATOX results against observed results within the AQUATOX interface is coming as part of Release 3.



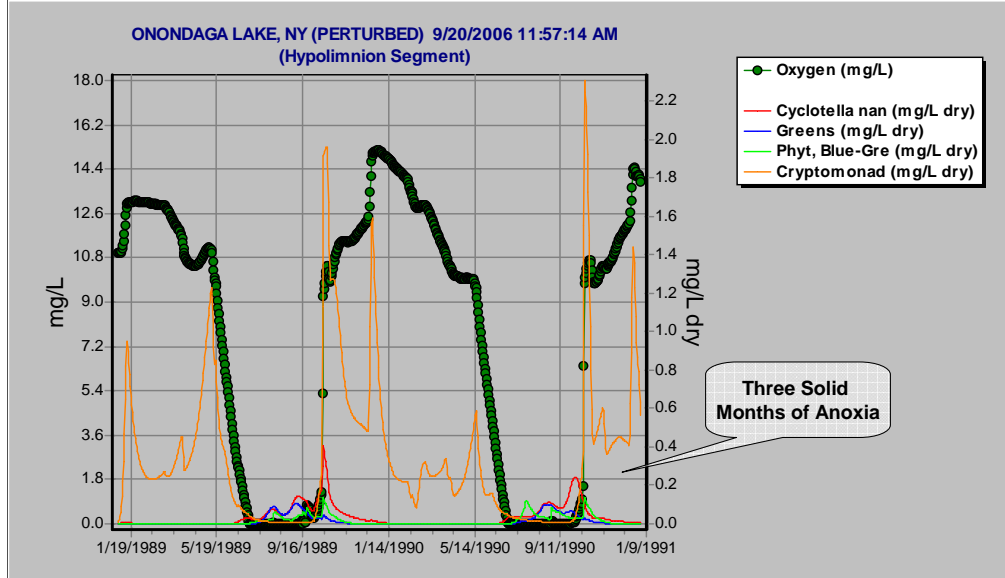
## What nutrient levels correspond to no anoxia? Control simulation eliminates WWTP discharge



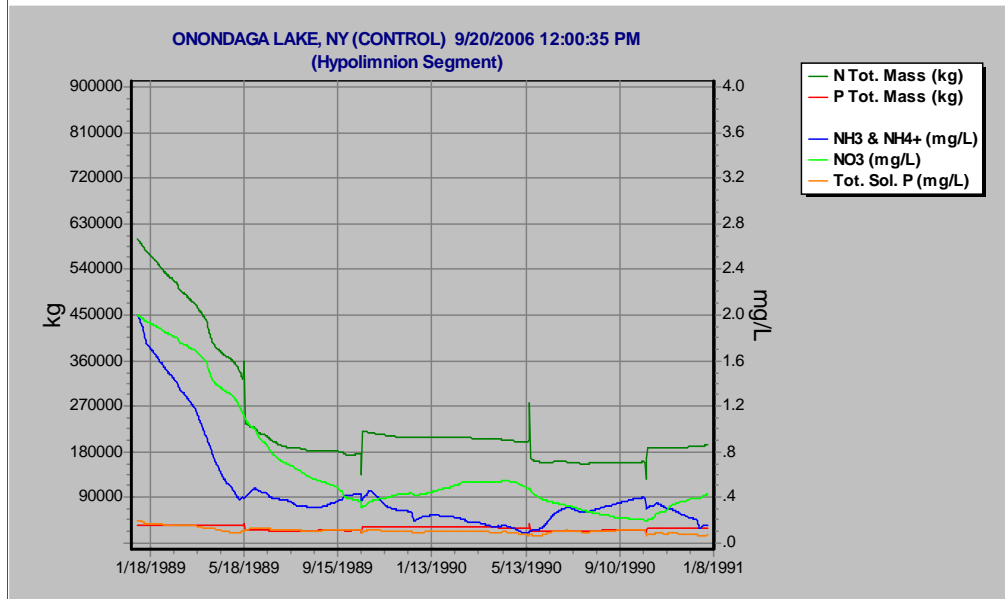
Now that we have a calibrated simulation, we can start to play “what if” games with it.

