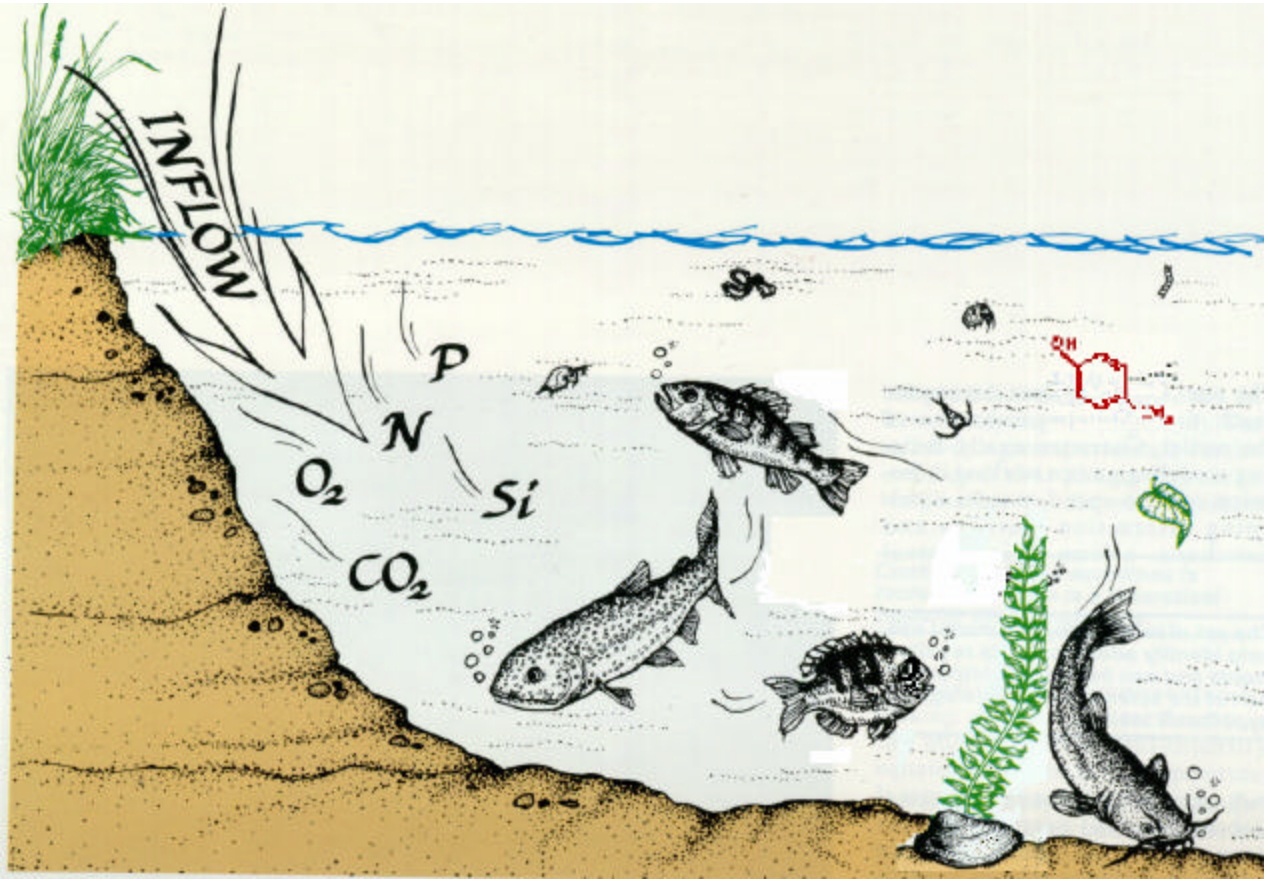
Predicting the Fate & Effects of Pollutants in Freshwater and Estuarine Environments with AQUATOX



Richard A. Park, Eco Modeling, Diamondhead MS
Marjorie C. Wellman, US EPA, Office of Science & Technology

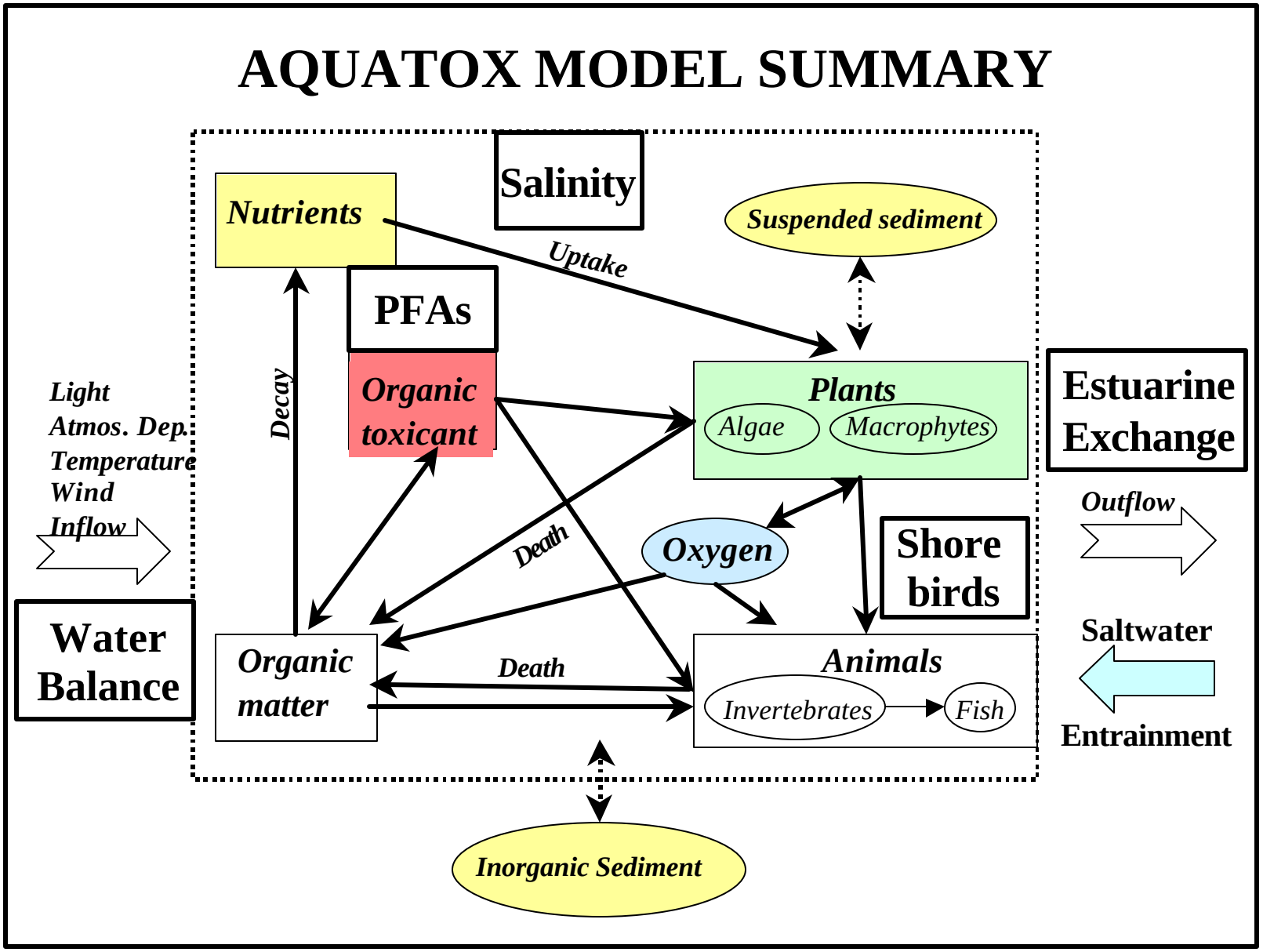
What is AQUATOX?

