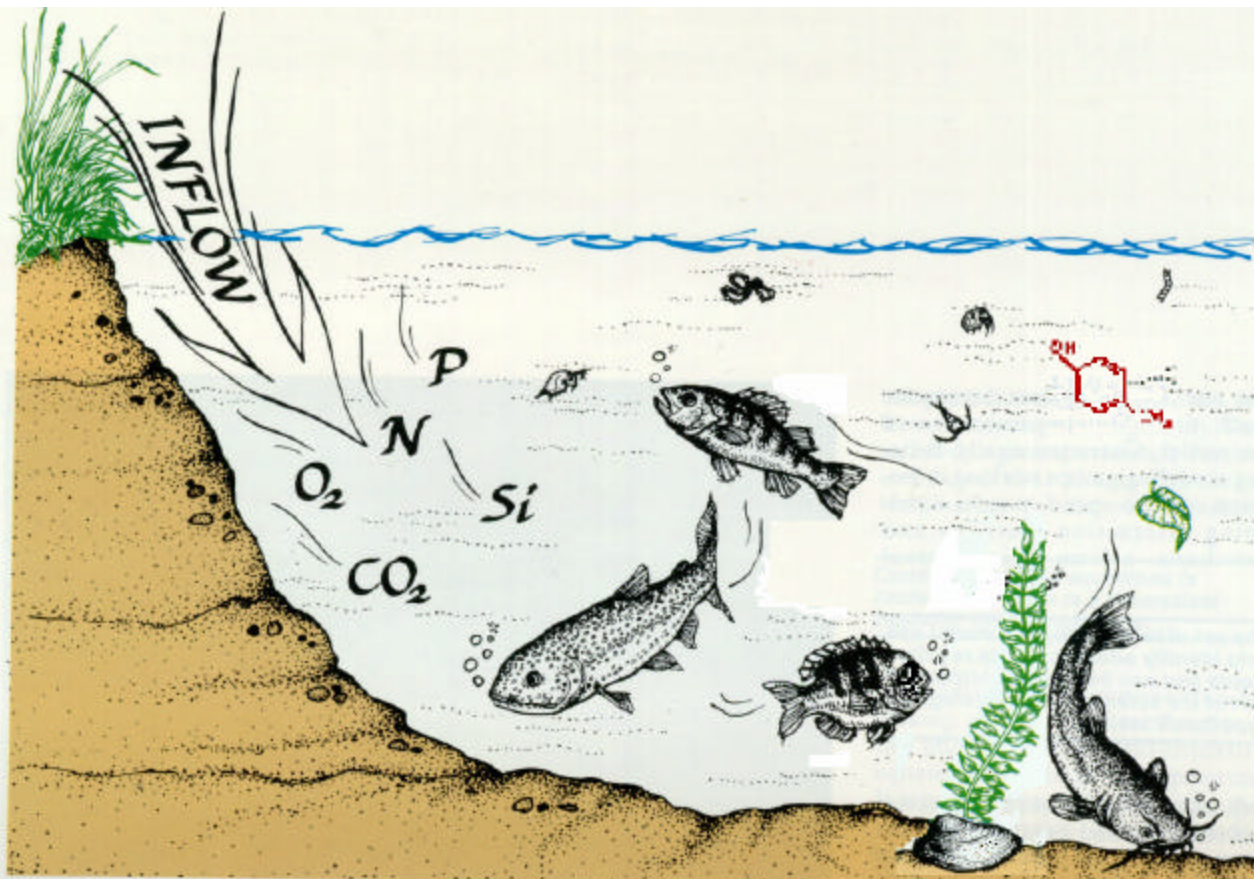


Predicting the Fate & Effects of Pollutants in Freshwater and Estuarine Environments with AQUATOX



Richard A. Park, Eco Modeling, Diamondhead MS

Marjorie C. Wellman, US EPA, Office of Science & Technology

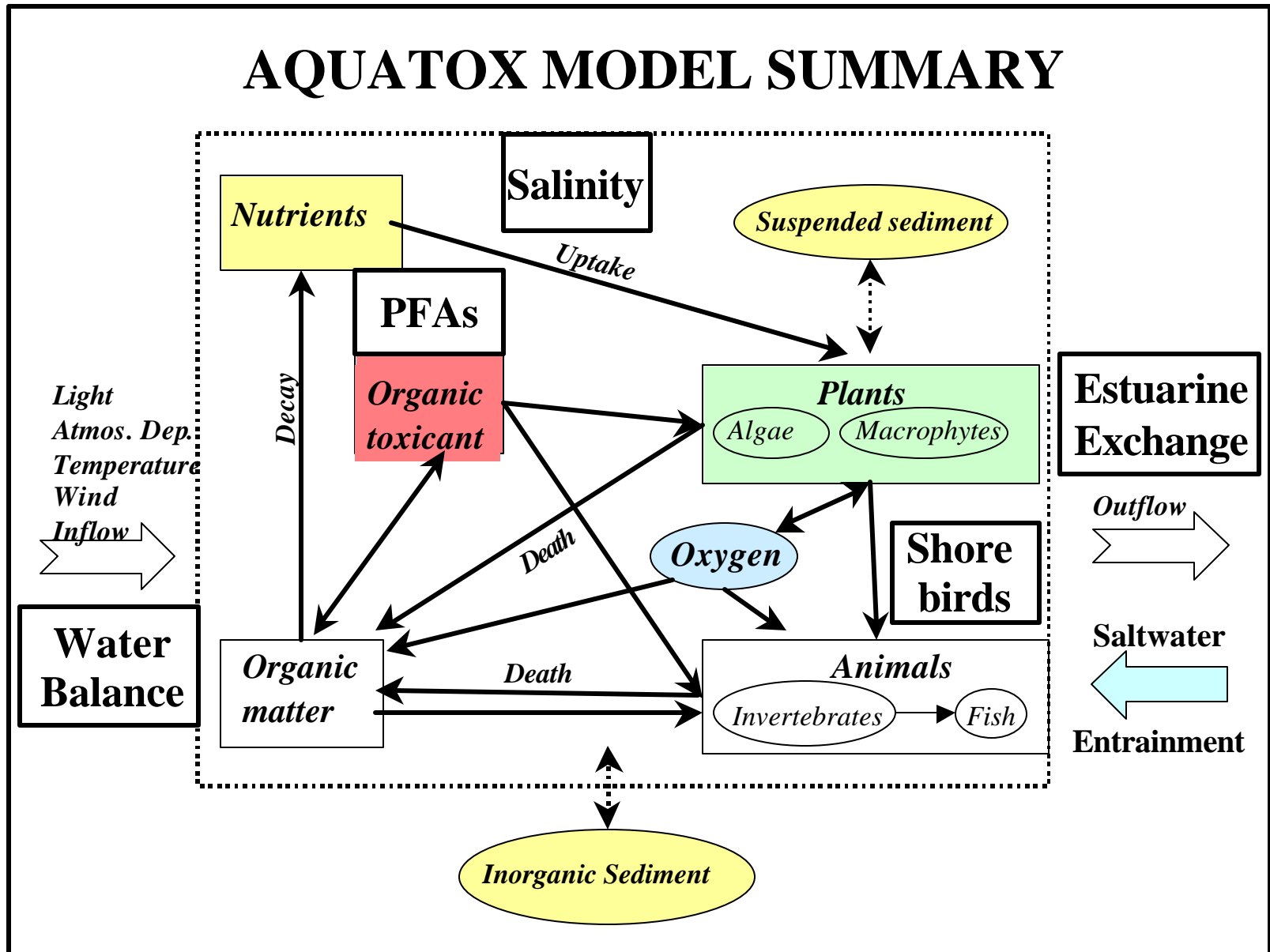
What is AQUATOX?

- **Simulation model that links pollutants to aquatic life**
- **Integrates fate & ecological effects**
 - **Fate & bioaccumulation of organics**
 - **Food web & ecotoxicological effects**
 - **Nutrient & eutrophication effects**
- **Predicts effects of multiple stressors**
 - **Nutrients, organic toxicants**
 - **Temperature, suspended sediment, flow, salinity**
- **Can be evaluative (with “canonical” environments) or site-specific**
- **Peer reviewed by independent panel and in two published model reviews**

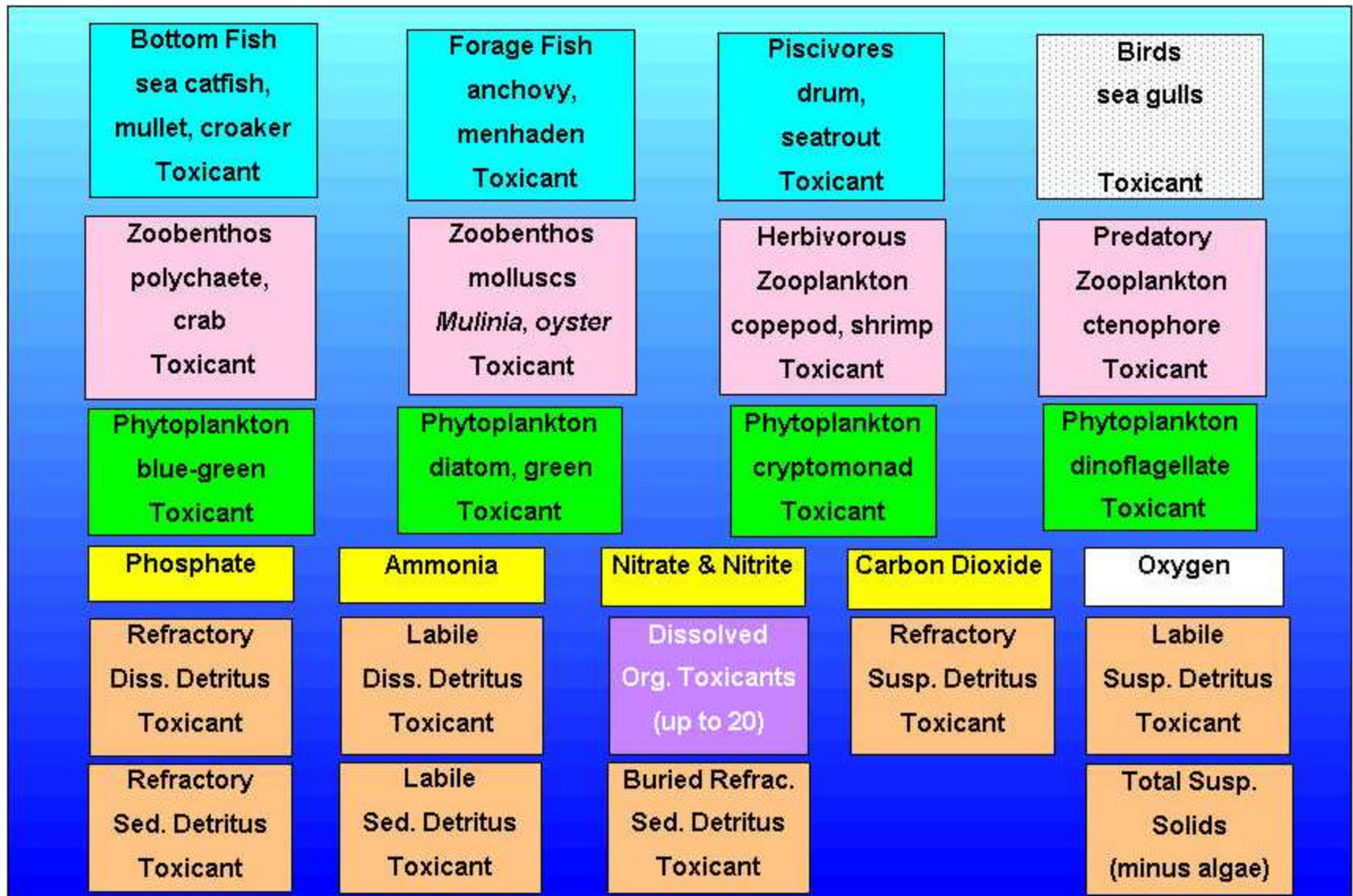
AQUATOX Structure

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

AQUATOX Ecosystem Representation



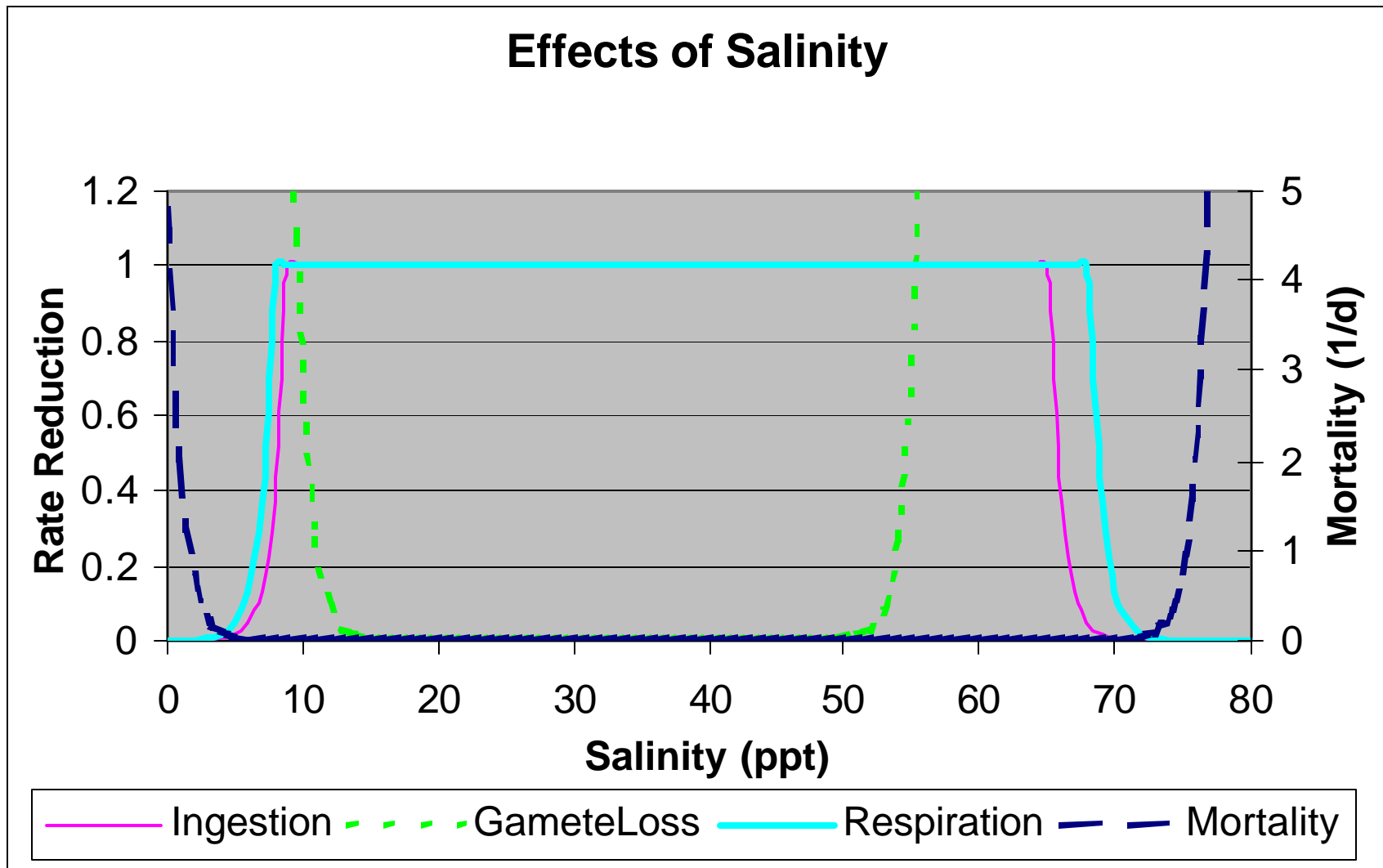
Galveston Bay, Texas, compartments



Processes Simulated

- **Bioenergetics**
 - feeding, assimilation
 - growth, promotion, emergence
 - reproduction
 - mortality
 - trophic relations
 - toxicity (acute & chronic)
- **Environmental fate**
 - nutrient cycling
 - oxygen dynamics
 - partitioning to water, biota & sediments
 - bioaccumulation
 - chemical transformations
 - biotransformations
- **Environmental effects**
 - direct & indirect

