

# AQUATOX Training Workshop (Day 3)

Web Training Materials, August 2012

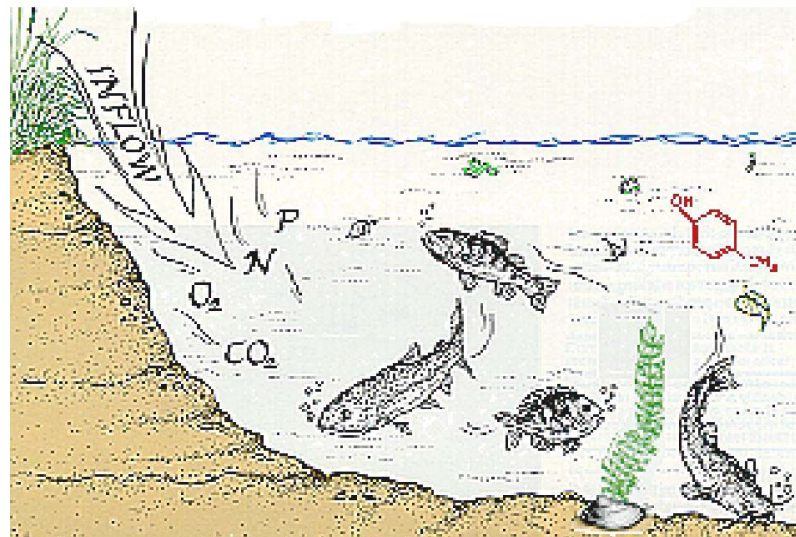
Based on Workshop Given for EPA Region 6, Dallas, Texas, December 2010  
and Columbia River Intertribal Fish Commission, November 2011



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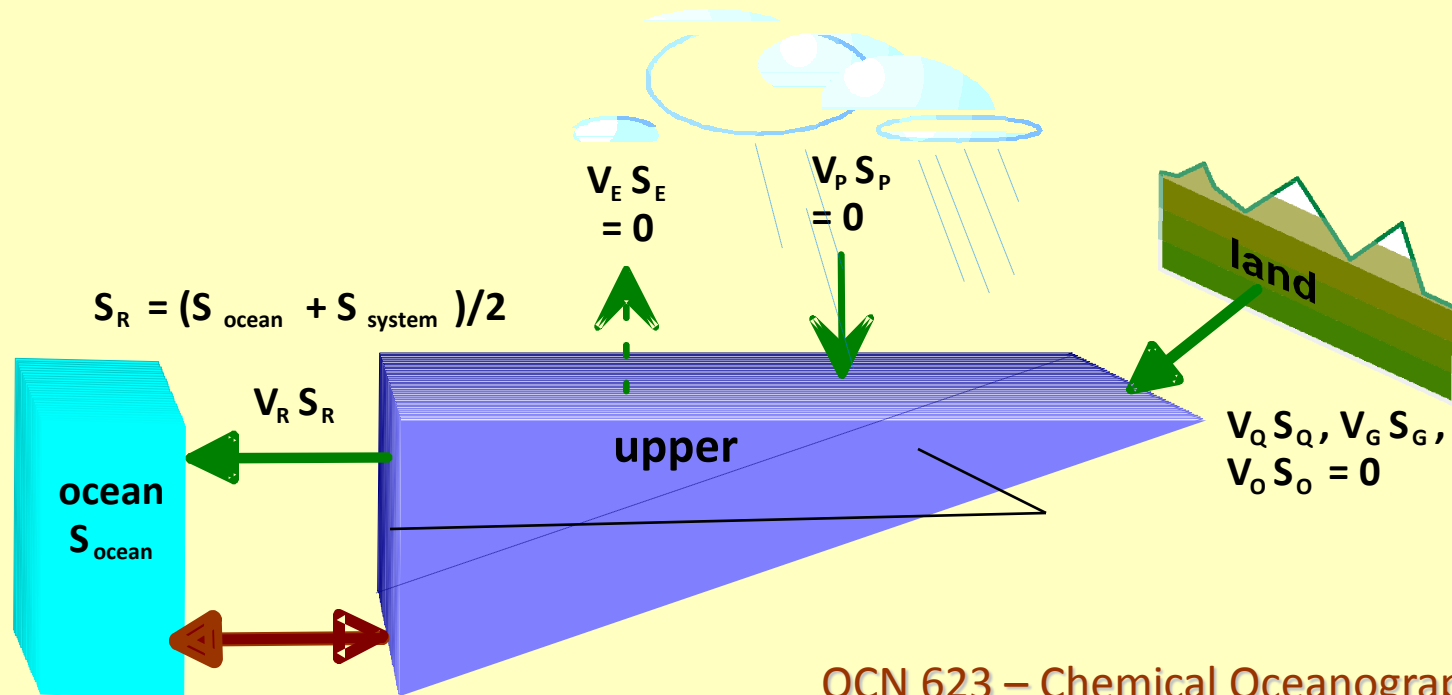