- **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**

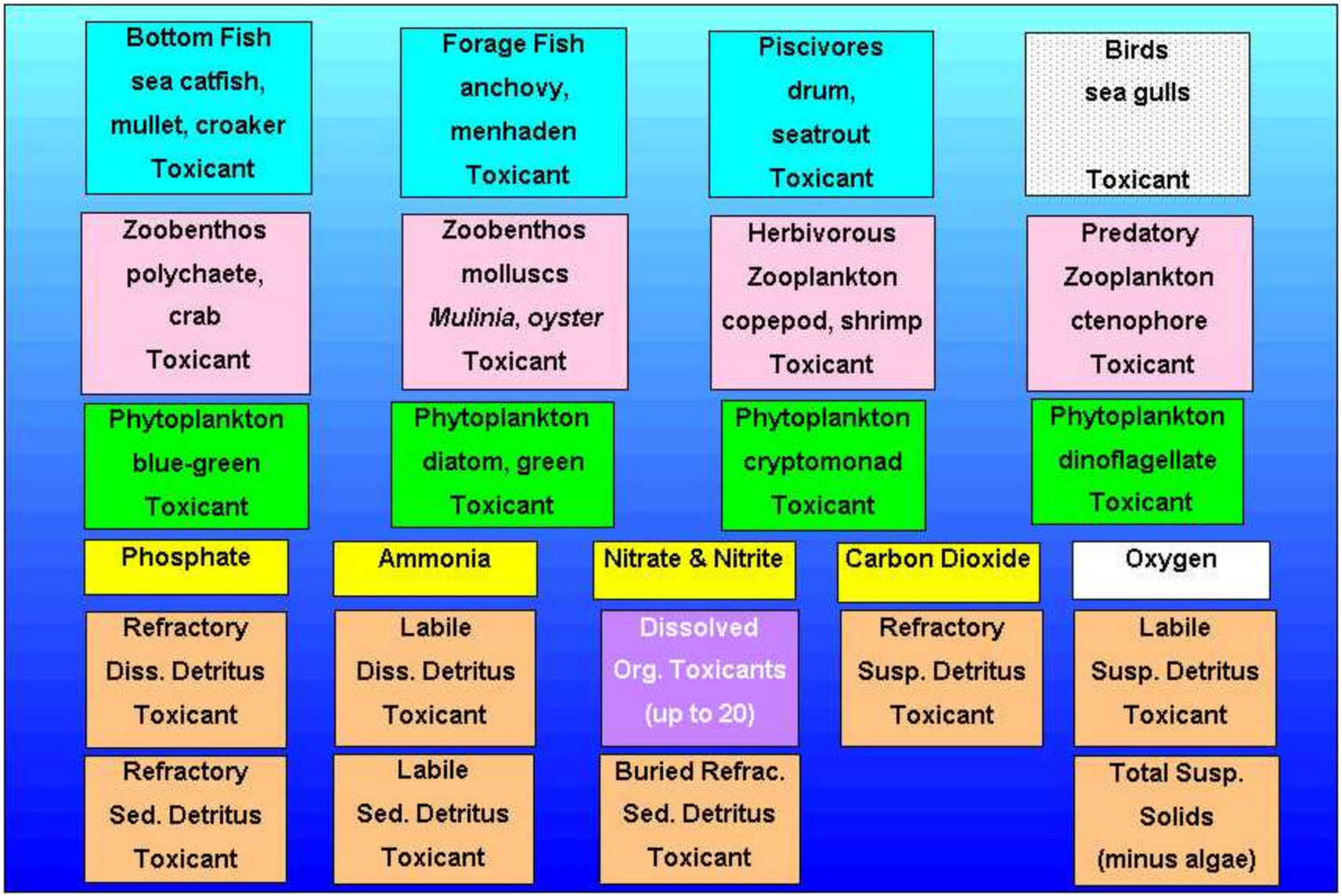
AQUATOX Structure

- **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



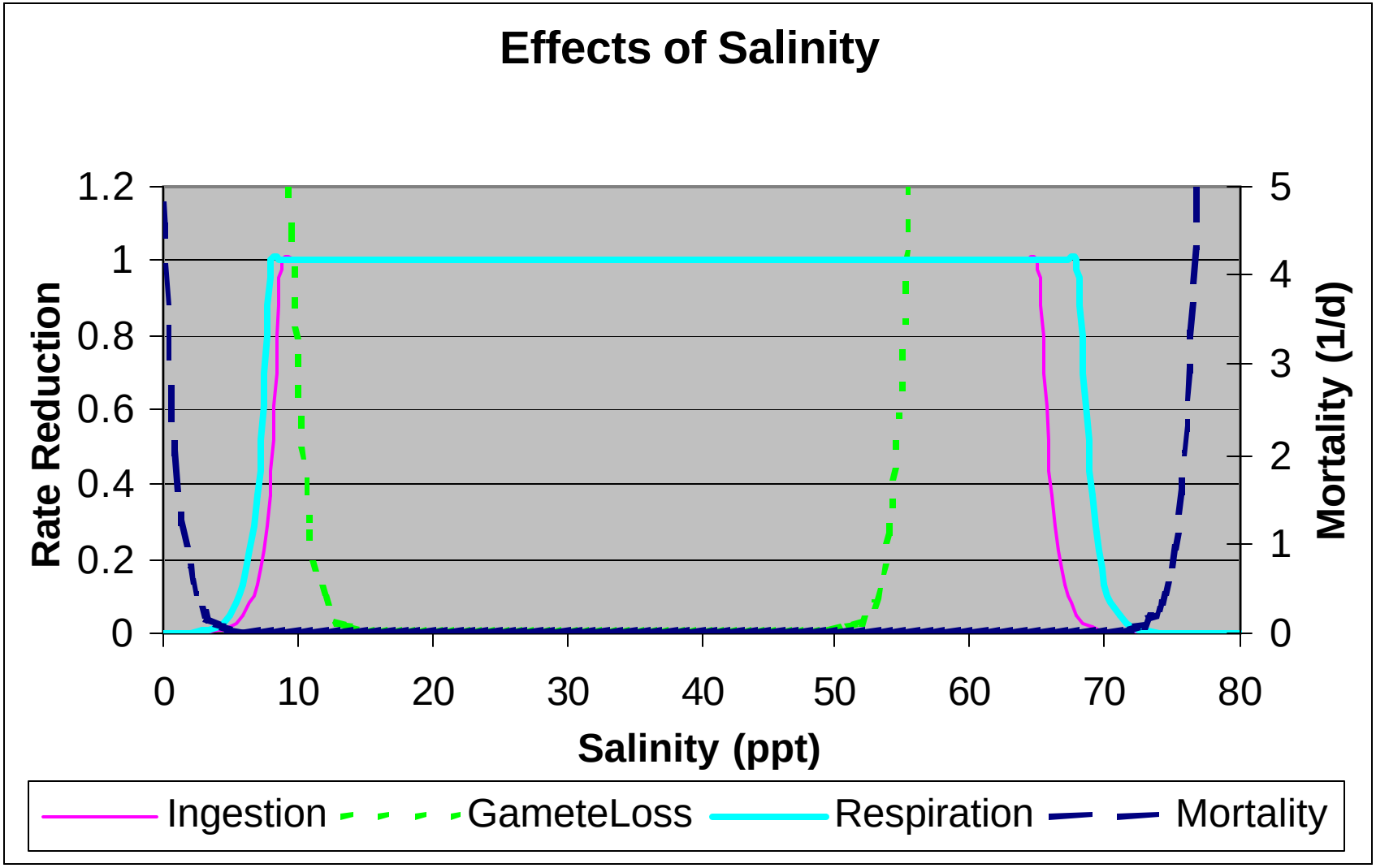
Galveston Bay, Texas, compartments



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

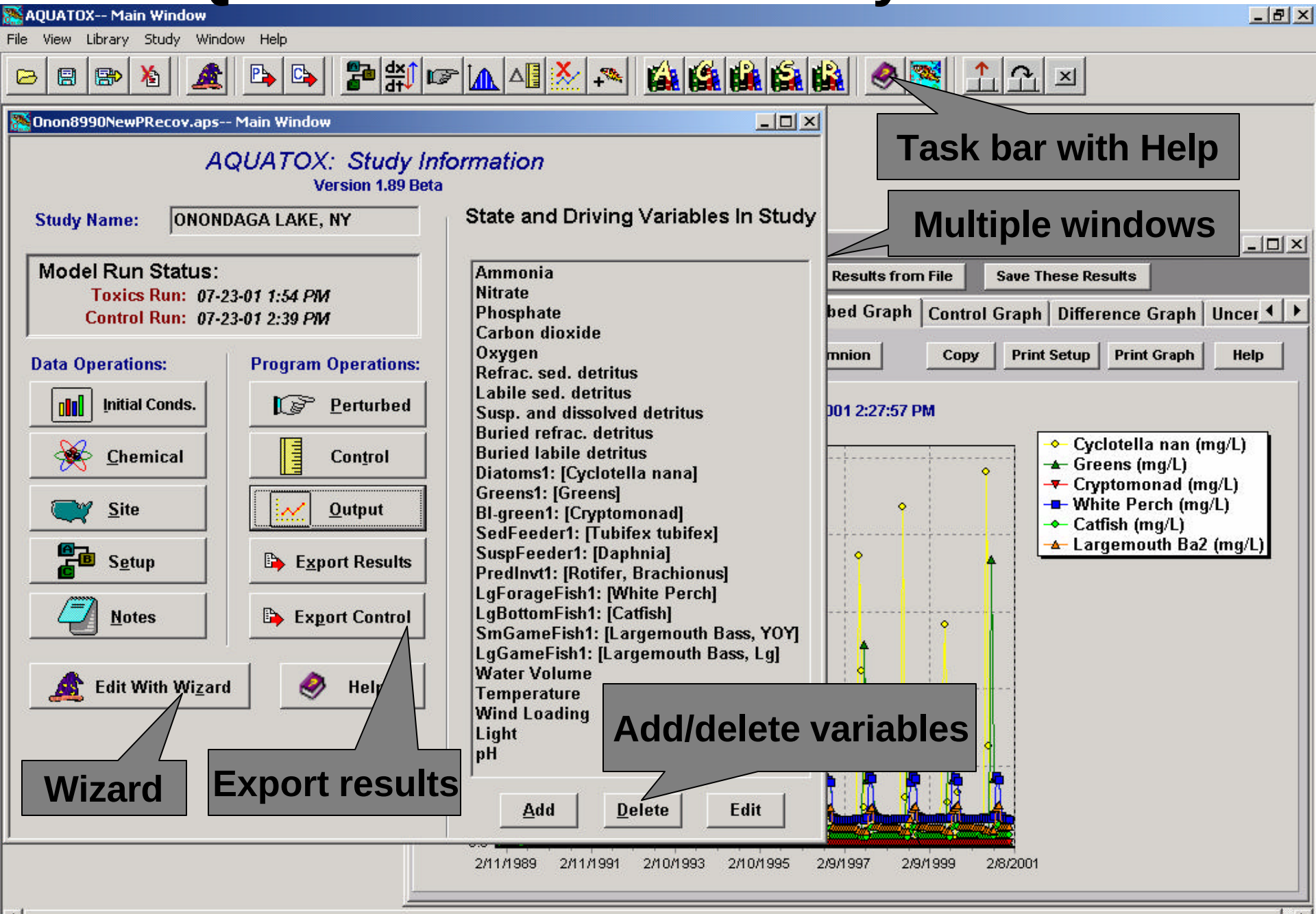


AQUATOX Capabilities

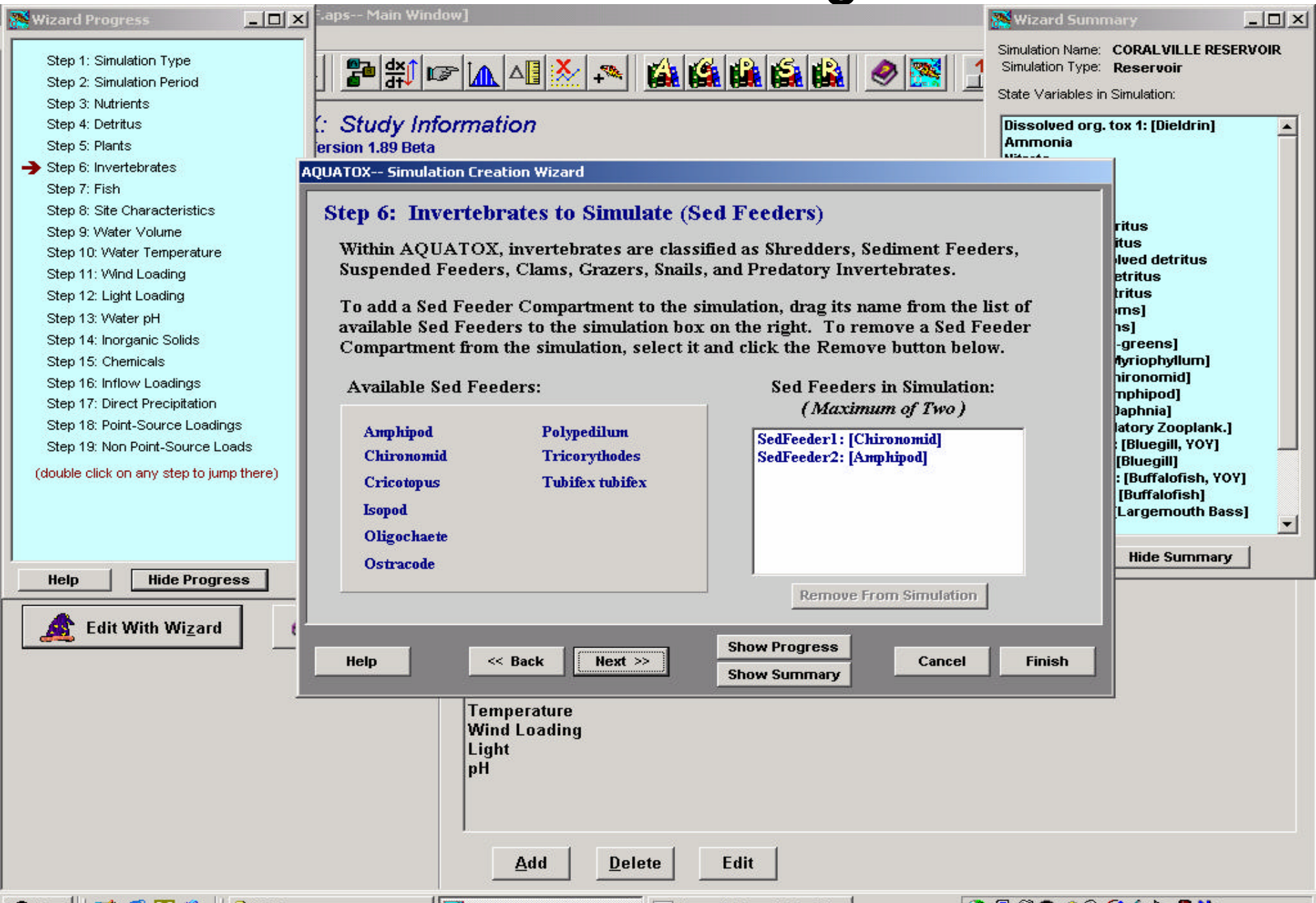
new capabilities in blue and red

- 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



Wizard is available for guidance

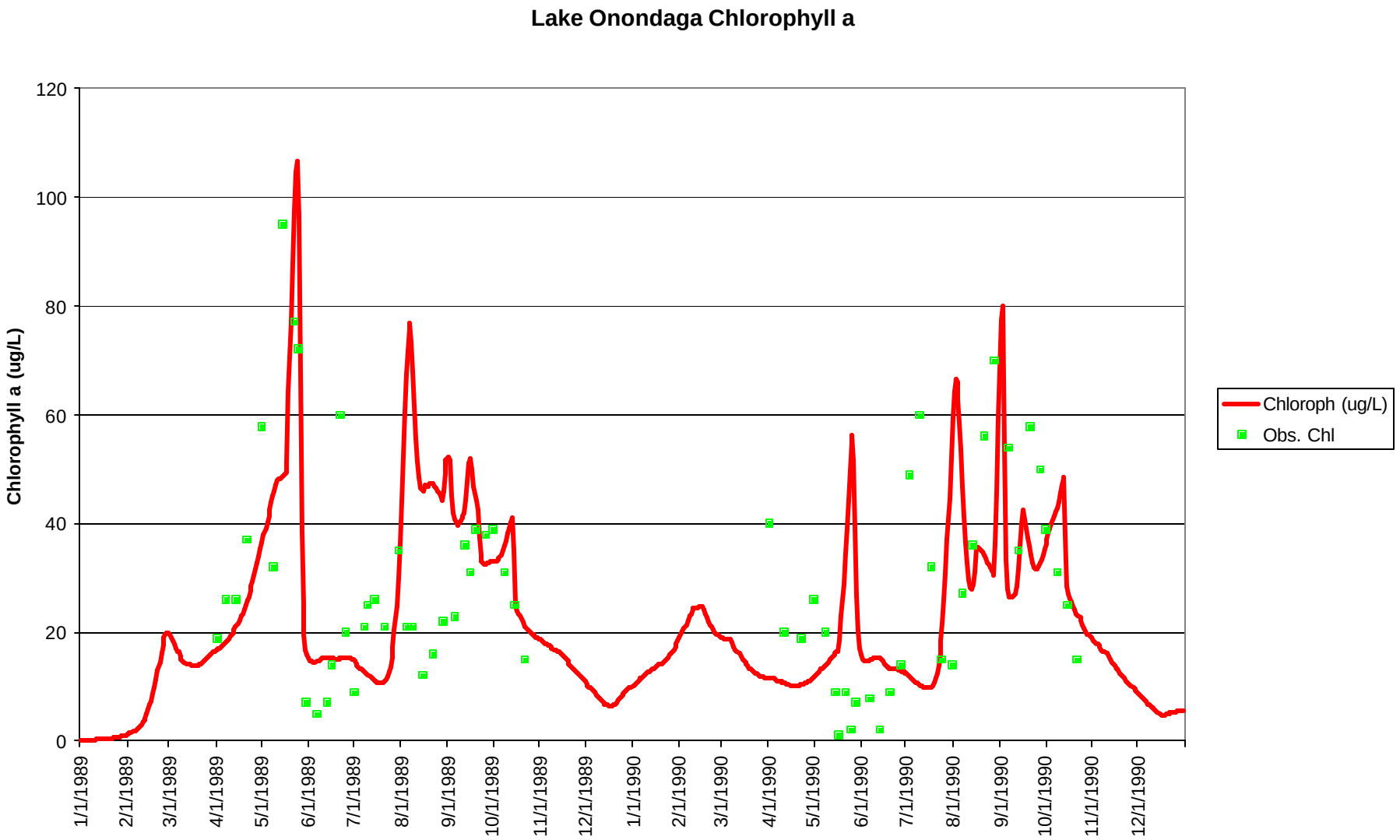