Salinity is an integral part of estuarine version



AQUATOX Capabilities

new capabilities in blue and red

- Riffle, run, and pool habitats for streams
- Completely mixed, thermal stratification, or **salinity stratification**
- **Linked segments & multiple sediment layers with pore waters** (in one version)
- Biota represented by guilds, key species
- Constant or variable loads
- Latin hypercube uncertainty analysis (**all parameters**)
- **Wizard & help files, multiple windows, task bar**
- **Links to HSPF and SWAT in BASINS**
- Can be linked to hydrodynamic model
- Ponds, lakes, reservoirs, streams, rivers, **estuaries**

AQUATOX Release 2 Study Overview

The screenshot displays the AQUATOX software interface. At the top, the title bar reads "AQUATOX-- Main Window". Below it is a menu bar with "File", "View", "Library", "Study", "Window", and "Help". A toolbar contains various icons for file operations and data analysis. The main window is titled "Onon8990NewPRecov.apr-- Main Window" and contains the following sections:

- AQUATOX: Study Information**
Version 1.89 Beta
- Study Name:** ONONDAGA LAKE, NY
- State and Driving Variables In Study**
 - Ammonia
 - Nitrate
 - Phosphate
 - Carbon dioxide
 - Oxygen
 - Refrac. sed. detritus
 - Labile sed. detritus
 - Susp. and dissolved detritus
 - Buried refrac. detritus
 - Buried labile detritus
 - Diatoms1: [Cyclotella nana]
 - Greens1: [Greens]
 - Bl-green1: [Cryptomonad]
 - SedFeeder1: [Tubifex tubifex]
 - SuspFeeder1: [Daphnia]
 - PredInvt1: [Rotifer, Brachionus]
 - LgForageFish1: [White Perch]
 - LgBottomFish1: [Catfish]
 - SmGameFish1: [Largemouth Bass, YOY]
 - LgGameFish1: [Largemouth Bass, Lg]
 - Water Volume
 - Temperature
 - Wind Loading
 - Light
 - pH
- Model Run Status:**
 - Toxics Run: 07-23-01 1:54 PM
 - Control Run: 07-23-01 2:39 PM
- Data Operations:**
 - Initial Conds.
 - Chemical
 - Site
 - Setup
 - Notes
- Program Operations:**
 - Perturbed
 - Control
 - Output
 - Export Results
 - Export Control
 - Edit With Wizard
 - Help
- Results from File** (tabbed interface):
 - bed Graph
 - Control Graph
 - Difference Graph
 - Uncer
 - Copy
 - Print Setup
 - Print Graph
 - Help
- Graph:** A line graph showing data from 2/11/1989 to 2/8/2001. The legend includes:
 - Cyclotella nan (mg/L)
 - Greens (mg/L)
 - Cryptomonad (mg/L)
 - White Perch (mg/L)
 - Catfish (mg/L)
 - Largemouth Ba2 (mg/L)
- Buttons:** Add, Delete, Edit

Task bar with Help

Multiple windows

Wizard

Export results

Add/delete variables

Wizard is available for guidance

The screenshot displays the AQUATOX Simulation Creation Wizard in Step 6: Invertebrates to Simulate (Sed Feeders). The main window behind it shows the simulation progress and various toolbars.

Wizard Progress

- Step 1: Simulation Type
- Step 2: Simulation Period
- Step 3: Nutrients
- Step 4: Detritus
- Step 5: Plants
- Step 6: Invertebrates
- Step 7: Fish
- Step 8: Site Characteristics
- Step 9: Water Volume
- Step 10: Water Temperature
- Step 11: Wind Loading
- Step 12: Light Loading
- Step 13: Water pH
- Step 14: Inorganic Solids
- Step 15: Chemicals
- Step 16: Inflow Loadings
- Step 17: Direct Precipitation
- Step 18: Point-Source Loadings
- Step 19: Non Point-Source Loads

(double click on any step to jump there)

Wizard Summary

Simulation Name: CORAL VILLE RESERVOIR
Simulation Type: Reservoir
State Variables in Simulation:
Dissolved org. tox 1: [Dieldrin]
Ammonia

AQUATOX-- Simulation Creation Wizard

Step 6: Invertebrates to Simulate (Sed Feeders)

Within AQUATOX, invertebrates are classified as Shredders, Sediment Feeders, Suspended Feeders, Clams, Grazers, Snails, and Predatory Invertebrates.

To add a Sed Feeder Compartment to the simulation, drag its name from the list of available Sed Feeders to the simulation box on the right. To remove a Sed Feeder Compartment from the simulation, select it and click the Remove button below.

Available Sed Feeders:	Sed Feeders in Simulation: (Maximum of Two)
Amphipod	SedFeeder1: [Chironomid]
Chironomid	SedFeeder2: [Amphipod]
Cricotopus	
Isopod	
Oligochaete	
Ostracode	
Polypedilum	
Tricorythodes	
Tubifex tubifex	

Remove From Simulation

Buttons: Help, Hide Progress, Edit With Wizard, Show Progress, Show Summary, Cancel, Finish, Add, Delete, Edit.

Temperature
Wind Loading
Light
pH

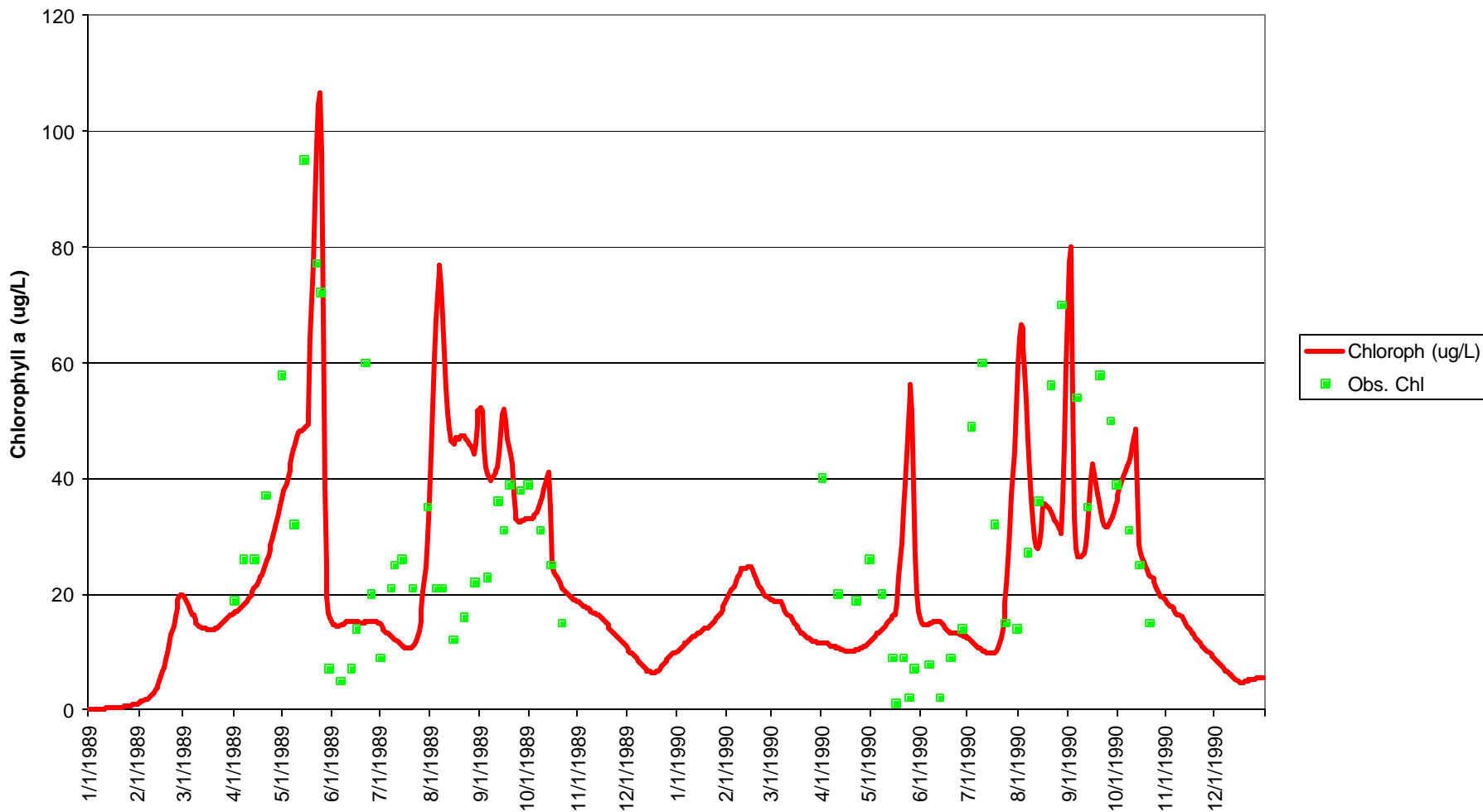
Loadings to AQUATOX

- Multiple sources
 - Atmospheric deposition
 - Nonpoint-source pollution
 - Point-source pollution
 - Upstream loadings
- Variable or constant loadings
- External file import or manual input
 - USGS stream flow data
 - Excel files
 - dBase and Paradox files
 - Comma- and tab-delimited files
 - Linkage through BASINS