# Modeling Estuarine Conditions

- 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

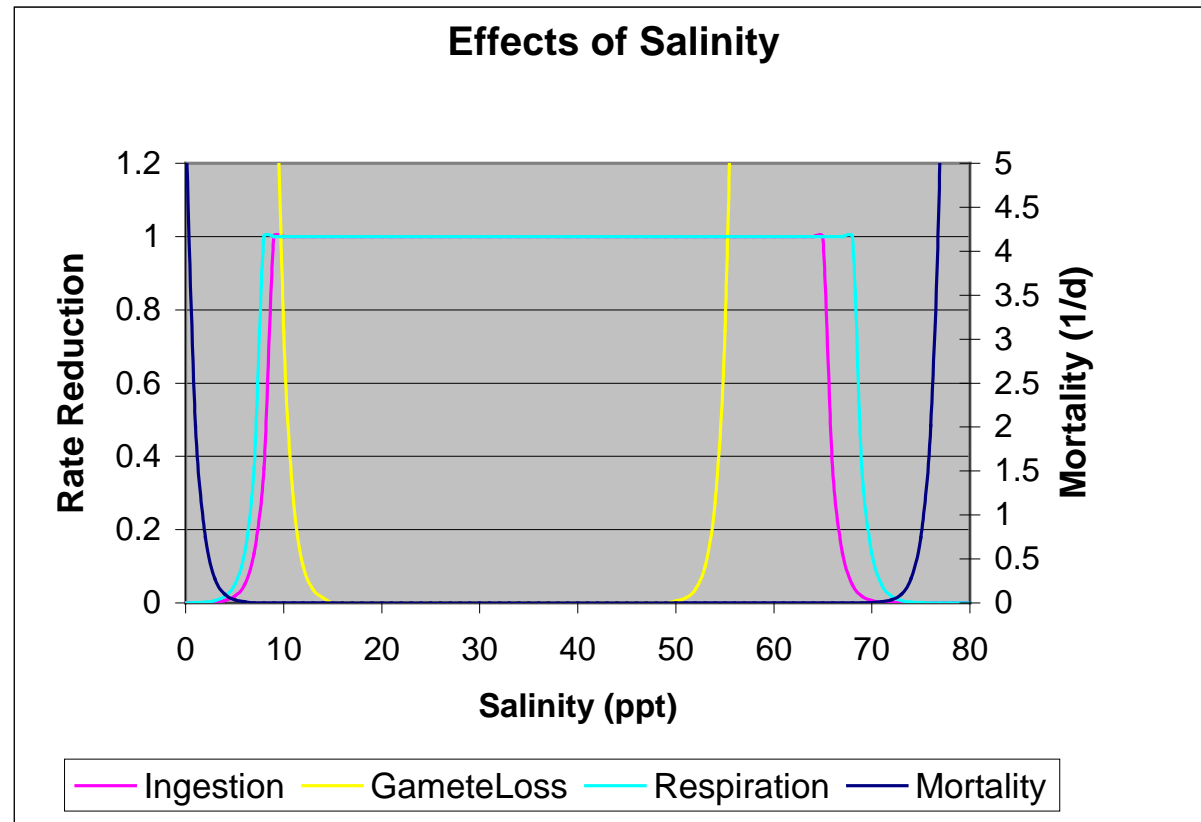
# Estuarine Features