Loadings to AQUATOX

- 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

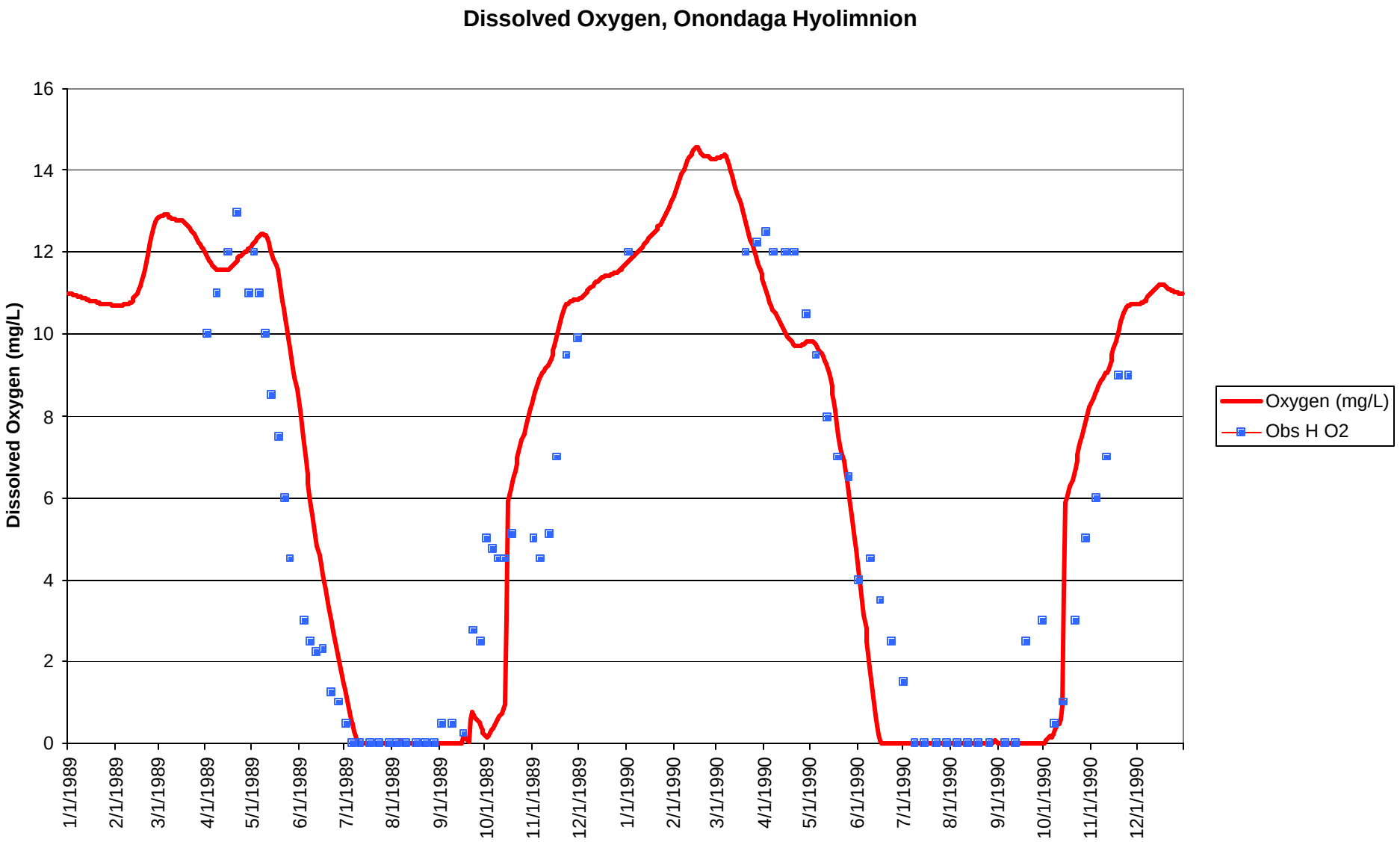
Lake Onondaga NY

Reasonable Simulation of Chlorophyll a



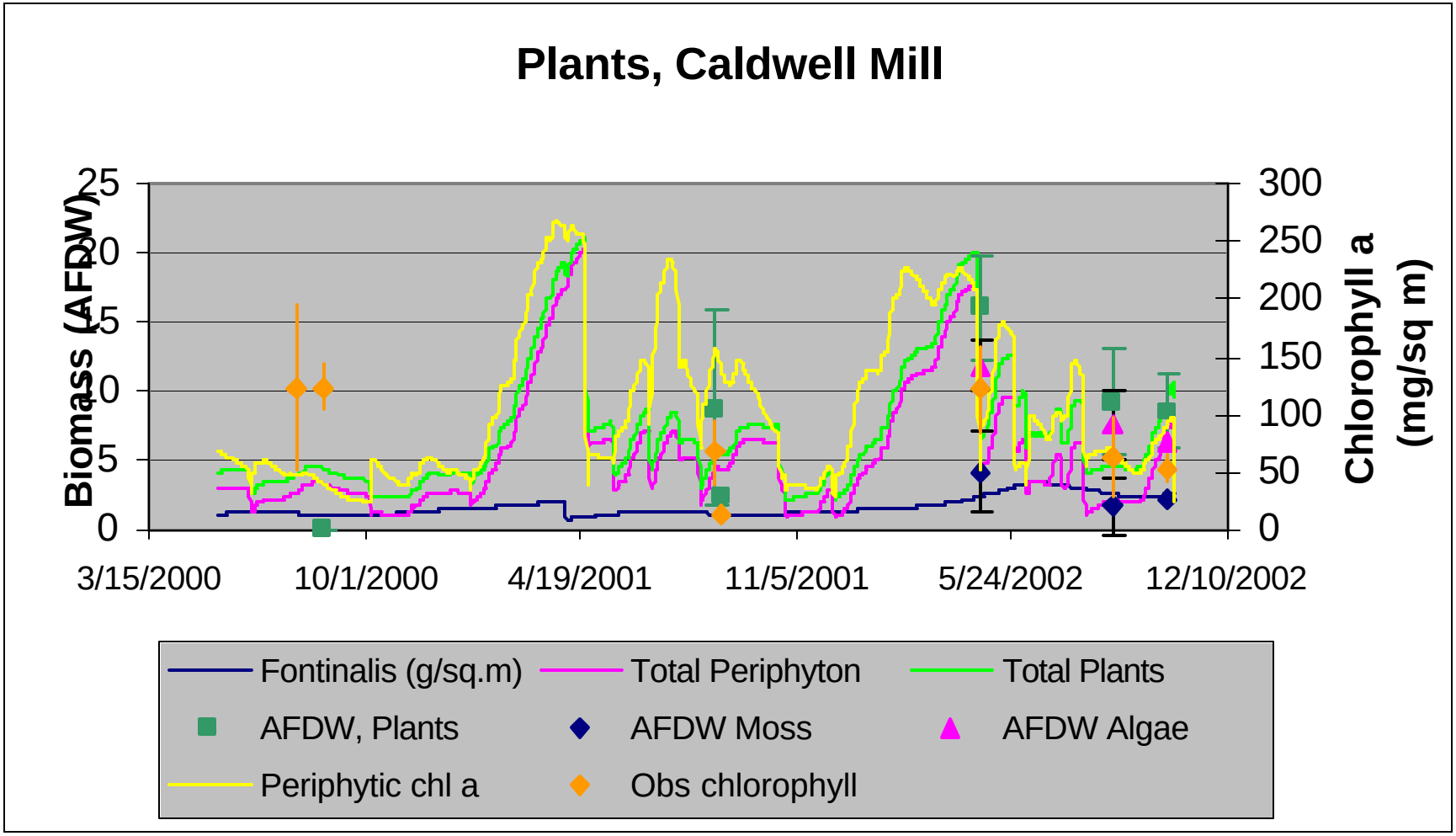
Lake Onondaga NY

Reasonable Simulation of Hypolimnetic DO

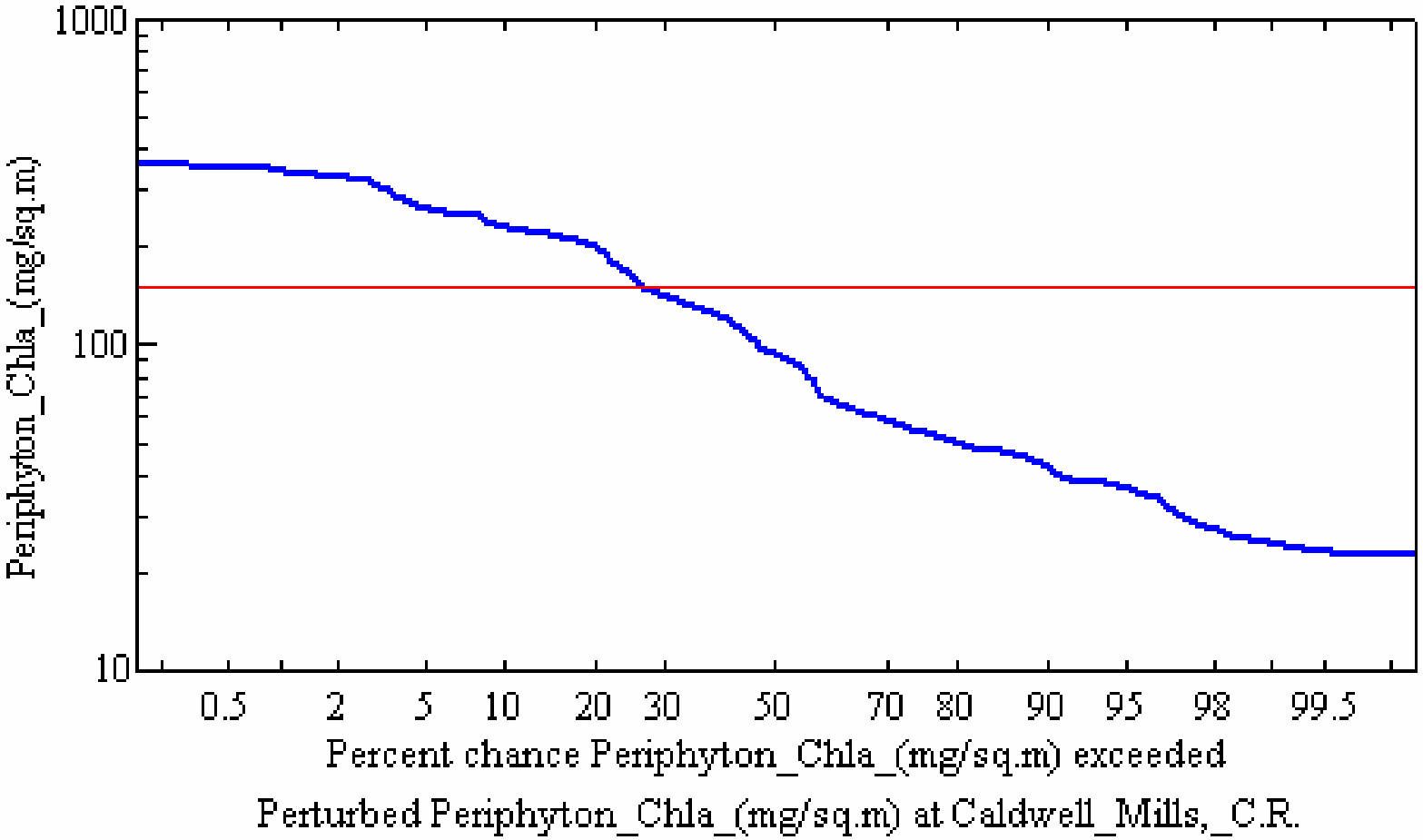


The model was calibrated for Caldwell Mill, Cahaba River, Ala.

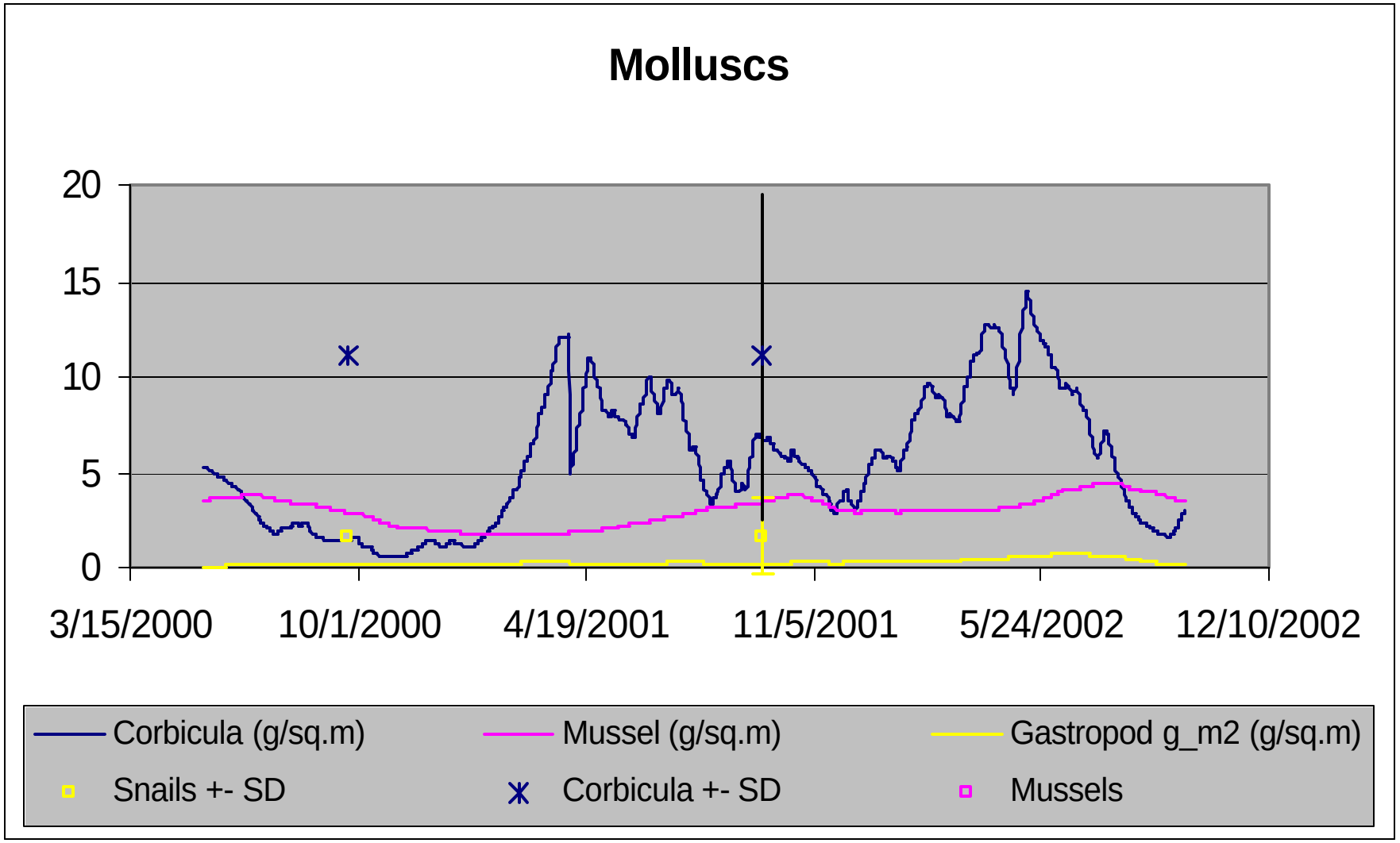
Once past the transient conditions of 2000, the fit was acceptable



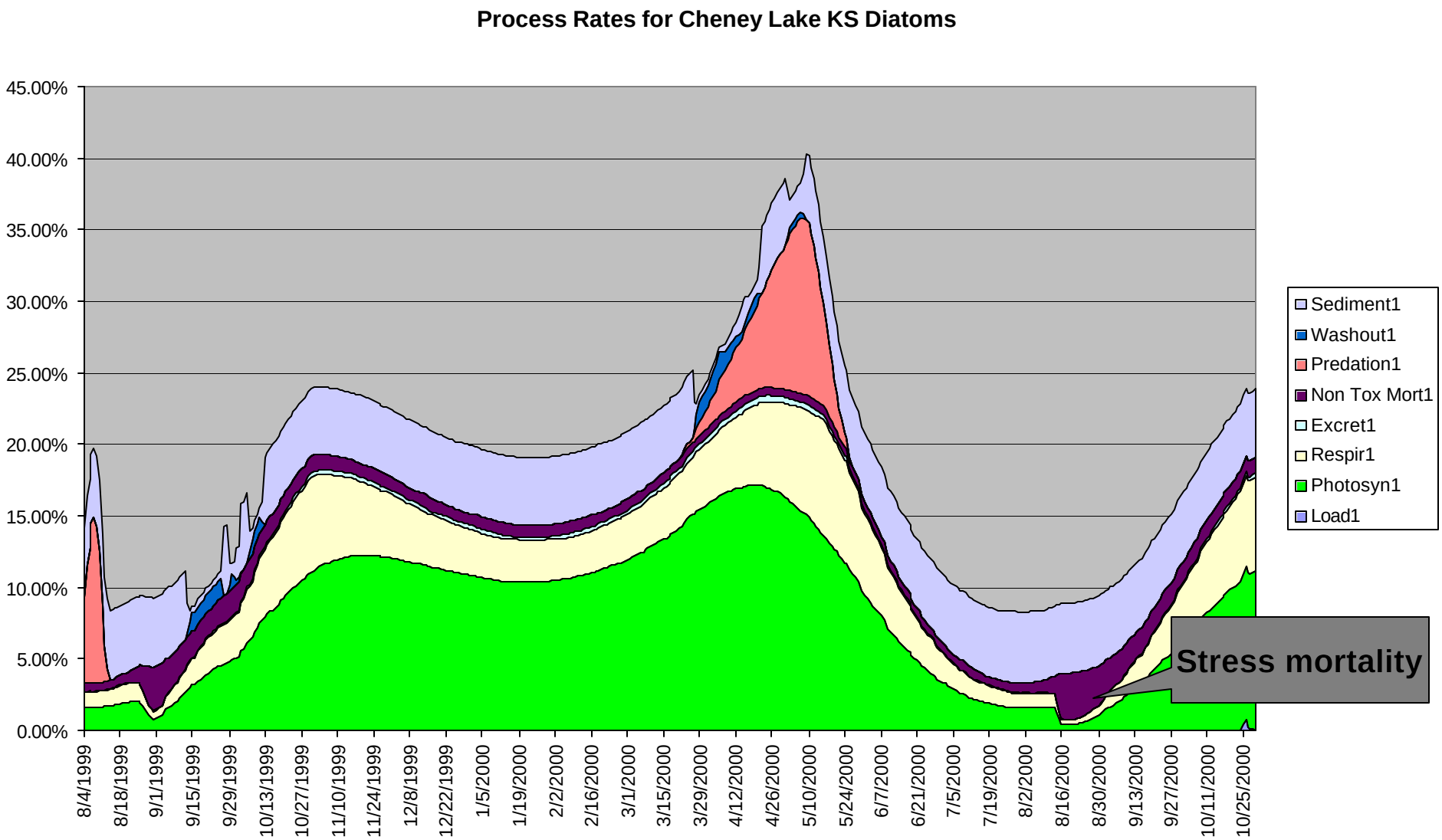
Linked with GenScn program for analyses such as exceedance plots



