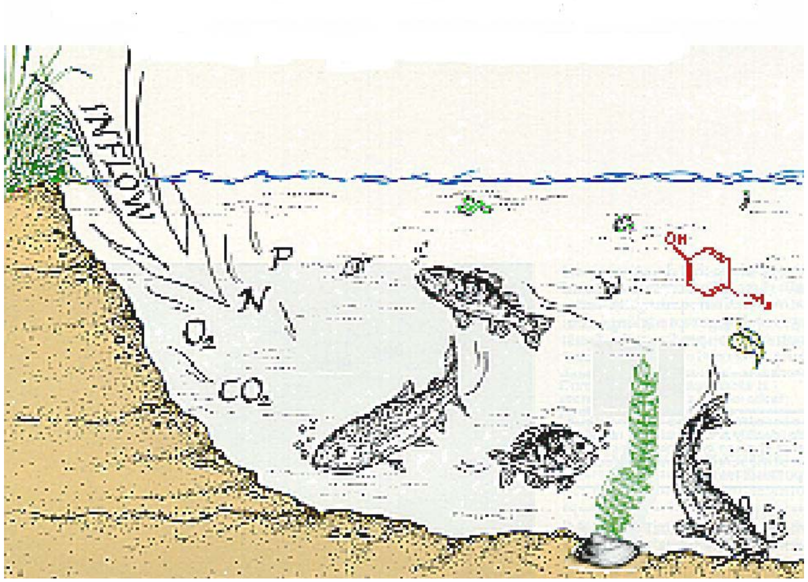
AQUATOX Training Workshop (Day 3)

Web Training Materials, August 2012

Based on Workshop Given for EPA Region 6, Dallas, Texas, December 2010
and Columbia River Intertribal Fish Commission, November 2011

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



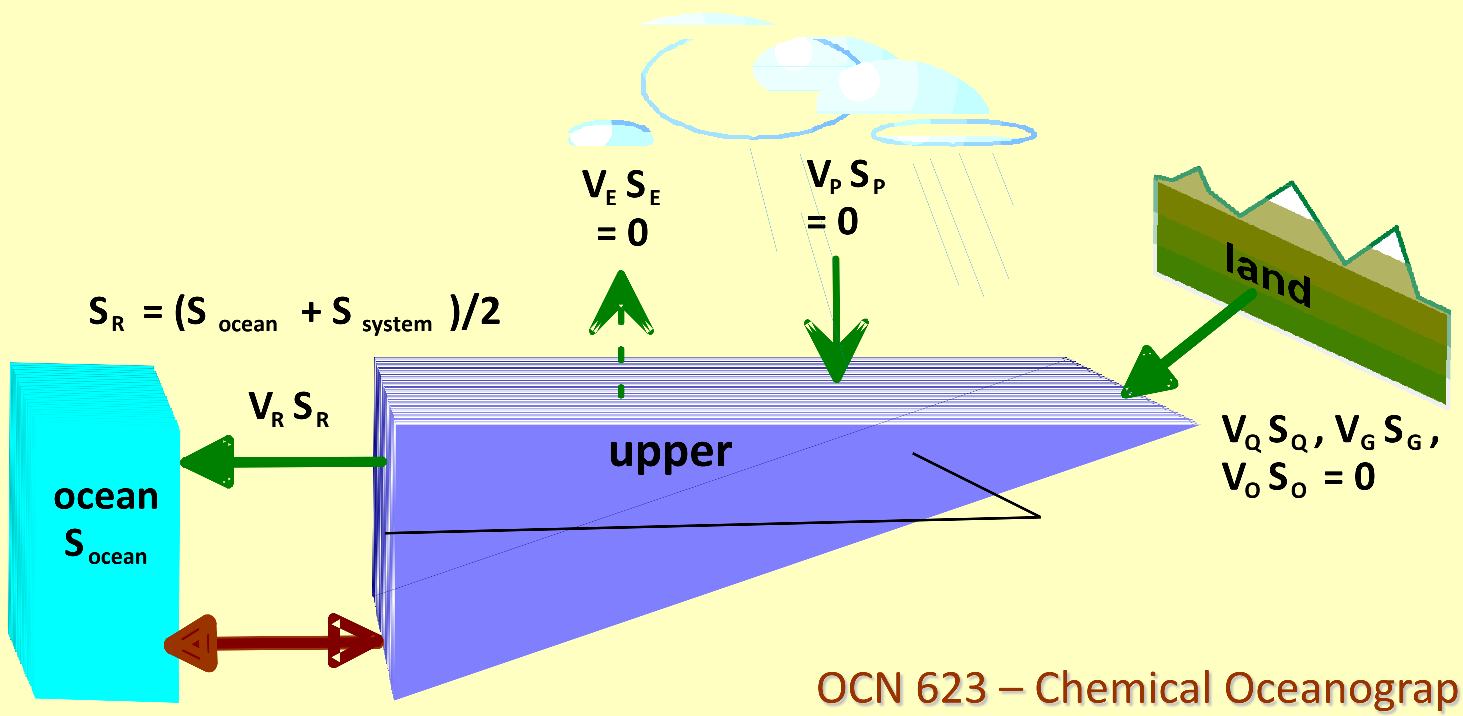
Modeling Estuarine Conditions

- Salt-balance submodel
- Estuarine species
- Shorebird bioaccumulation

- Alternatively, salinity can be included in a linked-segment model; in that case water exchange is the responsibility of the user

Estuarine Features

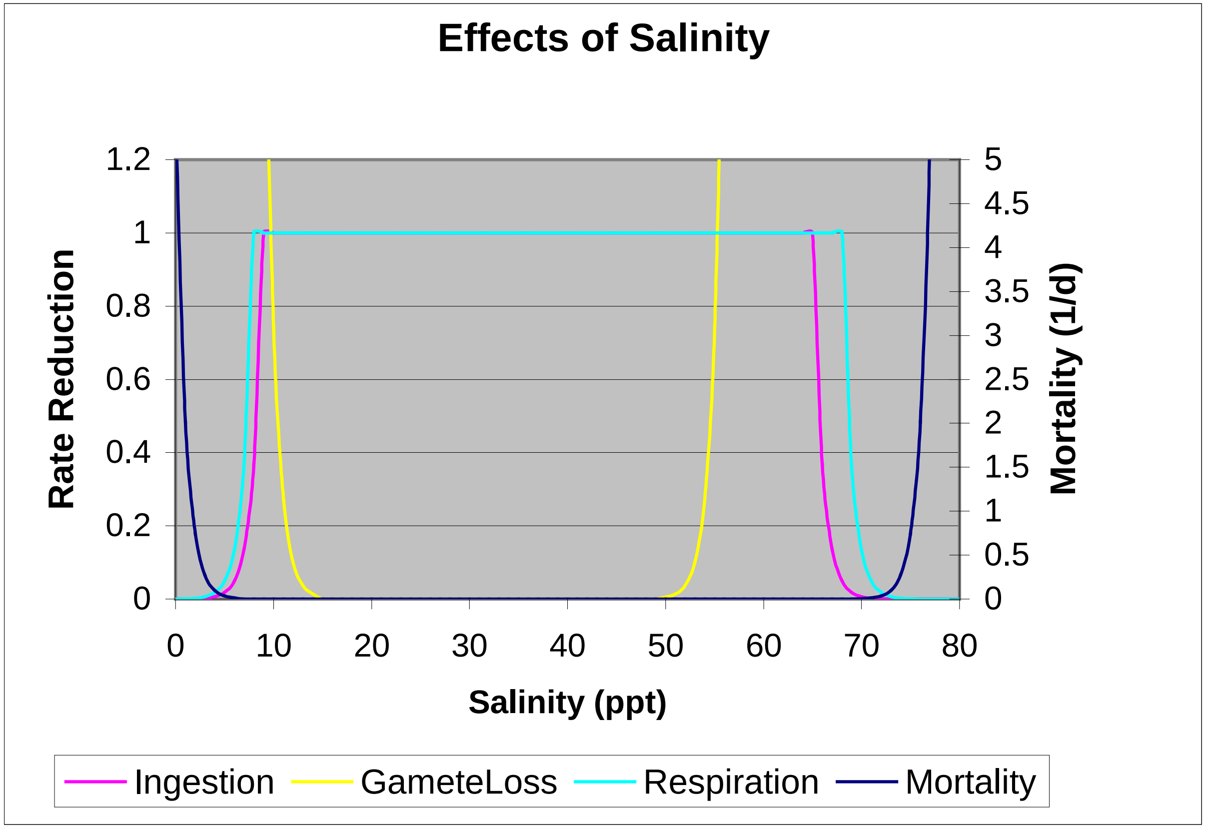
- Stratification – salt wedge
- Water Balance – salt balance approach
- Entrainment Process – lower to upper layers



OCN 623 – Chemical Oceanography
University Hawaii

Estuarine Features

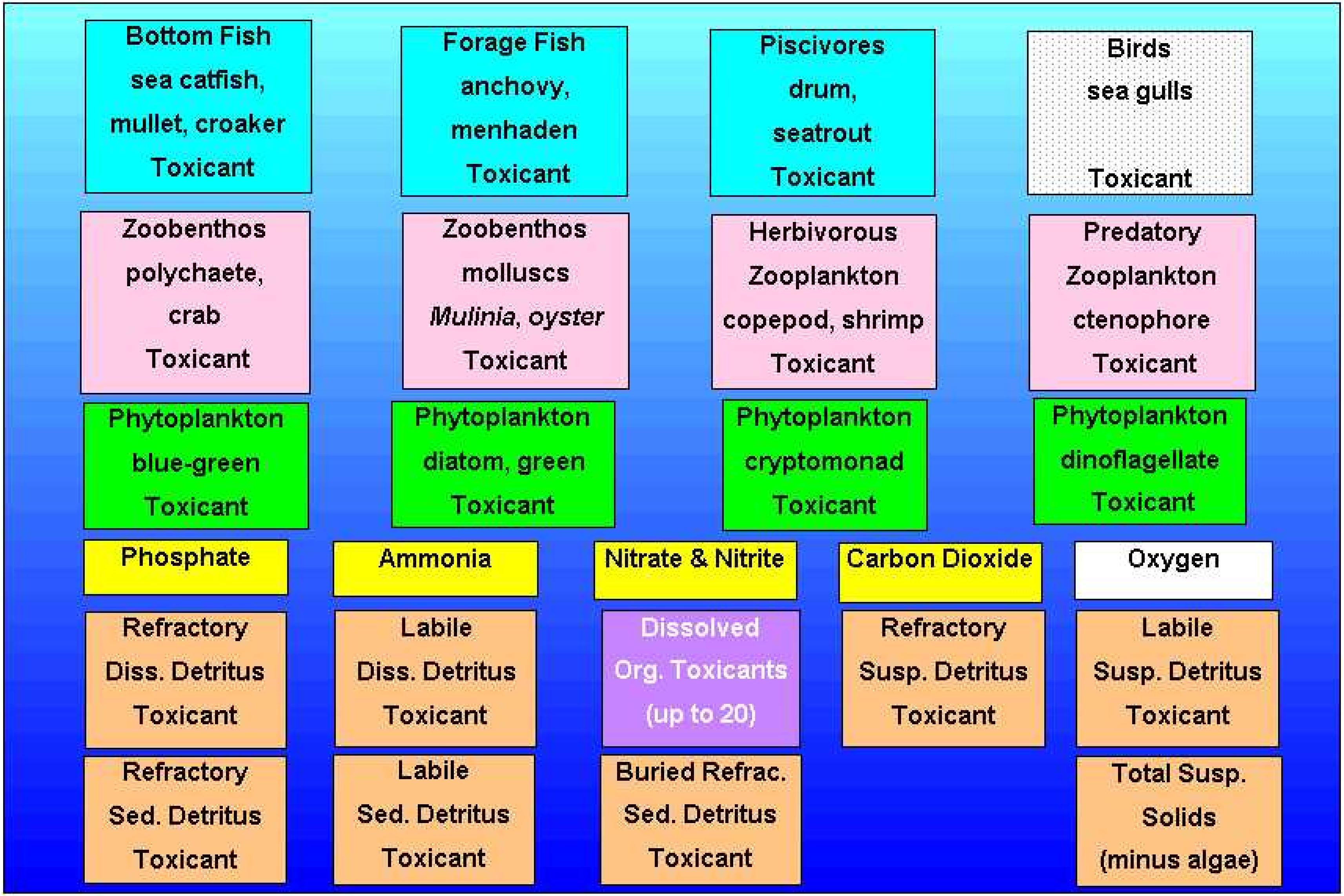
- Salinity Effects
  - Mortality/gamete loss
  - Photosynthesis, respiration, ingestion
  - Sinking
  - Volatilization
  - Reaeration



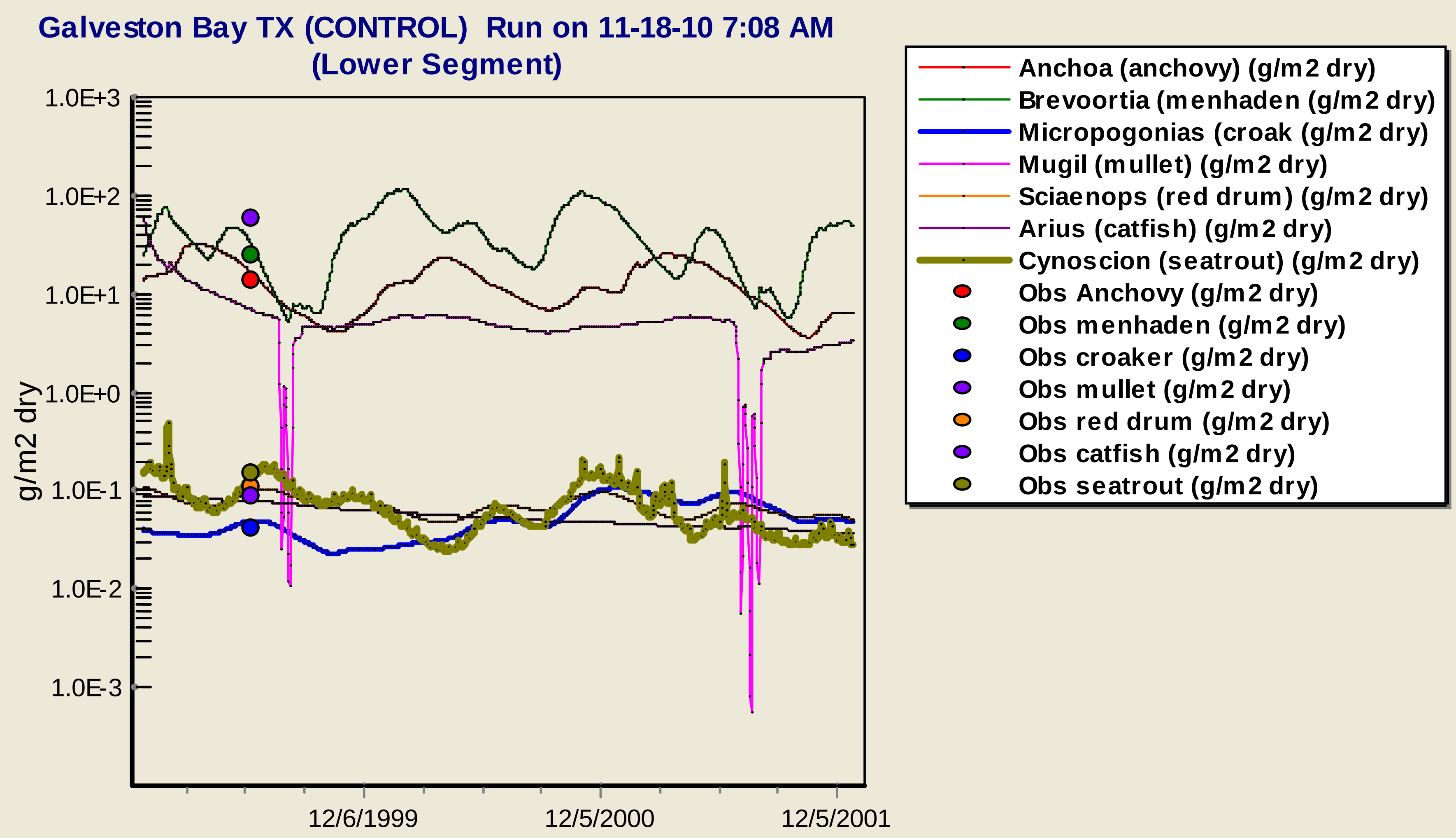
Estuarine version roughly calibrated for Galveston Bay, Texas, to evaluate toxicants