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



# Estuarine Features

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

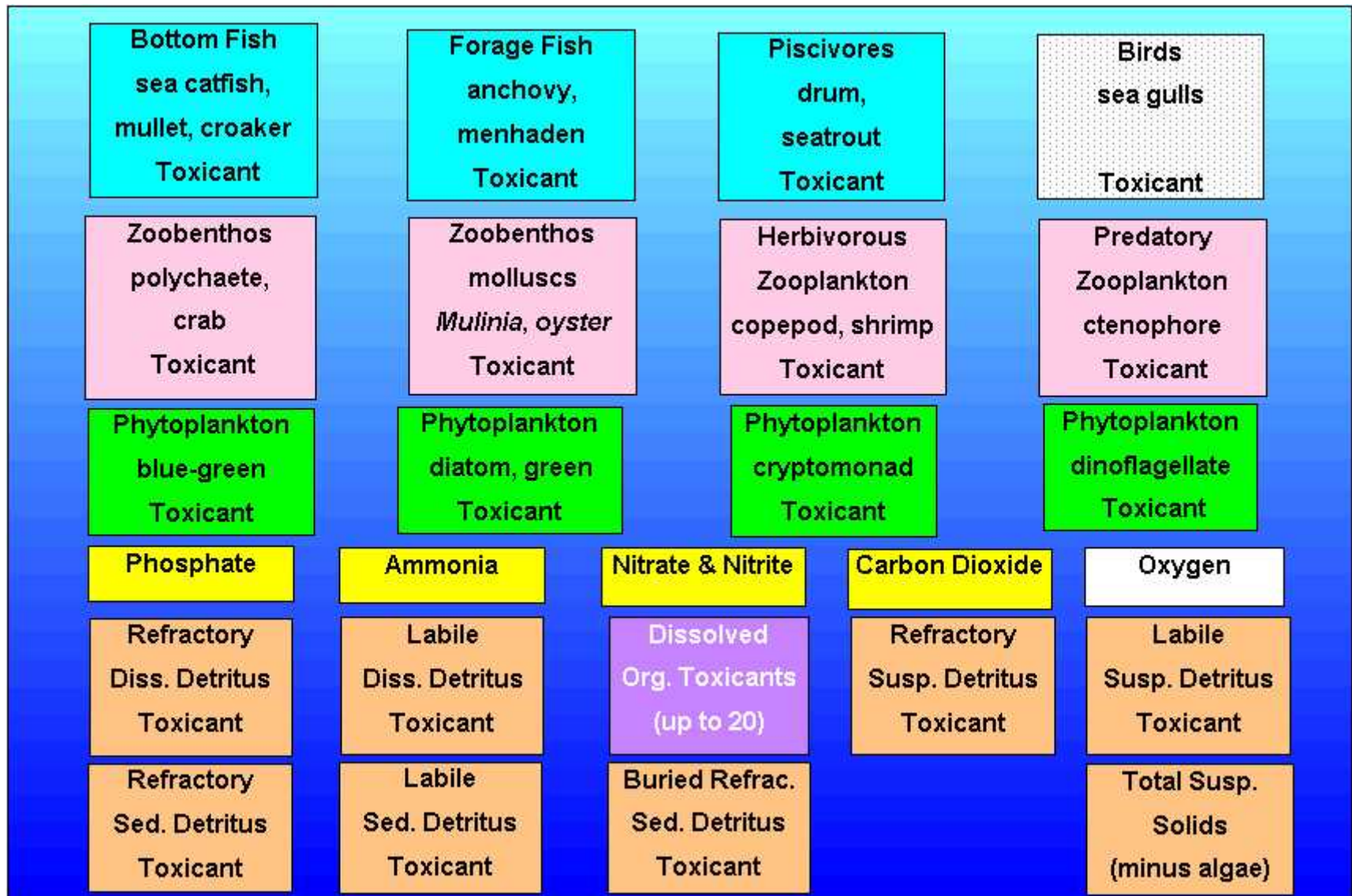