Lake Onondaga NY

Reasonable Simulation of Chlorophyll a

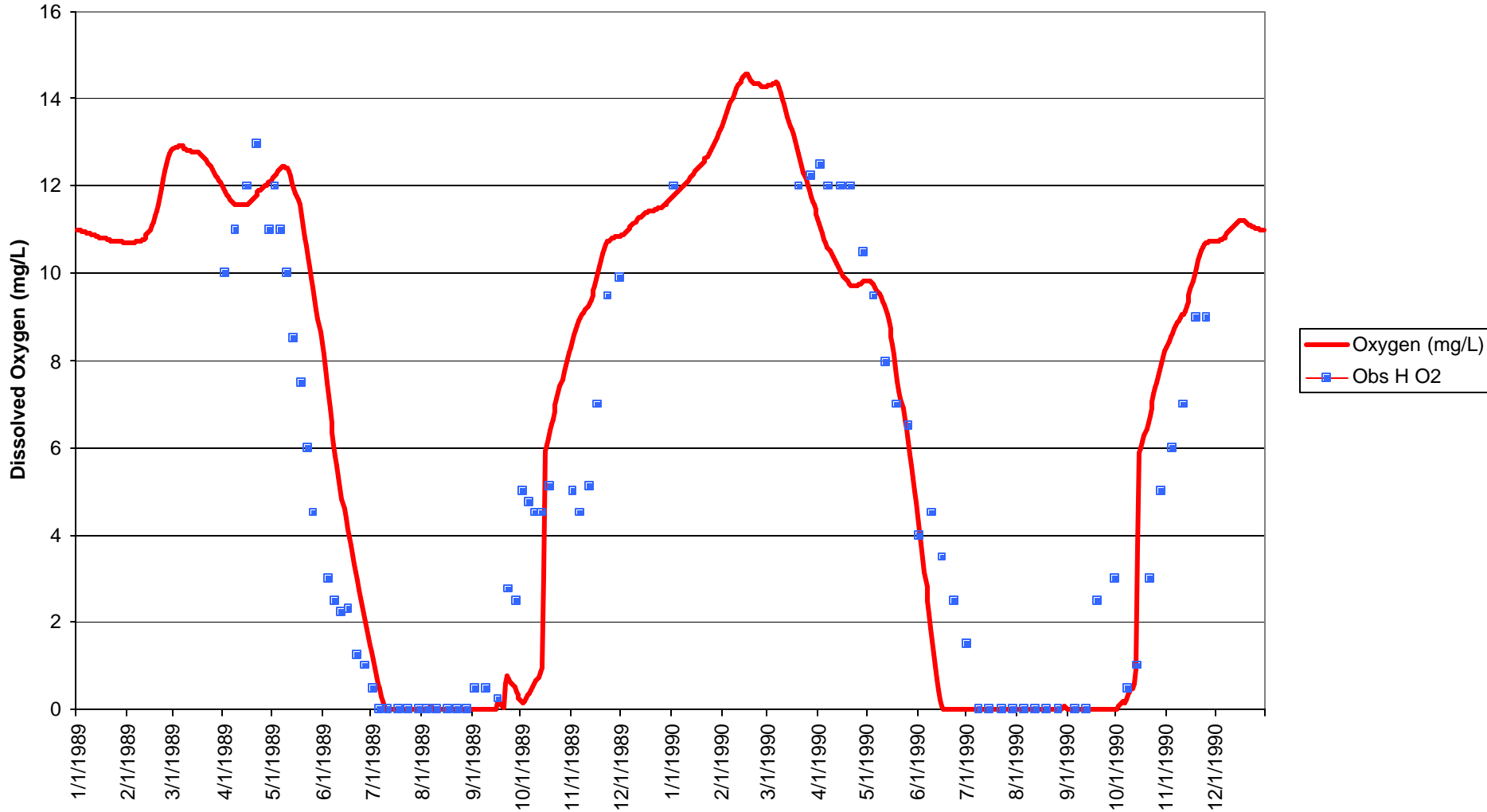
Lake Onondaga Chlorophyll a



Lake Onondaga NY

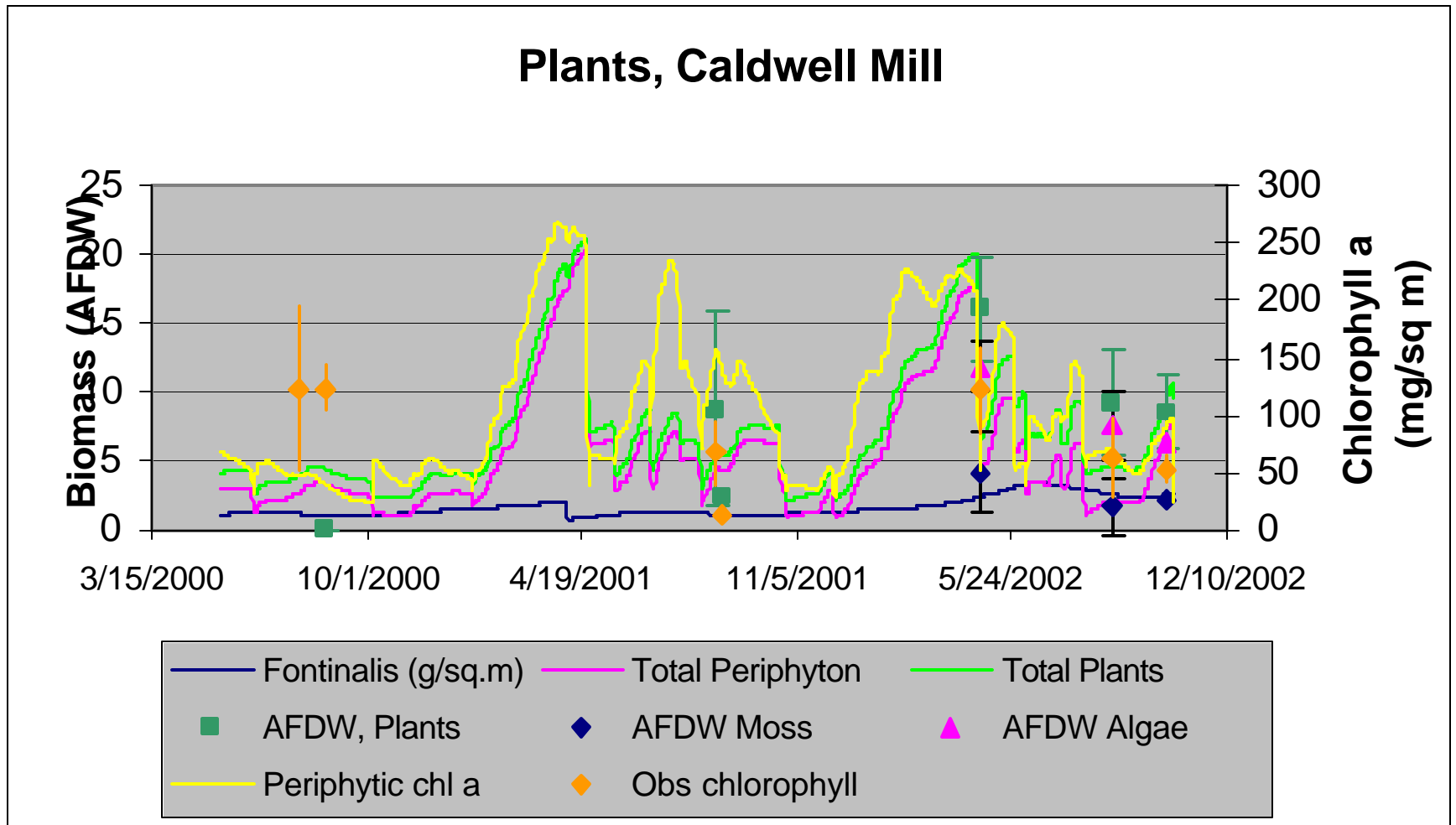
Reasonable Simulation of Hypolimnetic DO

Dissolved Oxygen, Onondaga Hyolimnion

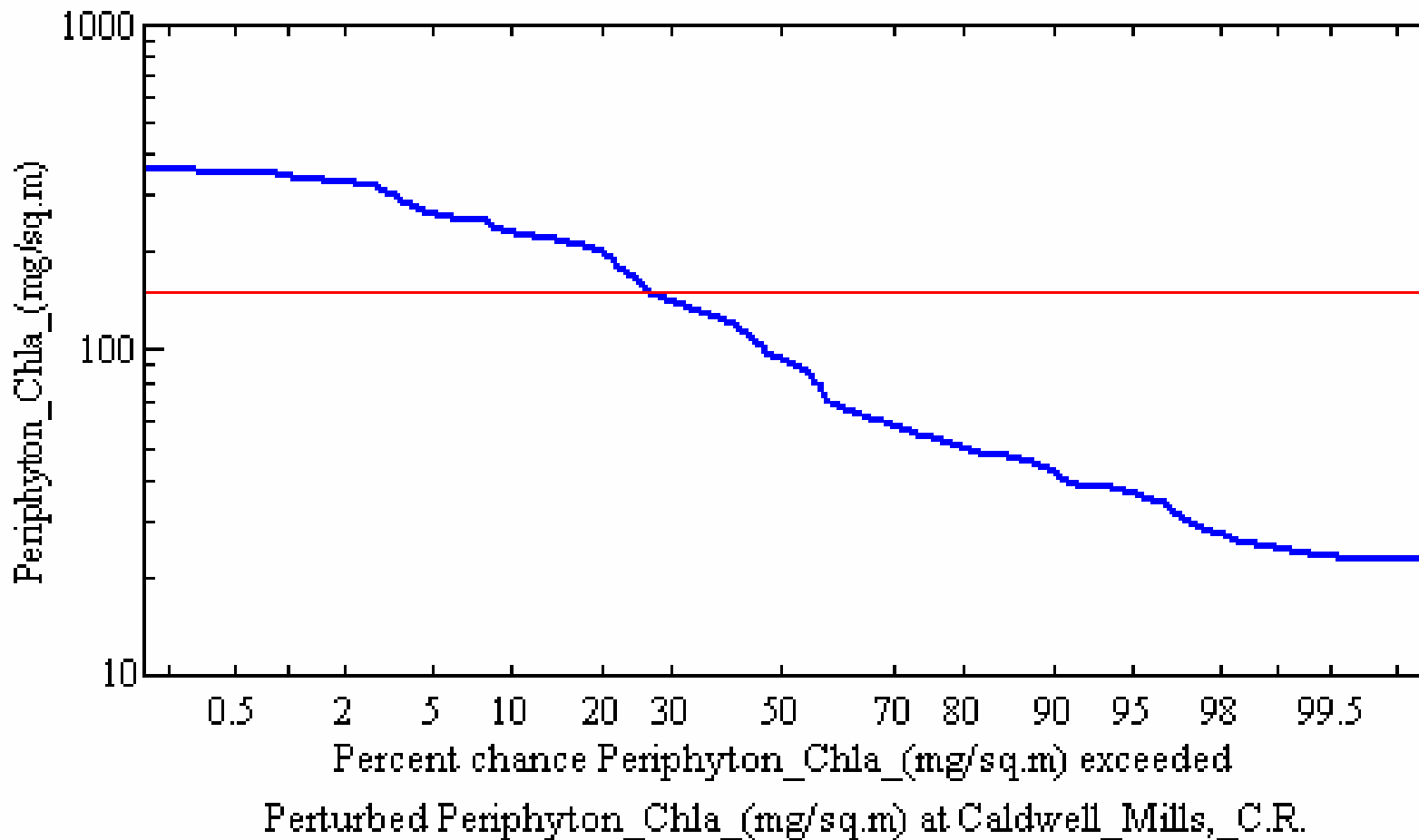


The model was calibrated for Caldwell Mill, Cahaba River, Ala.

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

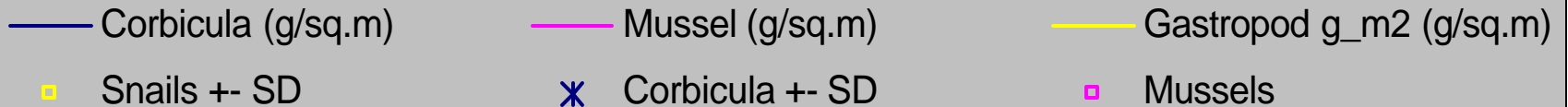
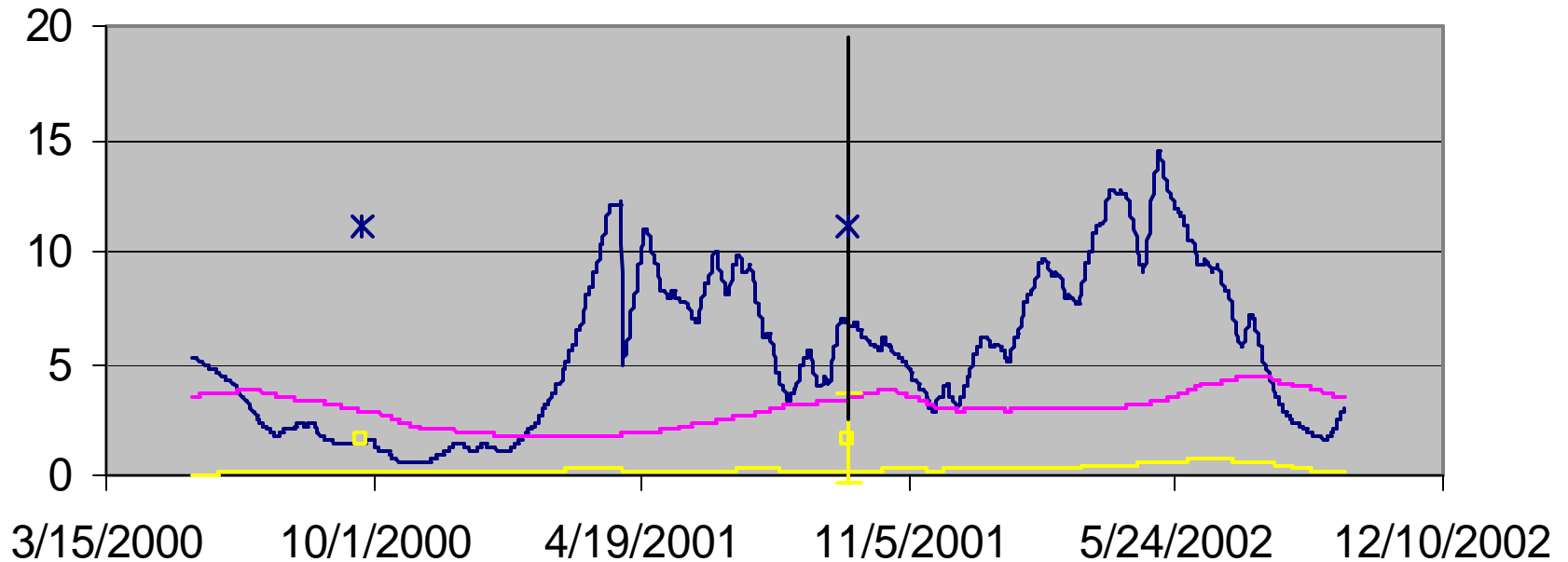


Linked with GenScn program for analyses such as exceedance plots



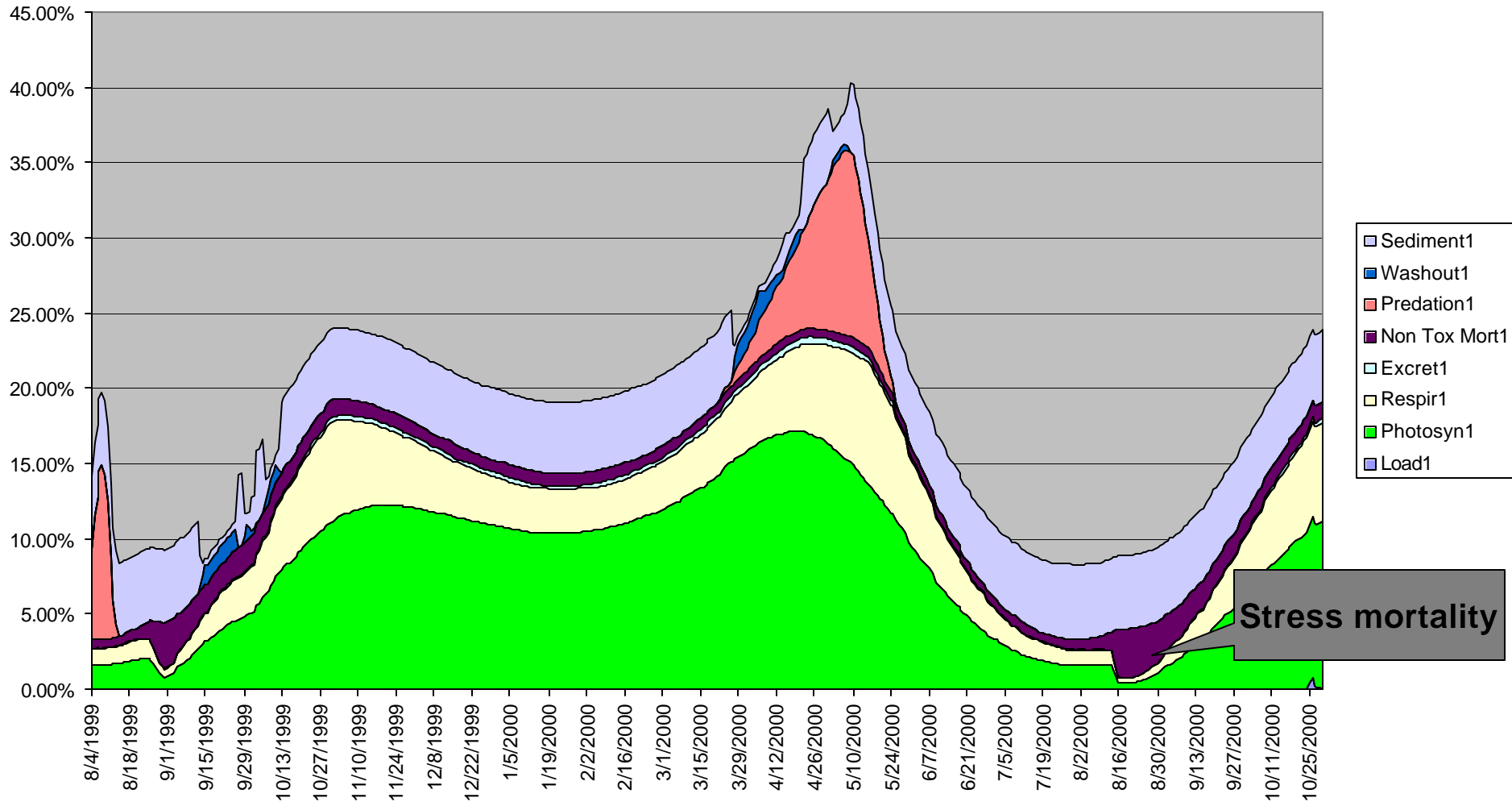
In Cahaba River AL, food, predation, and physical environment control animals