Photo Courtesy NASA Johnson Space Center

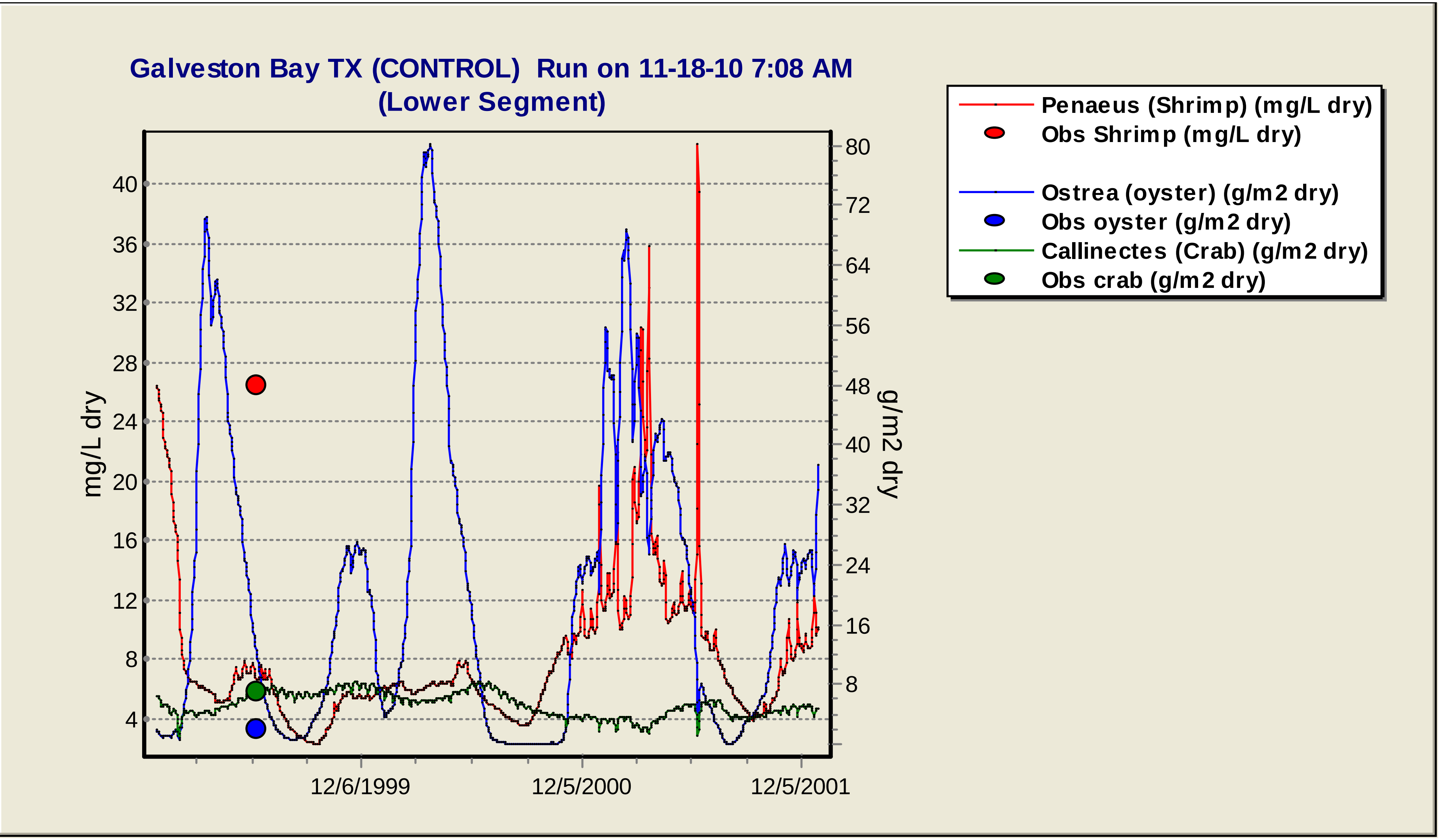
Galveston Bay, Texas, compartments



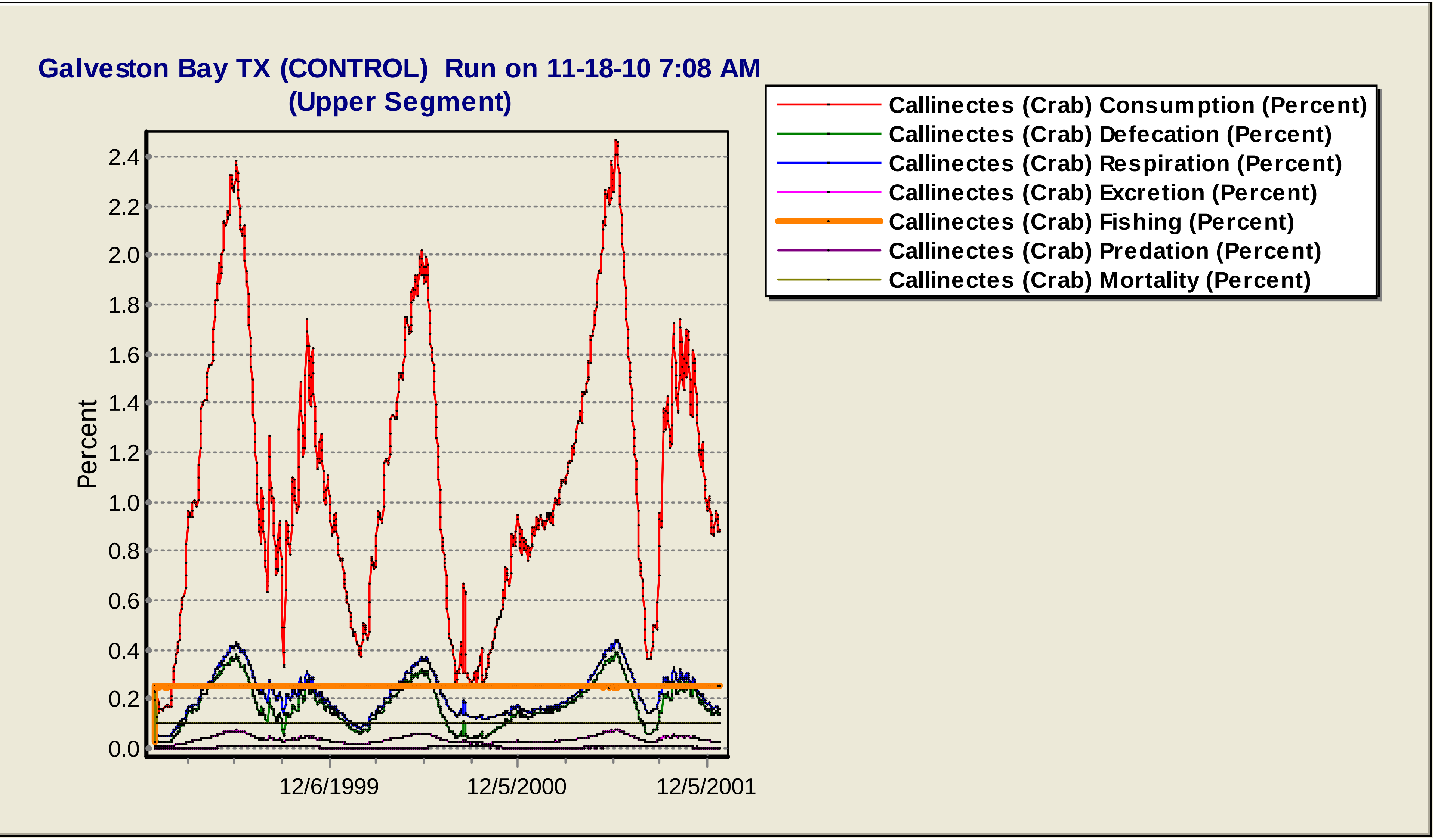
Can model biomass of commercial and other species of fish



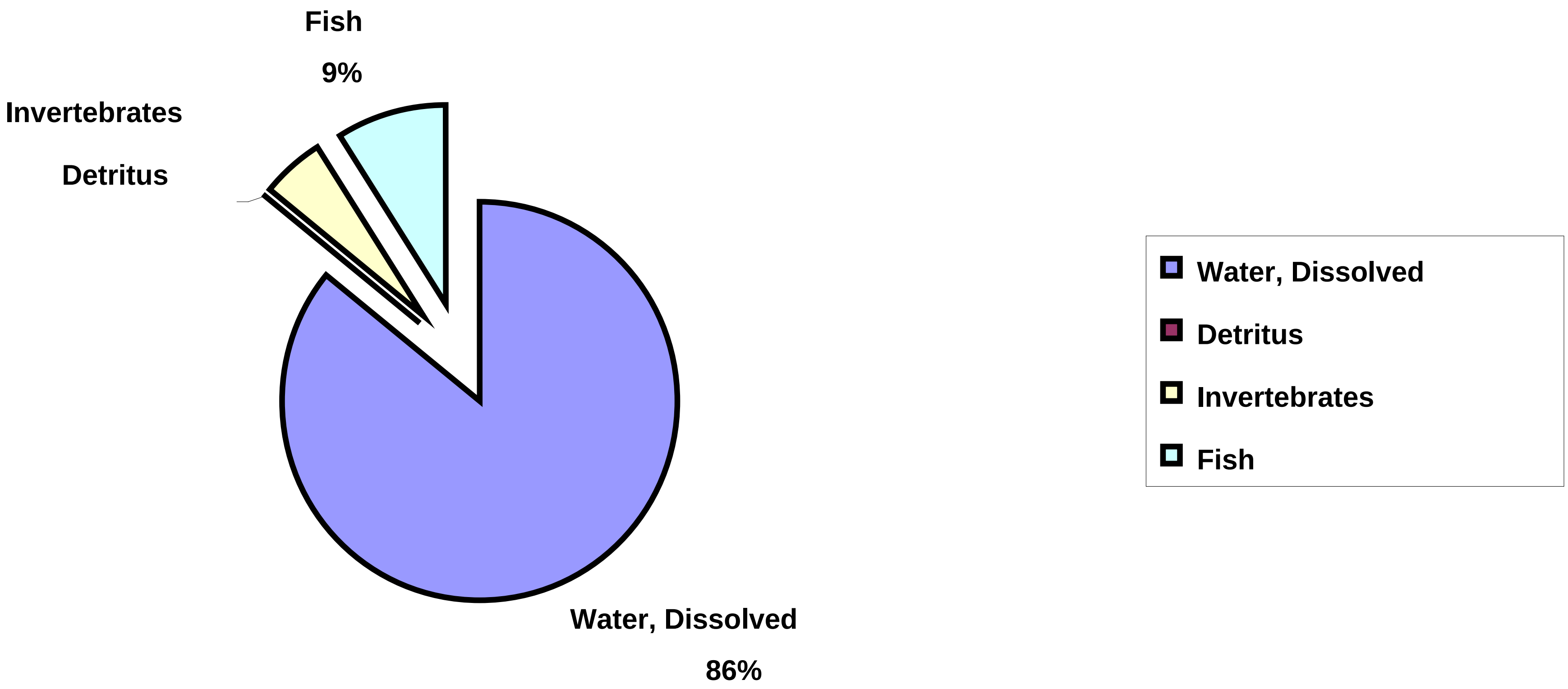
Can also model biomass of shrimp, oysters, and other invertebrates



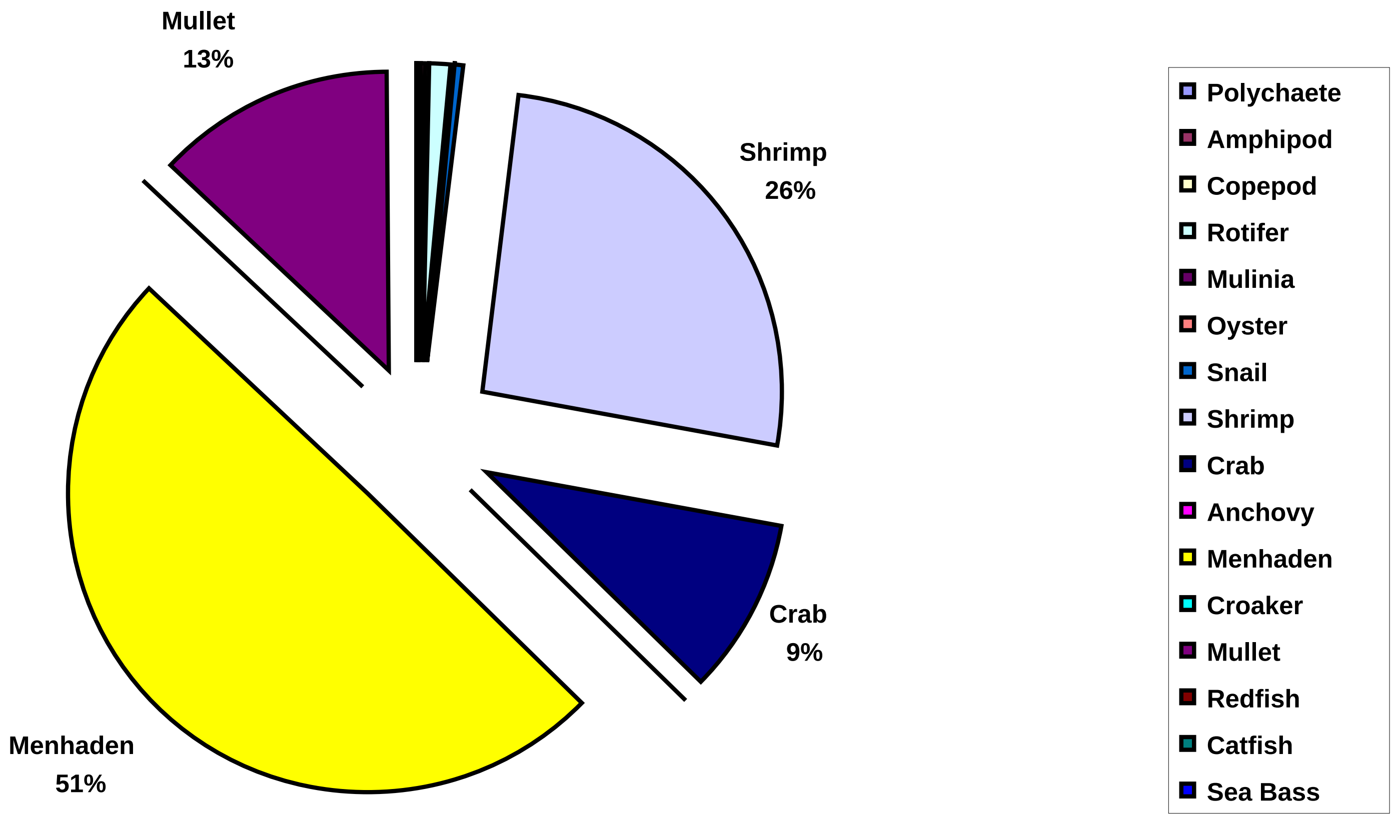
Predicted rates for crabs
(as % of biomass)



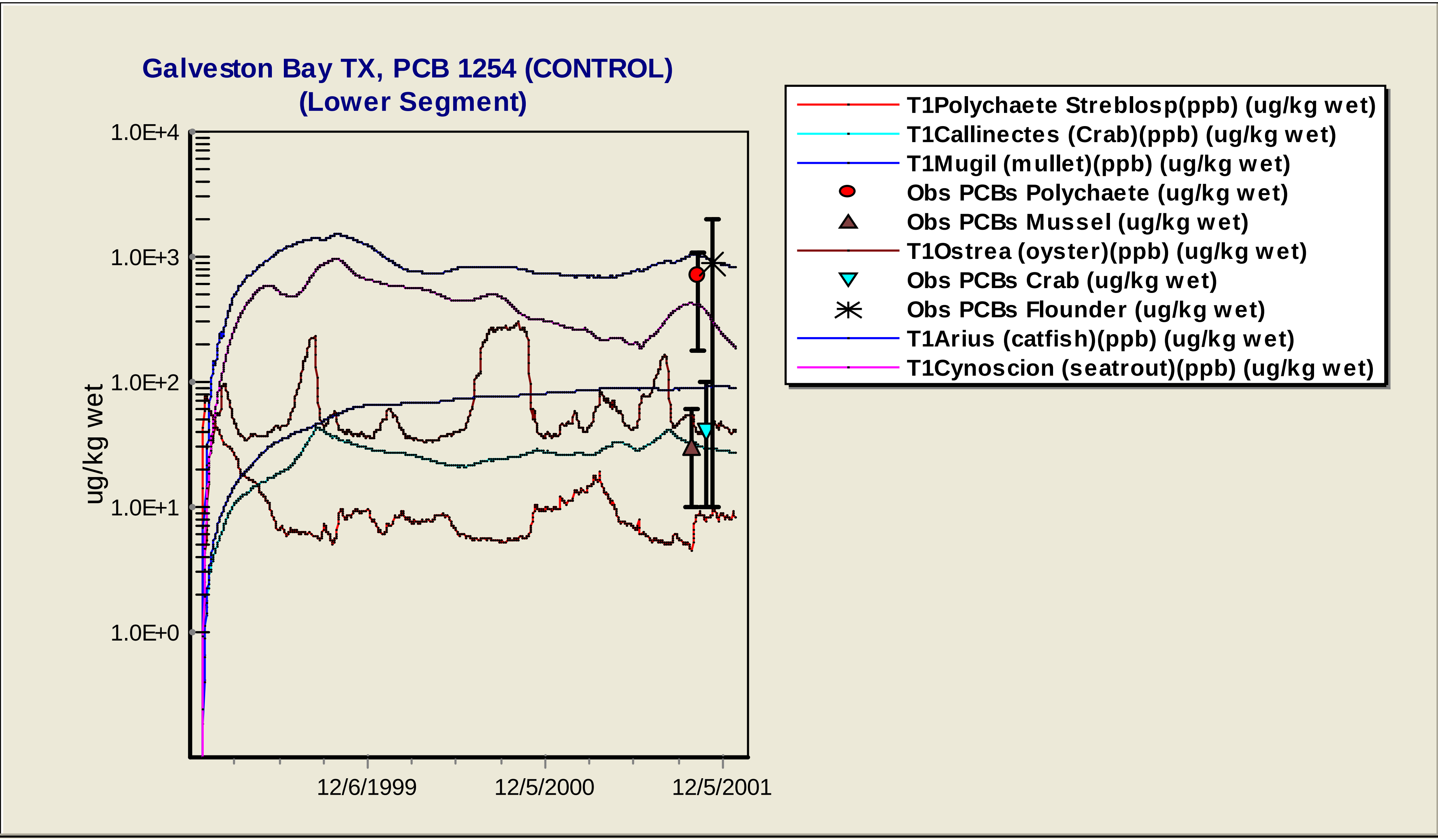
Predicted distribution of PFOS among major compartments in Galveston Bay at end of year



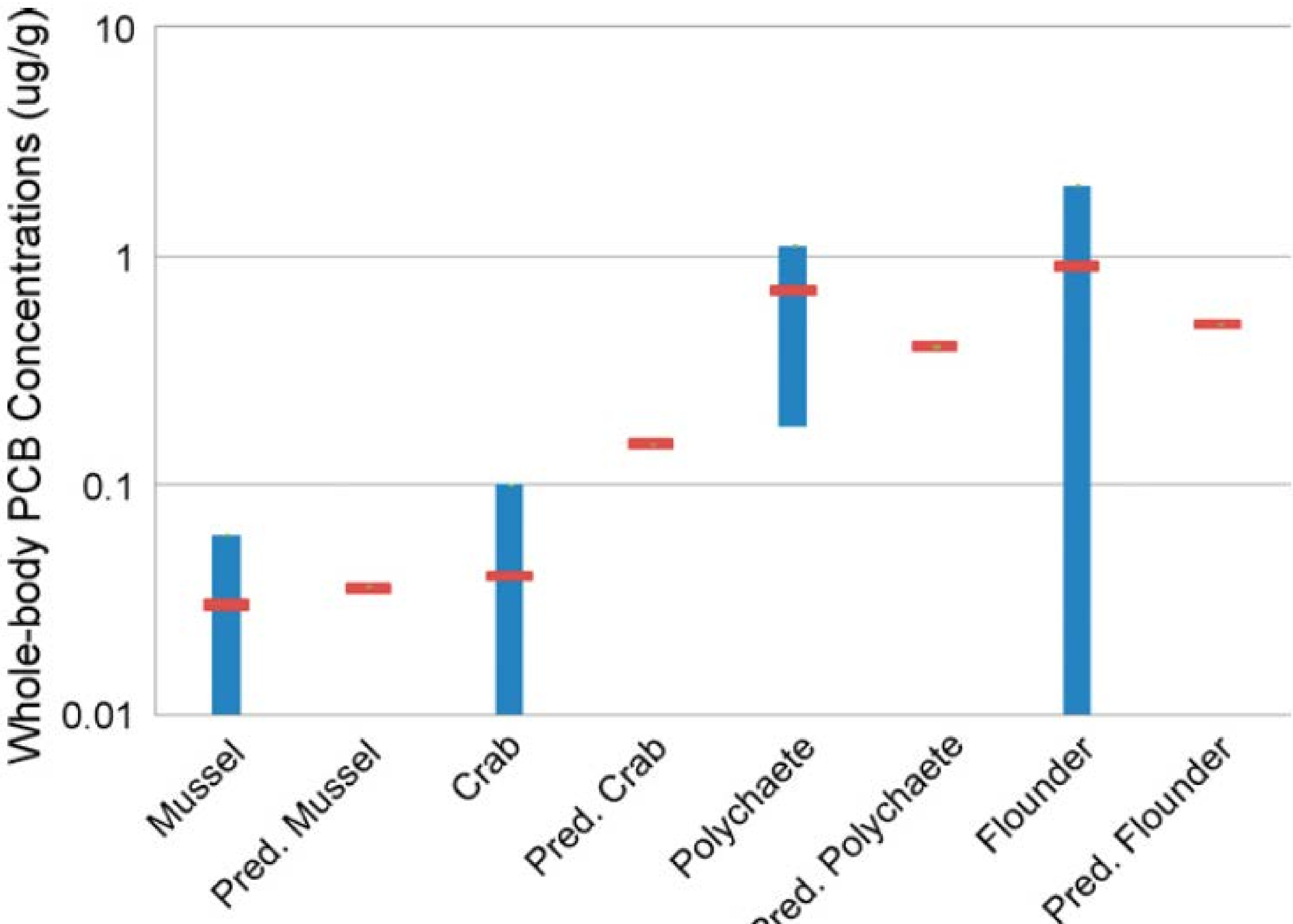
Distribution of PFOS among biotic compartments at end of year



New Bedford Harbor MA observed data: predicted PCB values in TX are comparable



Validation: New Bedford Harbor MA, observed & predicted PCB values are comparable



Park et. al, 2008, Figure 7, data from Connolly, 1991

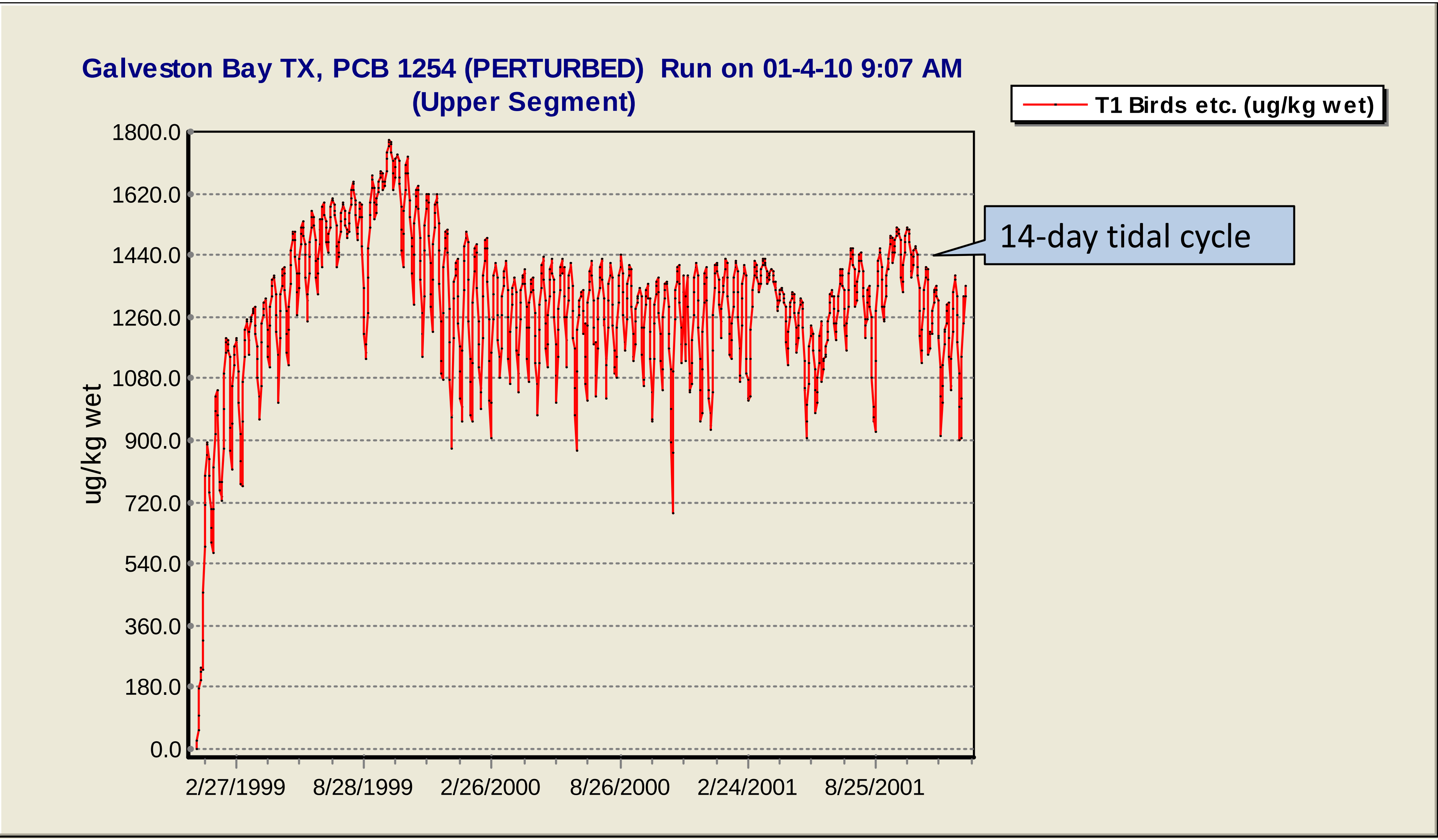
Estuarine Model Data Requirements

- Time Series of “Upper Layer” and “Lower Layer” Salinities for Salt Wedge Model
- Tidal Range Model Parameters
  - “harmonic constants”, often available from NOAA website
- Estuary Site Width
- Loadings of Freshwater Inflow