# **Estuarine version roughly calibrated for Galveston Bay, Texas, to evaluate toxicants**



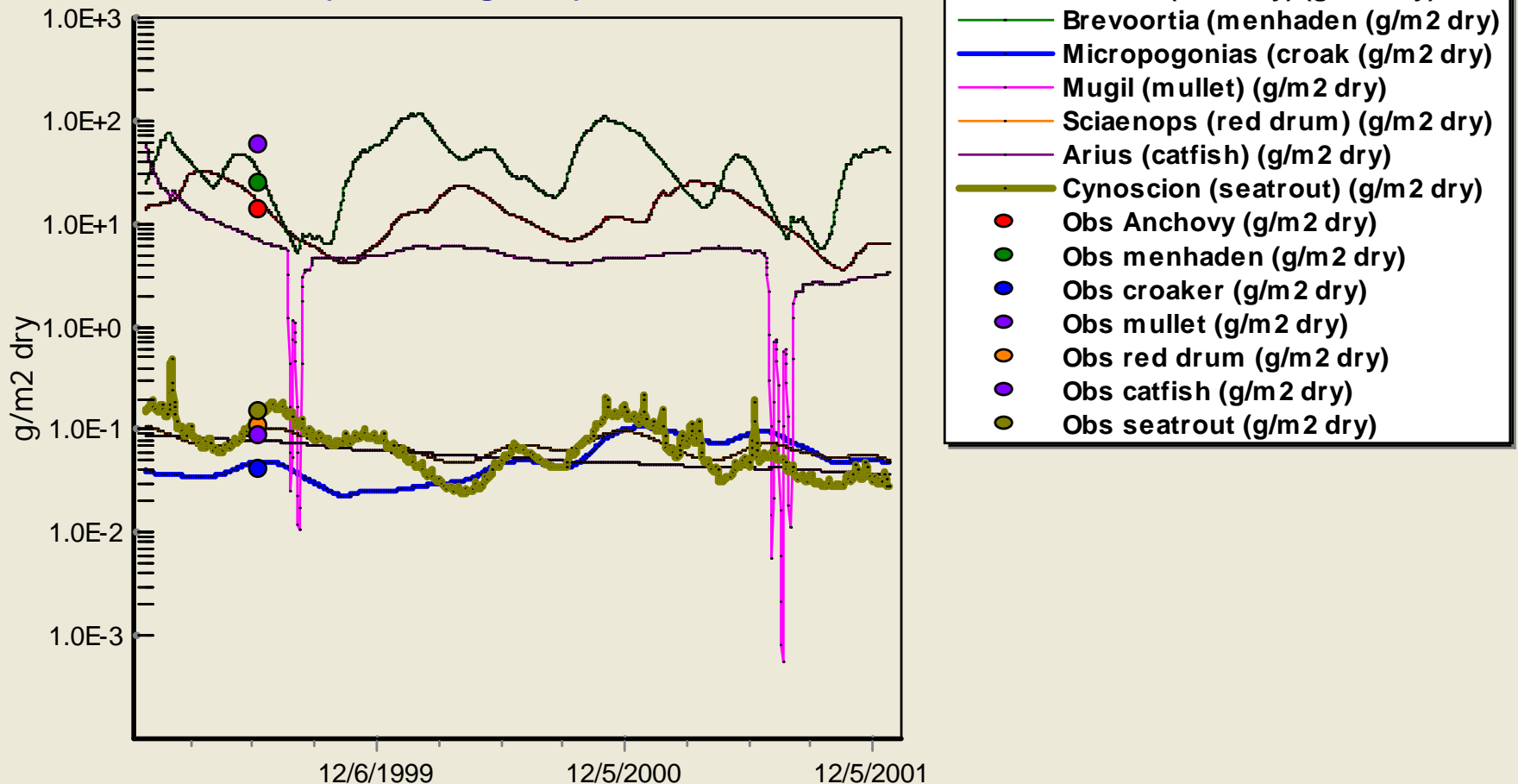
Photo Courtesy NASA Johnson Space Center