One of the proposals to clean up Onondaga Lake is to eliminate WWTP discharge into the lake, instead routing it directly to the Seneca River. We can quickly see the predicted consequences of such a proposed diversion. In **Setup, Control Setup**, check the *Omit Point Source Loadings* for both Nutrients and Detritus. Run **Perurbed** and run **Control** simultaneously. You’ll see that there is less anoxia in the second summer when the discharge is diverted. If you only divert the nutrients and not the detritus (think BOD), the recovery will not be as great.

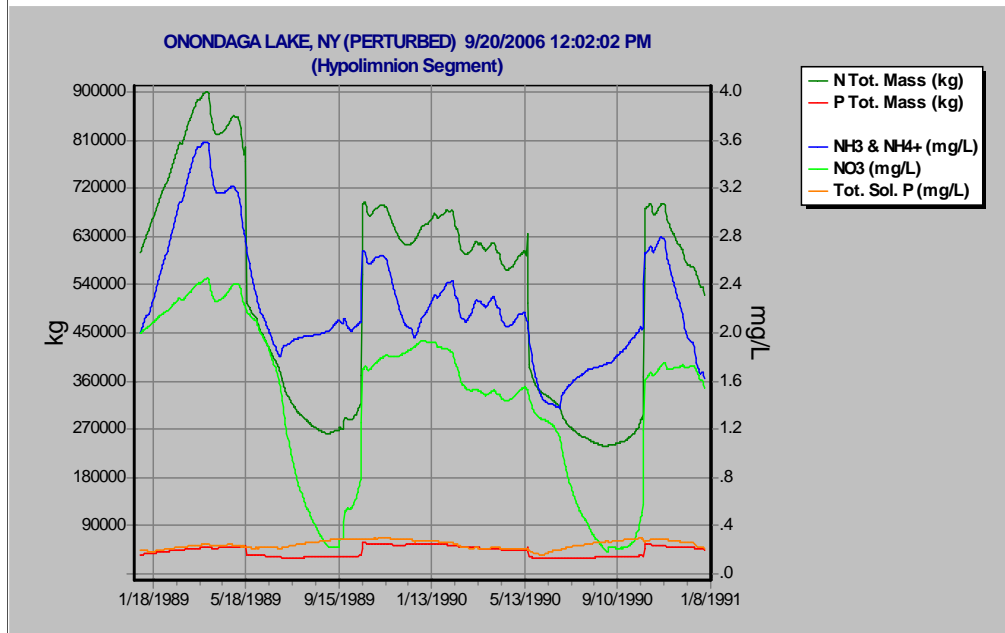
# Anoxia with Waste Water Treatment Plant Perturbed simulation includes WWTP discharge



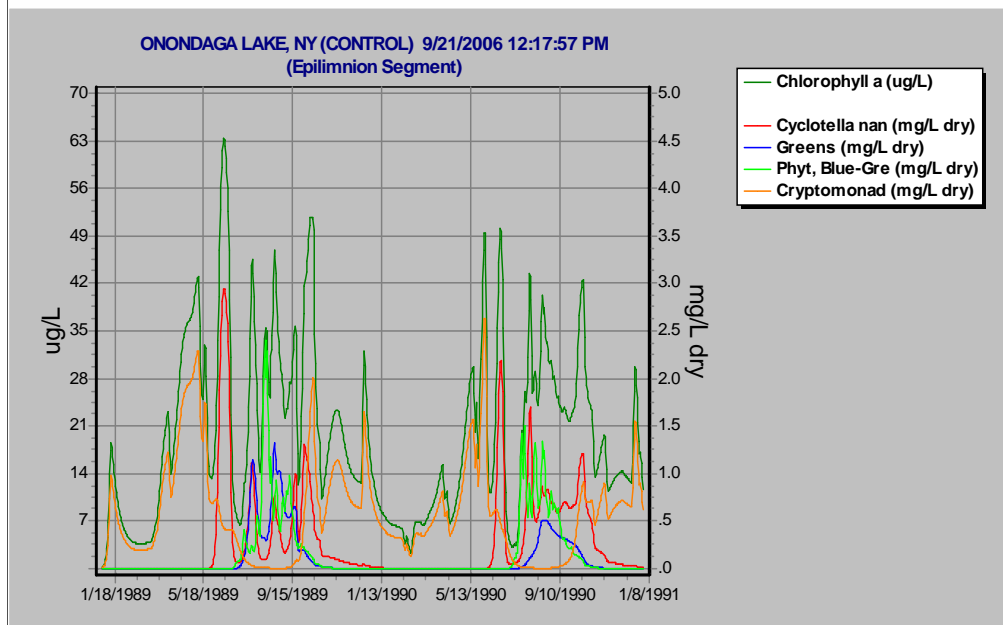
# Decrease in nutrients from initial conditions N drops to roughly 1/4 of its initial level