Aquatic-Feeding Vertebrates

- Originally developed as part of estuarine model
- Inputs:
  - Dietary preferences of the aquatic-dependent vertebrates
  - Biomagnification Factors (BMFs)
- Outputs:
  - Contaminant concentrations within aquatic-dependent vertebrates

PCB Bioaccumulation in Shorebirds



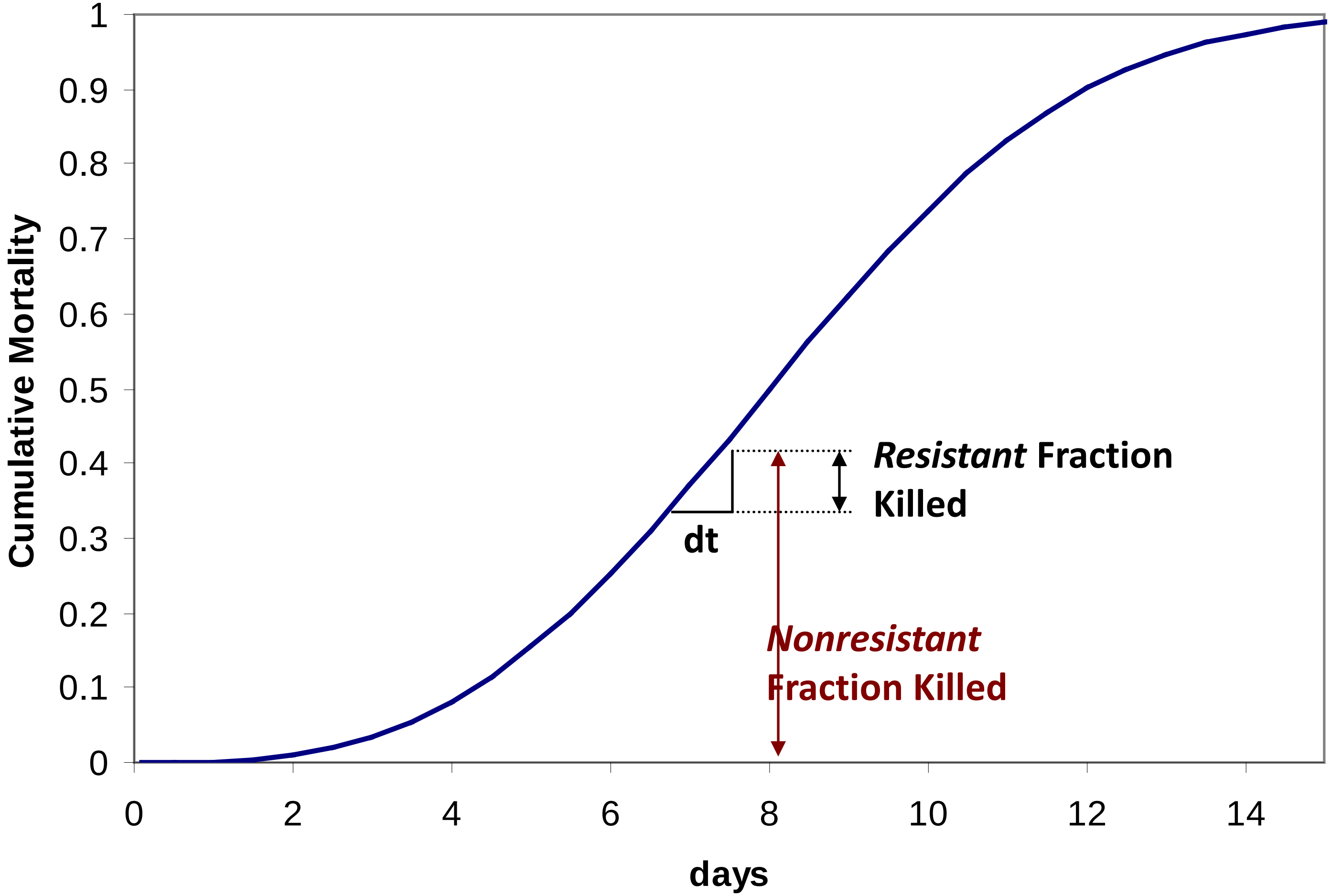
Modeling Toxicity of Chemicals

- Lethal and sublethal effects are represented
- Chronic and acute toxicity are both represented
- Effects based on total internal concentrations
- Uses the critical body residue approach (McCarty 1986, McCarty and Mackay 1993)
- Can also model external toxicity
  - Useful if uptake and depuration are very fast (as with herbicides)

Steps Taken to Estimate Toxicity

- Enter LC_{50} and EC_{50} values
  - 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
- Sublethal toxicity is related to lethal toxicity through an application factor
- Option has been added to use external concentration.

Disaggregation of Cumulative Mortality



Option to Model with External Concentrations

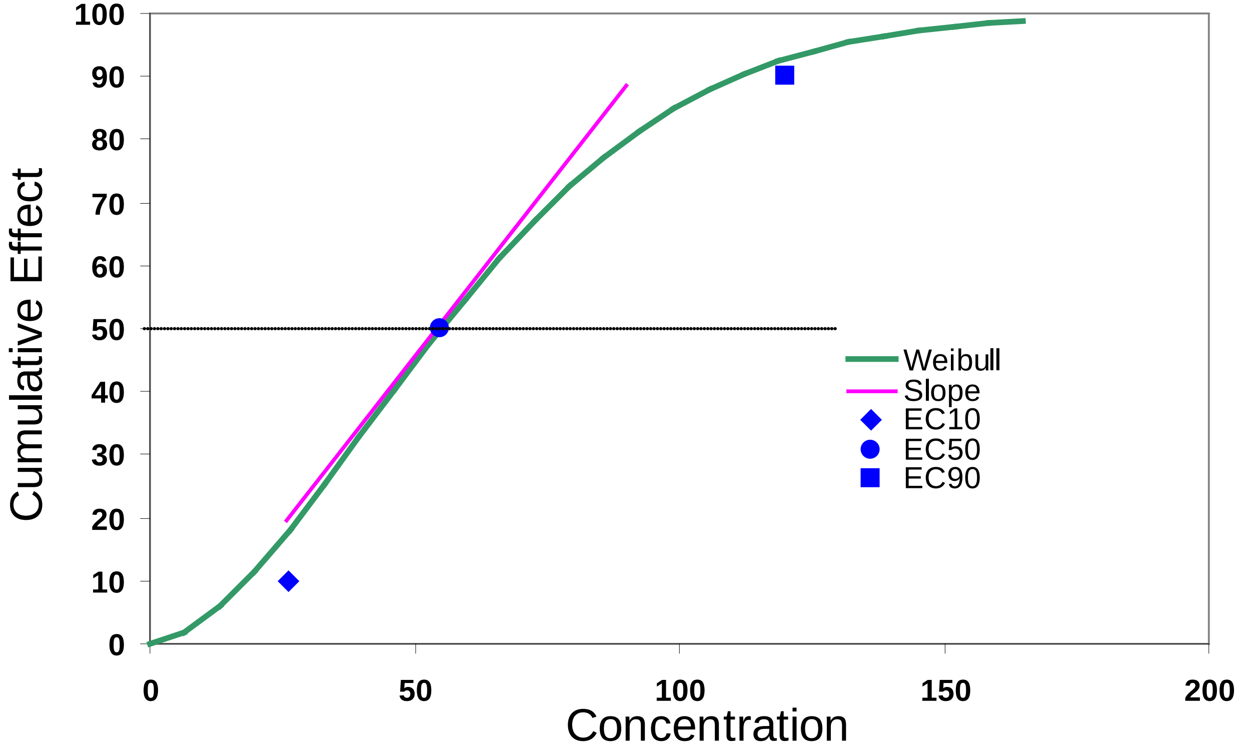
Two-parameter Weibull distribution as in Christiensen and Nyholm (1984)

$$CumFracKilled = 1 - \exp(-kz^{\eta})$$

Two Required Parameters:

LC50 (or EC50)

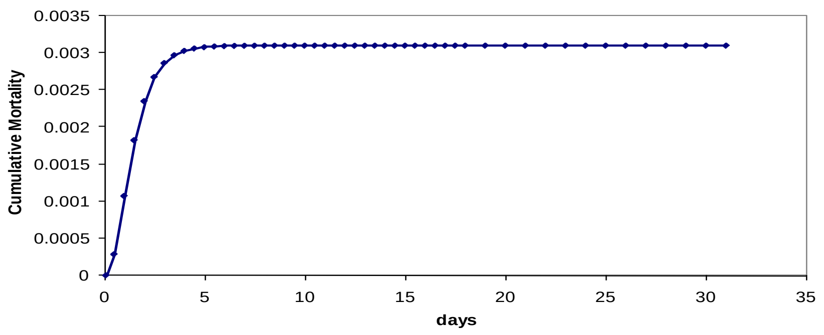
“Slope Factor” = Slope at LC50 multiplied by LC50

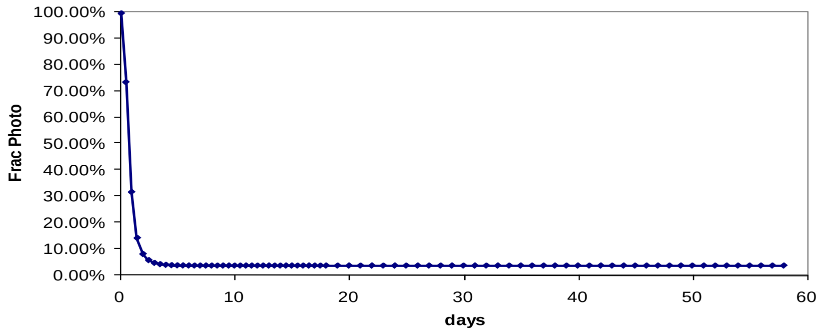


Spreadsheet Demo

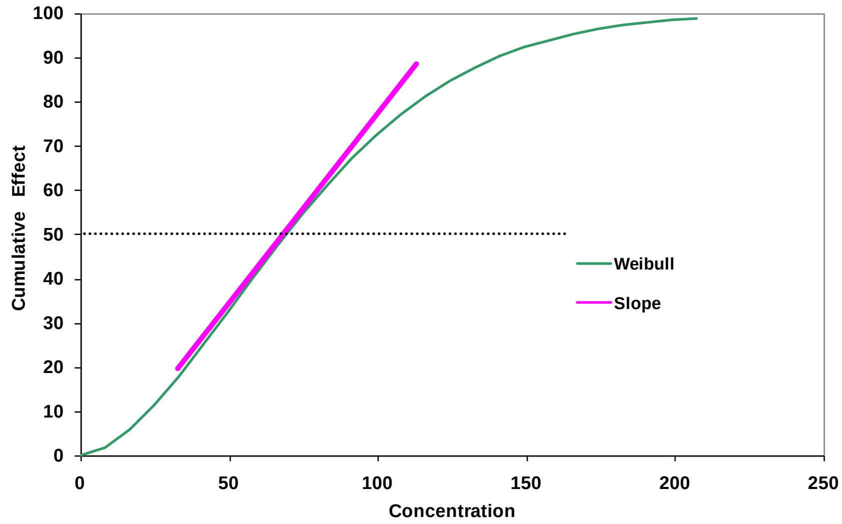
Materials for this short-course include two spreadsheets useful in understanding the model's toxicity components

AQUATOX_Internal_Toxicity_Model.xls

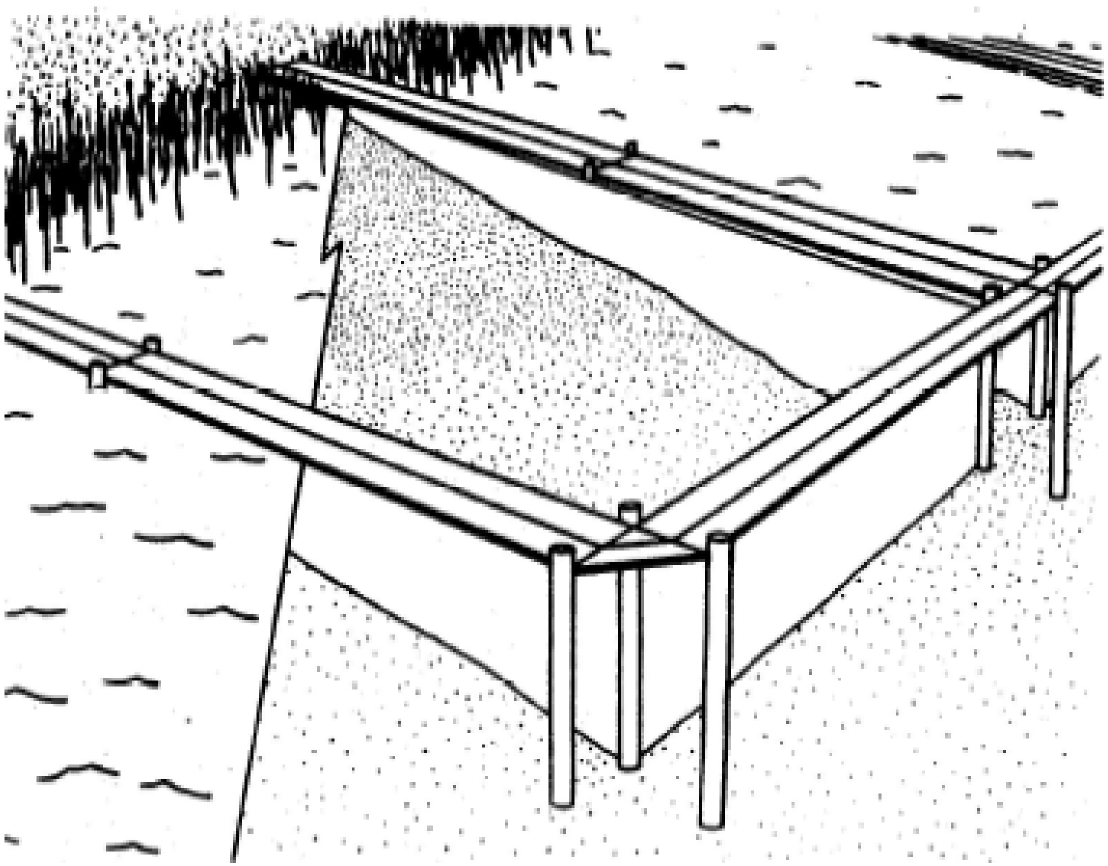




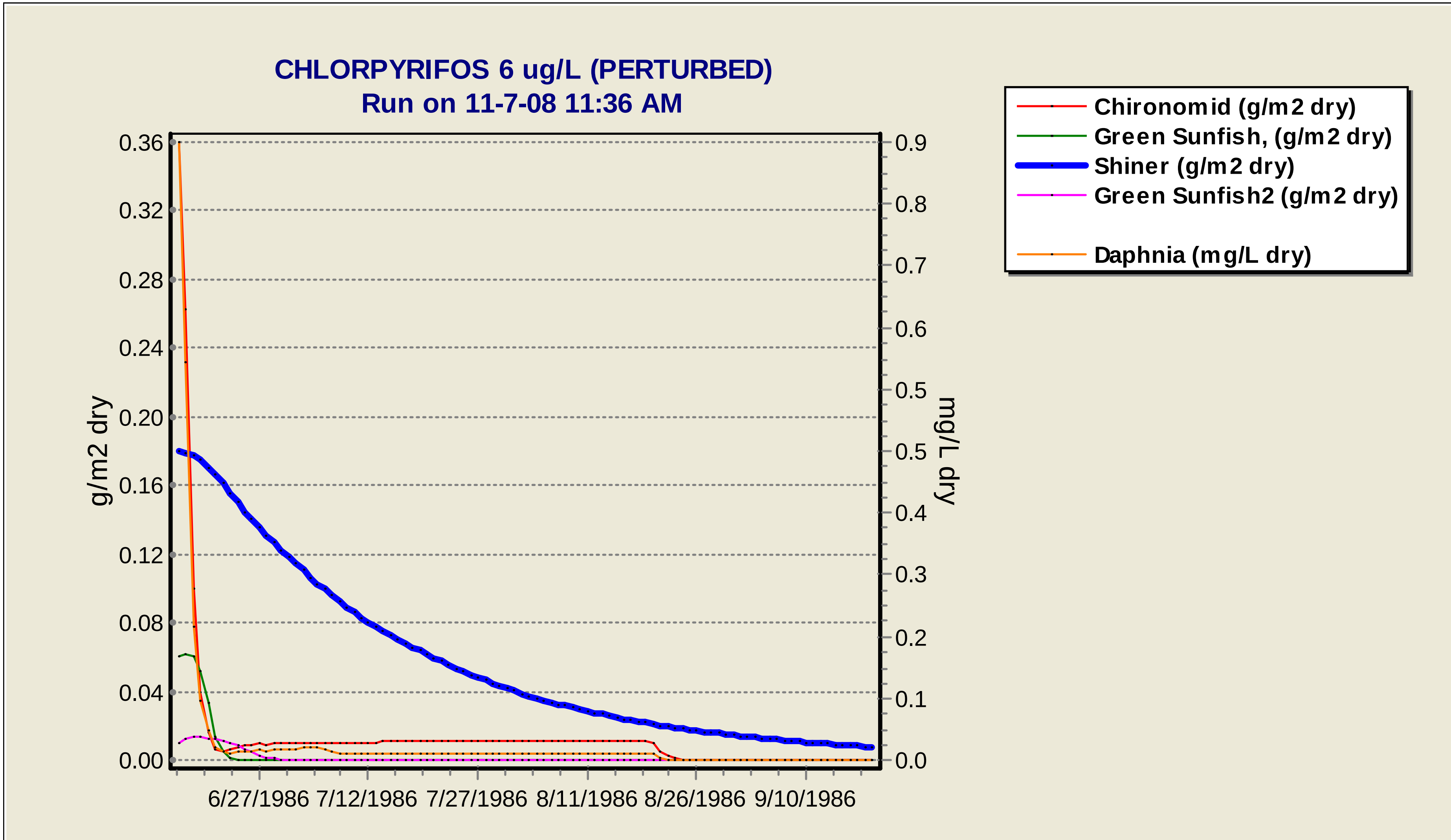
AQUATOX_External_Toxicity_Model.xls



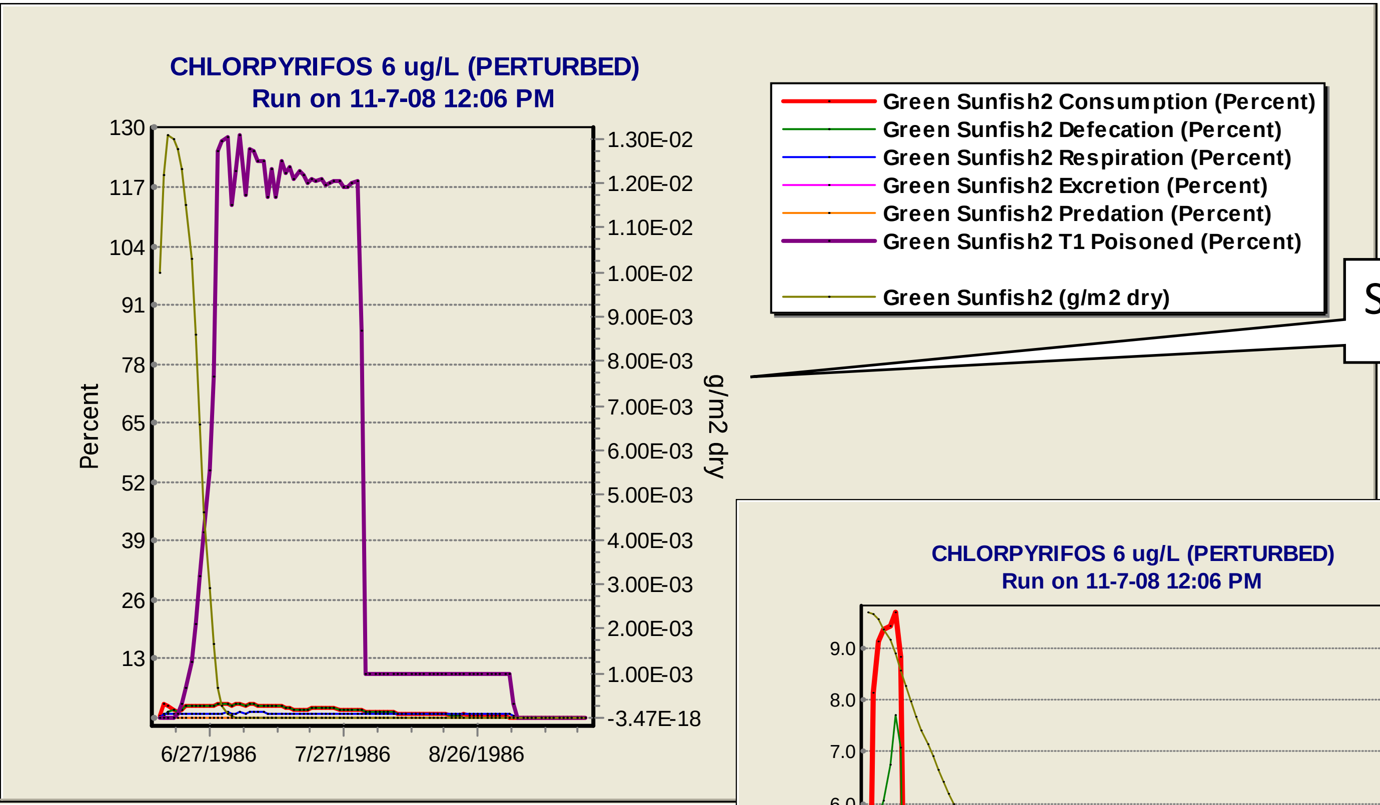
Returning to the Enclosure in Duluth MN . . .