Molluscs



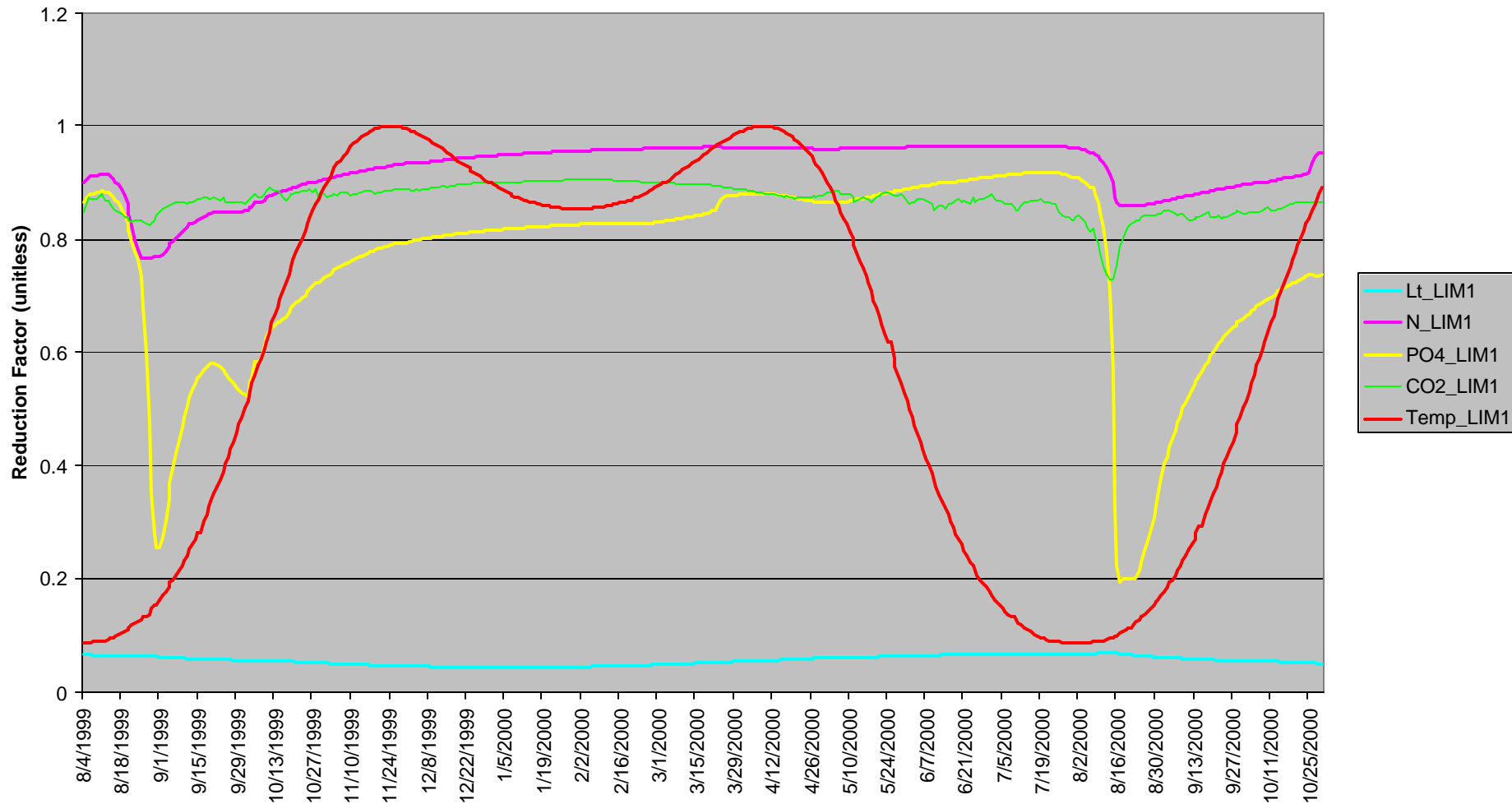
Rates can be saved and plotted for all processes

Process Rates for Cheney Lake KS Diatoms



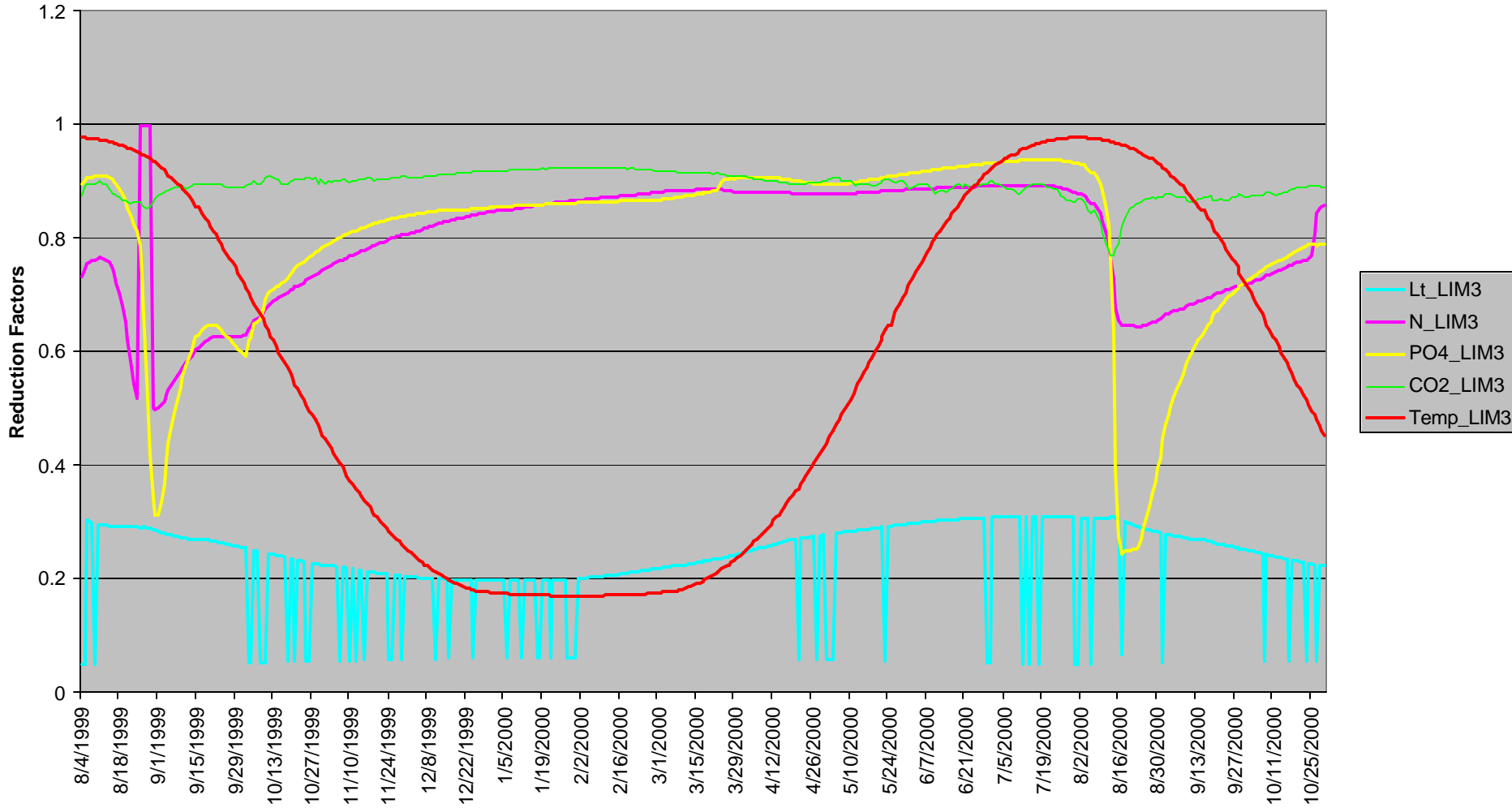
Time-varying limitations to photosynthesis also can be analyzed