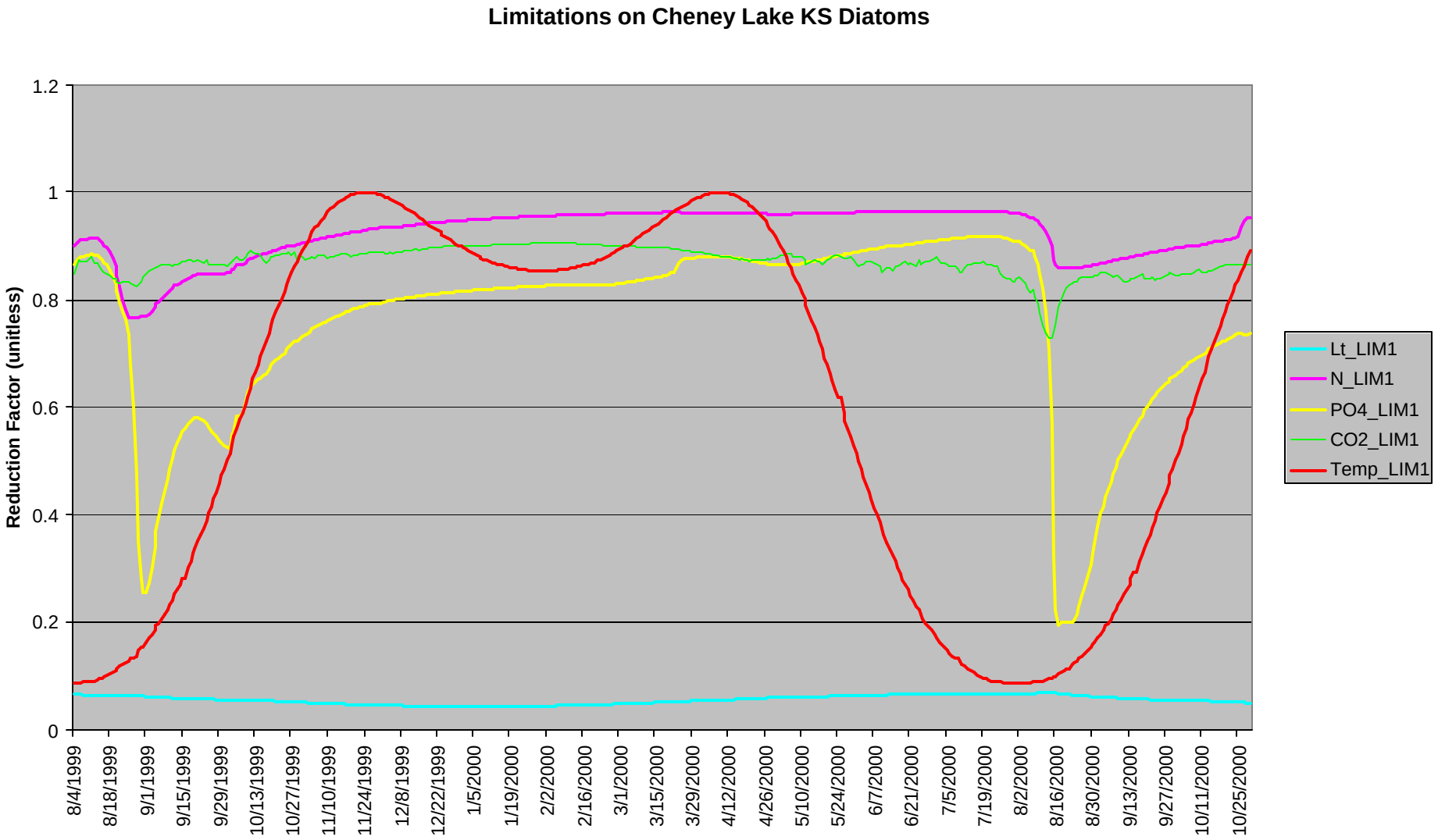
In Cahaba River AL, food, predation, and physical environment control animals



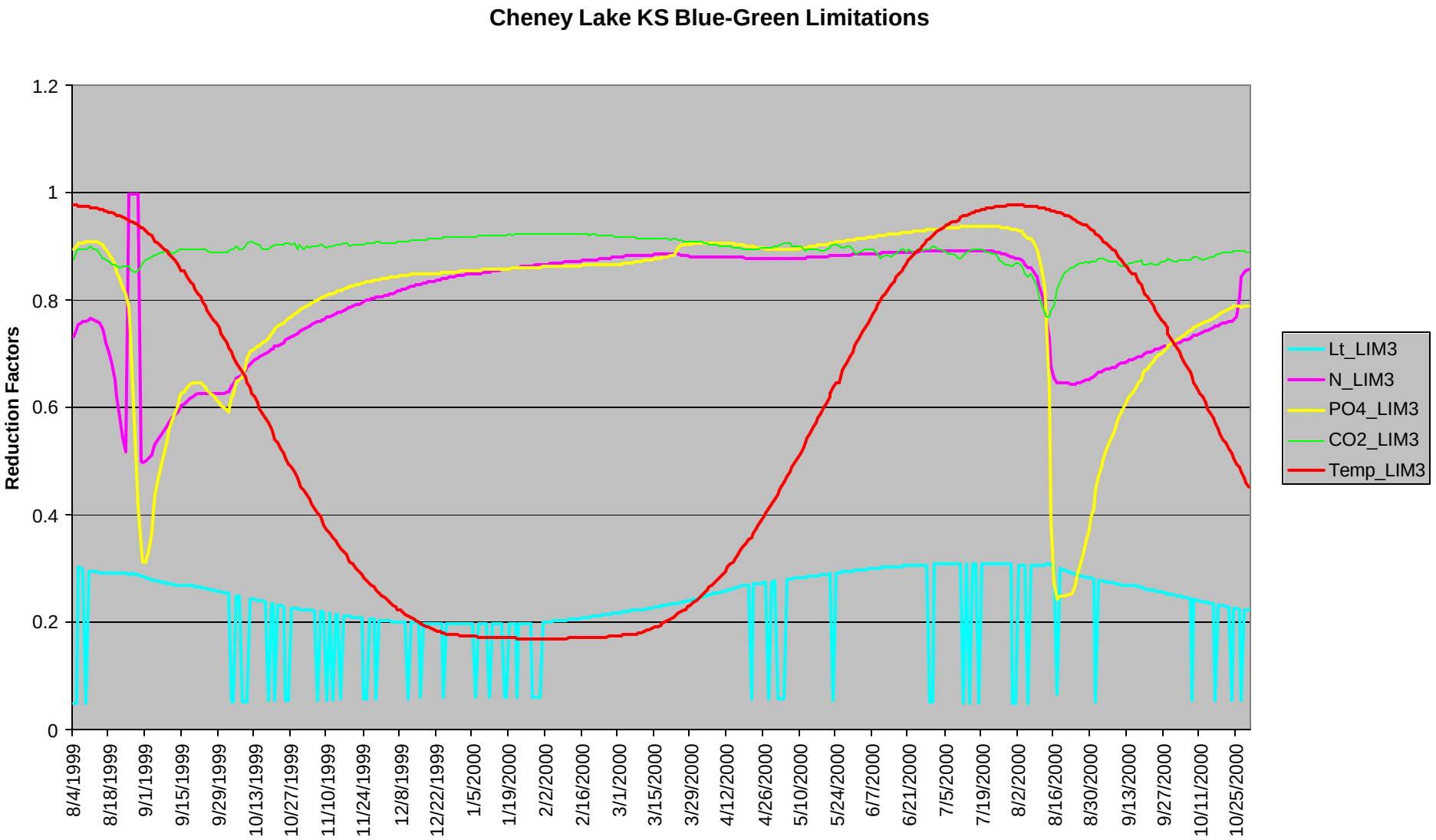
Rates can be saved and plotted for all processes



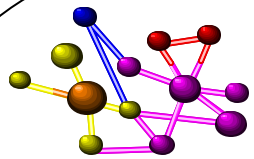
Time-varying limitations to photosynthesis also can be analyzed



Limitations on various groups can be compared

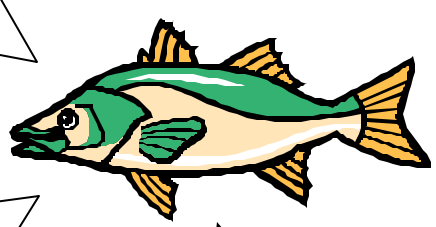


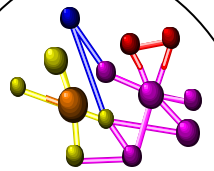
Bioaccumulation in AQUATOX



Toxicant in water:
- ionization
- volatilization
- hydrolysis
- photolysis
- microbial degradation

Uptake through gill:
- respiration rate
- assimilation efficiency

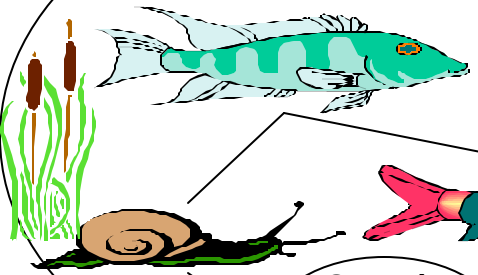




Losses of toxicant:
- predation
- mortality
- depuration
- spawning
- promotion
- emergence

Partitioning

Toxicant in food sources



- Organic sediments
- Algae

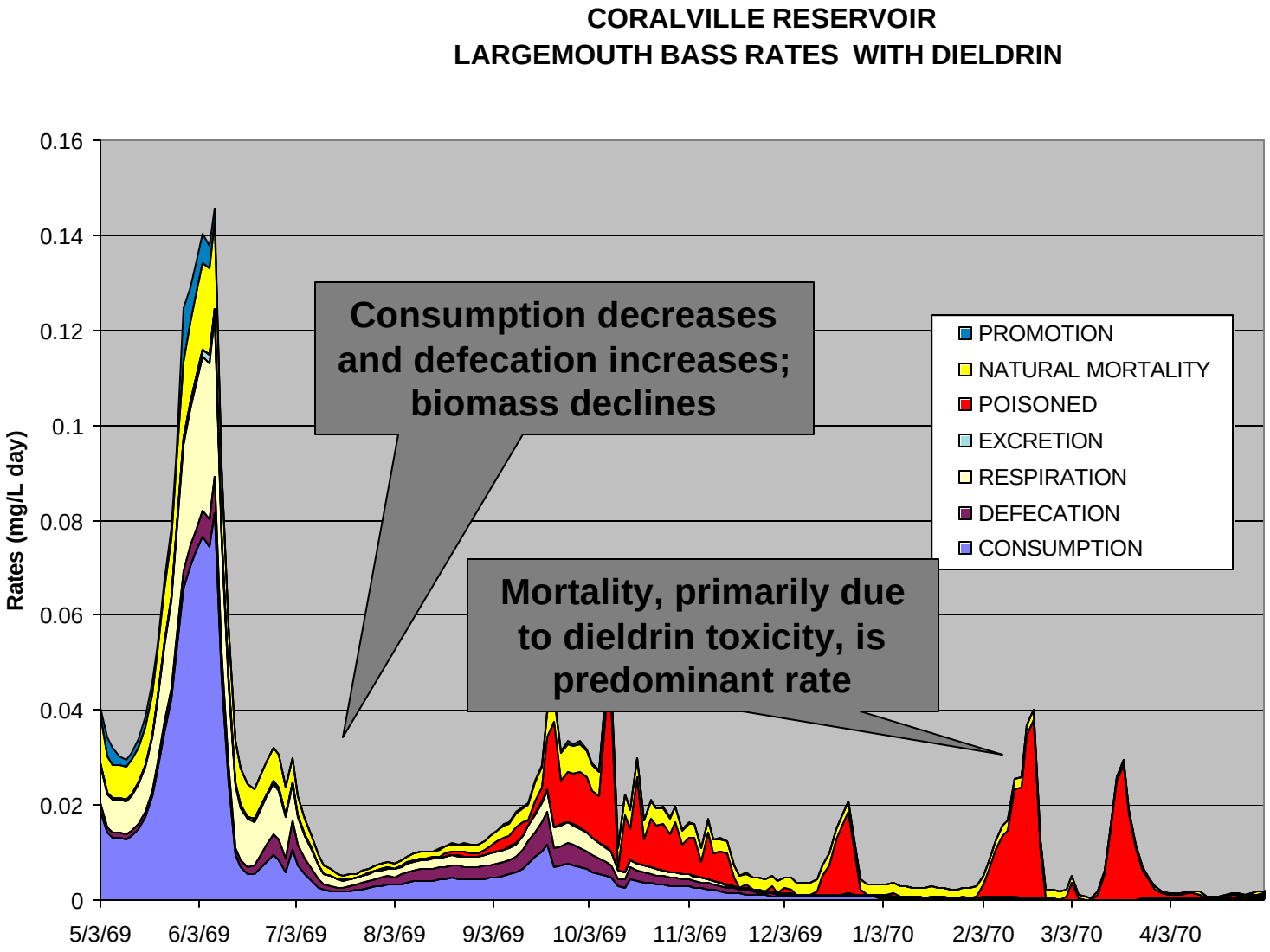
Uptake from diet
- consumption rates
- assimilation efficiency
- growth rates
- toxicity
- lipid content