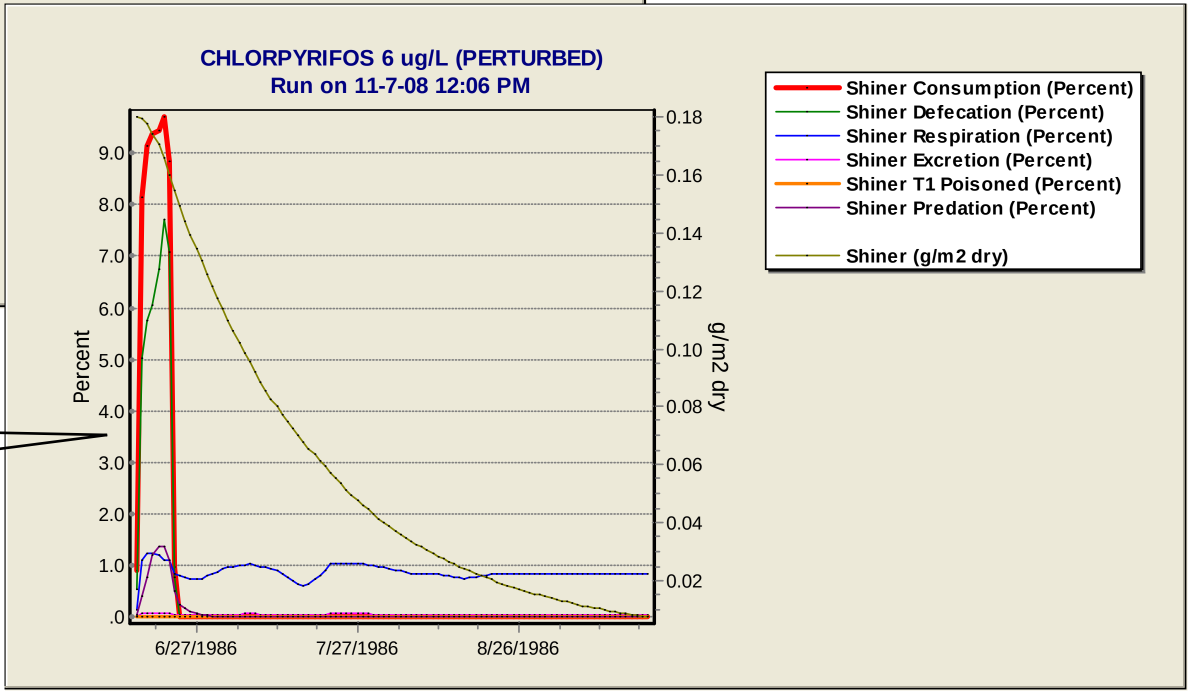
Animals all decline at varying rates following a single initial dose of chlorpyrifos



Sunfish have lethal effects, shiners have sublethal effects from chlorpyrifos

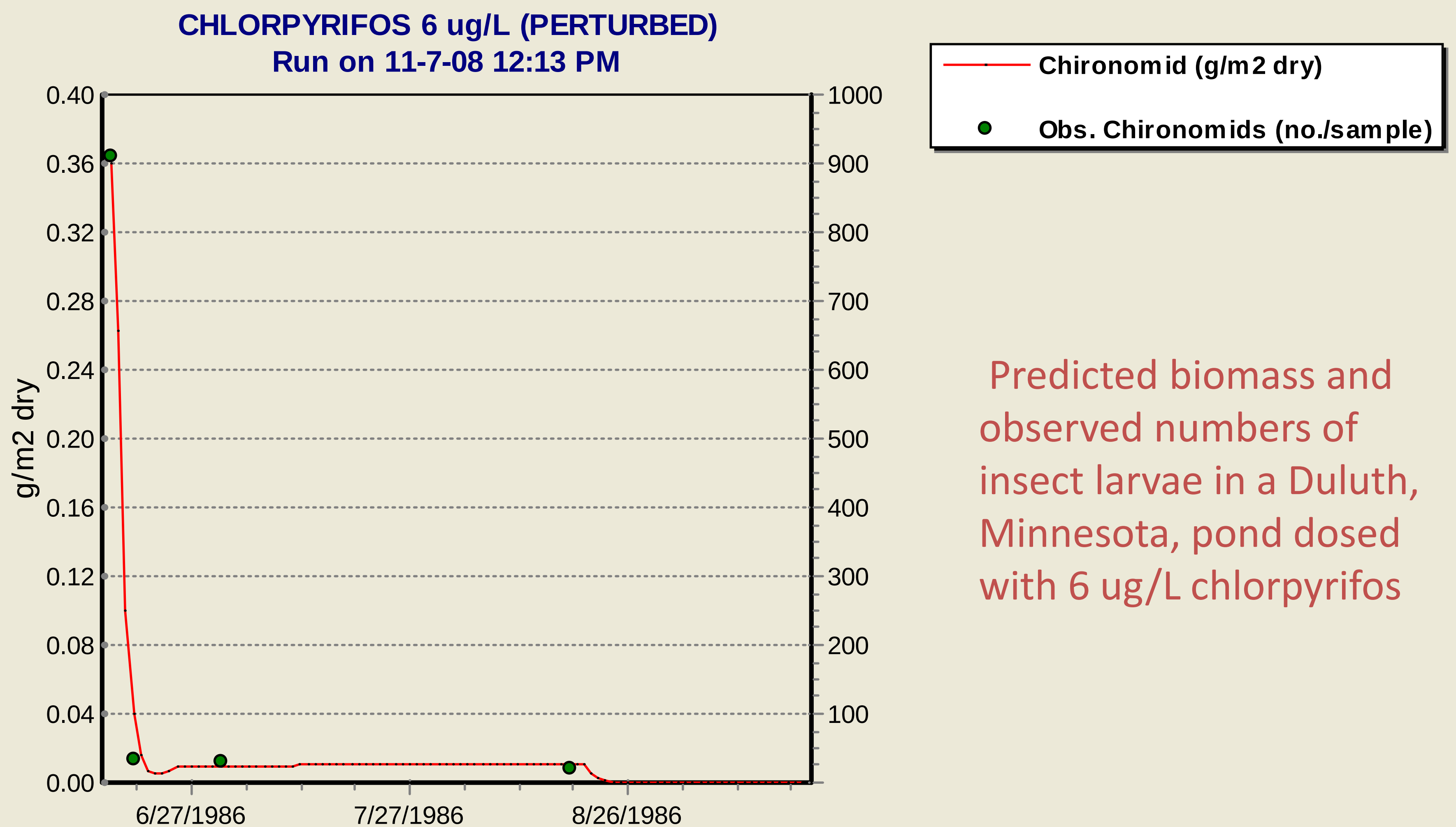


Sunfish with lethal effects



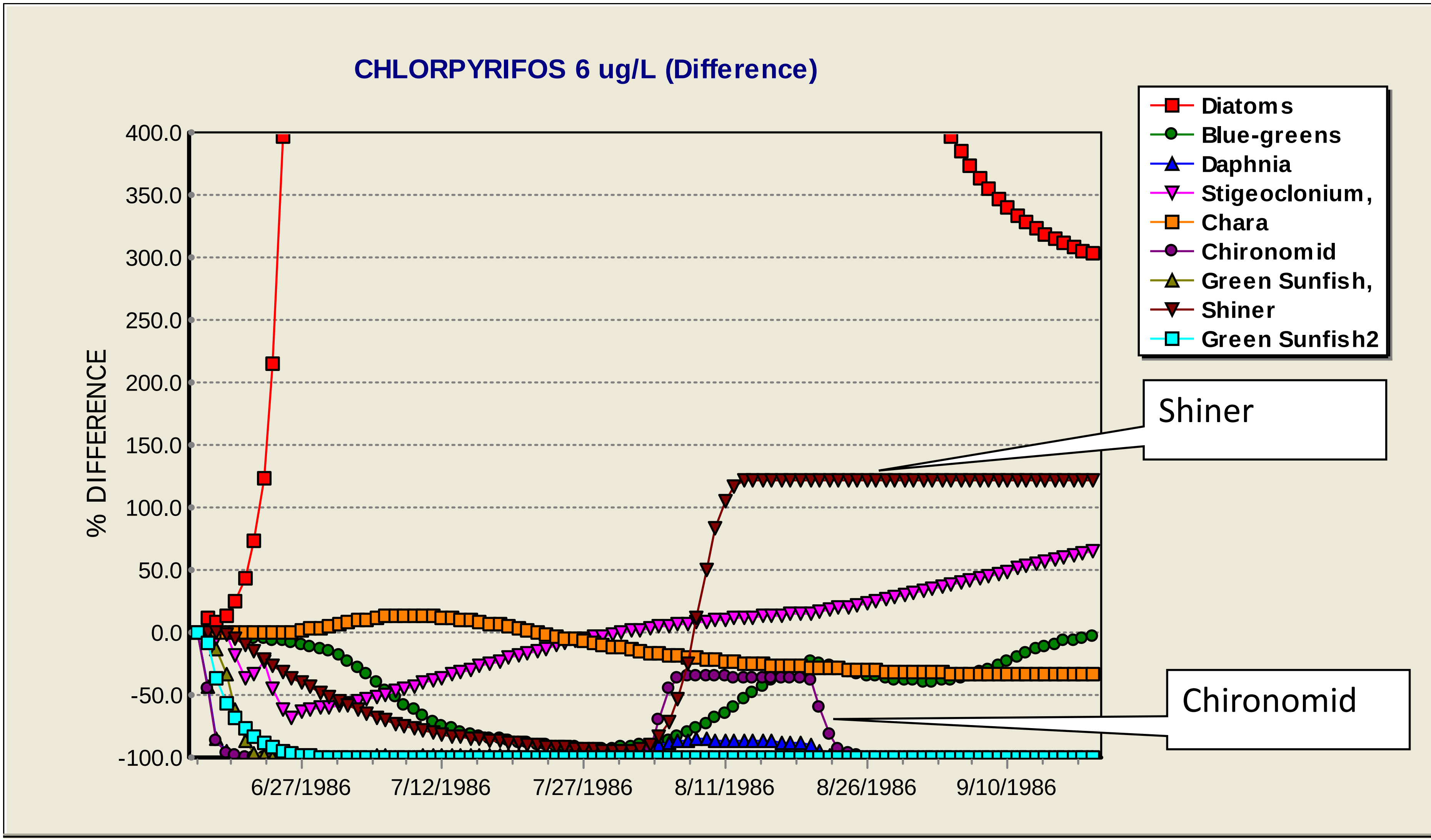
Shiner with sublethal effects only

Toxic effects of Chlorpyrifos in Duluth pond

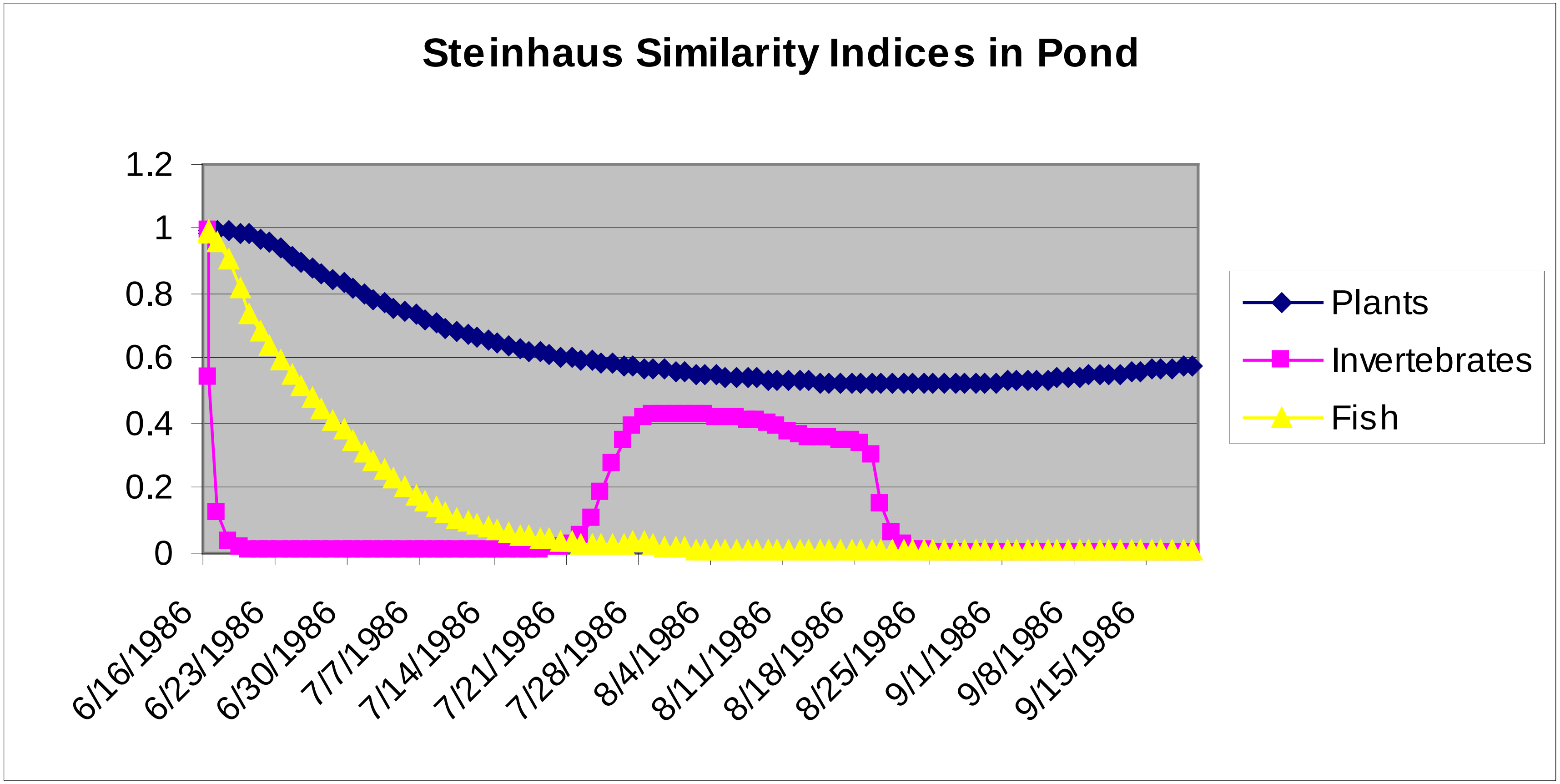


Predicted biomass and observed numbers of insect larvae in a Duluth, Minnesota, pond dosed with 6 ug/L chlorpyrifos

% Difference Graph shows differences in species response to toxicant



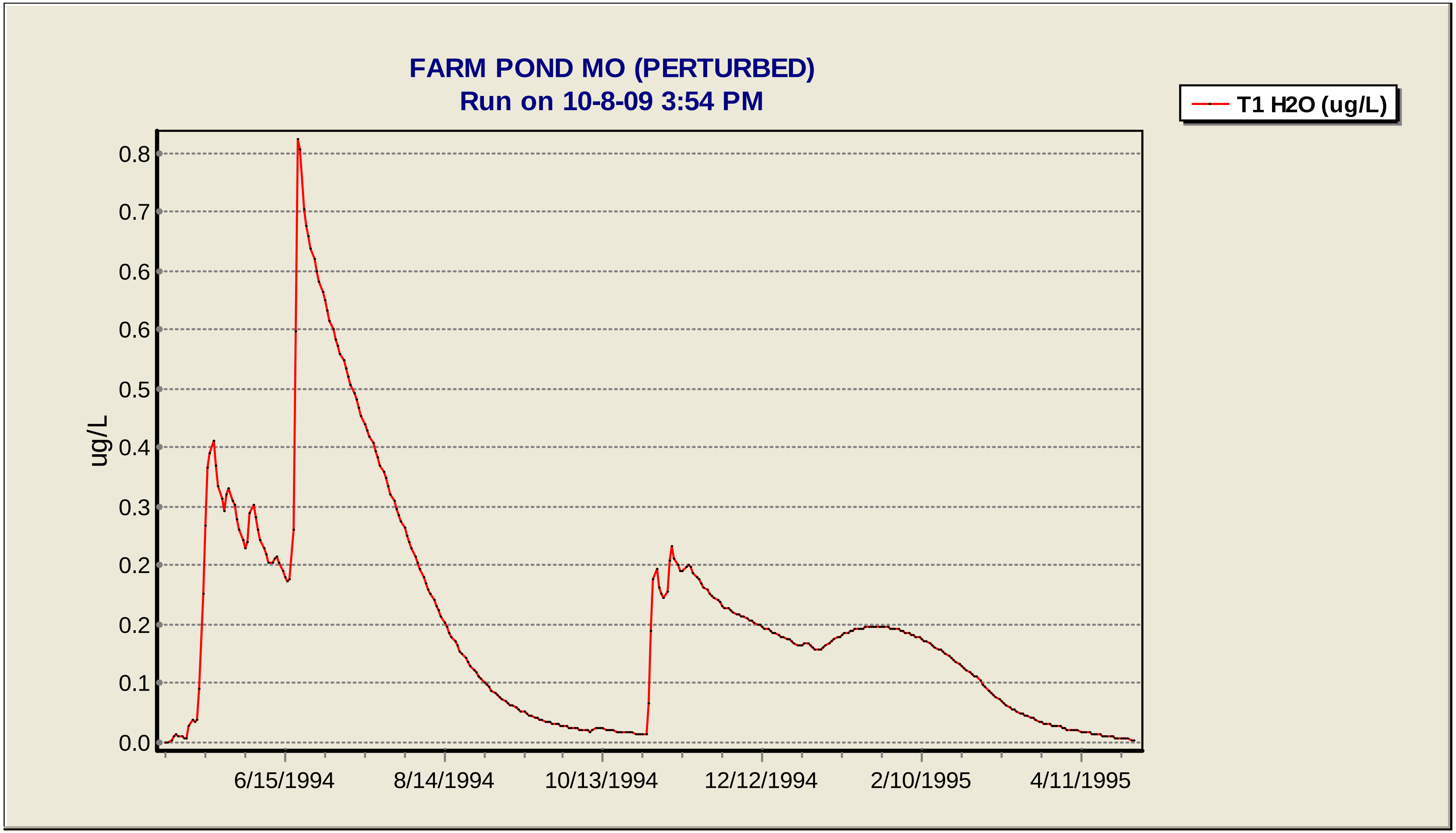
Steinhaus Indices show ecosystem impacts predicted by the model