Limitations on Cheney Lake KS Diatoms

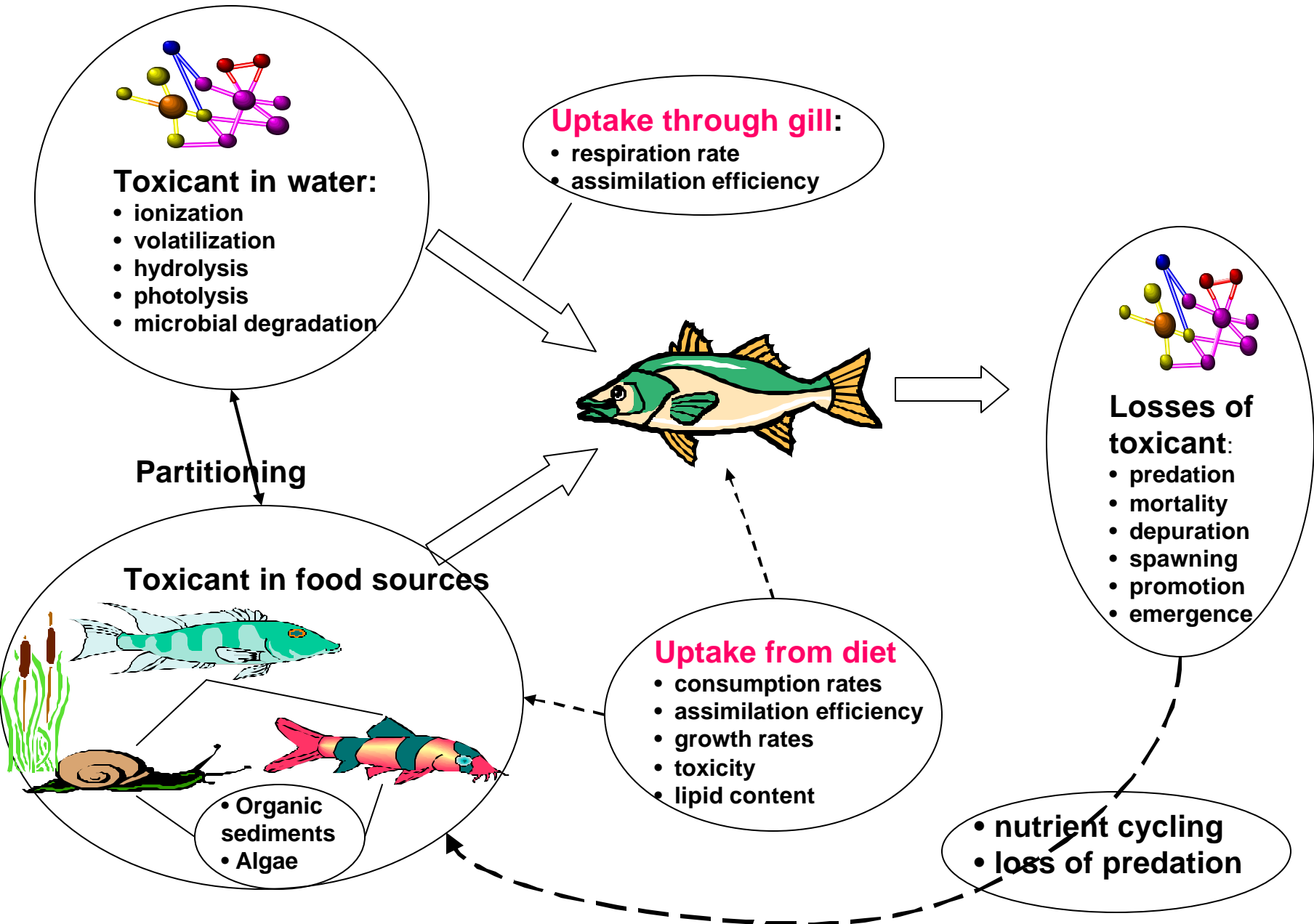


Limitations on various groups can be compared

Cheney Lake KS Blue-Green Limitations



Bioaccumulation in AQUATOX

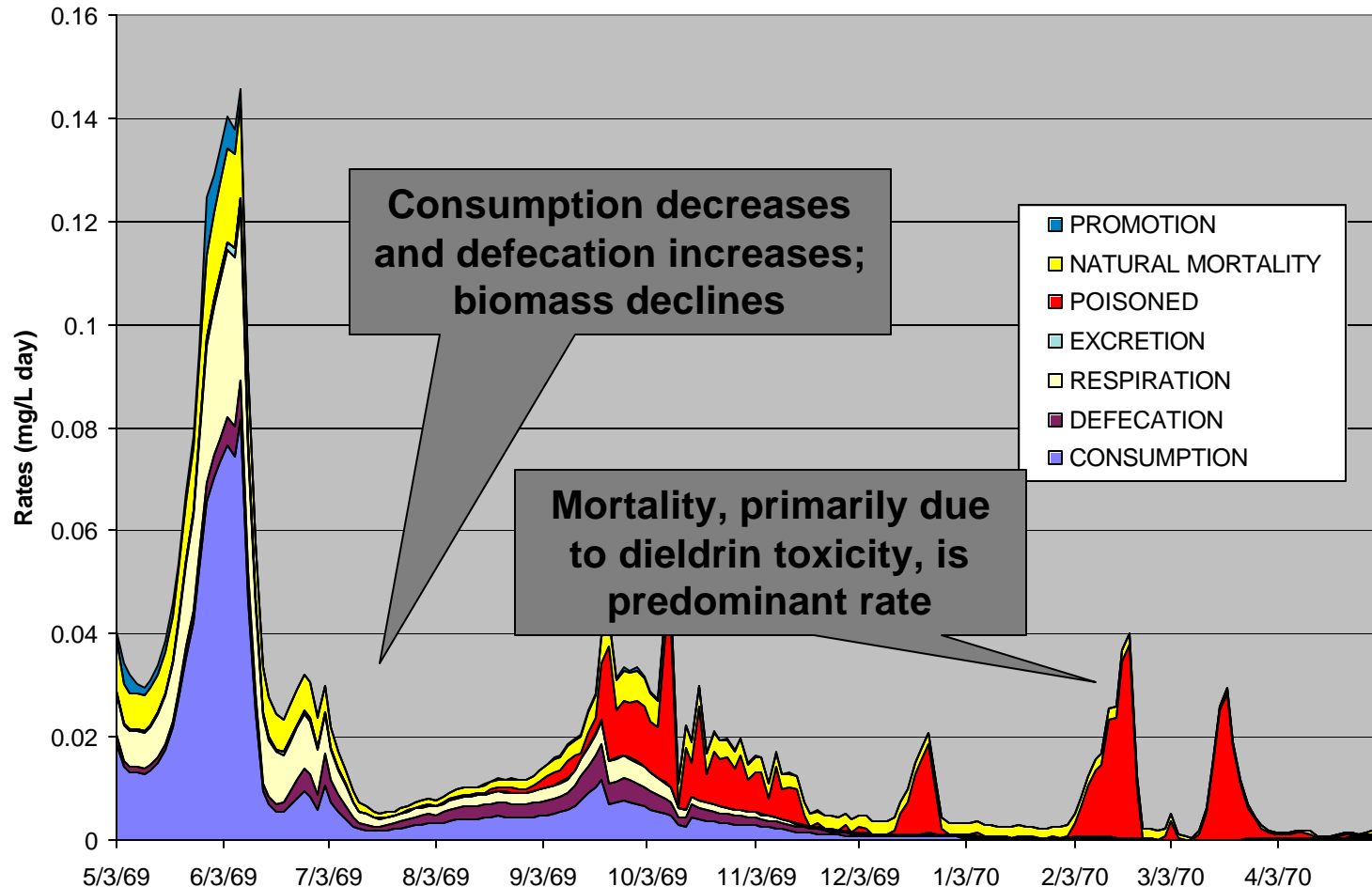


Steps Taken to Estimate Toxicity

- LC_{50} estimators are available for species
- Compute internal LC_{50}
- Compute infinite LC_{50} (time-independent)
- Compute t-varying internal lethal concentration
- Compute cumulative mortality
- Compute biomass lost per day by disaggregating cumulative mortality
- Chronic toxicity is related to acute toxicity through an application factor

With Bioaccumulation, Chronic Toxicity is Followed by Acute Toxicity

CORALVILLE RESERVOIR LARGEMOUTH BASS RATES WITH DIELDRIN



Can run perturbed & control simultaneously

AQUATOX: Study Information
Version 1.92

Study Name:

State and Driving Variables In Study

Model Run Status:
Toxics Run: *No Results Attached*
Control Run: *No Ctrl. Results Attached*

Data Operations:

- Initial Conds.
- Chemical
- Site
- Setup
- Notes
- Edit With Wizard

Program Operations:

- Perturbed**
- Control
- Output
- Export Results
- Export Control
- Help

Dissolved org. tox 1: [Dieldrin]

- Susp. Solids
- Refrac. sed. detritus
- Labile sed. detritus
- Susp. and dissolved detritus
- Buried refrac. detritus
- Buried labile detritus
- Diatoms1: [Diatoms]
- Greens1: [Greens]
- Bl-green1: [Blue-greens]
- Macrophyte1: [Myriophyllum]
- SedFeeder1: [Chironomid]
- SedFeeder2: [Oligochaete]
- SuspFeeder1: [Daphnia]
- PredInvt1: [Predatory Zooplank.]
- LgForageFish1: [Bluegill]
- LgForageFish2: [Shad]
- LgBottomFish1: [Buffalofish]
- SmGameFish1: [Largemouth Bass, YOY]
- LgGameFish1: [Largemouth Bass, Lg]
- LgGameFish2: [Walleye]
- Water Volume
- Temperature
- Wind Loading
- Light
- pH

Control and perturbed

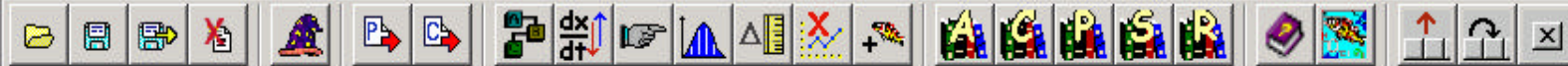
Add Delete Edit

Start | Marjorie Wellman ... | Creative PlayCenter | Microsoft PowerP... | AQUATOX | 12:05 PM

Scenario Management with Control Setup

AQUATOX-- Main Window

File View Library Study Window Help



CoralvilleNewPrms.apr-- Main Window

Control Run Options

All Organic Toxicants:

- Zero-Out Initial Conditions
- Omit Inflow Loadings
- Omit Point Source Loadings
- Omit Direct Precipitation Loadings
- Omit Non-Point Source Loadings
- Omit Toxicant in Organisms
- Omit Buried Toxicants
- Set Multiply-Loadings Factors to 1.0

Nutrients: (Ammonia, Nitrate, and Phosphate)

- Zero-Out Initial Conditions
- Omit Inflow Loadings
- Omit Point Source Loadings
- Omit Direct Precipitation Loadings
- Omit Non-Point Source Loadings
- Set Multiply-Loadings Factors to 1.0

Sand / Silt / Clay:

- Zero-Out Initial Conditions
- Omit Inflow Loadings
- Omit Point Source Loadings
- Omit Direct Precipitation Loadings
- Omit Non-Point Source Loadings
- Set Multiply-Loadings Factors to 1.0

Select conditions to eliminate in "control" simulation

- Zero-Out Initial Conditions
- Omit Inflow Loadings
- Omit Point Source Loadings
- Omit Direct Precipitation Loadings
- Omit Non-Point Source Loadings
- Omit Toxicant in Organisms
- Omit Buried Toxicants
- Set Multiply-Loadings Factors to 1.0

Detritus:

- Zero-Out Initial Conditions
- Omit Inflow Loadings
- Omit Point Source Loadings
- Omit Direct Precipitation Loadings
- Omit Non-Point Source Loadings
- Set Multiply-Loadings Factors to 1.0

Study Name: DIE

Model Run Status

Toxics Run: (

Control Run: (

Data Operations:

Initial Conds.

Chemical

Site

Setup

Notes

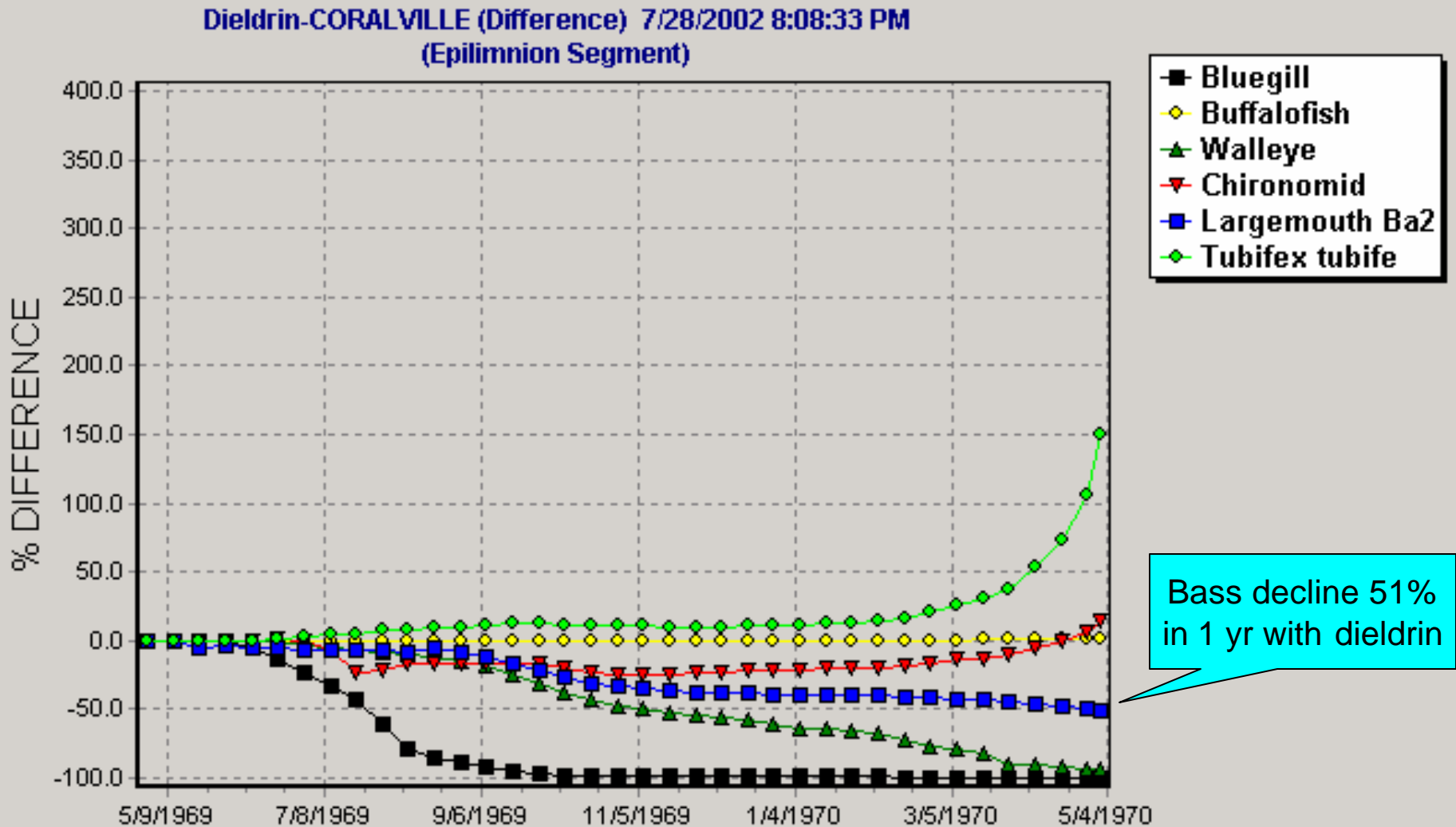
Edit With Wizard

Help

OK

Cancel

Percent Difference Graph emphasizes differences between ctl. & pert. simulations



All parameters and loadings subject to uncertainty analysis

AQUATOX – Uncertainty Setup

Run Uncertainty Analysis Number of Iterations: 20 (integer)

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

All Distributions

Distributions by Parameter

Distributions by State Variable

Dissolved org. tox 1: [Dieldrin]

Chemical Parameters

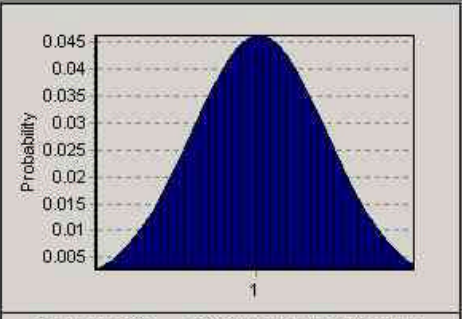
- T1: Molecular Weight
- T1: Dissociation Constant (pKa)
- T1: Solubility (ppm)
- T1: Henry's Law Const. (atm. m³/mol)
- T1: Vapor Pressure (mm Hg)
- T1: Octanol-Water Partition Coeff (Log Kow)
- T1: Sed/Detr-Water Partition Coeff (mg/L)
- T1: Activation Energy for Temp (cal/mol)
- T1: Anaerobic Microbial Degrn. (L/d)
- T1: Aerobic Microbial Degrn. (L/d)
- T1: Uncatalyzed Hydrolysis (L/d)
- T1: Acid Catalyzed Hydrolysis (L/d)
- T1: Base Catalyzed Hydrolysis (L/d)
- T1: Photolysis Rate (L/d)
- T1: Oxidation Rate Const (L/mol day)
- T1: Weibull Shape Parameter
- T1: Initial Condition (ug/L)
- T1: Const Load (ug/L)
- T1: Multiply Loading by
- T1: Mult. Direct Precip. Load by
- T1: Mult. Point Source Load by
- T1: Mult. Non-Point Source Load by

Toxicity Parameters

Ammonia as N

Distribution Information

T1: Multiply Loading by



Probability

0.045
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005

1

Probability Cumulative Distribution

Distribution Type:

- Triangular
- Uniform
- Normal
- Lognormal

Distribution Parameters:

Mean: 1

Std. Deviation: 0.4

For this parameter, in an Uncertainty Run:

- Use a Distribution
- Use a Point Estimate

Help OK Cancel

Help OK Cancel

Start ZoneAlarm... PPT timesheet.xls Inbox - Mic... Microsoft P... AQUATOX 7:08 PM