- nutrient cycling
- loss of predation

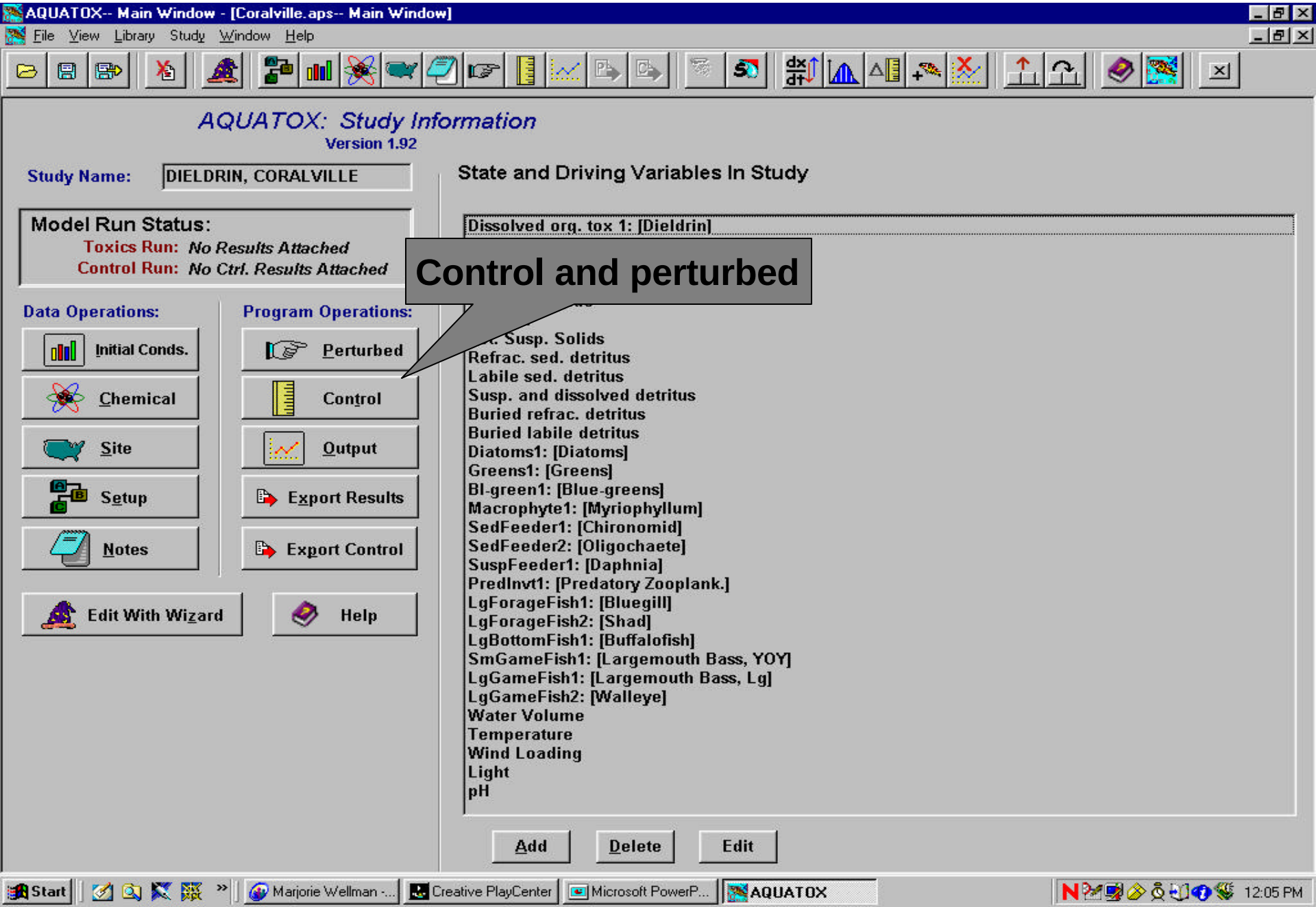
Steps Taken to Estimate Toxicity

- 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

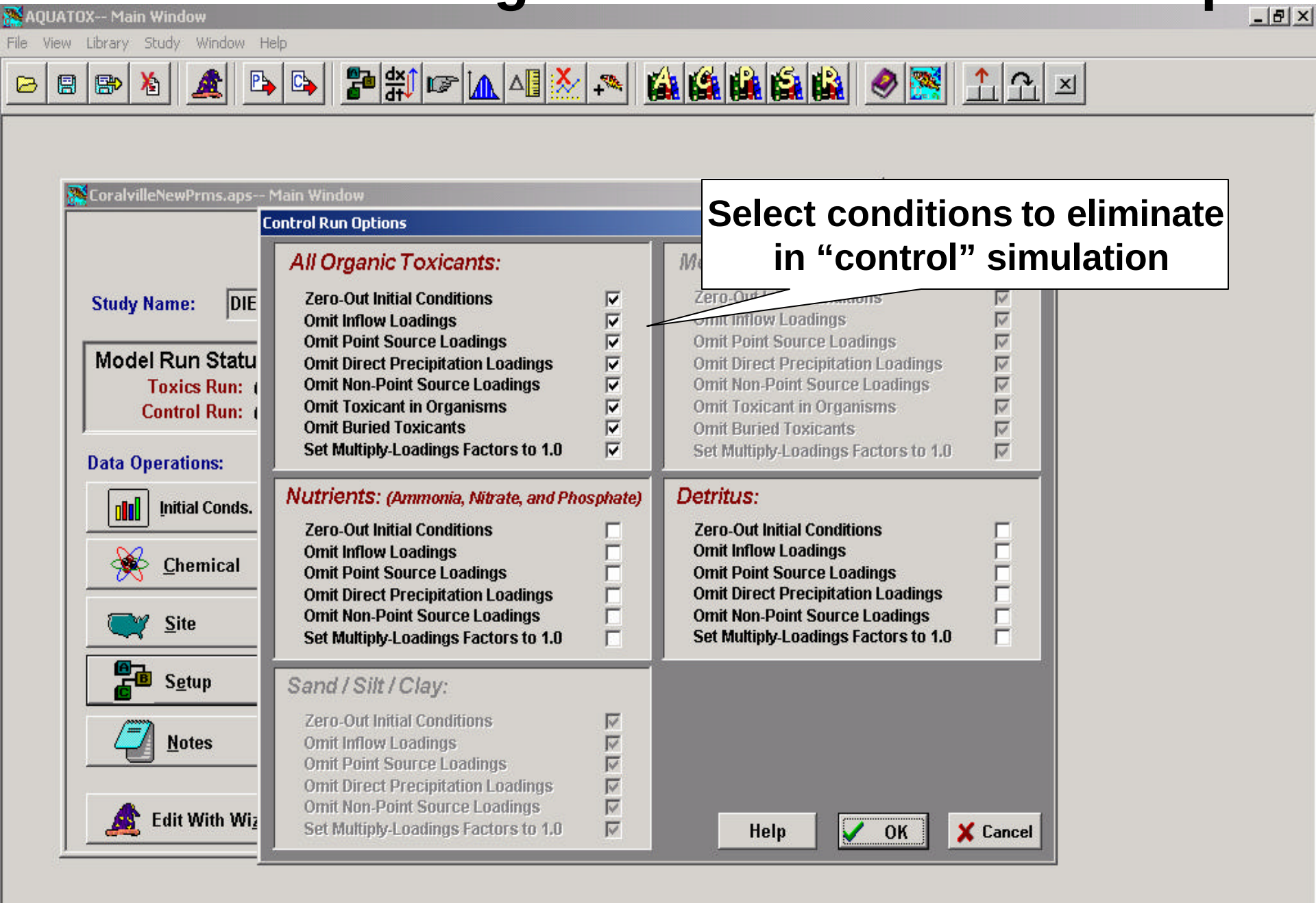
With Bioaccumulation, Chronic Toxicity is Followed by Acute Toxicity



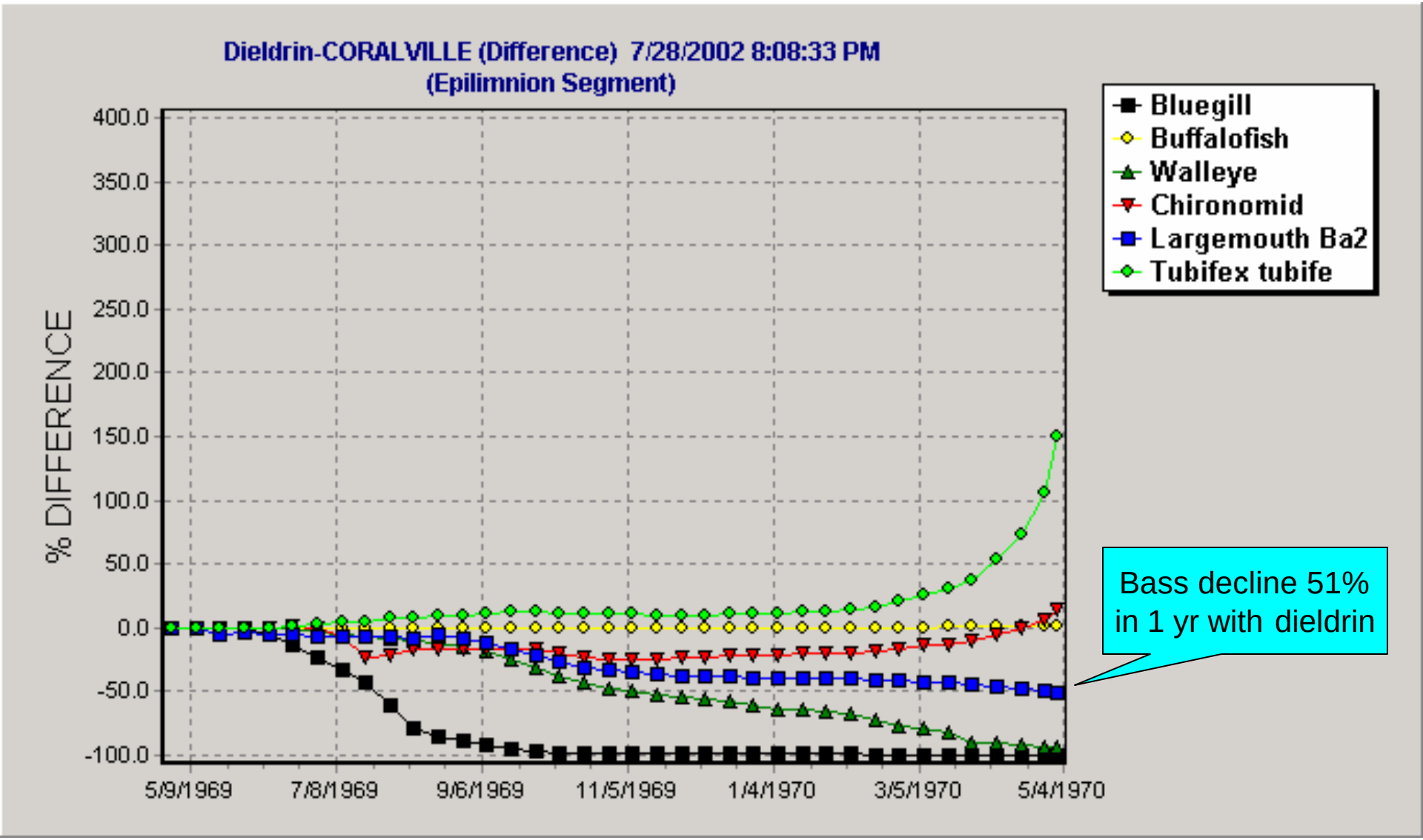
Can run perturbed & control simultaneously