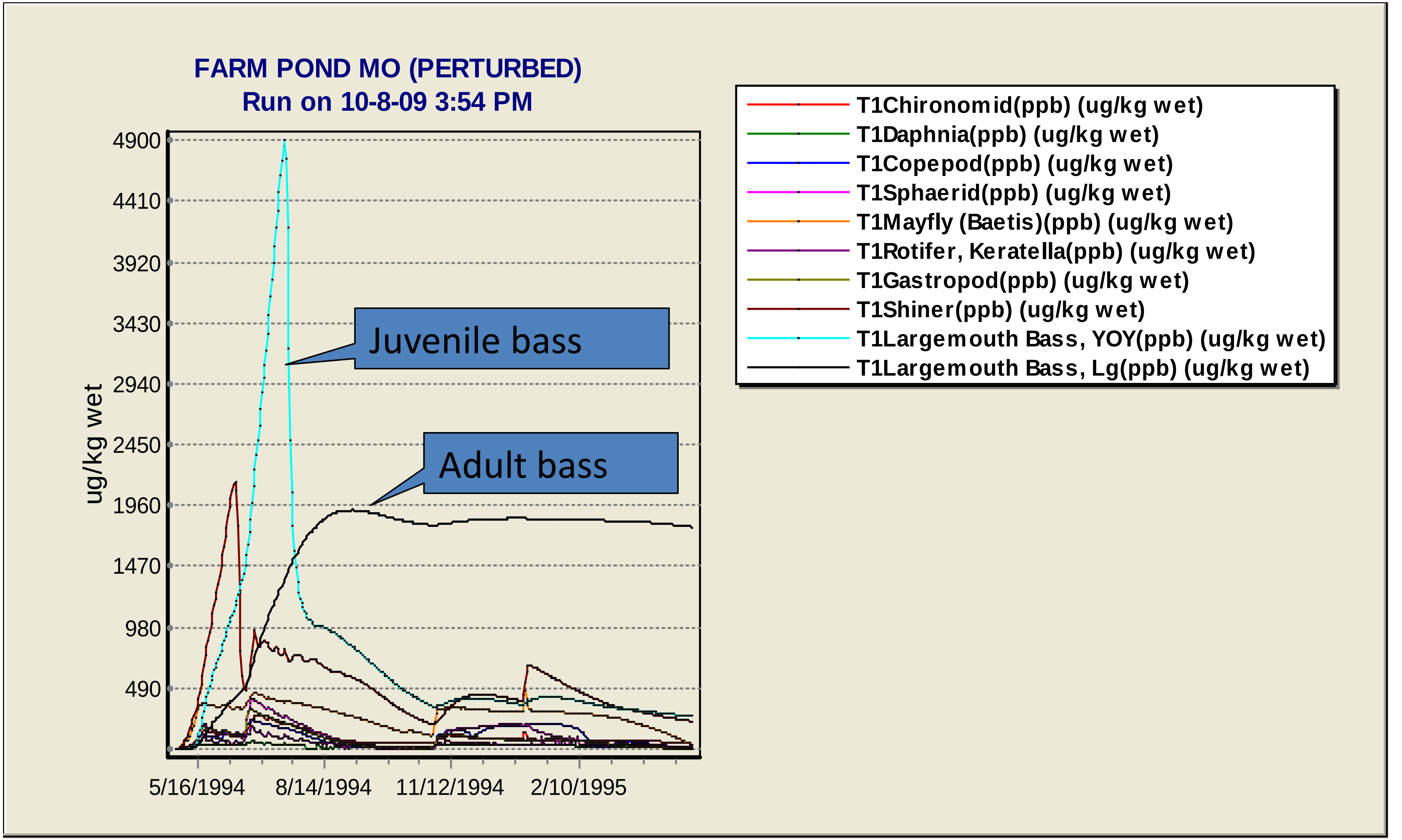
$$S = \frac{2 * \sum_{k=1}^{n} Min(a_{1,k}, a_{2,k})}{\sum_{k=1}^{n} a_{1,k} + \sum_{k=1}^{n} a_{2,k}}$$

Farm Pond MO, Esfenvalerate

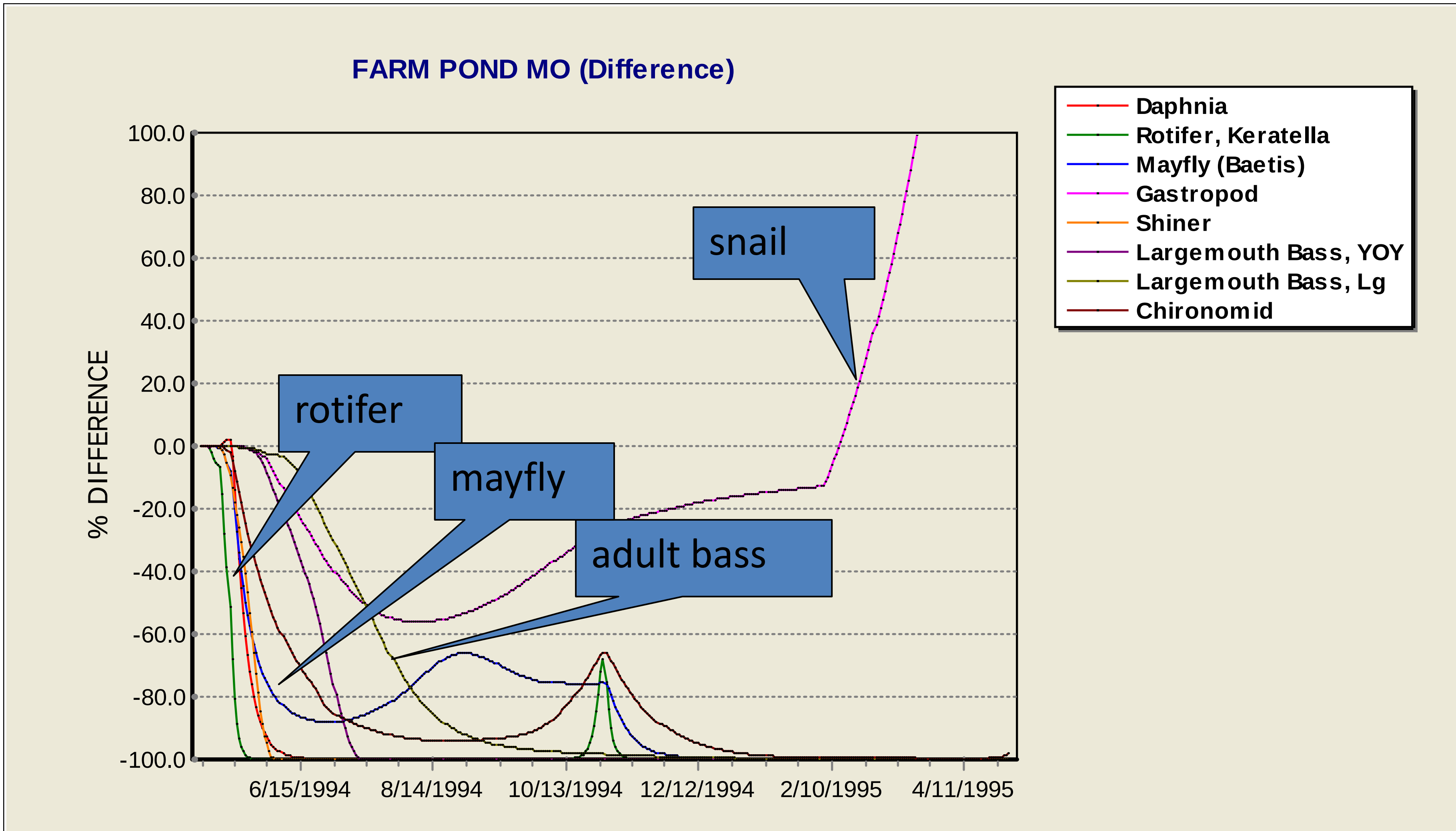
- Loadings from PRZM for adjacent cornfield
- Worst case scenario for runoff of pesticide predicted by PRZM



Farm Pond, Esfenvalerate Chemical Uptake in animals

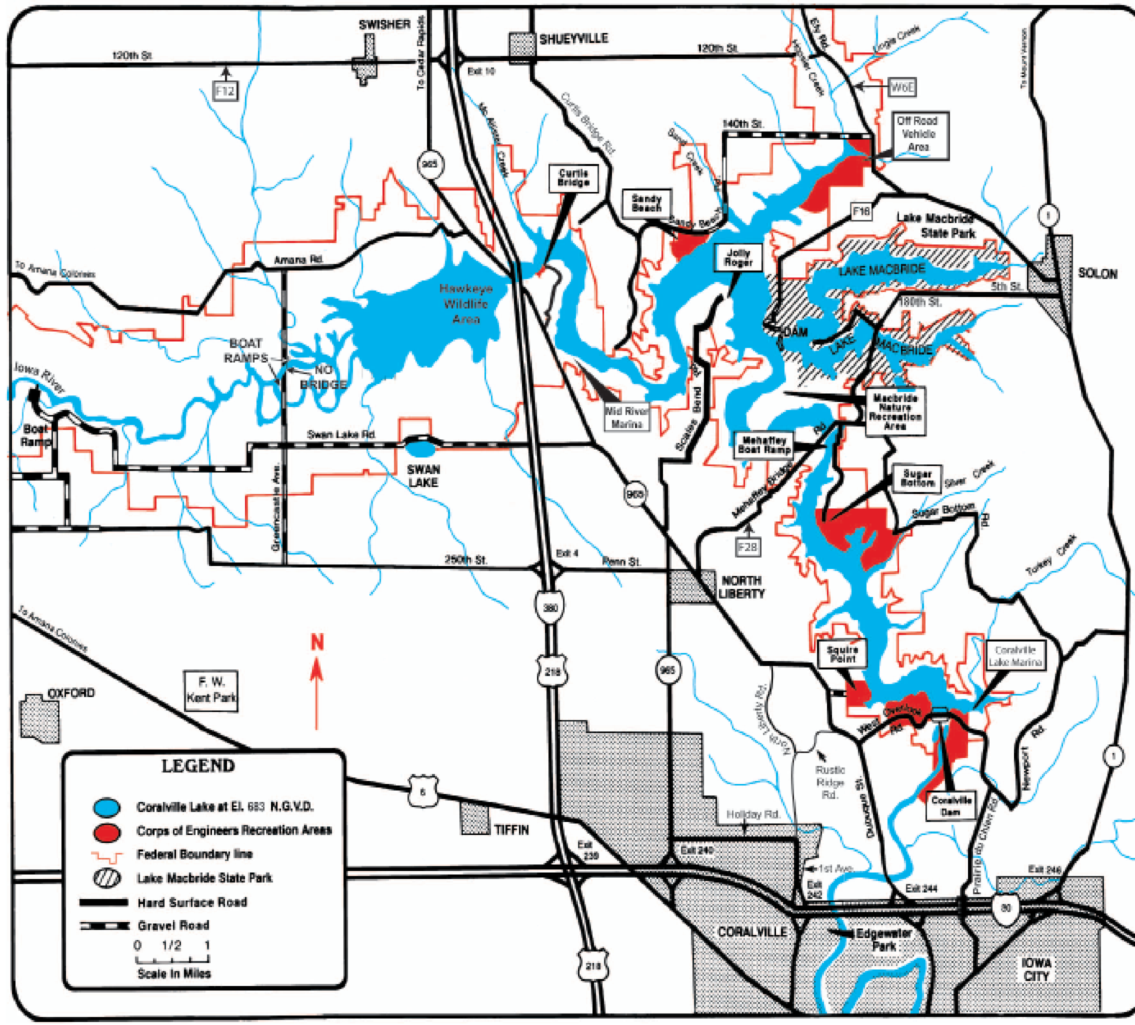


Farm Pond, Esfenvalerate Difference Graph

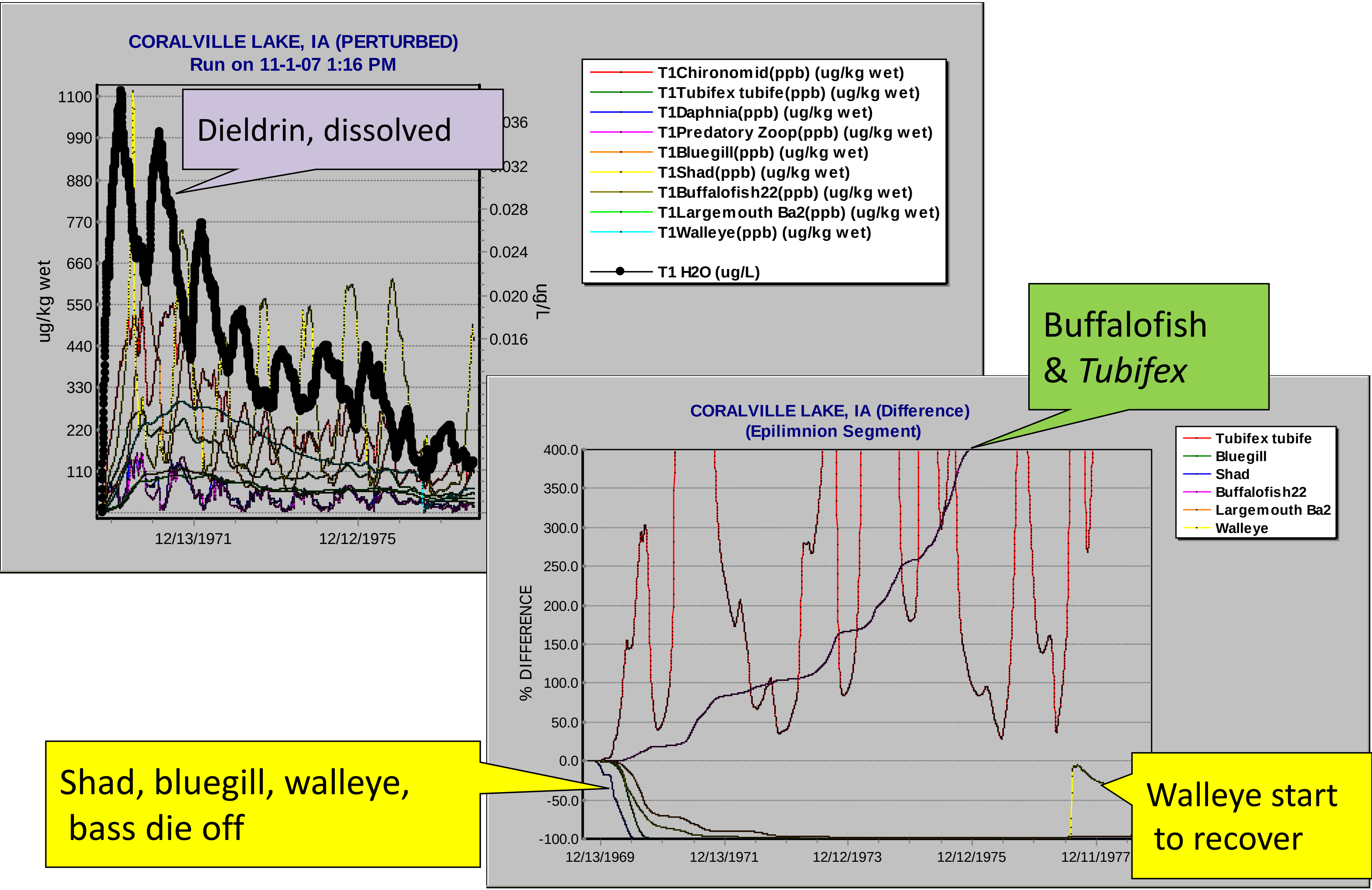


Coralville Reservoir Iowa
long-term contamination with dieldrin

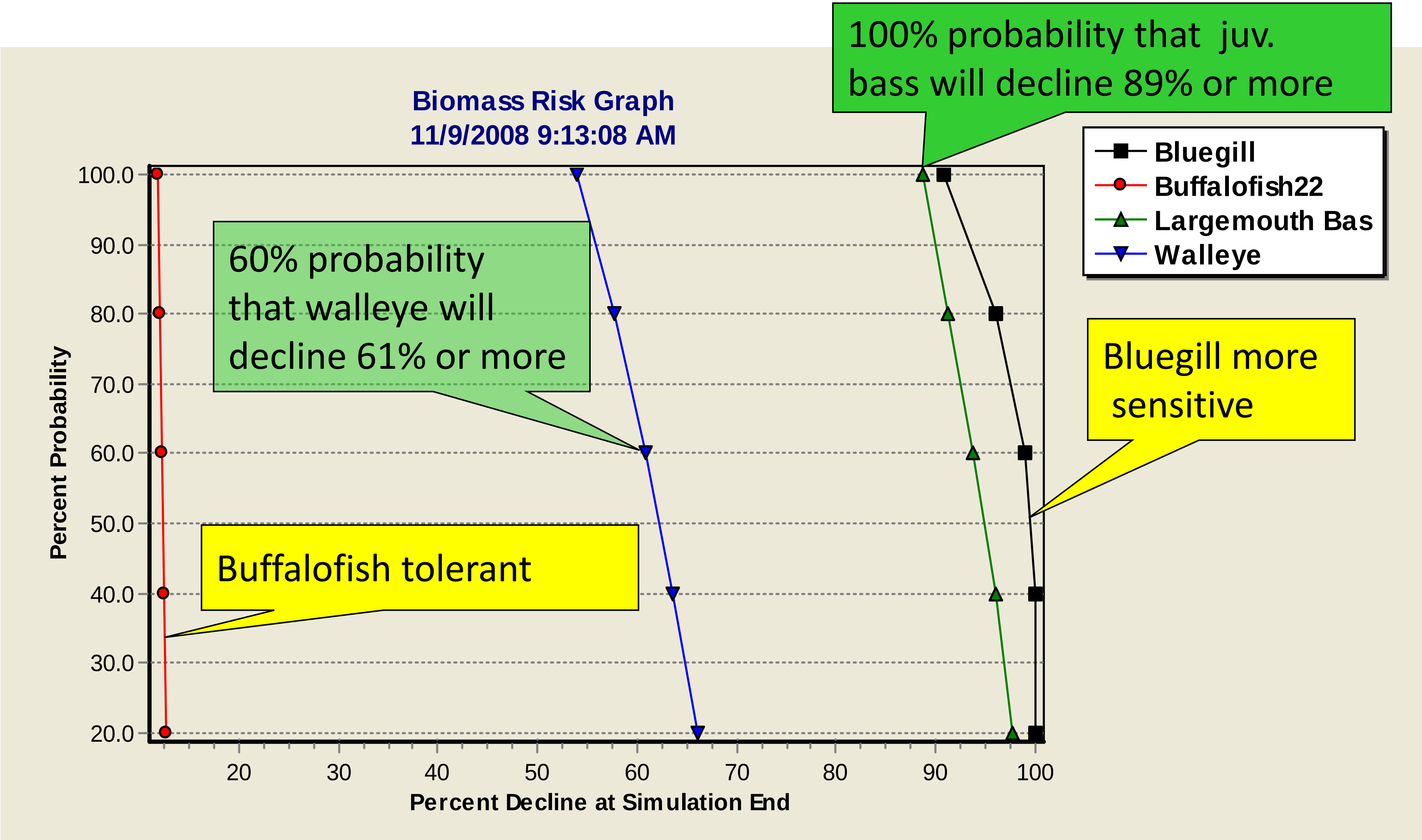
- Run-of-river
- Flood control
- 90% of basin in agriculture
  - Nutrients
  - Pesticides
  - Sediment