Sensitivity Analysis

View a Different Database

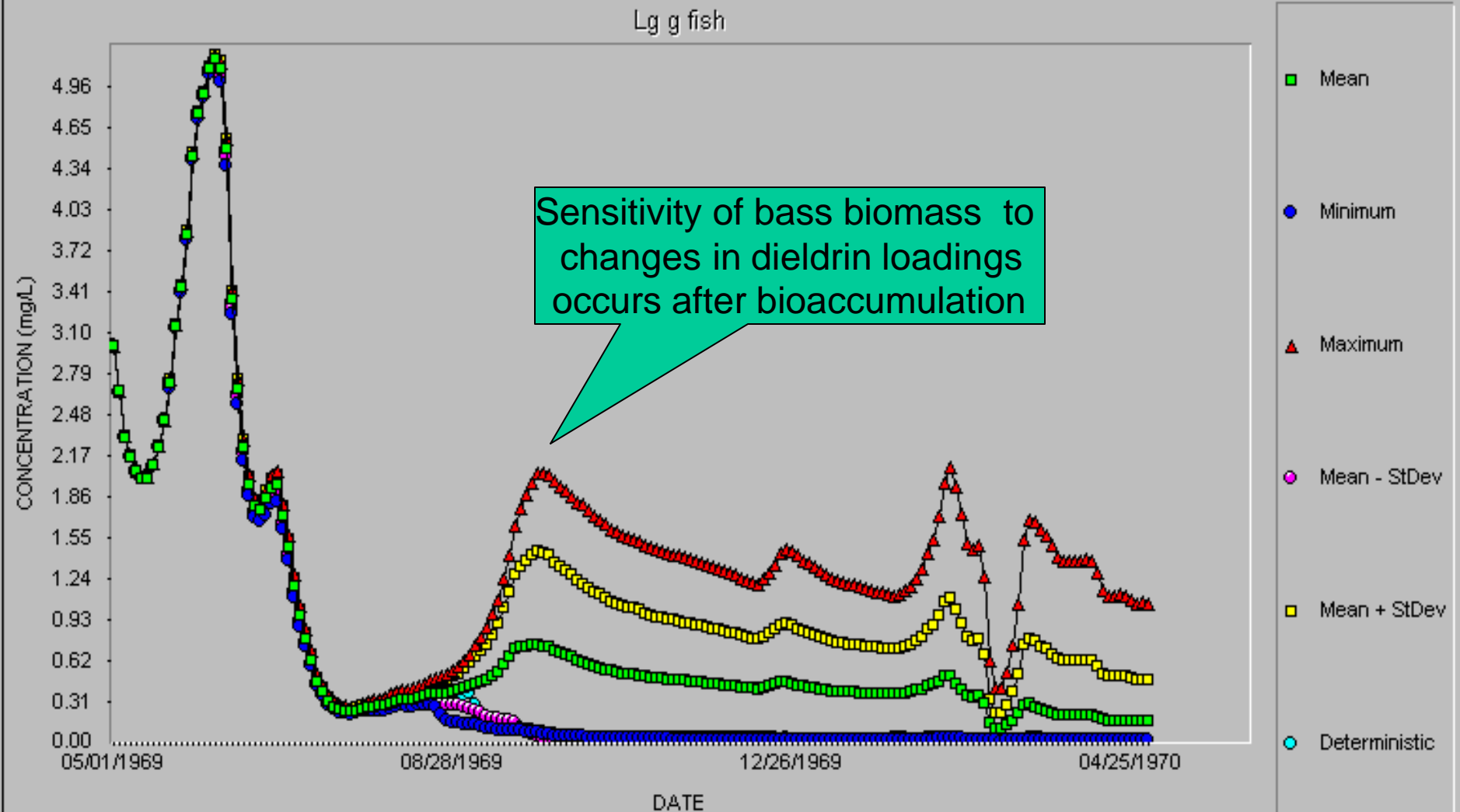
Organisms in mg/L, toxicant in $\mu\text{g/L}$ unless otherwise indicated.

Viewing Data in File: D:\Aqtx_168\Output\W_CoralvDieldr.dbf

Print Setup

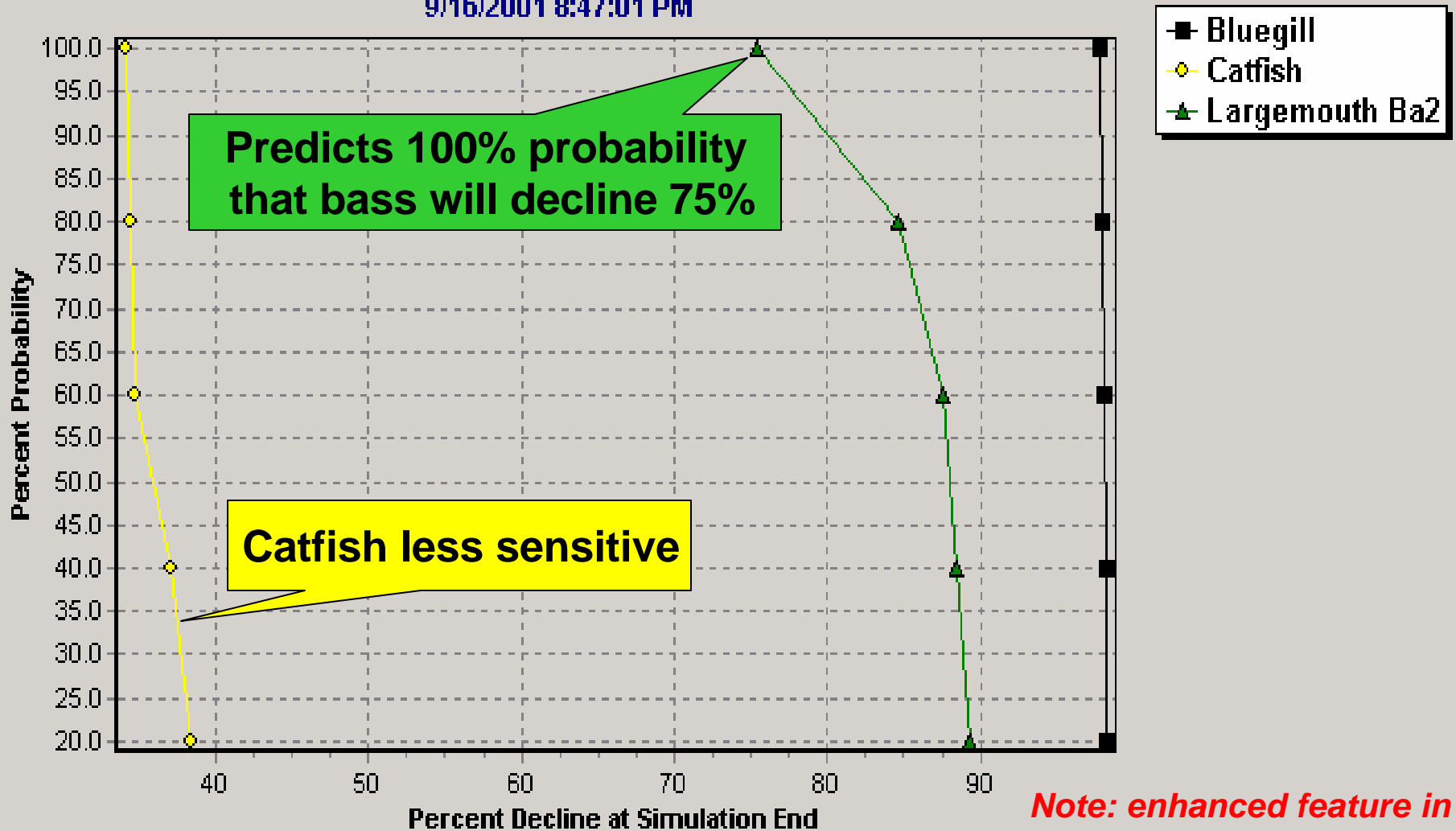
Print Chart

View a Different Variable

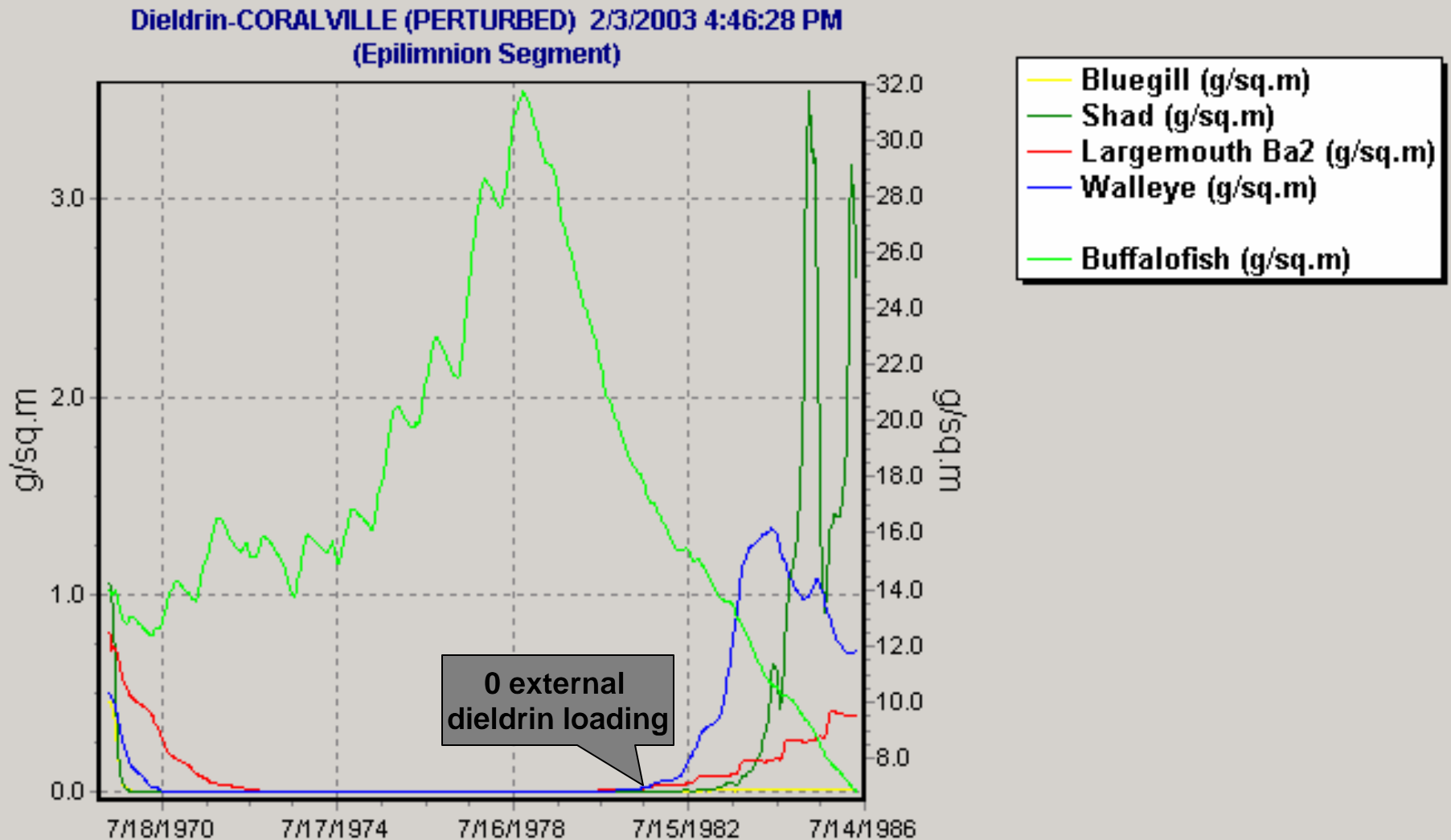


AQUATOX can estimate % probability of change in biomass

Biomass Risk Graph
9/16/2001 8:47:01 PM



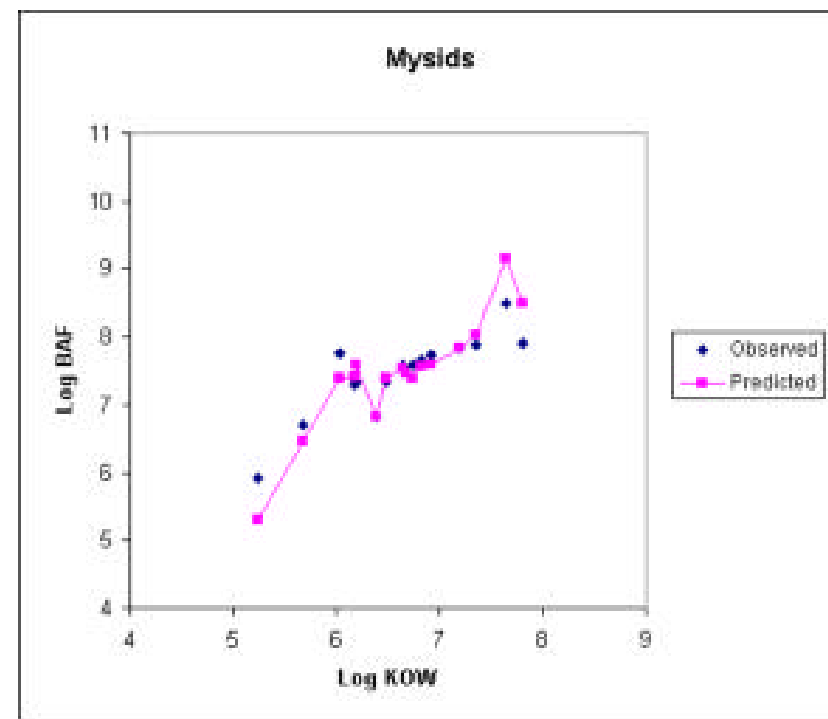
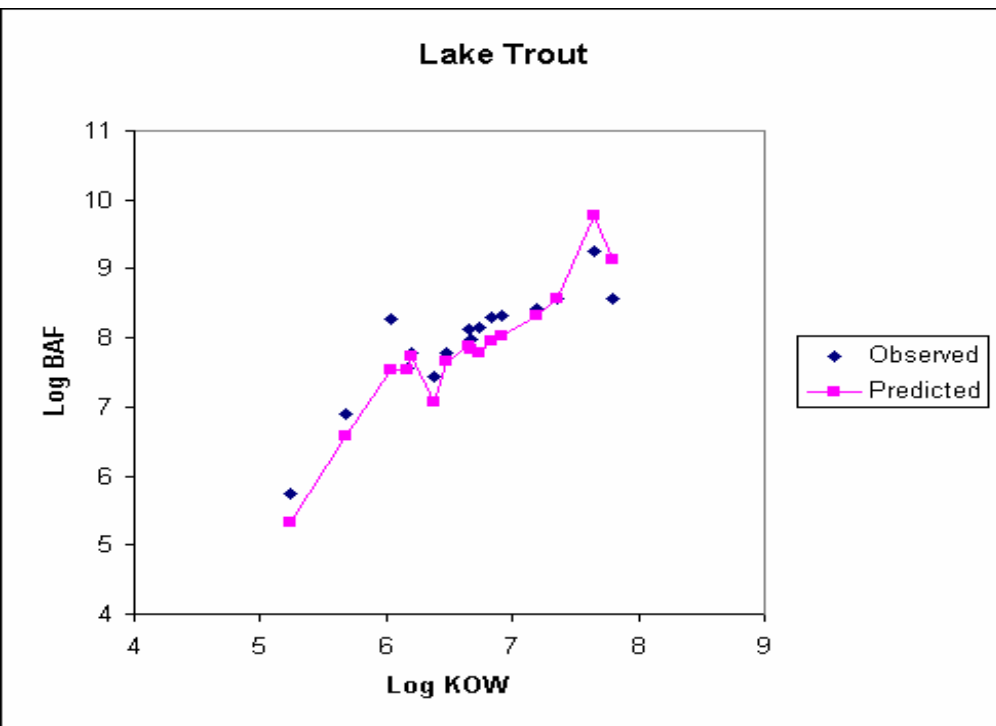
Recovery from pesticide in reservoir-- Coralville is now “best bass lake in Iowa”