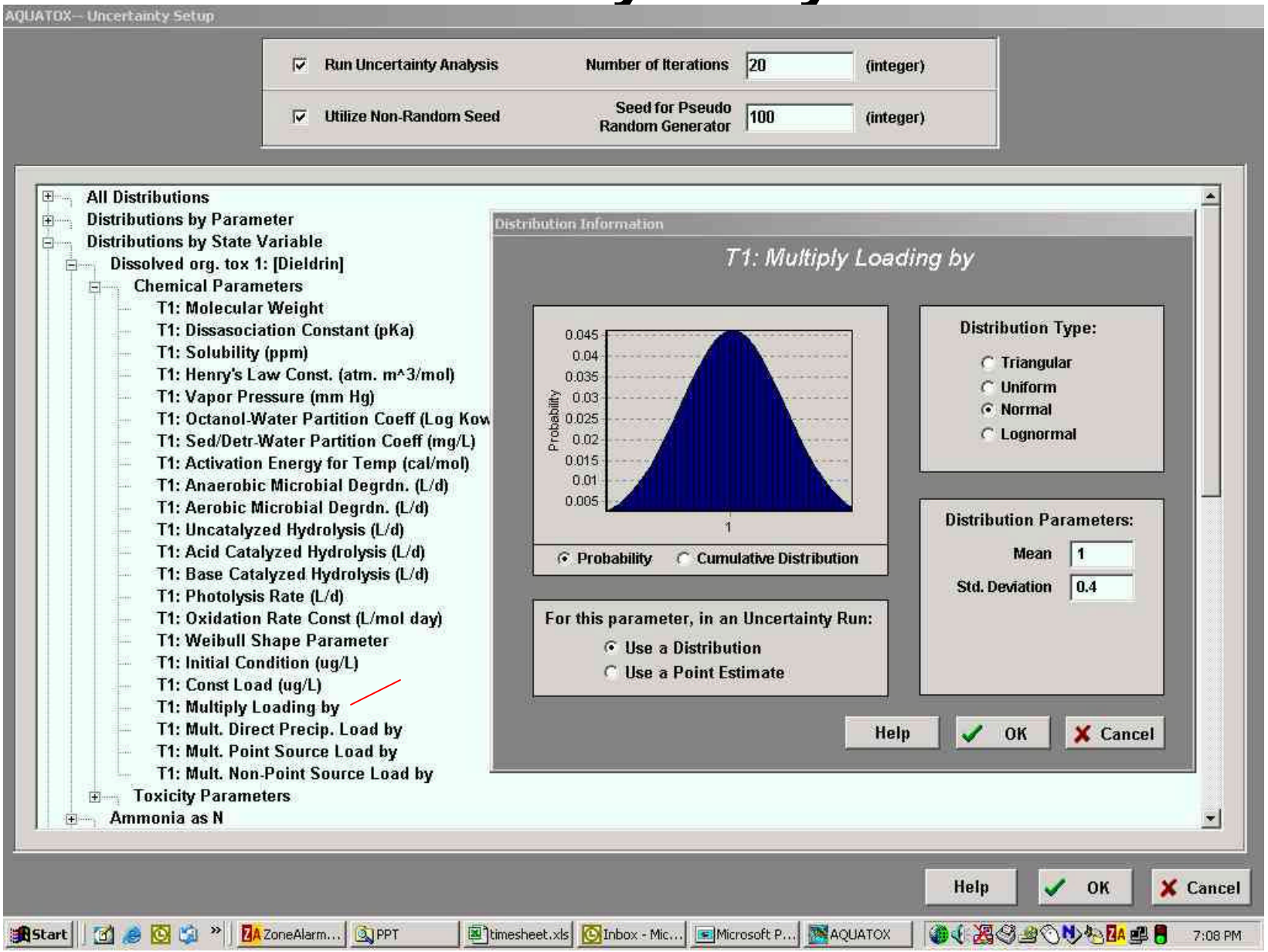
Scenario Management with Control Setup



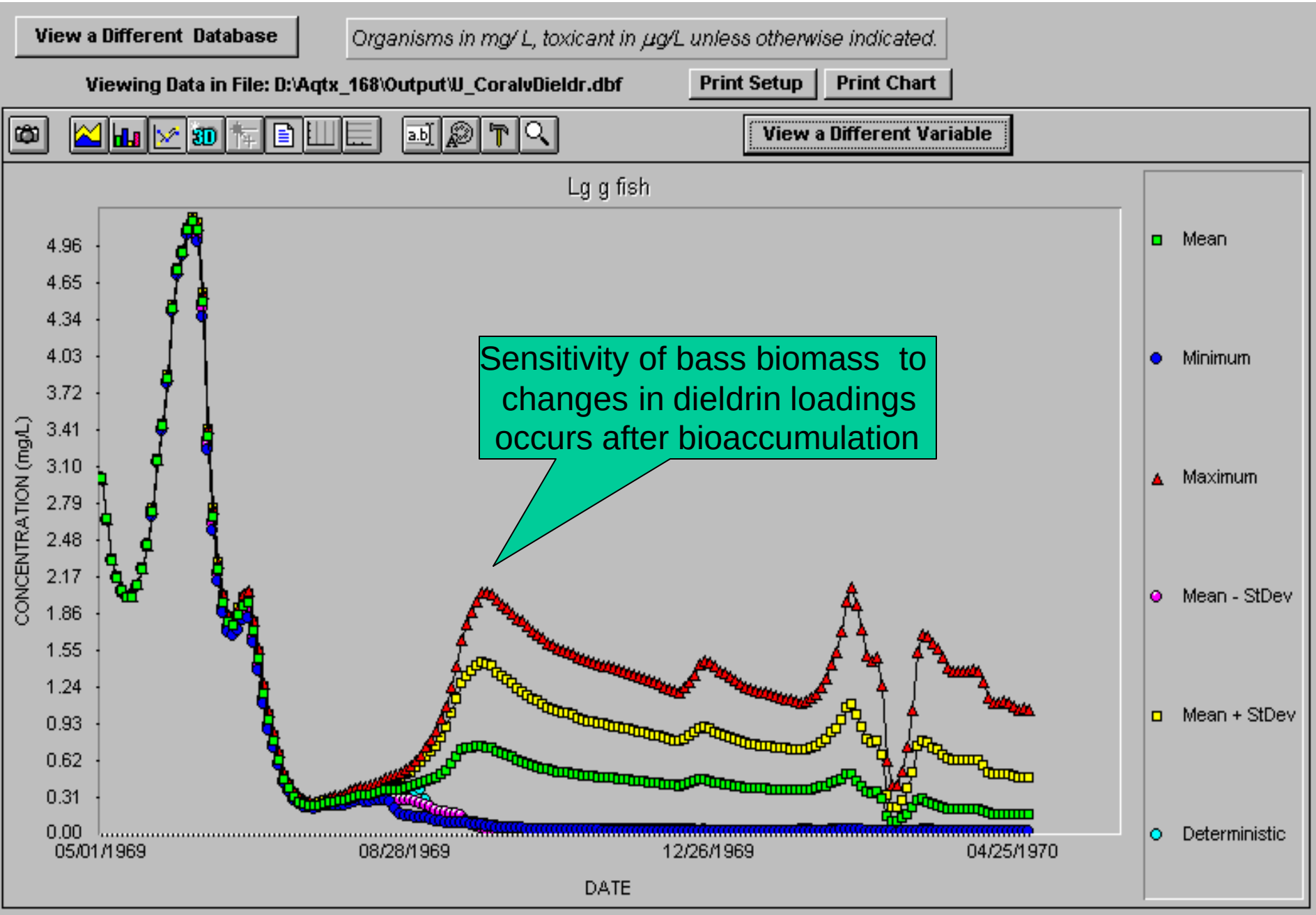
Percent Difference Graph emphasizes differences between ctl. & pert. simulations



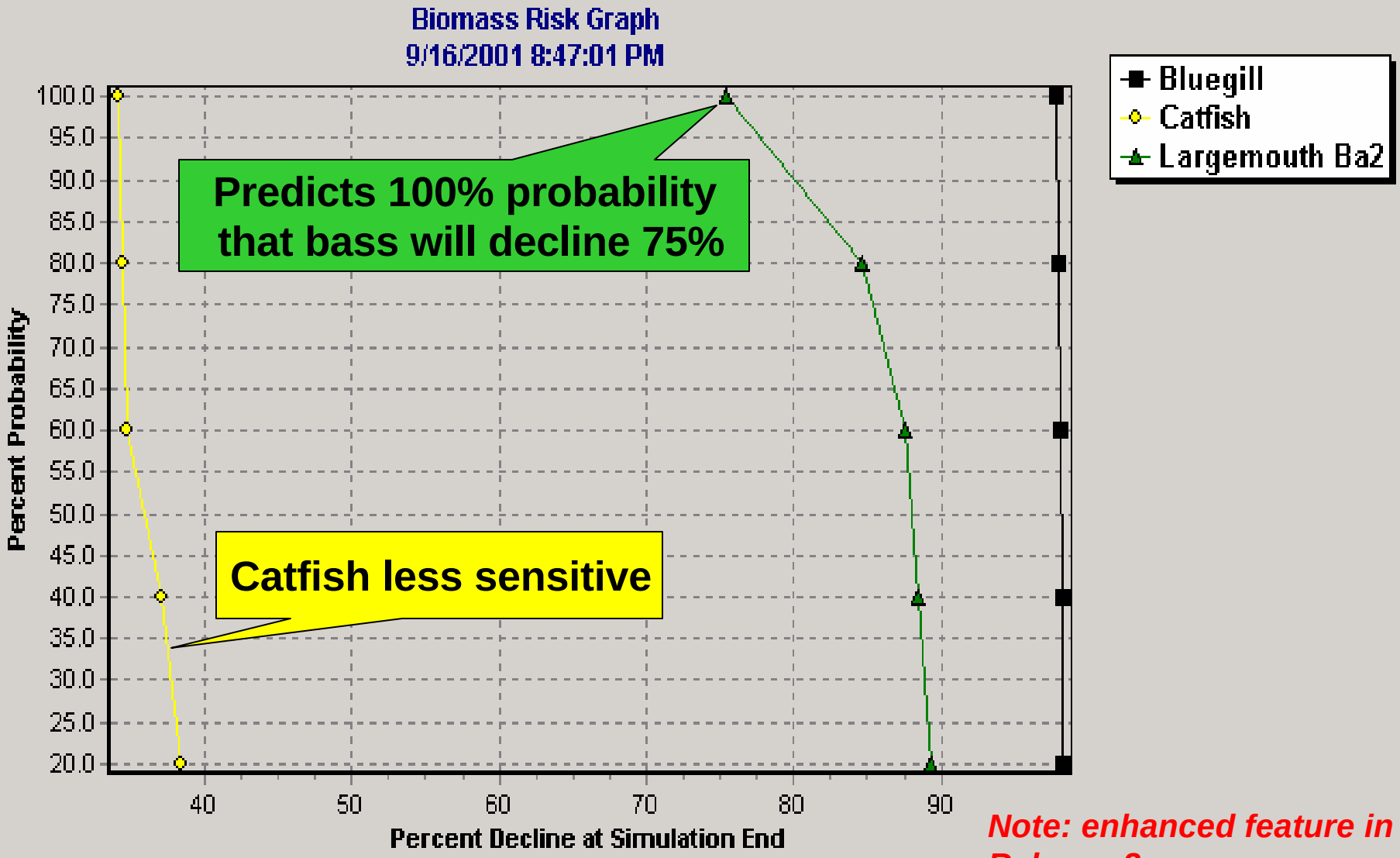
All parameters and loadings subject to uncertainty analysis



Sensitivity Analysis

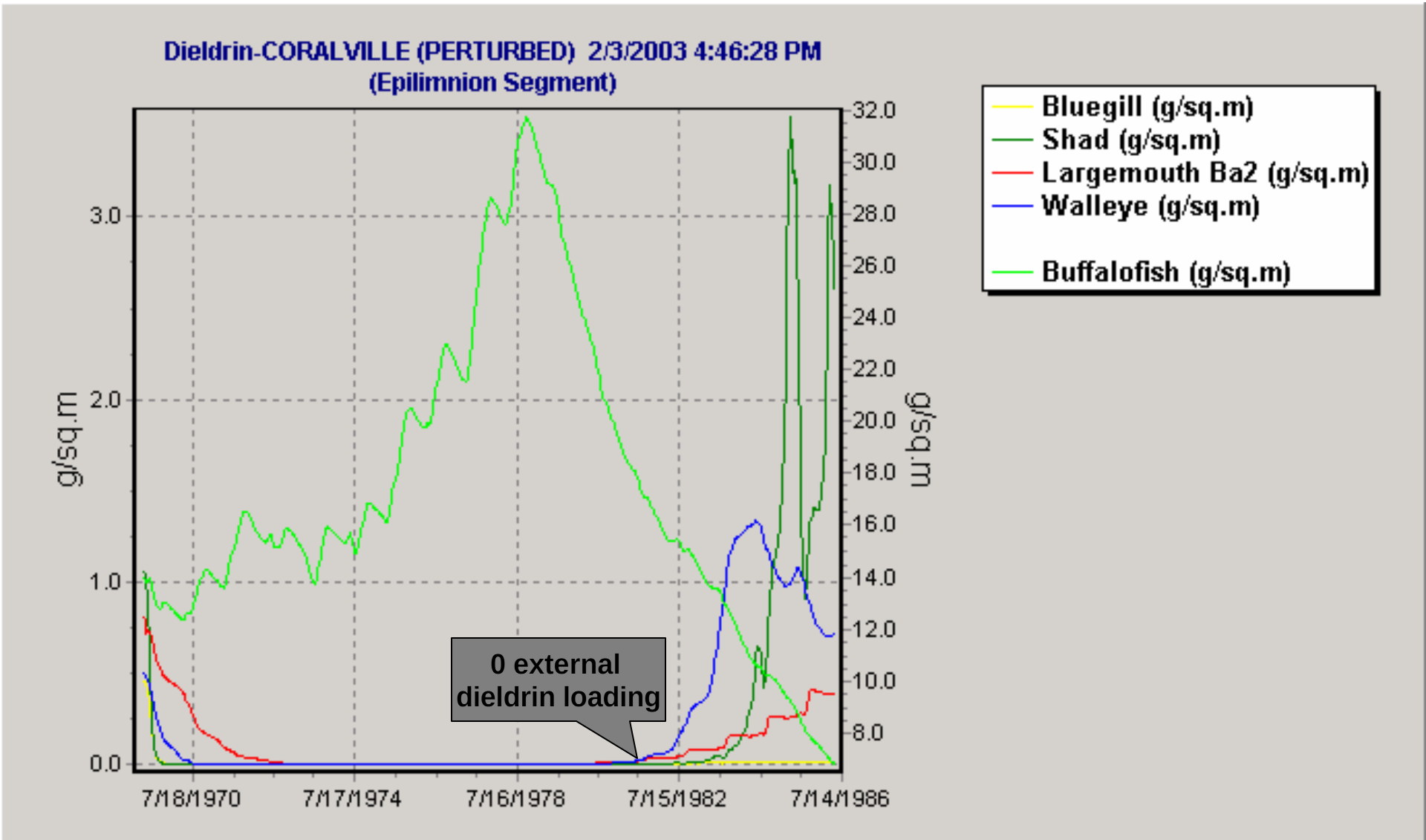


AQUATOX can estimate % probability of change in biomass



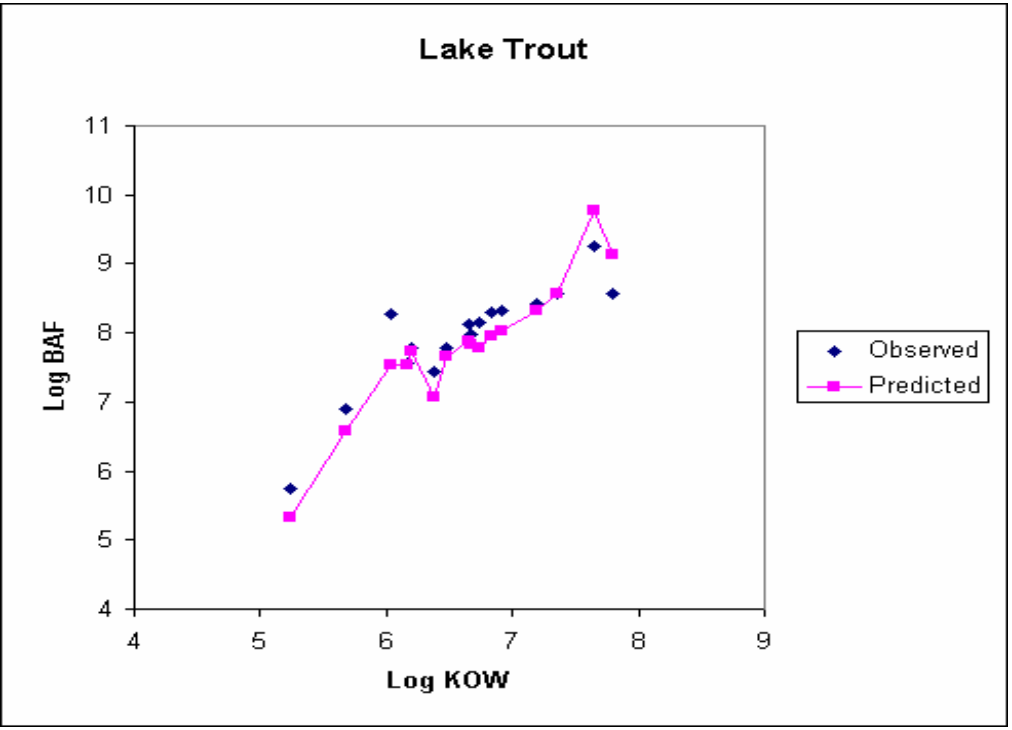
Note: enhanced feature in Release 2

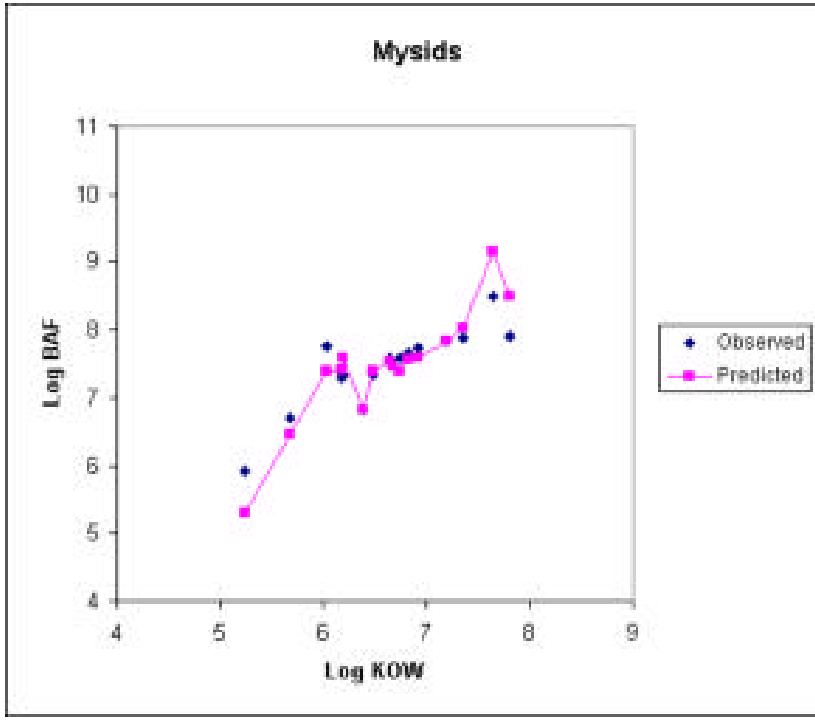
Recovery from pesticide in reservoir-- Coralville is now “best bass lake in Iowa”