## in contrast to predicted levels with WWTP



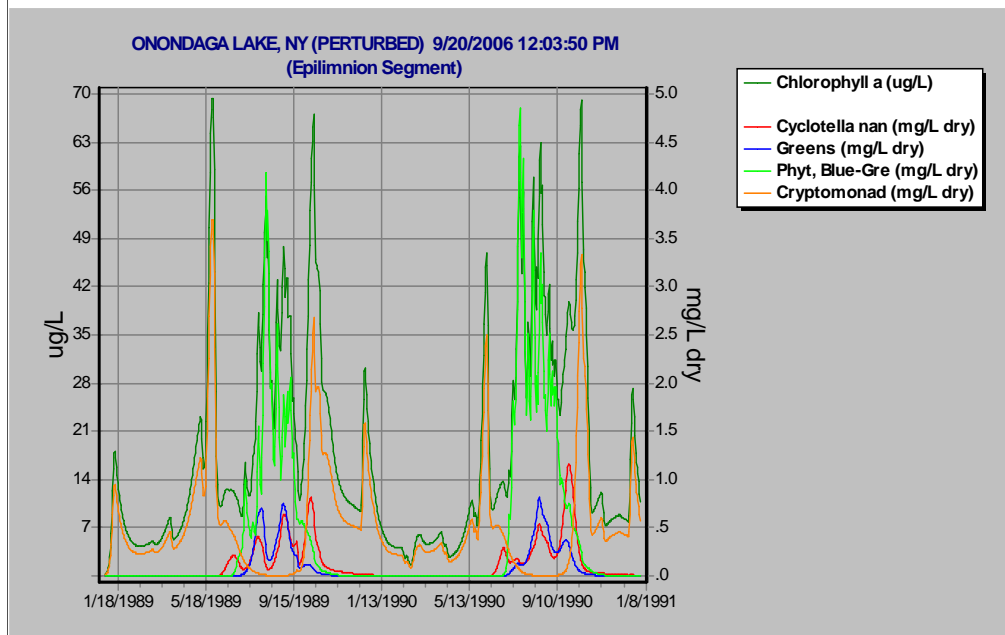
## Predict response to nutrient reduction: chl a decrease, dominant algae change



We also can see the predicted effects of the nutrient diversion on the algal community. The predicted algal biomass decreases significantly.

- Blue-greens blooms are significantly reduced
- Cryptomonad blooms are reduced.
- Overall Chlorophyll a concentrations are reduced

## Algal Composition with WWTP



Note the higher biomass and the composition of the algal community with existing effluent from the WWTP.

Blue-green blooms are prevalent during both summers.

## Lab 8: 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
- Analyze nutrient reduction effects

Objectives:

- analyze impacts of invasive plant species
- analyze effects of reducing inflow of nutrients

Assuming that we have a calibrated study, we can use it to answer “what if” questions about the site being modeled.

This lab is intended to introduce you to an analysis of the impacts of the invasive aquatic weed *Hydrilla*. Load **Clear Lake CA.aps**. This is based on, but not intended to faithfully represent, Clear Lake CA. The macrophyte *Hydrilla* was first found in the lake in 1994 and has been spreading rapidly since then. Eradication efforts have been underway since 1996. The purpose of this exercise is to analyze the impacts of this invasive aquatic weed. If *Hydrilla* were to spread to all of the lake what would be the impacts on the invertebrates, fish, and nutrients? How does it compare to another invasive species, *Myriophyllum*? How might it affect the widespread blue-green algal blooms? Why? What effect would a reduction in nutrient loadings have?