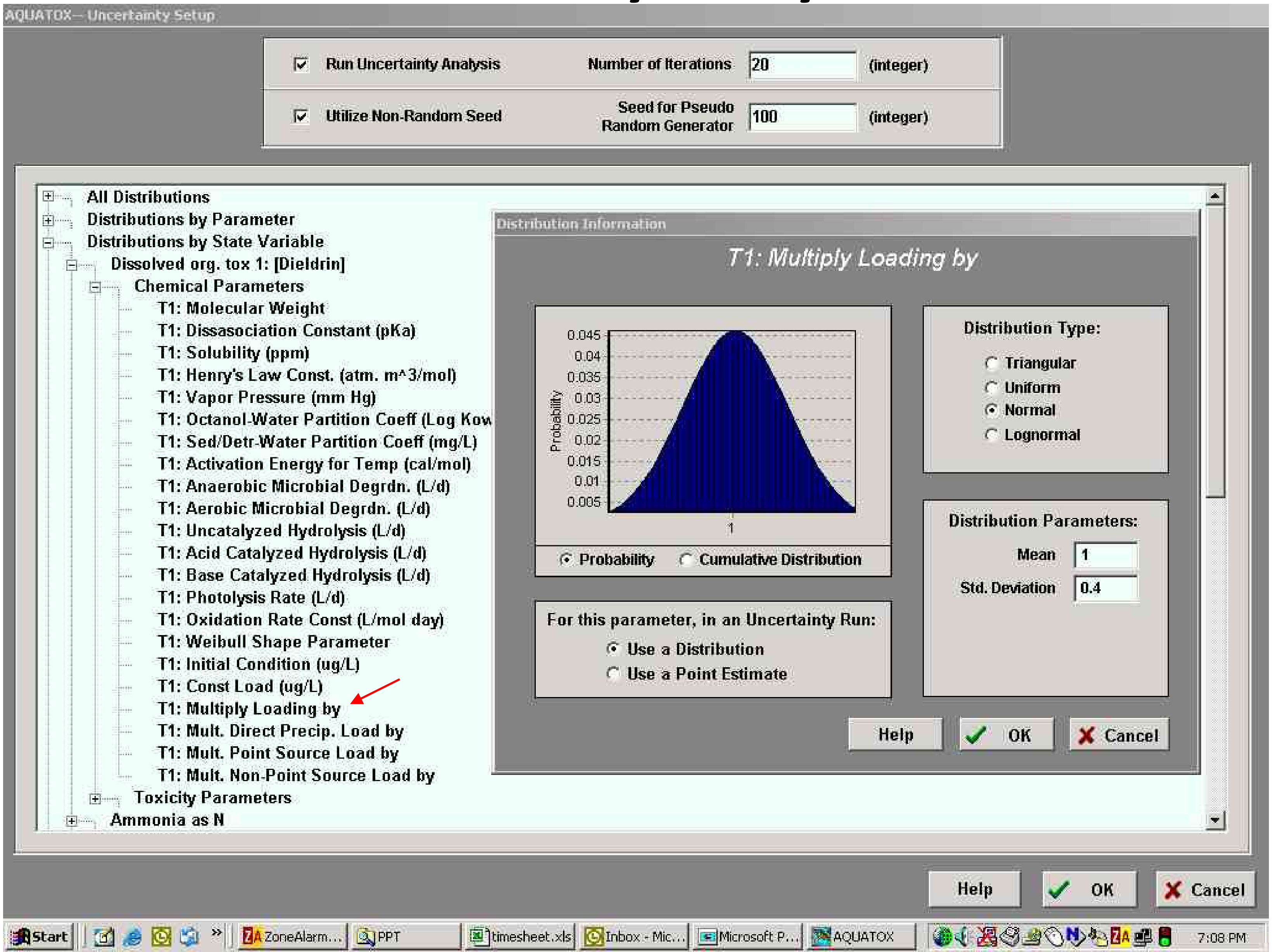
Dieldrin bioaccumulates & declines over 20 years with fish mortality, but tolerant buffalofish, *Tubifex* prosper



Probability of decline in biomass (end of 1st year) can be estimated based on uncertainty



Toxicant Parameters and Loadings are Subject to Uncertainty Analysis



Chemical Toxicity Screen

Chemical Toxicity Parameters -- Chlorpyrifos

Animal Toxicity Data | Add Animal Toxicity Record | Export Grid to Excel (to print)

To delete a record, press <Ctrl> <Del>

Drift Threshold only relevant to zoobenthos

Animal name	LC50 (ug/L)	LC50 exp. time (h)	LC50 comment	K2 Elim. rate const (1/d)	K1 Uptake const (L/kg d)	BCF (L/kg)	Biotrnsfm. rate (1/d)	EC50 growth (ug/L)	Gro
Trout	8.701	96	Regression on Bluegill	1.9E-03			0	0.71	
Bluegill	2.4	96	EPA Duluth '88, p. 124	7.6E-03			0	0.17	
Bass	9.849	96	Regression on Bluegill	3.3E-03			0	1.2439	
Catfish	387.174	96	Regression on Bluegill	3.7E-03			0	28	
Minnow	203	96	Holcombe et al., 1982	1.85E-02			0	20.3	
Daphnia	0.17	24	EPA '87, p. 42 (Duluth)	9.15E-02			0	0.09	
Chironomid	1.416	24	Regression on Daphnia	5.32E-02			0	0.5798	
Stonefly	10	96	Mayer & Ellersieck, 1982	4.03E-02			0	1	
Ostracod	2.055	24	Regression on Daphnia	6.93E-02			0	0.5776	
Amphipod	0.29	48	EPA '87, p. 42 (Duluth)	6.93E-02			0	0.011	
Other	0	96		0E+00			0	0	

- Enter or Estimate K2, Calculate K1 and BCF (default behavior)
- Enter K1 and K2, Calculate BCF
- Enter K1 and BCF, Calculate K2
- Enter K2 and BCF, Calculate K1

Plant Toxicity Data | Add Plant Toxicity Record | Export Grid to Excel (to print)

Plant name	EC50 photo (ug/L)	EC50 exp. time (h)	EC50 dislodge (ug/L)	EC50 comment	K2 Elim. rate const (1/d)	K1 Uptake Const (L/kg d)	BCF (L/kg)	Biotrnsfm. rate (1
Greens	0	96	0		2.4			
Diatoms	0	96	0		2.4			
Bluegreens	0	96	0		2.4			
Macrophytes	0	96	0		0.3247			

- Enter or Estimate K2, Calculate K1 and BCF (default behavior)
- Enter K1 and K2, Calculate BCF
- Enter K1 and BCF, Calculate K2
- Enter K2 and BCF, Calculate K1

K1, BCF entered on a dry weight basis; lipid frac. is wet wt.

Estimate Animal K2s using Kow | Estimate Plant K2s using Kow | Interspecies Toxicity Correlation Models

Estimate plant LC50s using EC50 to LC50 ratio

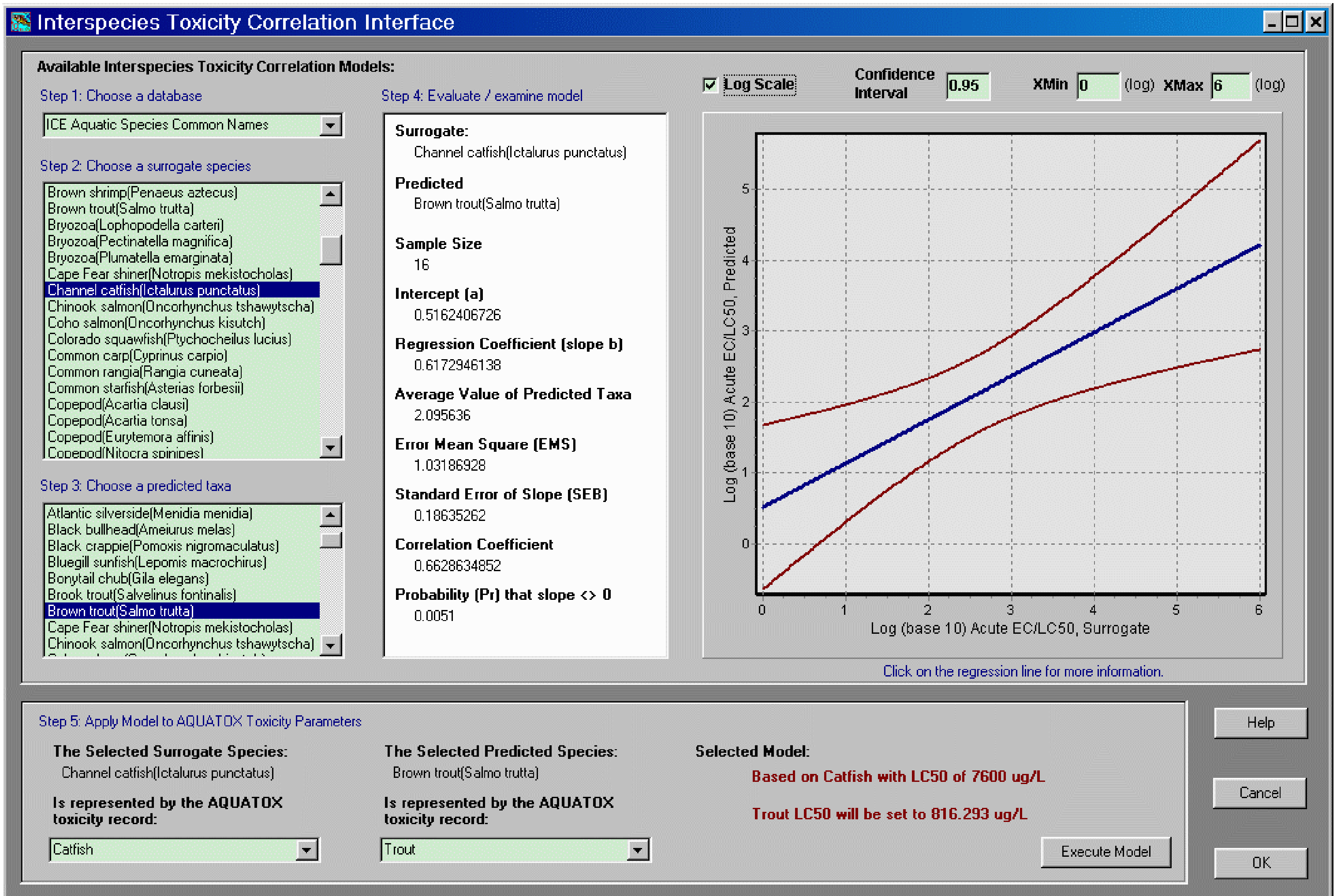
Estimate animal EC50s using LC50 to EC50 ratio | Help | O.K.

Interspecies Correlation Estimates (ICE Version 3.1, January 2010)

- Developed by EPA ORD
- Estimates the acute toxicity of a chemical to a species with no test data
- 1440 regression models derived
  - 180 species and 1266 chemicals
- Regressions on species, families, genus
- Goodness of fit information for regressions

Release 3: Additional Toxicity Features

- **Integration with ICE: a large EPA database of toxicity regressions**



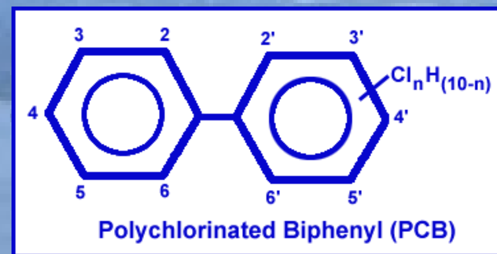
Lab 7: Risk Assessment of Insecticide in Ohio Stream

Objective: analyze direct and indirect ecotoxicological effects with model

- Assessment of chlorpyrifos in a generic stream
  - small stream in corn belt
  - drain tiles
- Open Ohio Stream.aps,
- Add chlorpyrifos, save as Ohio Stream chlor.aps
- Run, plot, analyze control/perturbed/ %difference
- Compare constant exposure vs. single dose

Lab 8: PCBs in Lake Hartwell, SC

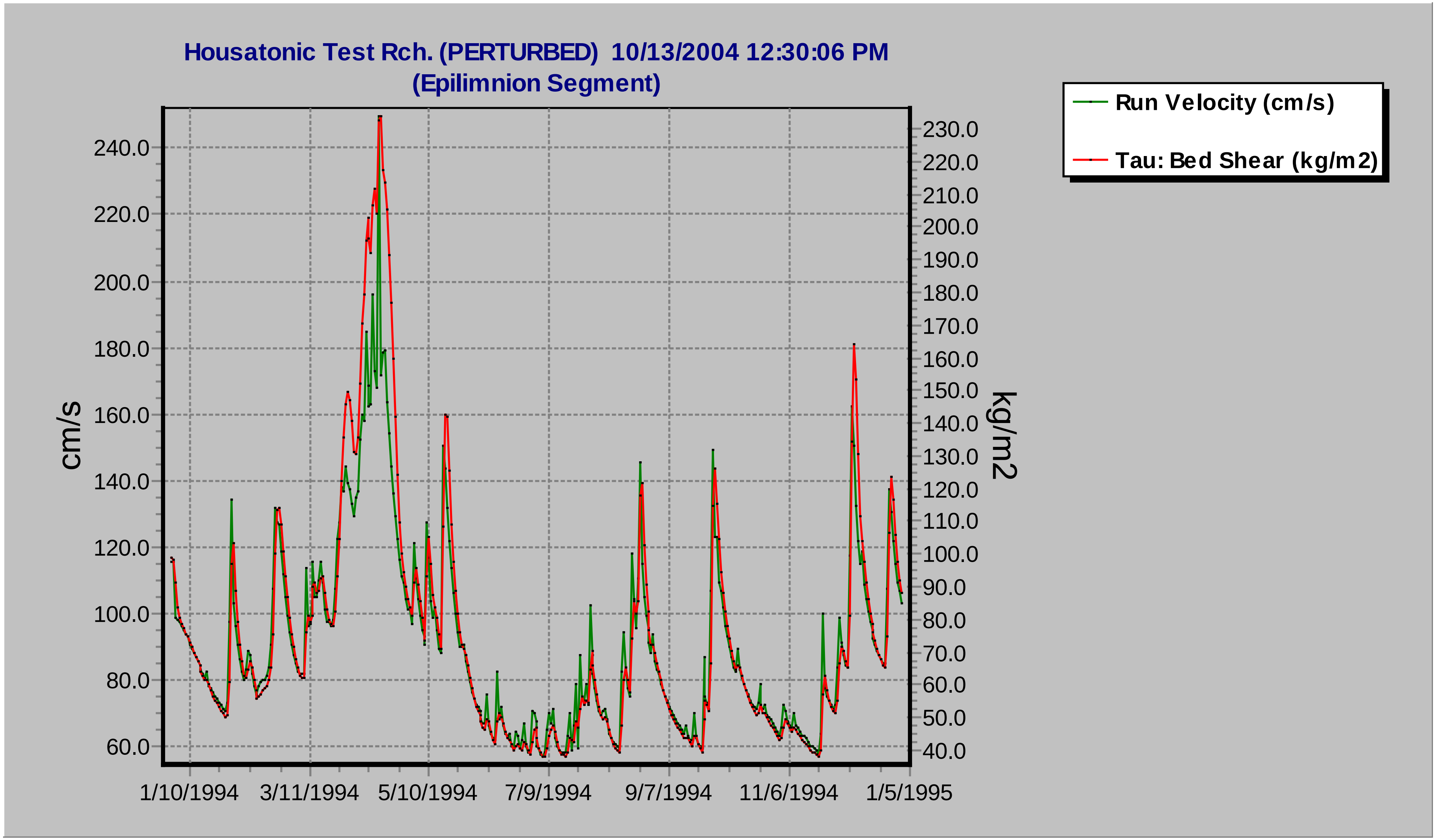
prepared by Brenda Rashleigh, ORD USEPA, Athens GA



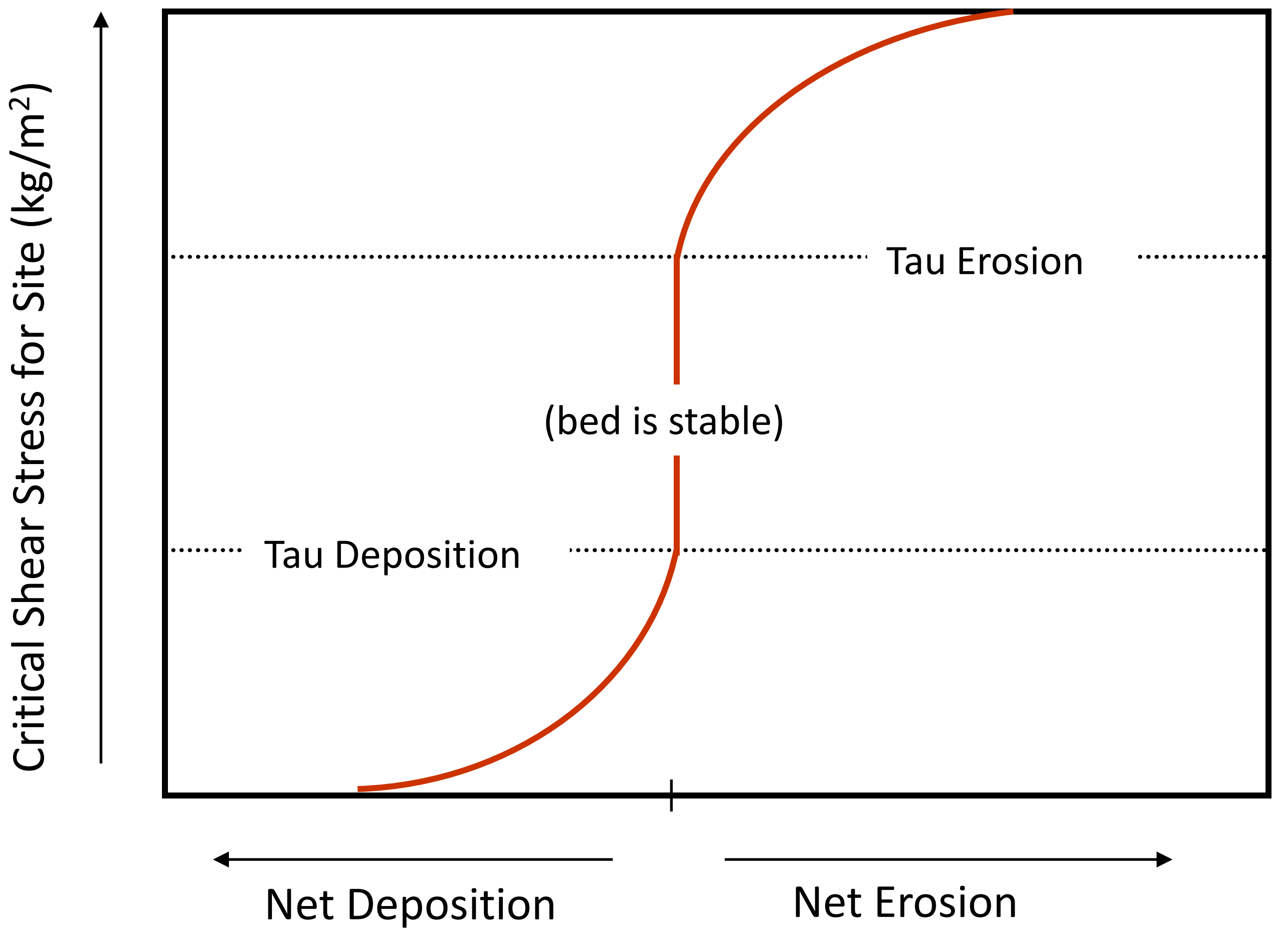
Modeling Inorganic Sediments
(sand, silt, and clay)

- Stream simulations only
- Scour, deposition and transport of sediments
- River reach assumed short and well mixed
- Daily average flow regime determines shear stresses
- Feedback to biota through light limitation, sequestration of chemicals, and now direct sediment effects