Model Validation
PCBs in Lake Ontario

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

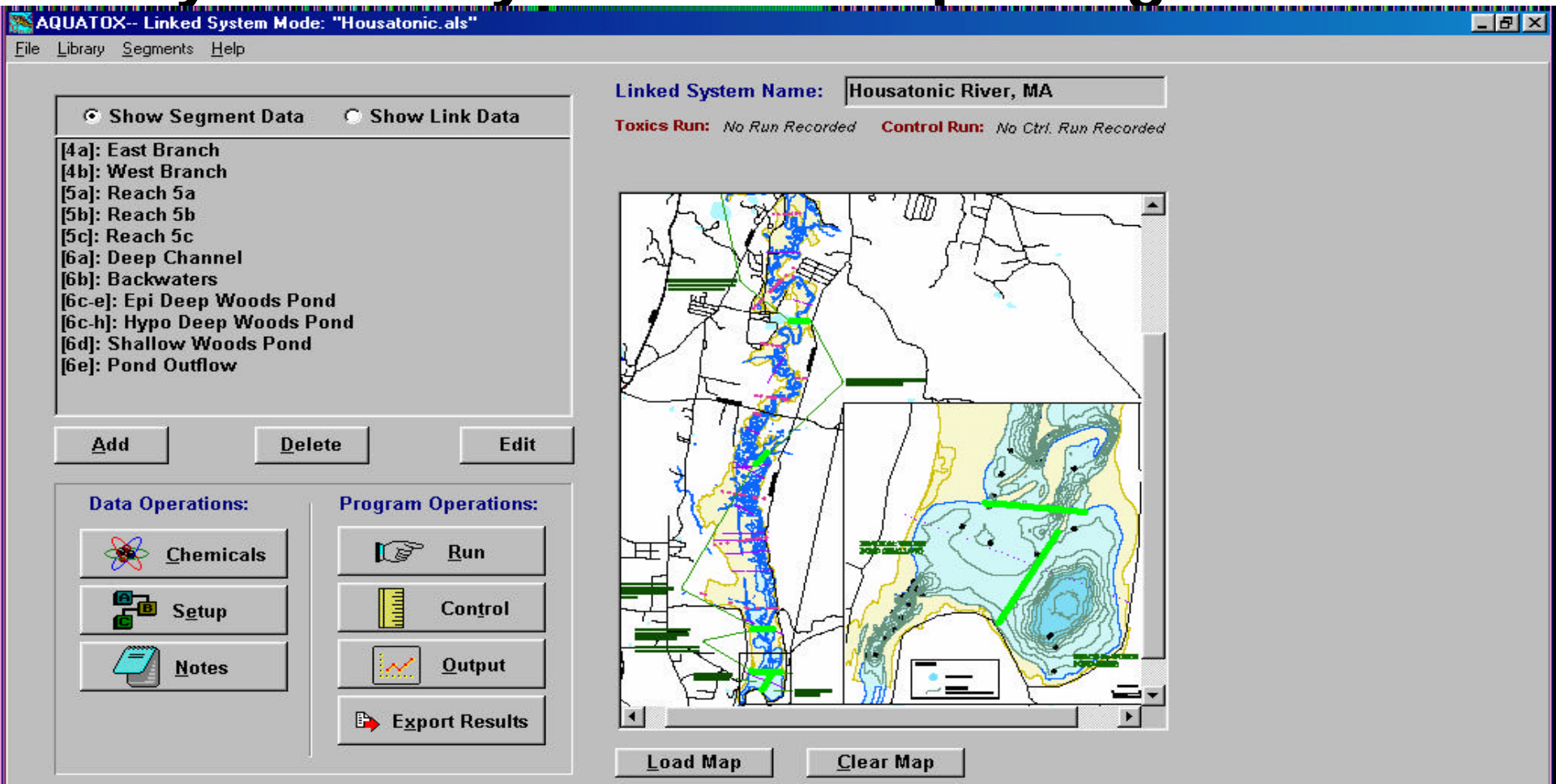




B.

Note: analysis done as part of model validation, using published data; not part of regulatory actions

Segmented version can represent dynamically linked multiple segments

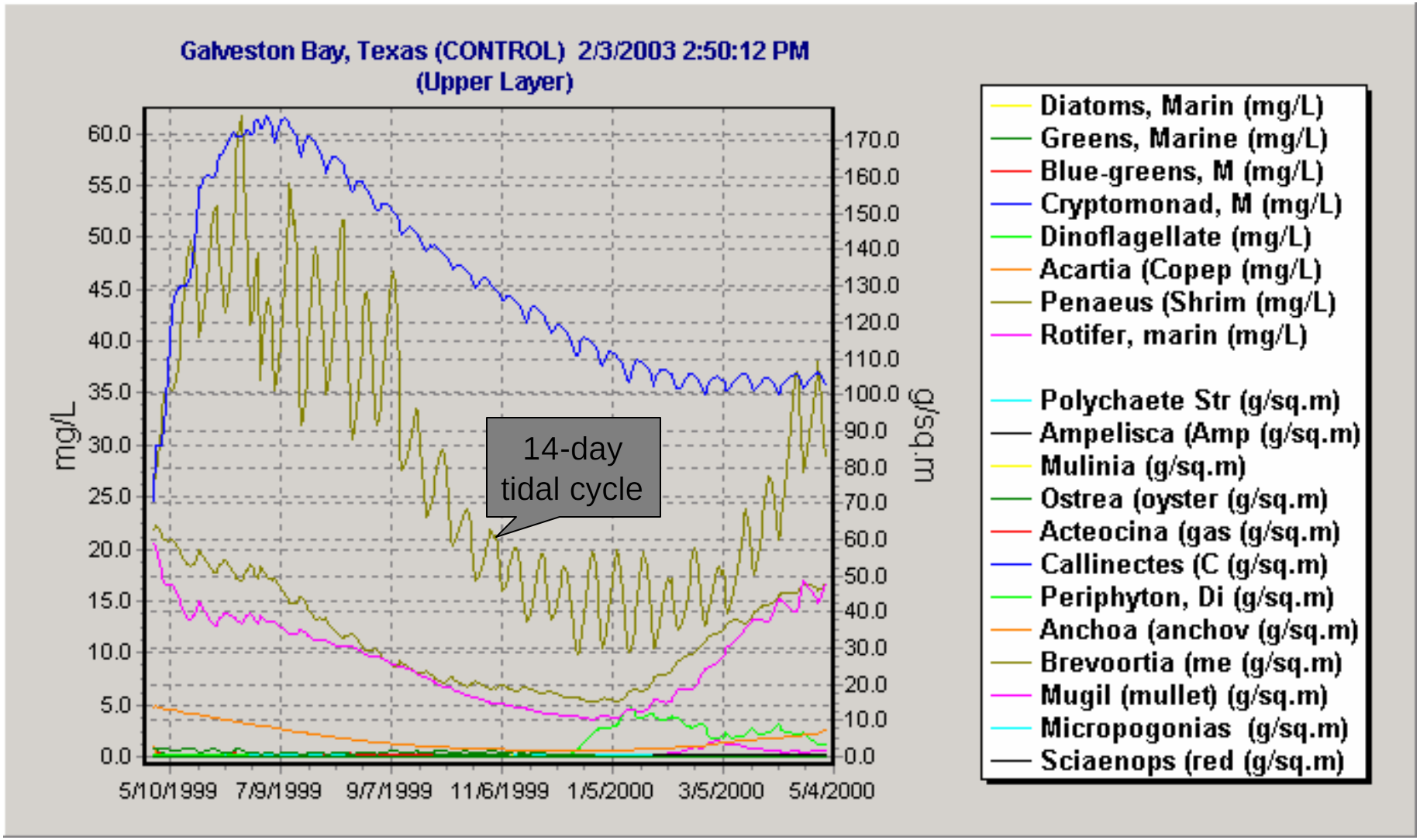


developed for Housatonic River MA project

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

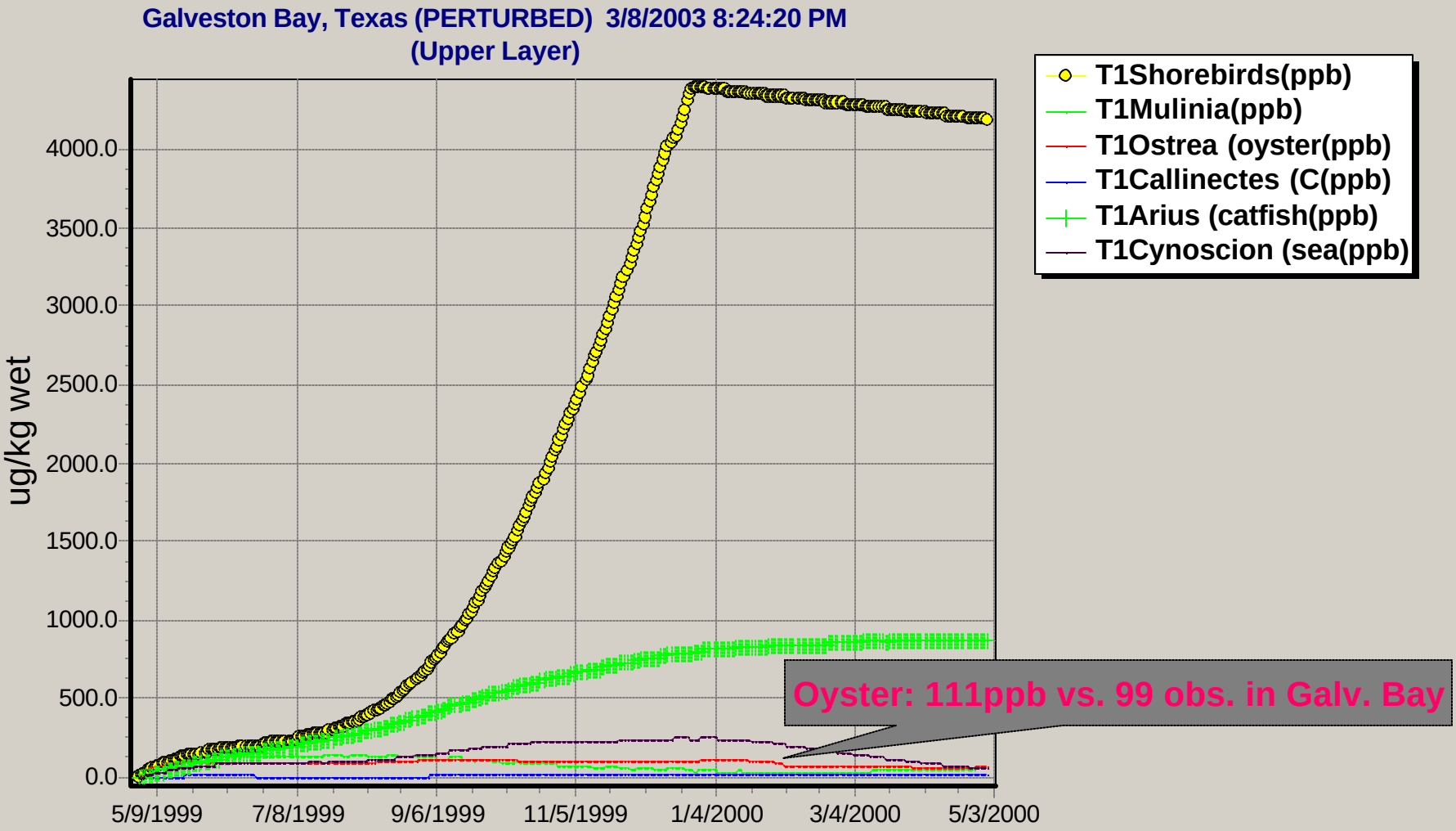
Photo Courtesy NASA Johnson Space Center