## **Run Control**

- Check Setup to make sure 3-year simulation (to go beyond transient conditions)
- Check Rate Specifications
  - considering objectives, are variables suitable?
- Run and inspect Control graph

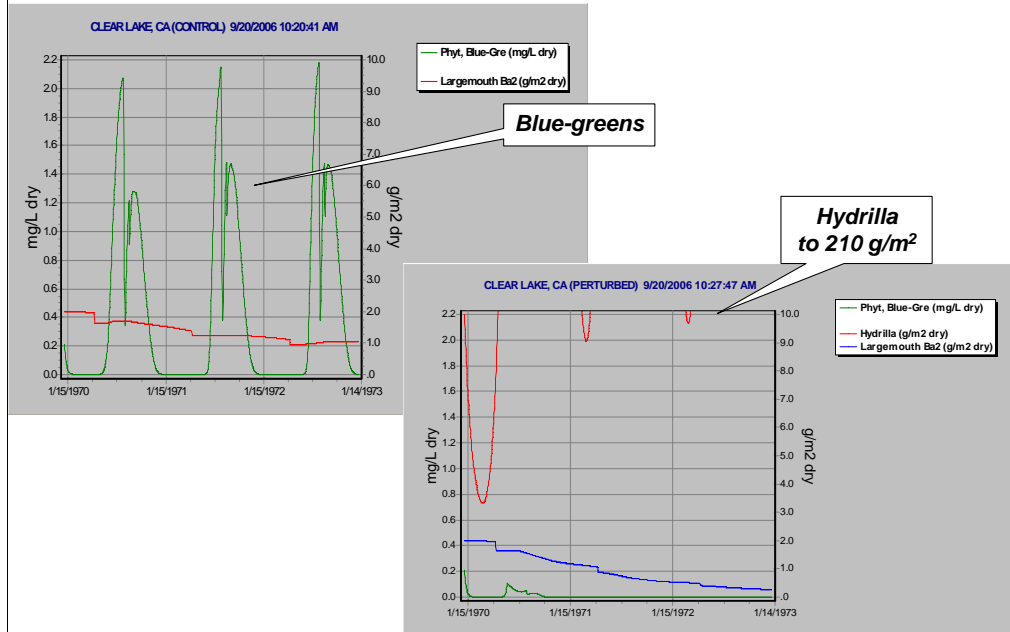


## **Add *Hydrilla***

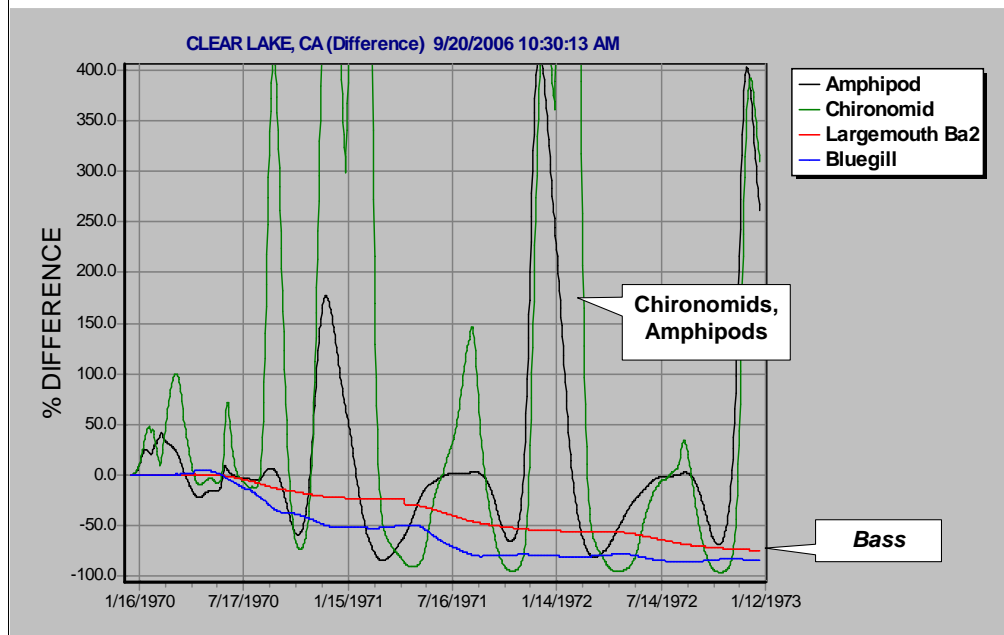
- Add Macrophyte2
- Choose *Hydrilla*
- Set initial biomass to 10 g/m<sup>2</sup> and loading to 1e-5
- (Check Trophic Interactions)
- Run and inspect Perturbed graph

It's always a good idea to check trophic interactions after adding a new state variable to make sure that the feeding matrix is set up properly.