Model Validation

PCBs in Lake Ontario

- Reasonable agreement of calculated BAFs with observed BAFs for some, not all, species



Note: analysis done as part of model validation, ^{B.} using published data; not part of regulatory actions

Segmented version can represent dynamically linked multiple segments

AQUATOX-- Linked System Mode: "Housatonic.als"

File Library Segments Help

Show Segment Data Show Link Data

- [4a]: East Branch
- [4b]: West Branch
- [5a]: Reach 5a
- [5b]: Reach 5b
- [5c]: Reach 5c
- [6a]: Deep Channel
- [6b]: Backwaters
- [6c-e]: Epi Deep Woods Pond
- [6c-h]: Hypo Deep Woods Pond
- [6d]: Shallow Woods Pond
- [6e]: Pond Outflow

Add Delete Edit

Data Operations:

- Chemicals
- Setup
- Notes

Program Operations:

- Run
- Control
- Output
- Export Results

Linked System Name:

Toxics Run: *No Run Recorded* Control Run: *No Ctrl. Run Recorded*

Load Map Clear Map

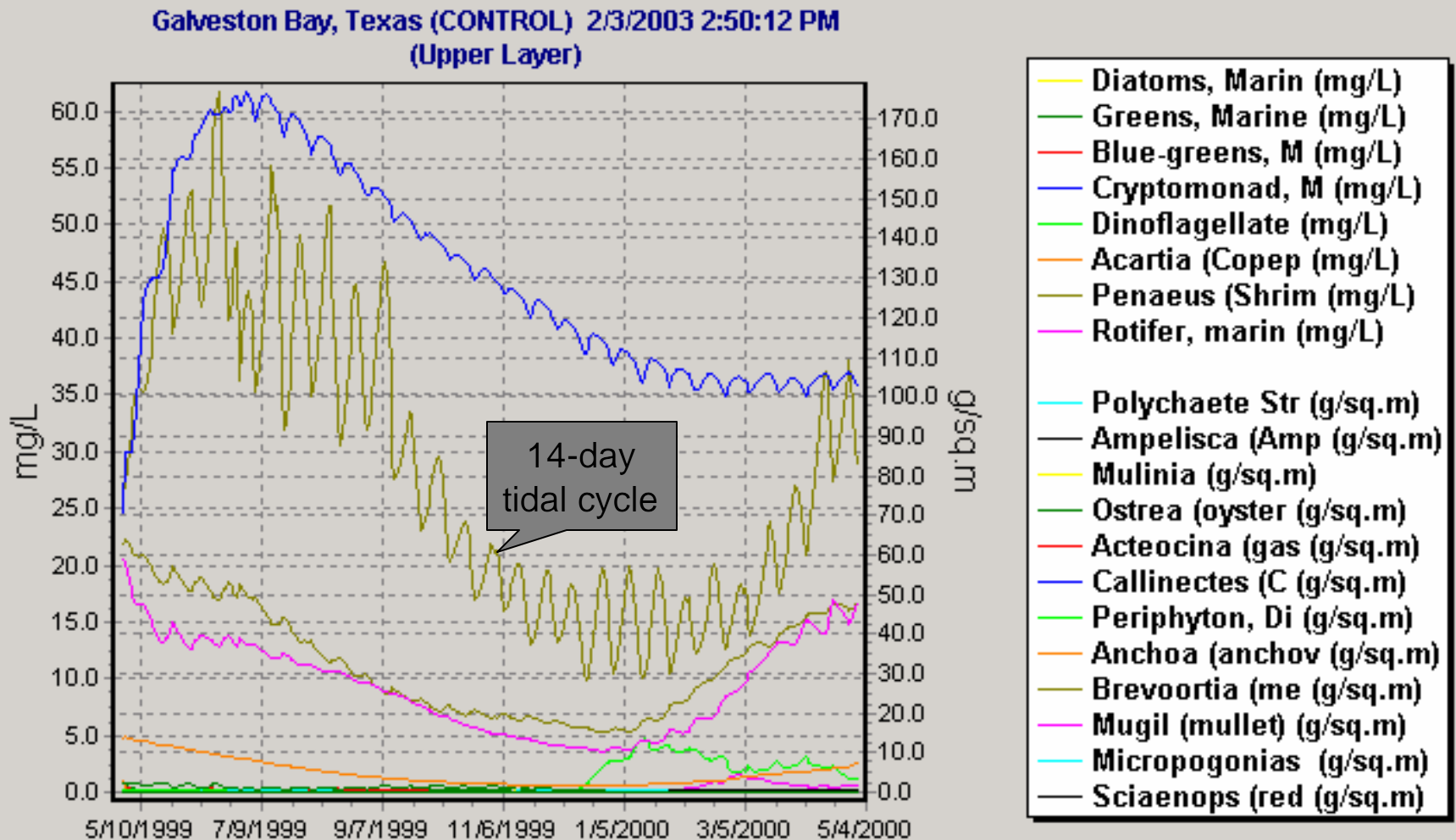
developed for Housatonic River MA project

Estuarine version calibrated for Galveston Bay, Texas, to evaluate toxicants



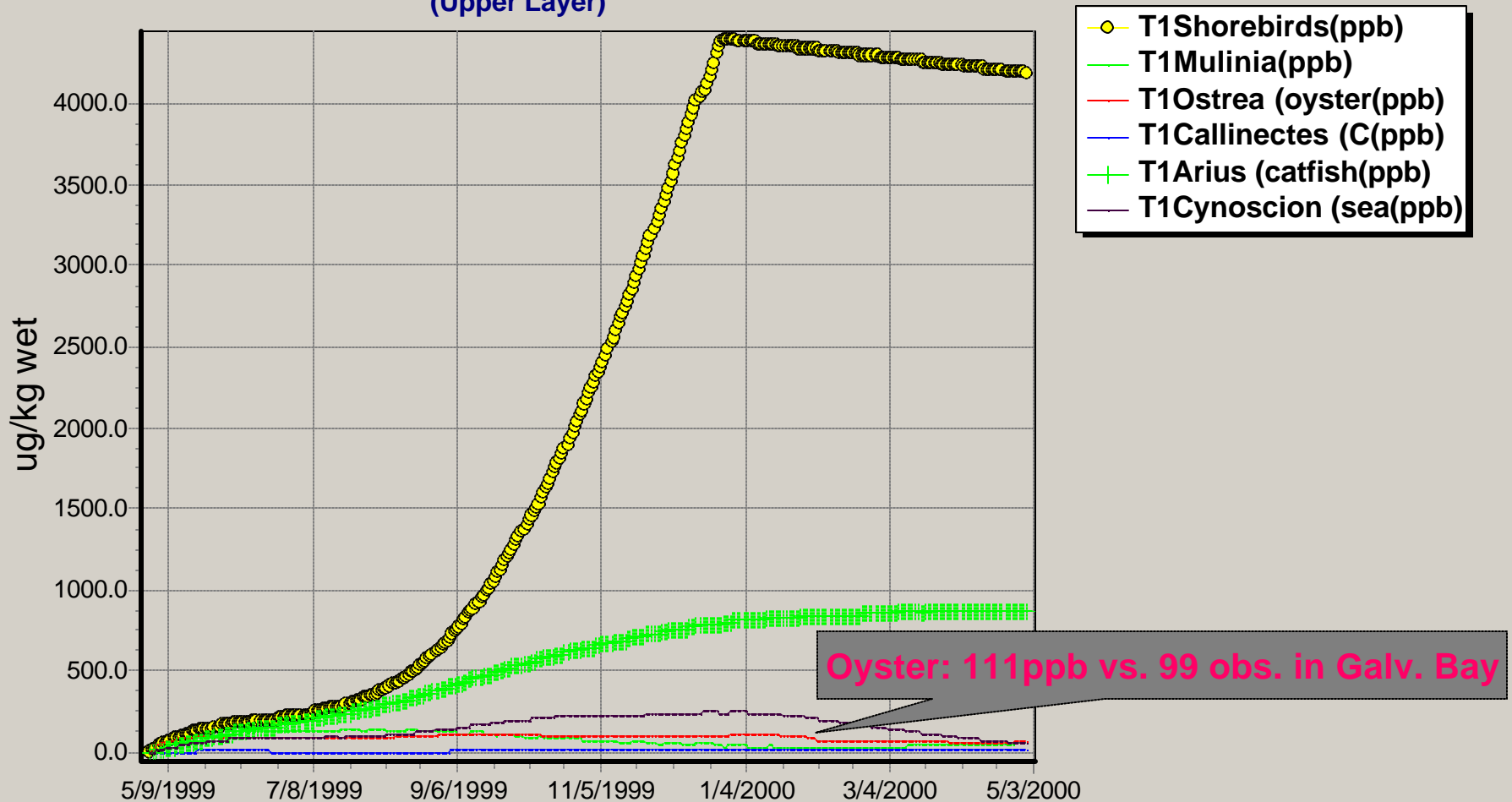
Photo Courtesy NASA Johnson Space Center

Can model biomass of commercial and other species in upper and lower layers



Can model bioaccumulation in plants, animals, and *shorebirds*; PFOS shown based on constant concentration of 1 ug/L

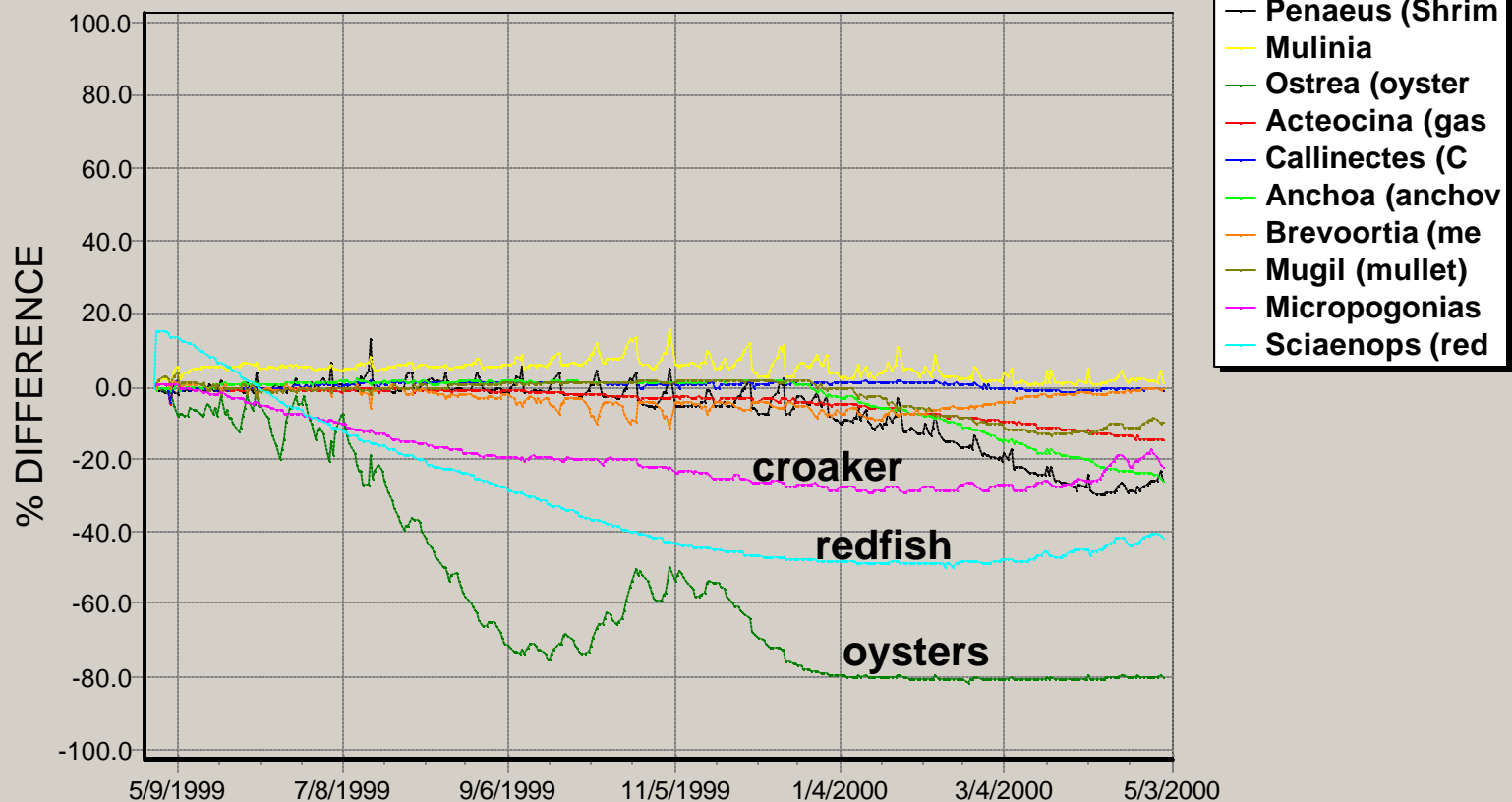
Galveston Bay, Texas (PERTURBED) 3/8/2003 8:24:20 PM
(Upper Layer)