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



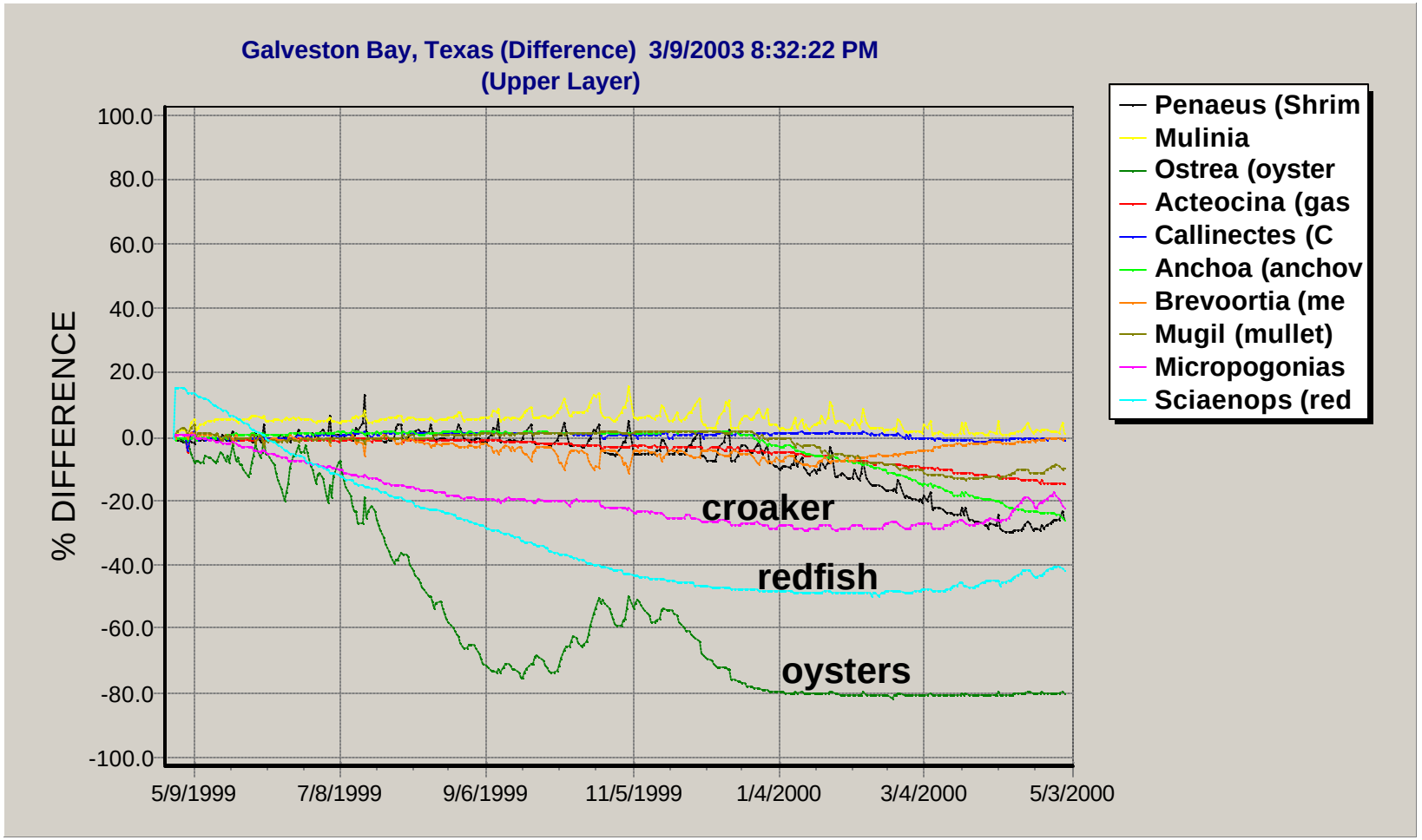
Can model bioaccumulation in plants, animals, and *shorebirds;* PFOS shown

based on constant concentration of 1 ug/L

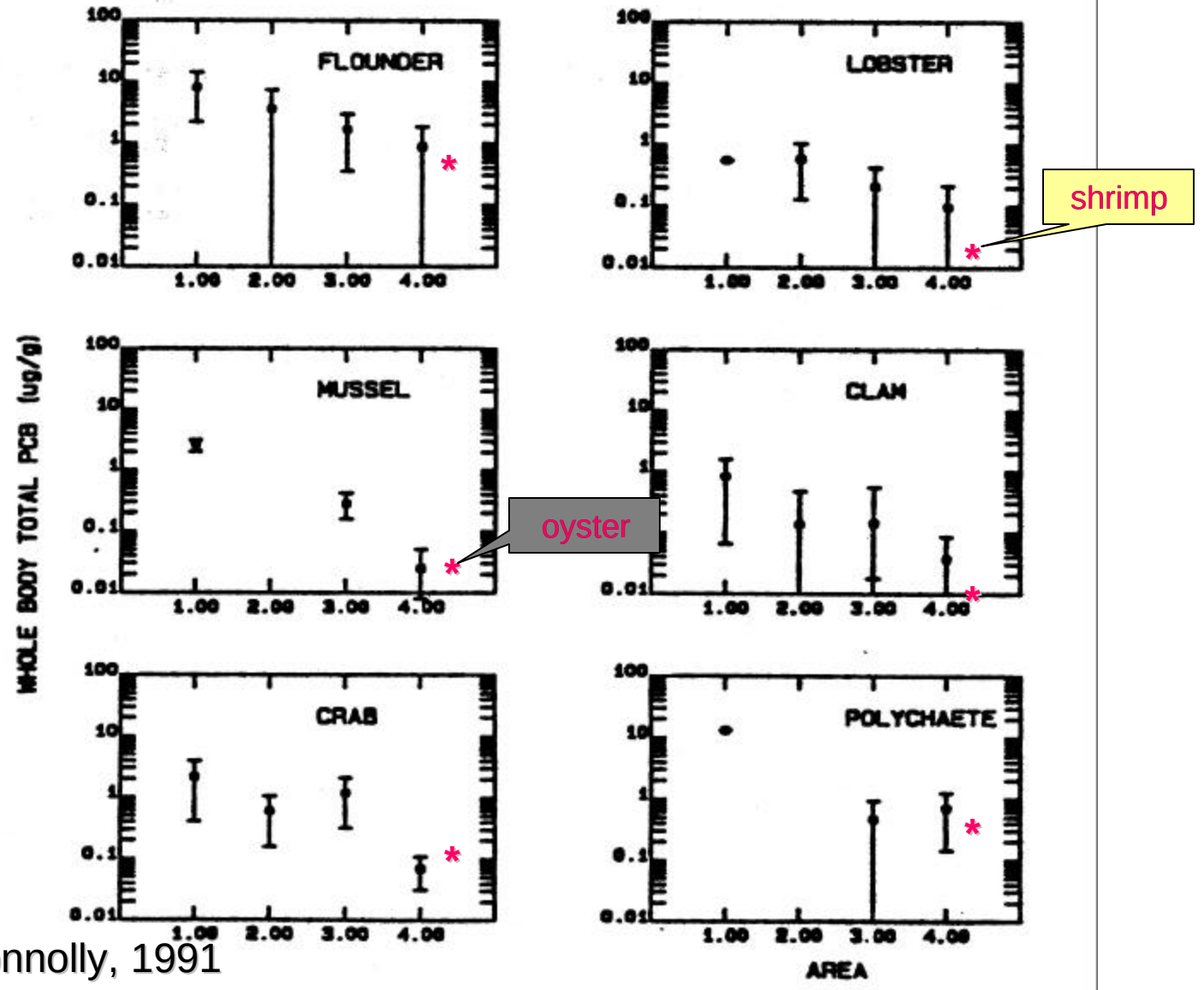


Model predicts decline of sensitive species with high PFOS levels

based on limited toxicology values



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



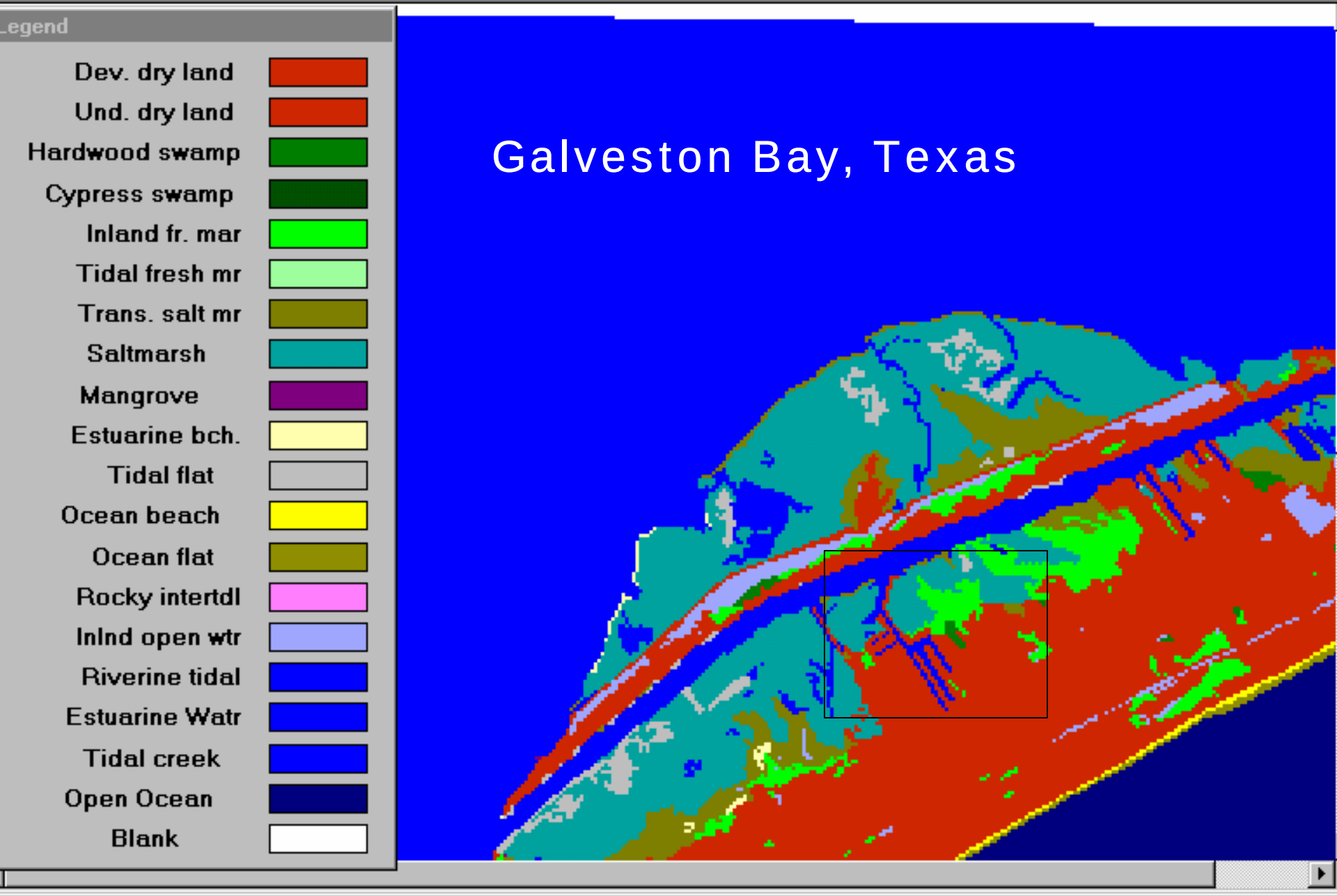
graphs from Connolly, 1991

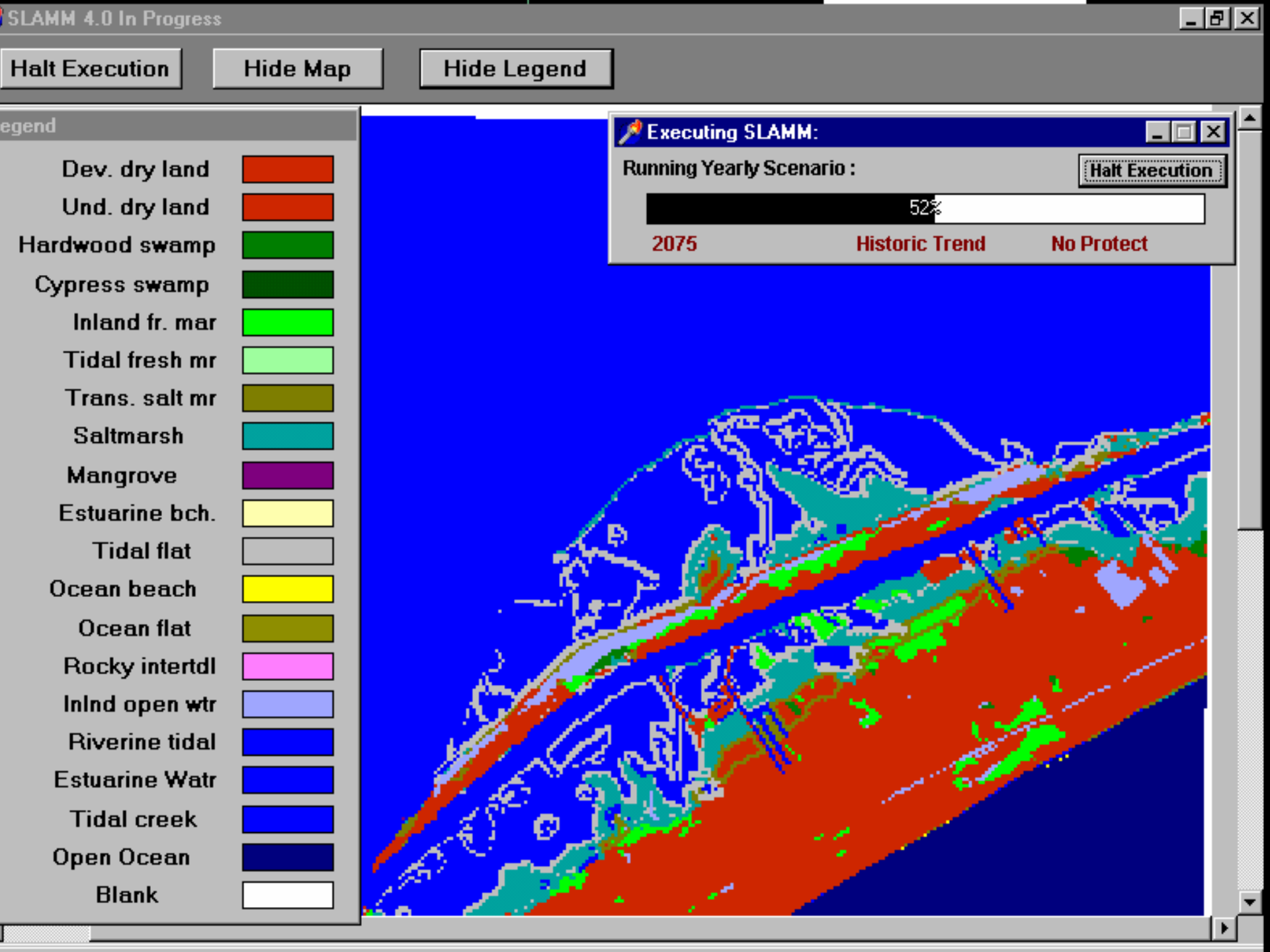
Potential Next Steps

- **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**

SLAMM 4.0 In Progress

Halt Execution | Hide Map | Hide Legend | Pixel Size: 1 2 3 4




SLAMM 4.0 In Progress
Halt Execution
Hide Map
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egend
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 :
Halt Execution
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)