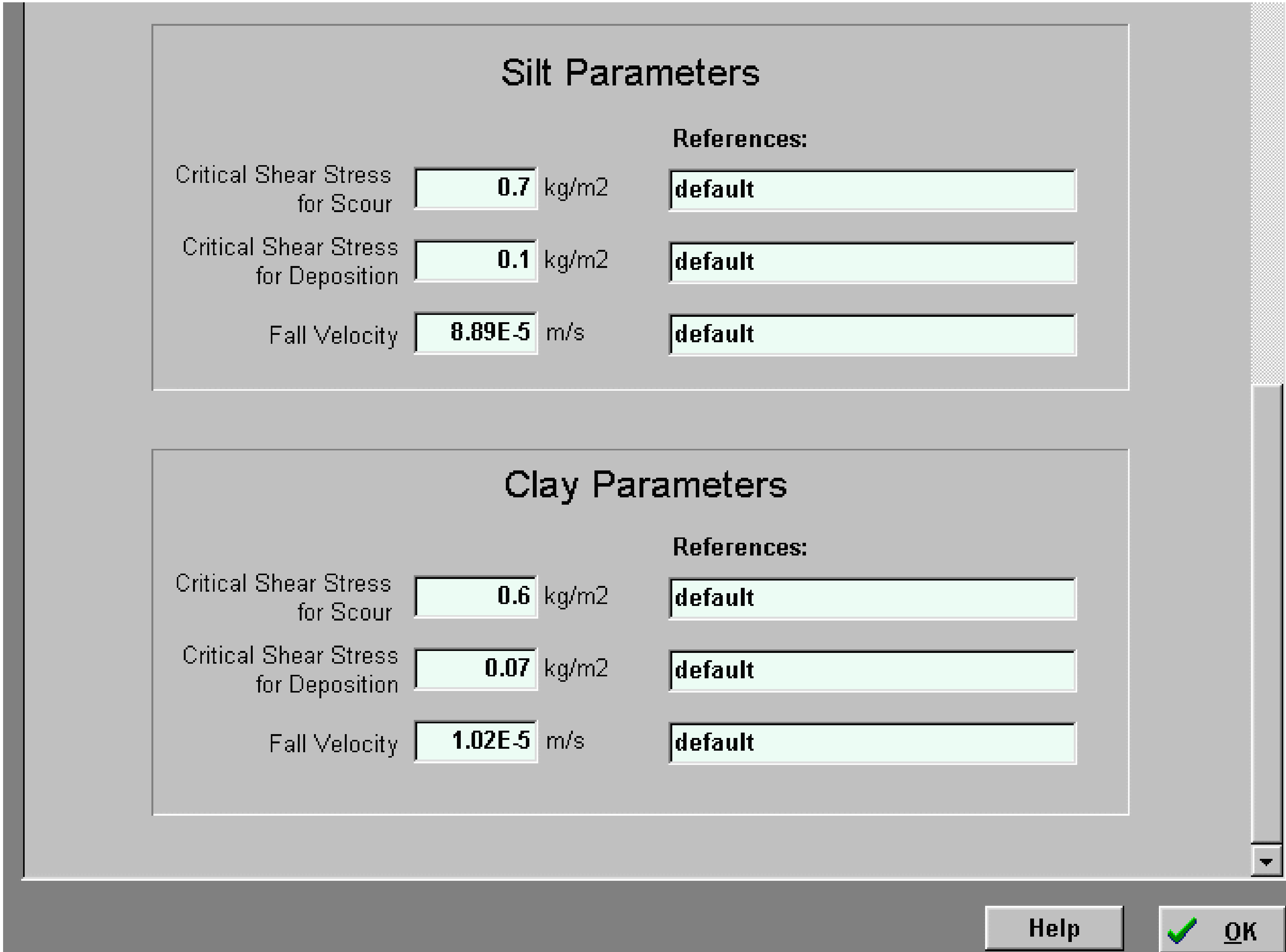
Bed Shear Stress (Tau) Closely Related to Water Velocity



Critical Shear Stress for Erosion and Deposition Key Parameters



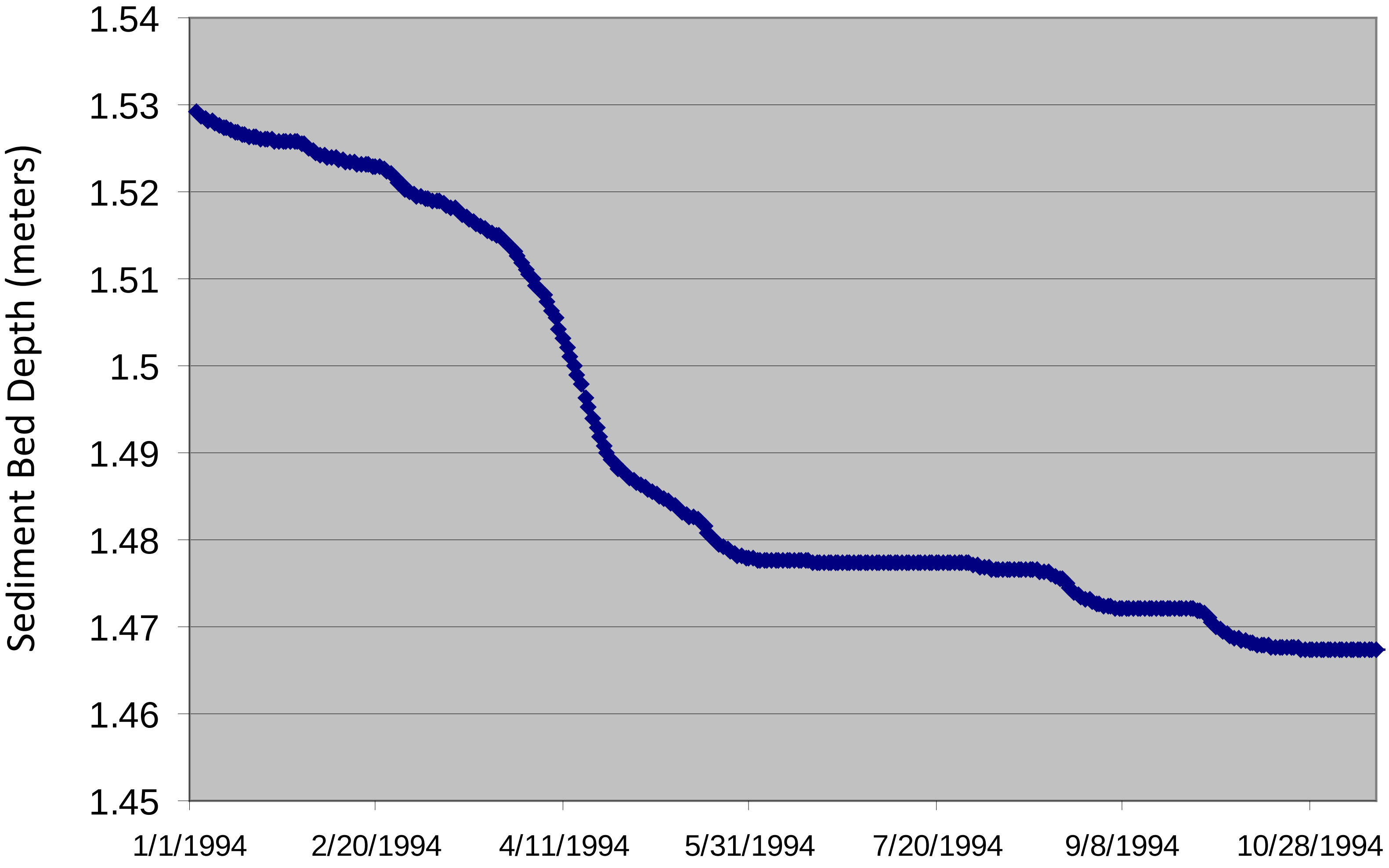
Sediment Model Parameters



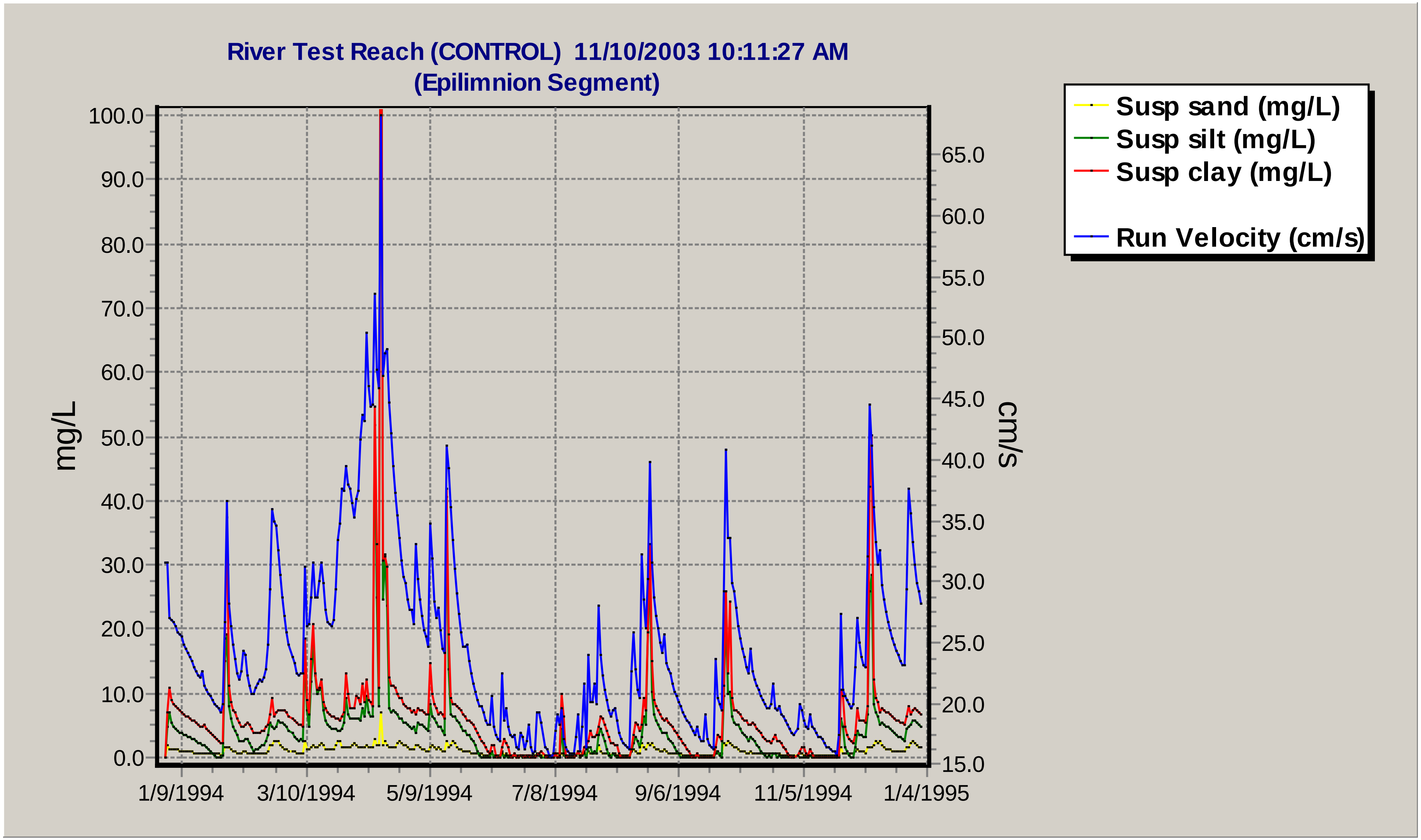
Sand Model

- No additional parameters / calibration required
- Potential concentration of sand in the water column is calculated as a function of water velocity and slope
- Uses Engelund and Hansen (1967) sediment transport relationships as presented by Brownlie (1981).

Sediment Bed Depth May be Plotted



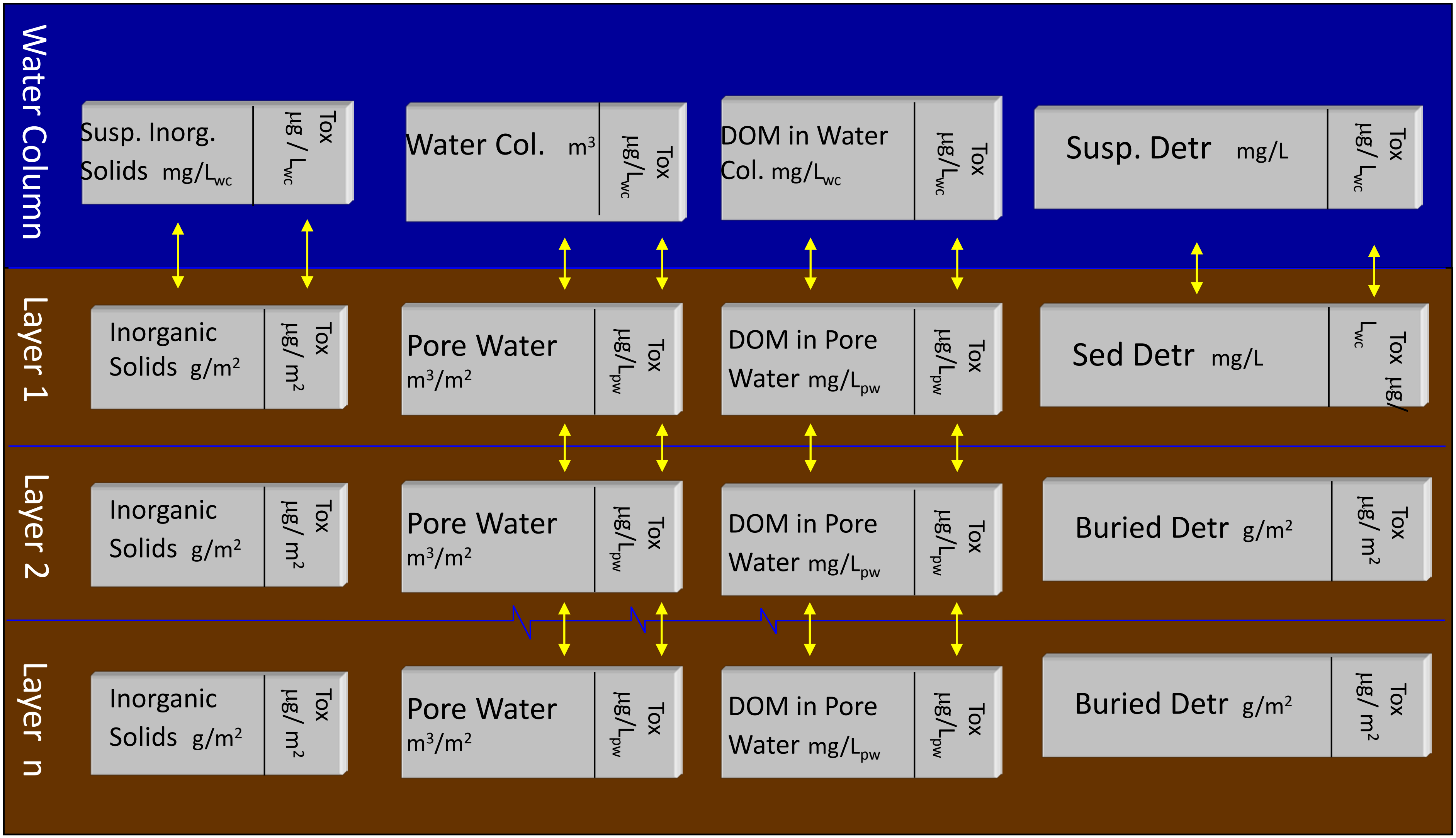
Suspended Sand, Silt, Clay may be Plotted



AQUATOX Multi-Layer Sediment Model

- Based on IPX version 2.7.4
- Developed as part of a Superfund project; now part of Release 3
- Can model up to ten distinct sediment layers on top of non-reactive hardpan.
- Each sediment layer assumed to be perfectly mixed.
- “Pez-dispenser” action avoids common numerical problems.

AQUATOX Multi-Layer Sediment Model based on the IPX module (Velleux et al. 2000)



Representation of Inorganic Sediments:

- **Cohesives:** particle size smaller than 63 mg (clay)
- **Non-Cohesives:** particle size from 63 to 250 mg (silt)
- **Non-Cohesives2:** particle size greater than 250 mg (sand)
- **Chemical sorption** to inorganic sediments may be modeled. (Multi-Layer sediment model only)

Composition of each Bed Layer

- Inorganic Sediments (and sorbed toxicants)
- Sedimented or Buried Detritus (and sorbed toxicants)
- Pore Waters (and dissolved toxicants)
- DOM in Pore Waters (and sorbed toxicants)

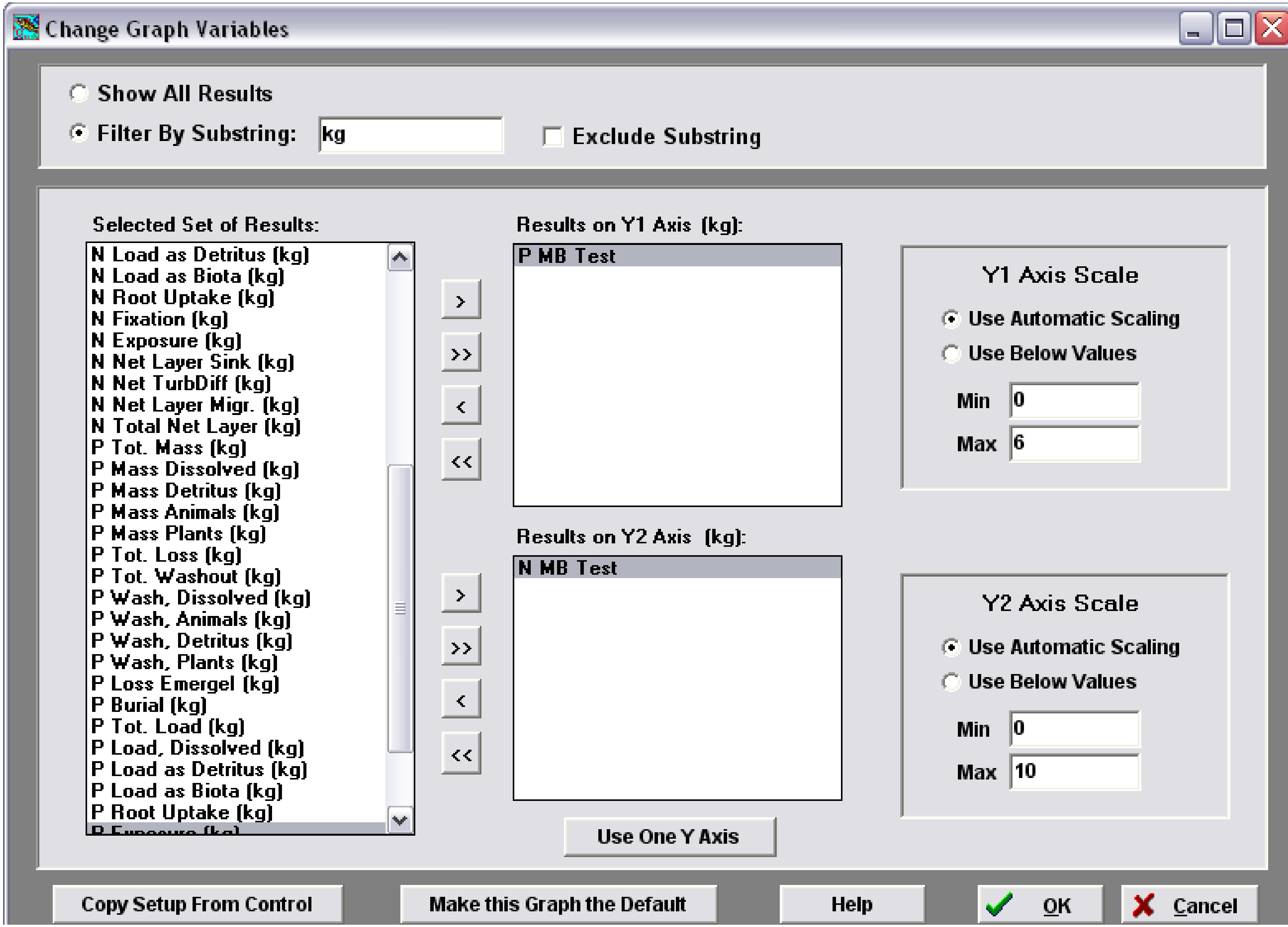
Sediment Model Data Requirements

- Densities of inorganic and organic sediments
- Sediment layer thicknesses
- Initial concentrations of each element and toxic exposure
- Each layer's porosity and density is calculated given densities and initial conditions
- Erosion/Deposition Velocities for inorganic sediments; alternatively erosion/deposition velocities may be internally calculated using HSPF-based model