# Clear Lake CA with and without *Hydrilla*



## Clear Lake CA with and without *Hydrilla*



The difference graph summarizes the effects of *Hydrilla*.

Bass are predicted to decline due to indirect foodchain effects. Interestingly, *Hydrilla* is sometimes planted in lakes to provide bass habitat, this (relatively uncalibrated) model indicates a potential downside of this management technique. (One possibility is that fishing is better at the edge of *Hydrilla* beds, but worse within the beds.) Sediment-dwelling detritivores (chironomids and amphipods) are predicted to increase, but the large biomass of *Hydrilla* interferes with predation.

## Analyze *Hydrilla* Impacts

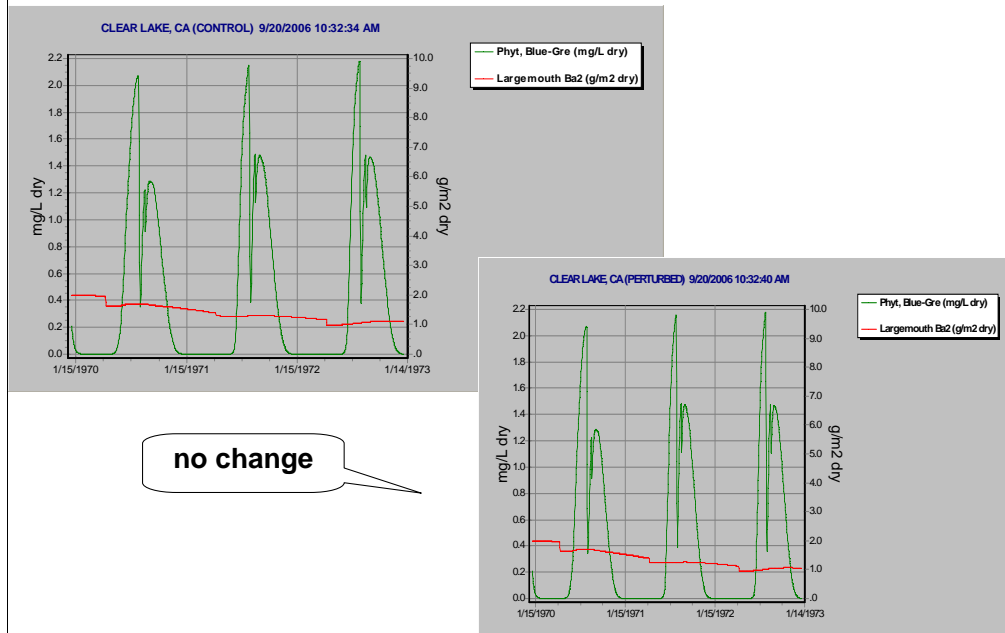
- What is the impact of *Hydrilla* on invertebrates and fish?
- How does *Hydrilla* affect the nutrient levels? Why?
  - hint: see *Tech Doc.* pp. 4-25, 5-12
  - confirm by looking at mass balance plots
- How does *Hydrilla* affect blue-green algae?
  - hint: plot control & perturbed blue-green limitations

## Analyze Nutrient Reduction

- Is it possible to reduce blue-green algal blooms in the absence of *Hydrilla*?
- Save study as **Clear Lake CA Hydrilla.aps**
- Delete *Hydrilla* and save as separate study (perhaps **Clear Lake CA nutrients.aps**)
- Check “Set Multiply-Loadings Factors to 1.0” in Control Setup
- Experiment with reduction factors in nutrient loadings; run Perturbed to see results
  - bracket reductions to speed up analysis
- Examine mass balance of nutrients

Assuming that nutrients could be reduced through land-use changes, would a reduction in loadings help to control blue-green algae? Be careful to save your previous work and use a new name for this study. As Marge has shown, the best way to tackle this question would be to link AQUATOX with a runoff model to represent what is possible. However, we'll just tackle it using fractional loading factors for the nutrient(s). Remember that the nutrient loadings for Clear Lake are Nonpoint-source Loadings. If you don't get a response, what would be the explanation?