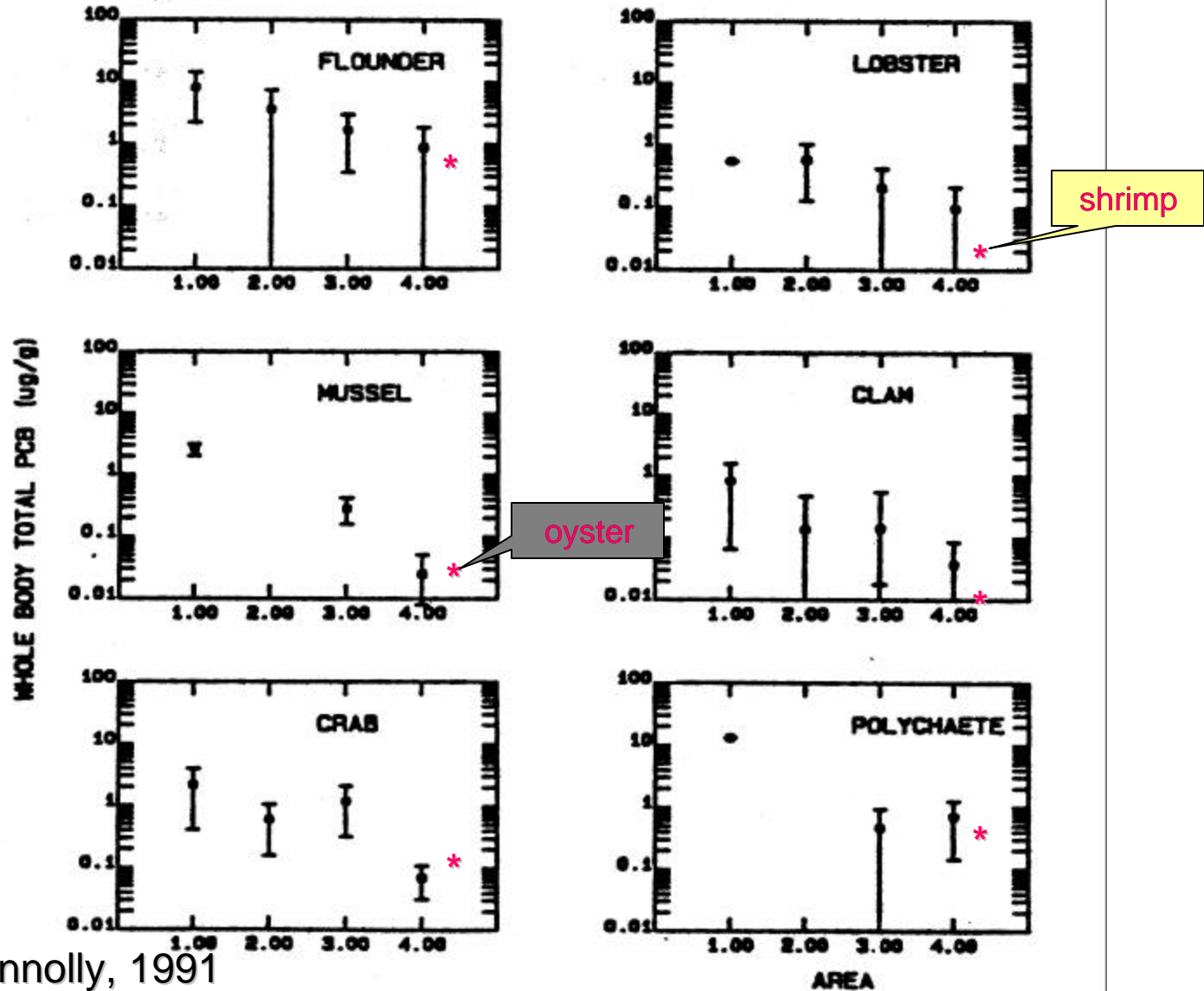
Model predicts decline of sensitive species with high PFOS levels

based on limited toxicology values

Galveston Bay, Texas (Difference) 3/9/2003 8:32:22 PM
(Upper Layer)



Validation: New Bedford Harbor MA, peak PCB values were comparable



graphs from Connolly, 1991

Potential Next Steps

- **Generalization of estuarine version**
- **Implementation of segmented version for estuaries**
- **Application to representative estuaries as template for site-specific simulations**
- **Linkage to SLAMM to predict effects of habitat loss on estuarine ecosystems**

Halt Execution

Hide Map

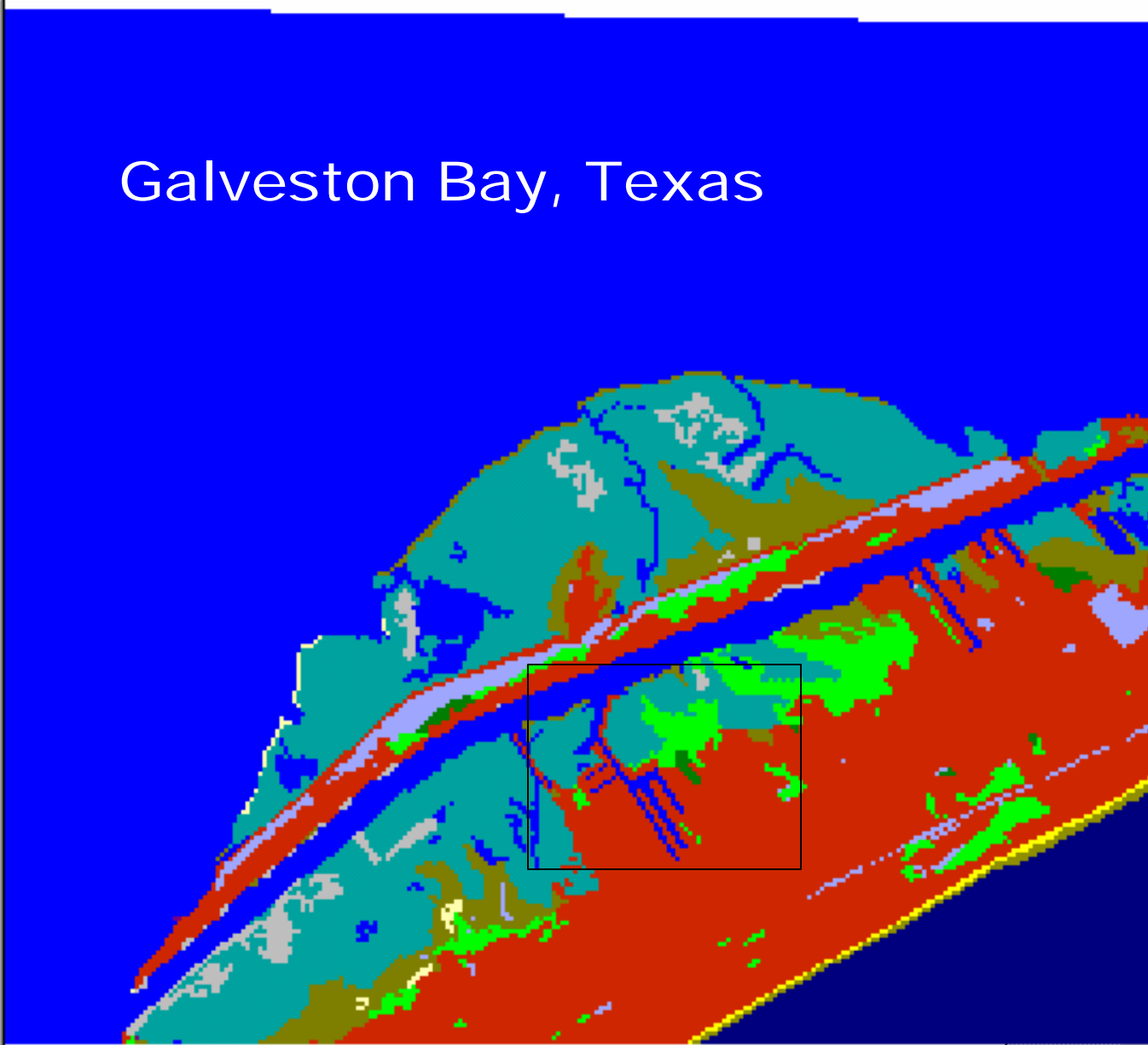
Hide Legend

Pixel Size: 1 2 3 4

Legend

Dev. dry land	
Und. dry land	
Hardwood swamp	
Cypress swamp	
Inland fr. mar	
Tidal fresh mr	
Trans. salt mr	
Saltmarsh	
Mangrove	
Estuarine bch.	
Tidal flat	
Ocean beach	
Ocean flat	
Rocky intertdl	
Inld open wtr	
Riverine tidal	
Estuarine Watr	
Tidal creek	
Open Ocean	
Blank	

Galveston Bay, Texas






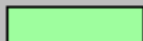
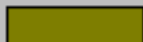
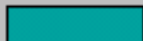
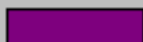
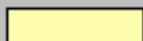


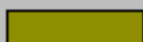
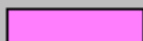
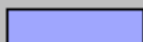


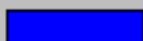




Halt Execution

Hide Map

Hide Legend

Legend

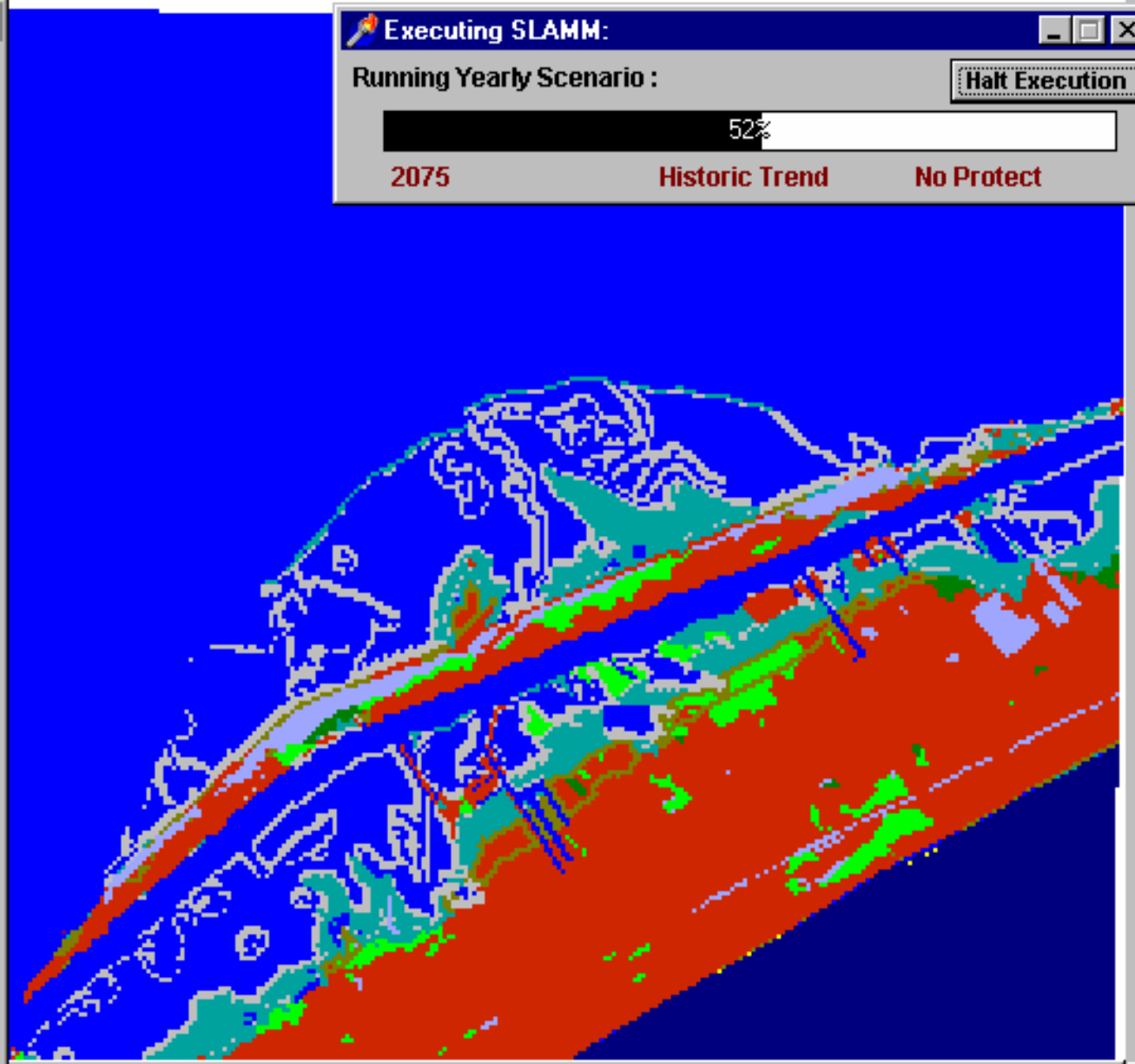
Dev. dry land	
Und. dry land	
Hardwood swamp	
Cypress swamp	
Inland fr. mar	
Tidal fresh mr	
Trans. salt mr	
Saltmarsh	
Mangrove	
Estuarine bch.	
Tidal flat	
Ocean beach	
Ocean flat	
Rocky intertdl	
Inlnd open wtr	
Riverine tidal	
Estuarine Watr	
Tidal creek	
Open Ocean	
Blank	

Executing SLAMM:

Running Yearly Scenario :

52%

2075 Historic Trend No Protect



To Obtain AQUATOX

- Download from Internet:
www.epa.gov/ost/models/aquatox
- Release 2 will be available in April (?) from OST
- For latest Release 2 beta test version:
www.myweb.cableone.net/dickpark/AQTXFacts.htm
- Estuarine version will be available from EPA
OPPT (Don Rodier)