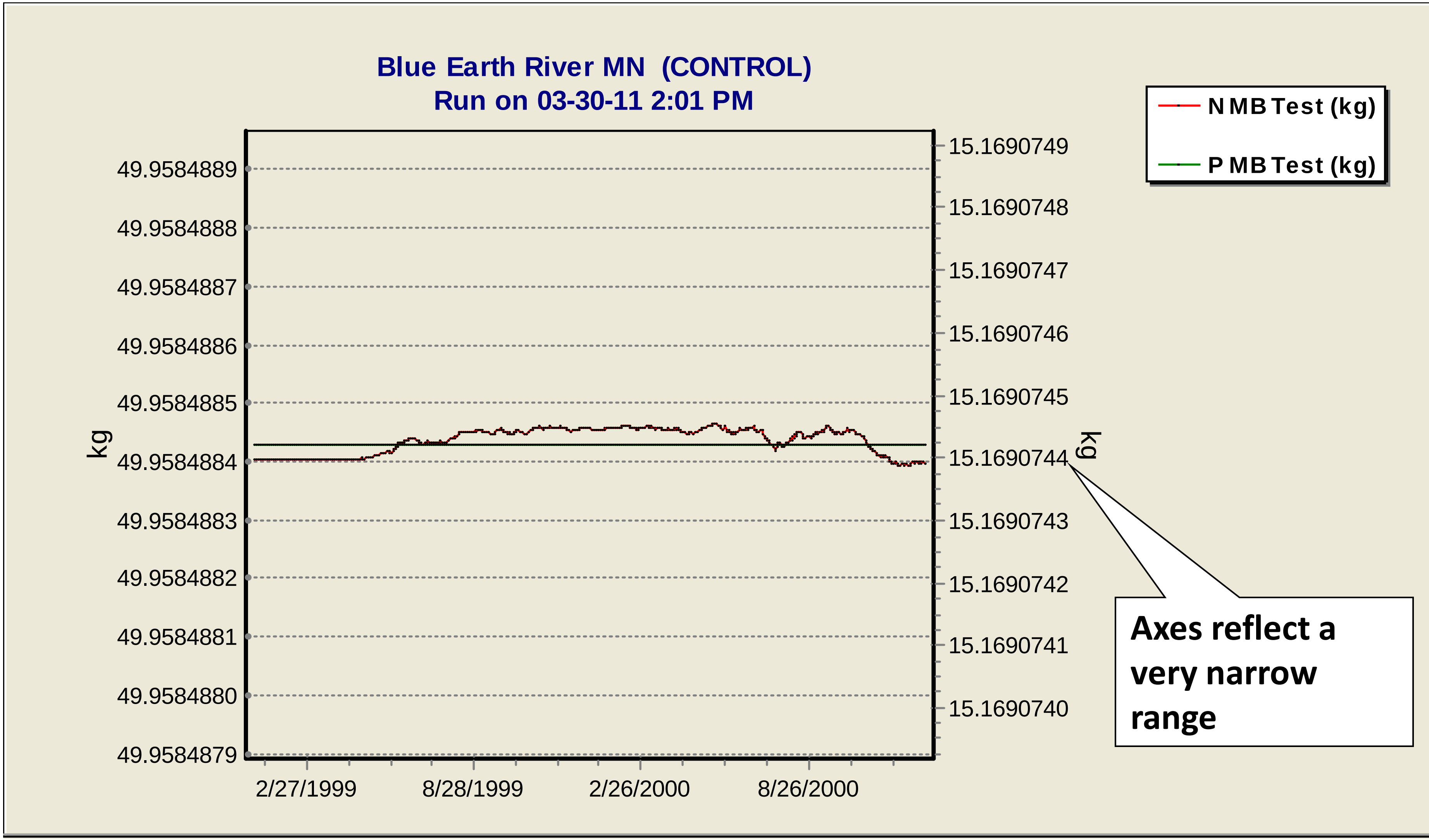
Demonstration: Stoichiometry and Mass Balance of Nutrients in Blue Earth River

- 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)

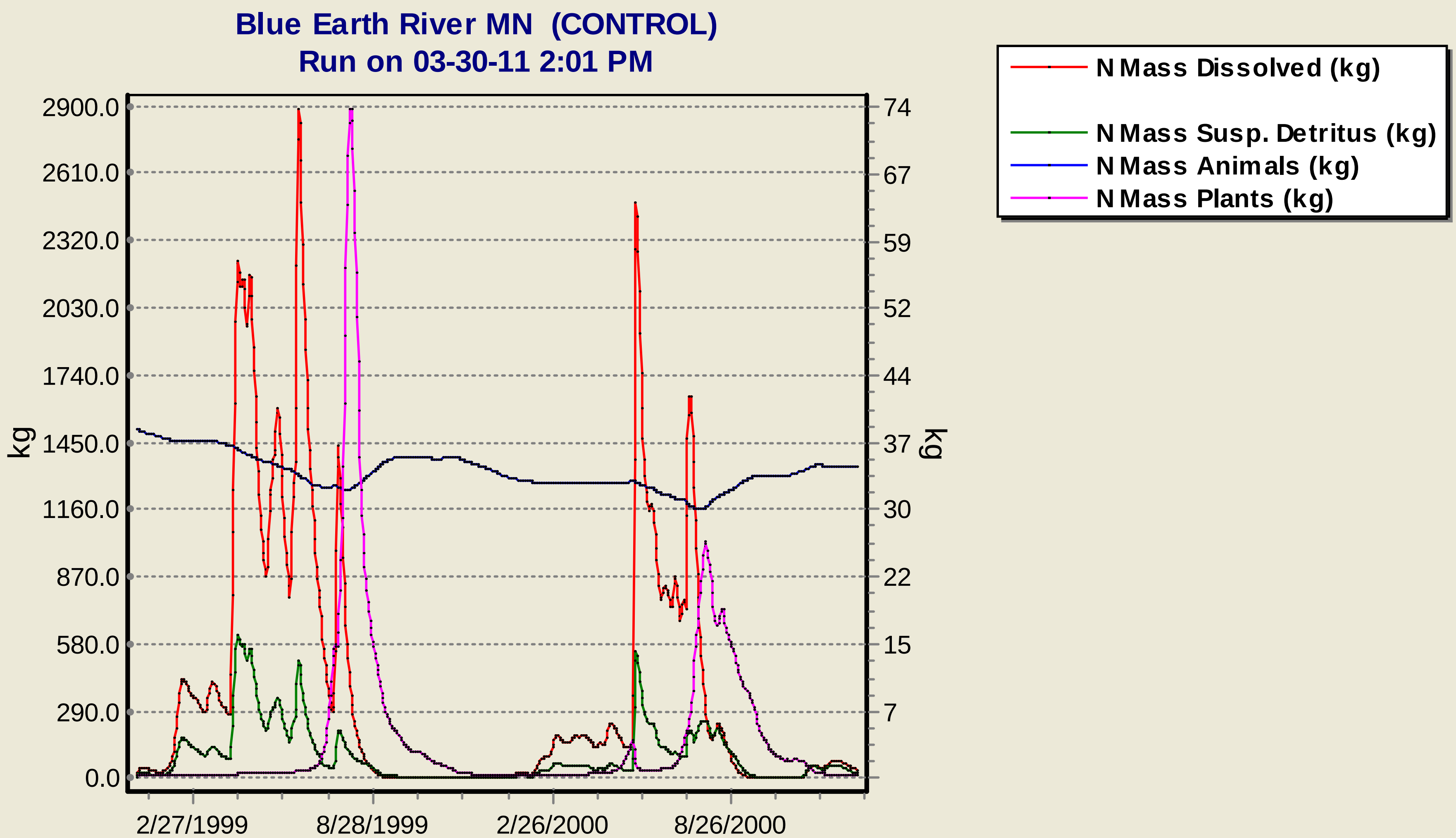
Nutrient Mass Balance Results Grouped



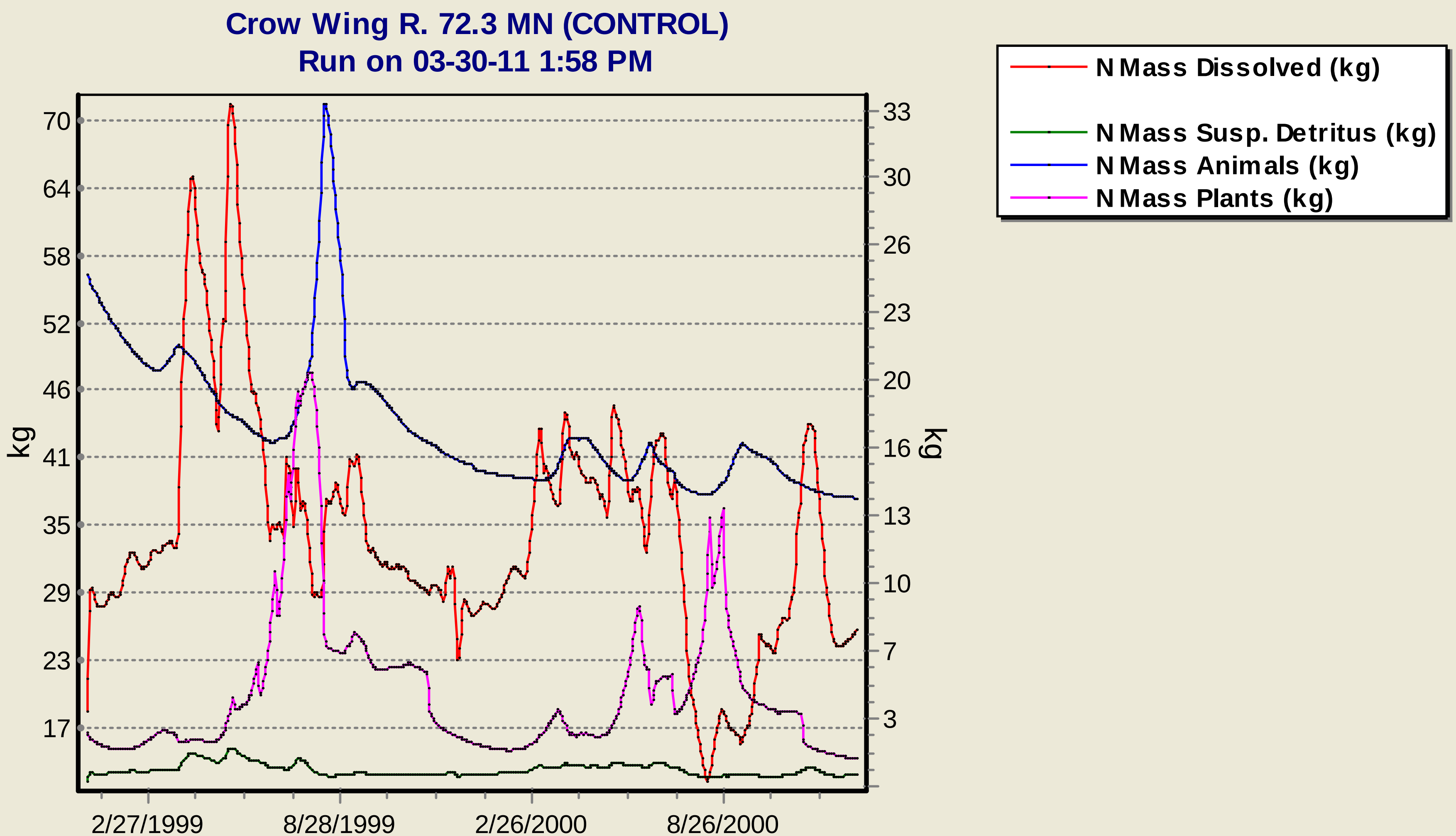
Mass is Balancing



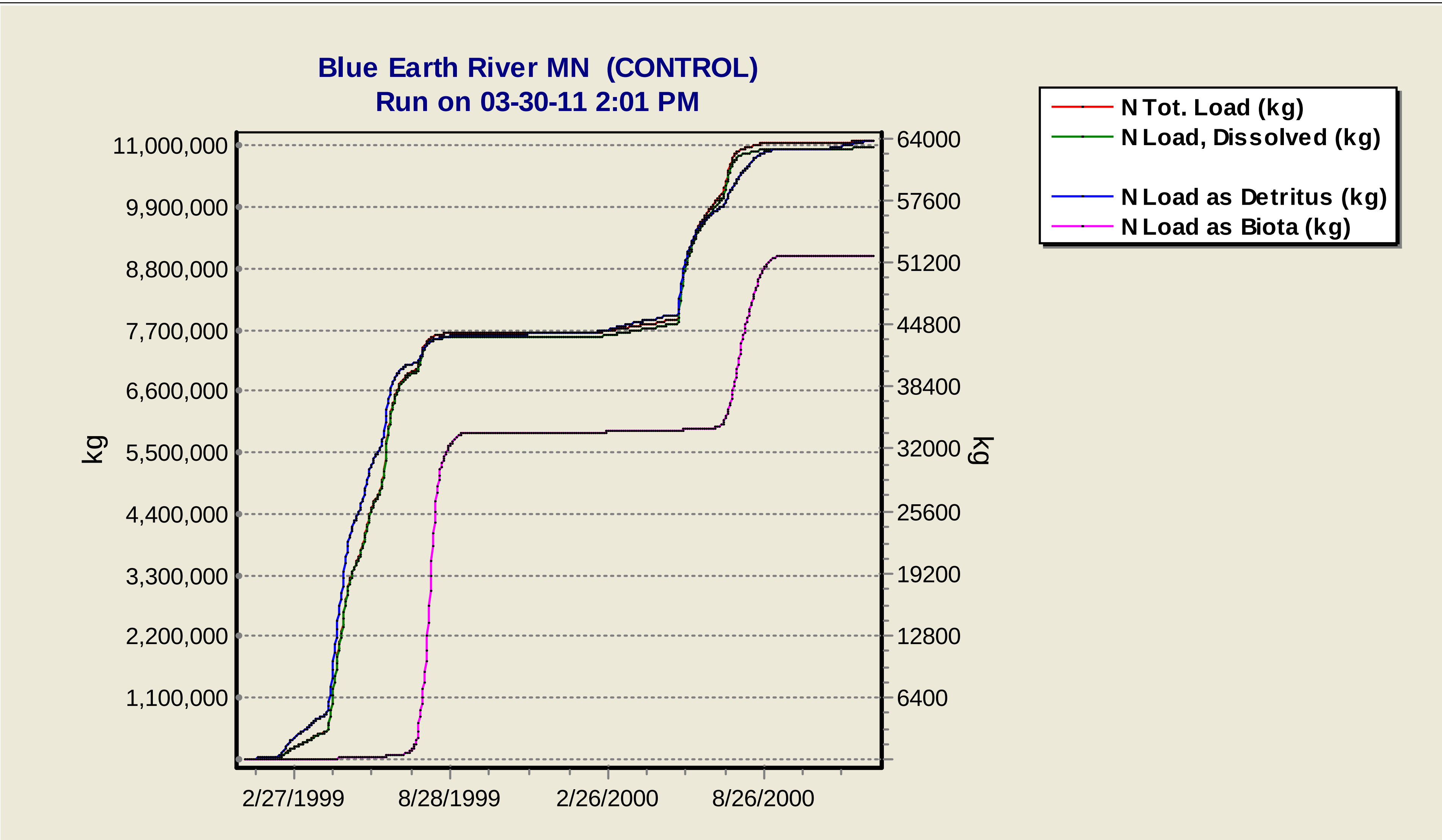
Where are the Nutrients within the System?



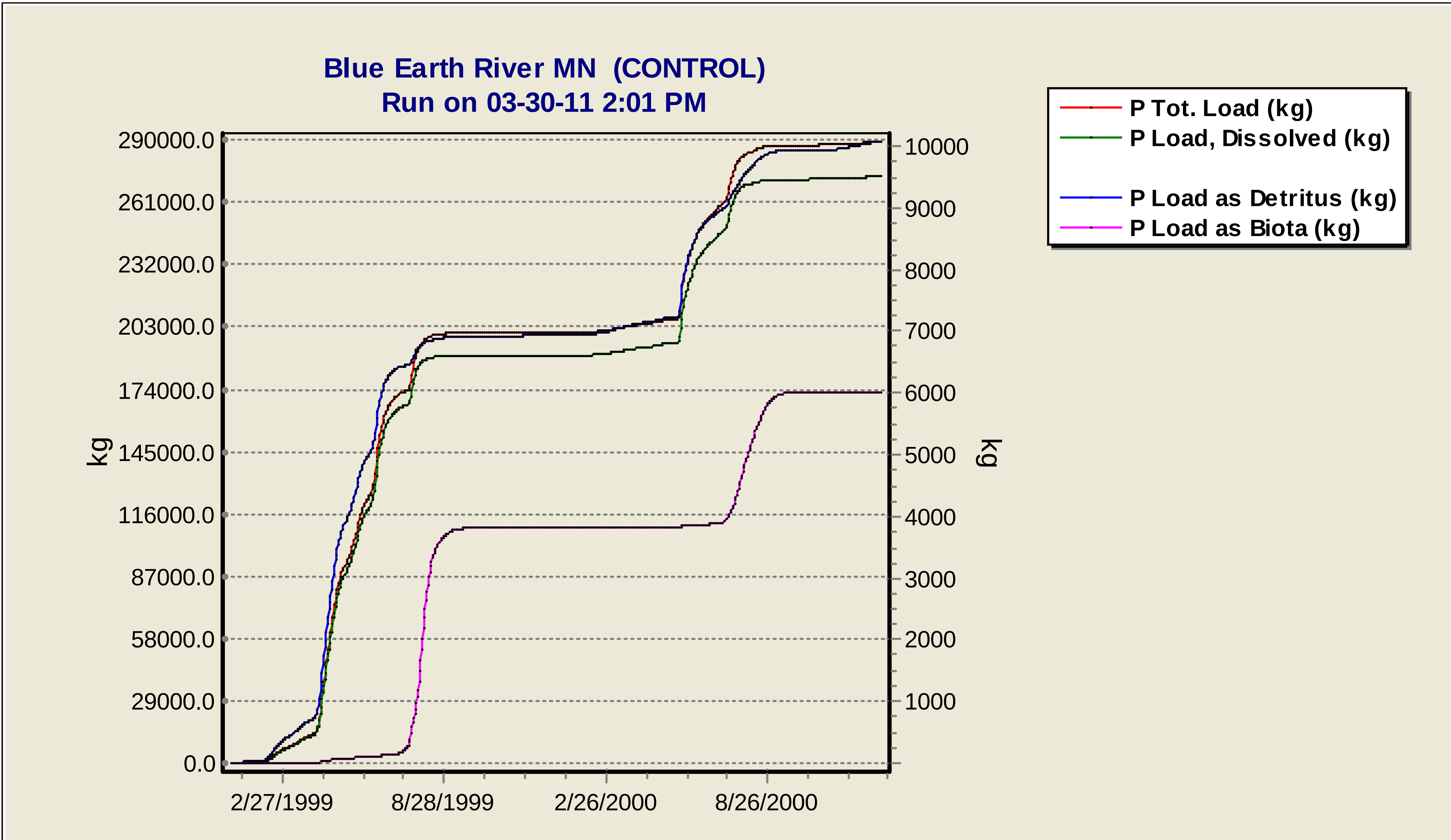
Contrast Blue Earth with the Crow Wing River



Nitrogen Loadings, Blue Earth River

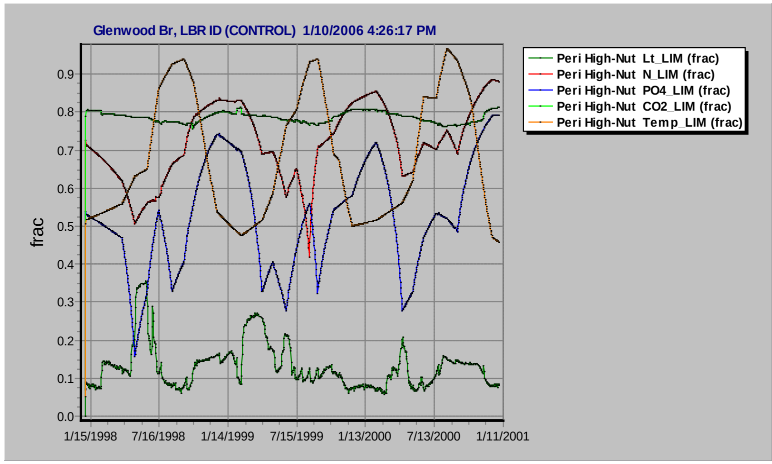


Phosphorus Loadings, Blue Earth River



Other Release 3 Notes

- Additional Output Categories
  - oxygen duration below a given threshold
  - minimum and maximum O_2
  - minimum and maximum un-ionized ammonia
- Chemical Mass Balance Testing
  - Tracks loadings of and fate of chemicals similar to nutrient mass balance covered earlier
- Trapezoidal Integration of Results
- Scientific Names in Databases
- Comprehensive Sensitivity Analysis



- Beta test version: www.warrenpinnacle.com/prof/AQUATOX

Summary, Wrap-up

What we've tried to cover in this course:

- What AQUATOX can do
- A start on how to do it
- In what situations you would want to use it

Value added of AQUATOX

- **Process-based approach yields better understanding of ecosystem**
  - feedback loops, indirect effects, trophic cascades
  - Relative importance of multiple stressors
- **Leads to better management decisions**
  - Compare different management options
  - Avoid unintended consequences
  - What stressor to control first
- **Get more bang from monitoring buck**
  - Fill in gaps between sampling periods
  - Identify monitoring needs

Challenges

- It's not an easy model to master!
  - Complex model reflects the complex ecosystem
  - Some processes omitted or imperfectly understood
- Calibration and parameterization are probably hardest tasks
  - Technical note(s), data sources on web site
- High data requirements
  - Many inputs and parameters
  - Continue to expand data libraries and utilities

Please Keep in Touch!

- Applications help drive enhancements, example studies and data libraries
- Growing user community builds robustness and confidence
- Continued model and user support
  - One-on-one technical support is available
  - AQUATOX listserver
- Visit the AQUATOX web site
  - http://water.epa.gov/scitech/datait/models/aquatox
  - Citations of articles using or reviewing AQUATOX
  - Data sources