# 80% reduction in P loading



*Hint:* look at mass balance of nutrients to see importance of various loadings (both P and N).

## Uncertainty and 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 is currently being performed (tornado diagram, p. 98, Lab 7, is an example).

EPA (U.S. Environmental Protection Agency). 1997. *Guiding Principles for Monte Carlo Analysis*. Risk Assessment Forum, U.S. Environmental Protection Agency. EPA/630/R-97/001. March 1997.

Saltelli, A. 2001. Unpublished manuscript. Sensitivity Analysis for Importance Assessment. Proceedings of a workshop held June 11-12, 2001, at North Carolina State on “Sensitivity Analysis Methods.” Joint Research Centre of the European Communities in Ispra. 36 <http://www.ce.ncsu.edu/risk/pdf/saltelli.pdf>

## Uncertainty Analysis

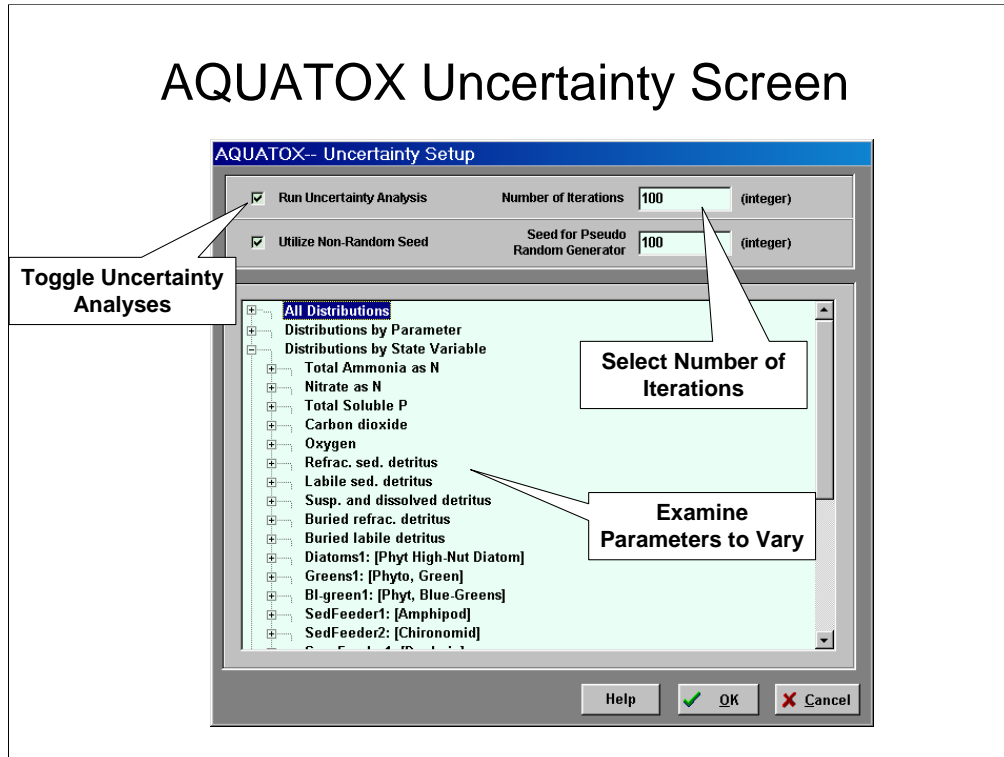
- Uncertainty analyses describe sources of uncertainty and variability in model simulations
- There are many sources of uncertainty e.g.
  - parameter uncertainty
  - model uncertainty due to necessary simplification of real-world processes
- Monte Carlo analysis is a statistical sampling technique that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

EPA (U.S. Environmental Protection Agency). 1997. *Guiding Principles for Monte Carlo Analysis*. Risk Assessment Forum, U.S. Environmental Protection Agency. EPA/630/R-97/001. March 1997.

A formal uncertainty analysis often follows a sensitivity analysis as the modelers may limit the parameters they are varying to those that have proven to be sensitive over the range of uncertainty.



## AQUATOX Uncertainty Screen



Start by loading **Clear Lake CA.aps**

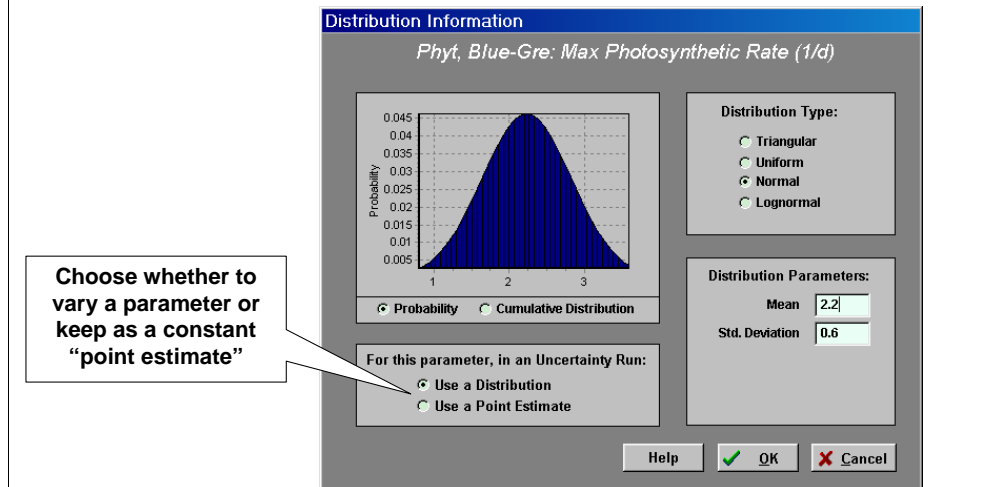
Get to the uncertainty screen by clicking on the “Setup” button and then clicking on the “Uncertainty Setup” button or by using the uncertainty analysis tool-button.

Nearly all parameters may be varied within the uncertainty analysis, trophic interactions being the one exception.

Select 100 iterations and to “Run Uncertainty Analysis.” Next we will choose which parameters to vary in this analysis.

## 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.



Our “sensitivity analysis” indicated that the model is not sensitive to non point-source loadings of phosphate, so we will try a different variable.

To look at the parameters you may modify for the blue greens state variable choose the “+” next to “Distributions by State Variable”. Then choose the “+” next to “BI-green1: [Phyt, Blue-Greens]”

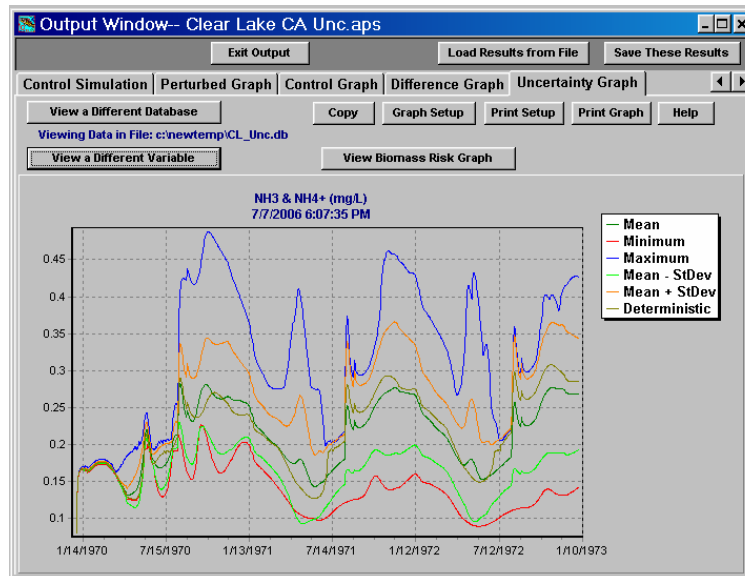
I chose to modify the PMAX (Max Photosynthetic Rate) as there is often some uncertainty surrounding this particular parameter. For my simulation I’m choosing a normal distribution with a **mean of 2.2** (this is the “best estimate” used in the simulation) and a **standard deviation of 0.6**.

Run the simulation and save the output set as a “db” file. ( Release 3 will have the capability to save uncertainty output as an Excel file as well.) This set of 100 simulations will probably take about 1.5 hours.

Note, the distributions chosen can reflect variability in various scientific studies that attempt to quantify the given parameter.

You may select as many parameters to vary as you’d like. However, note that the more parameters that you choose to vary, the more iterations are required to produce an output distribution that is stable (i.e. that reflects the true effects of all of the input distributions combined).

## Using the Uncertainty Tab on the Output Screen



AQUATOX Uncertainty Output consists of several files:

{filename}.db - A database file with the minimum, maximum, mean, deterministic, and standard deviation for each variable for each day of the simulation.

{filename}2.db – These databases only support so much width so additional variables may need to be saved in additional files.

{filename}.TXT– A text file that indicates what variable draws were chosen for each iteration and the timing of the simulations.

{filename}\_decline.CSV – A text file that contains data for the biomass risk graph.

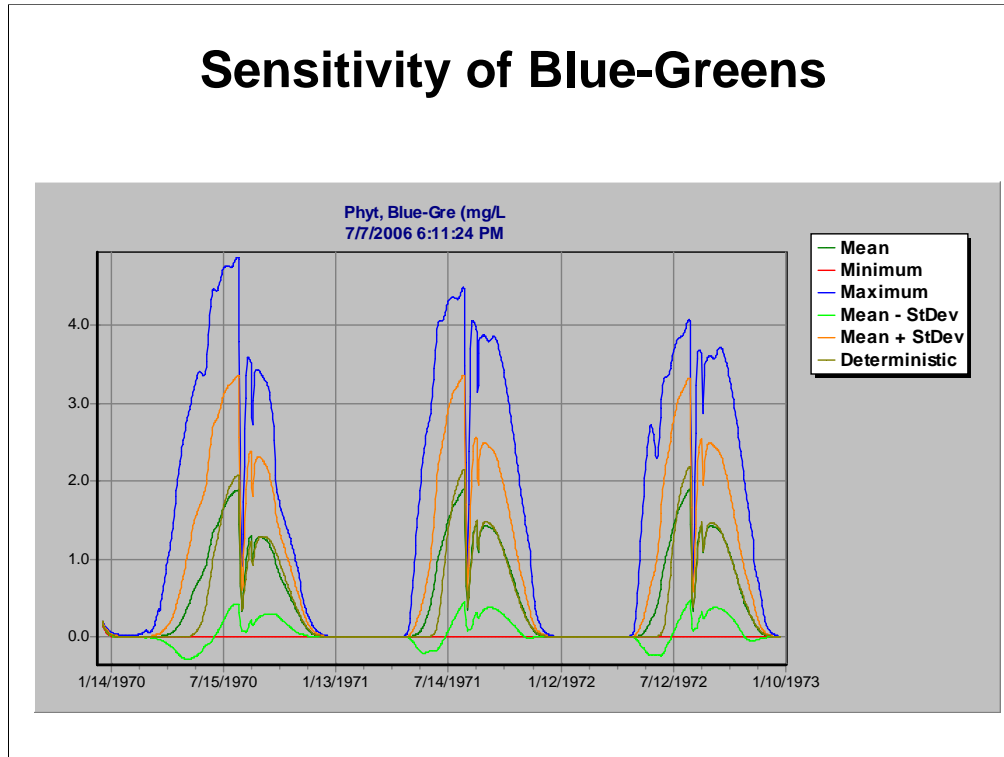
A “deterministic” run is performed without including random draws from the uncertainty analysis, i.e. the deterministic run uses point estimates for all model parameters.

Click on “View a different Variable” to see the other variables within the current db file.

Click on “View a different Database” to see if other db files have been created with uncertainty results.

The uncertainty graph gives the user an idea of the spread of the resultant distribution over the entire time-period of the simulation. The results here, for ammonia, show strong indirect effects to the PMAX parameter in Blue-Greens.

## Sensitivity of Blue-Greens



Click on the “View a Different Variable” and select “Phyt, Blue-Greens” The difference in the size of the blue-greens blooms are considerable indicating that blue-greens are indeed quite sensitive to the PMAX parameter.

On your own time, view various different variables and see if you can figure out why or why not the results for these variables are sensitive to the change in the size of the blue-greens bloom.