# Galveston Bay, Texas, compartments

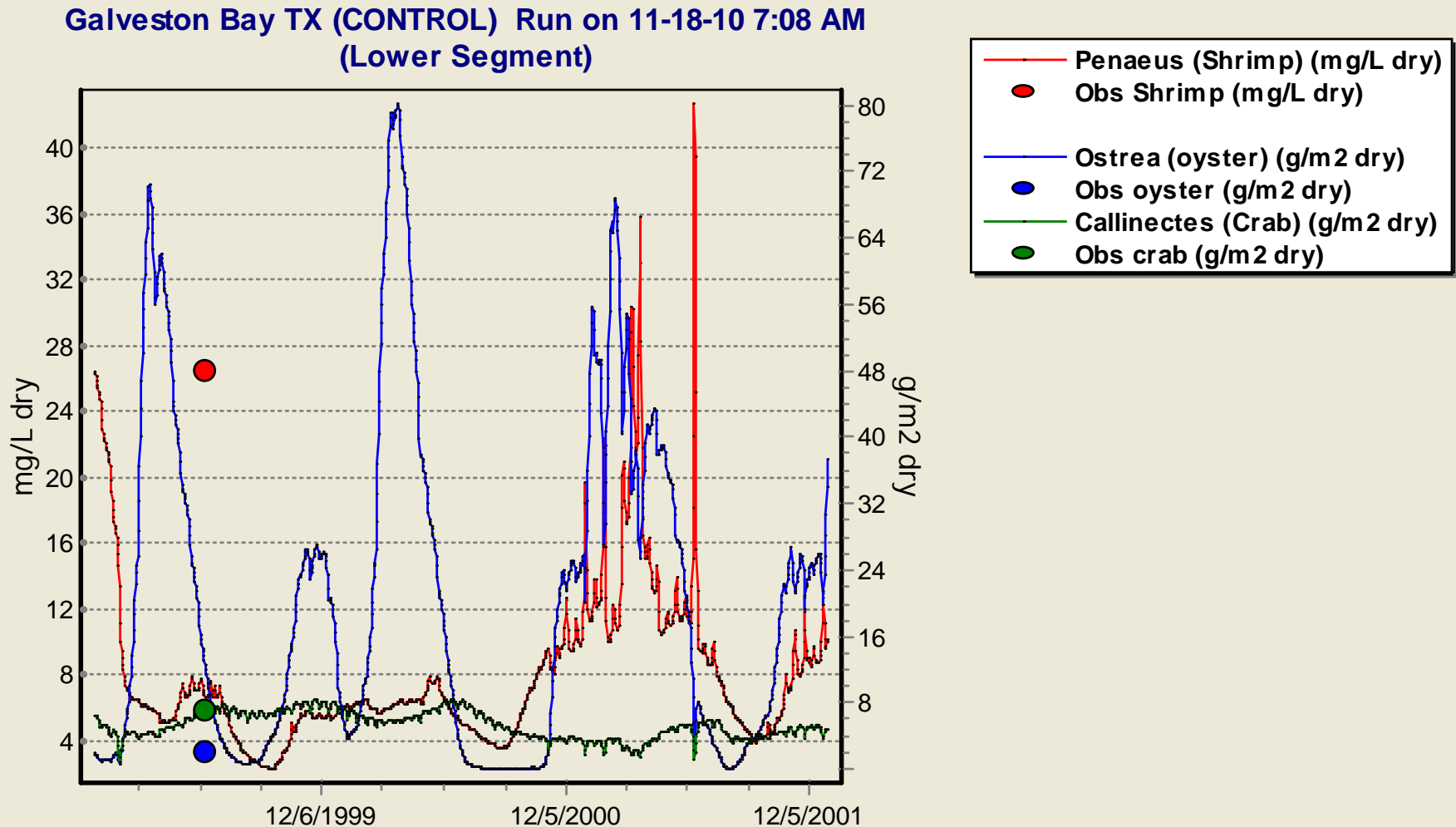


# Can model biomass of commercial and other species of fish

Galveston Bay TX (CONTROL) Run on 11-18-10 7:08 AM  
(Lower Segment)



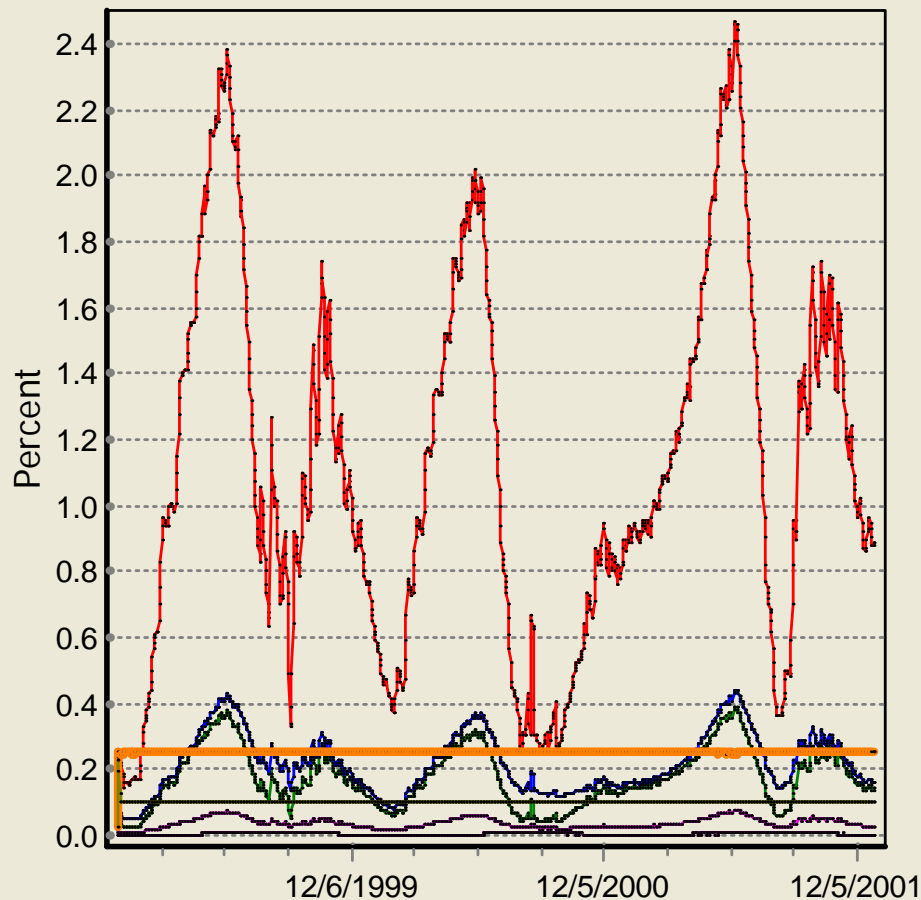
# Can also model biomass of shrimp, oysters, and other invertebrates





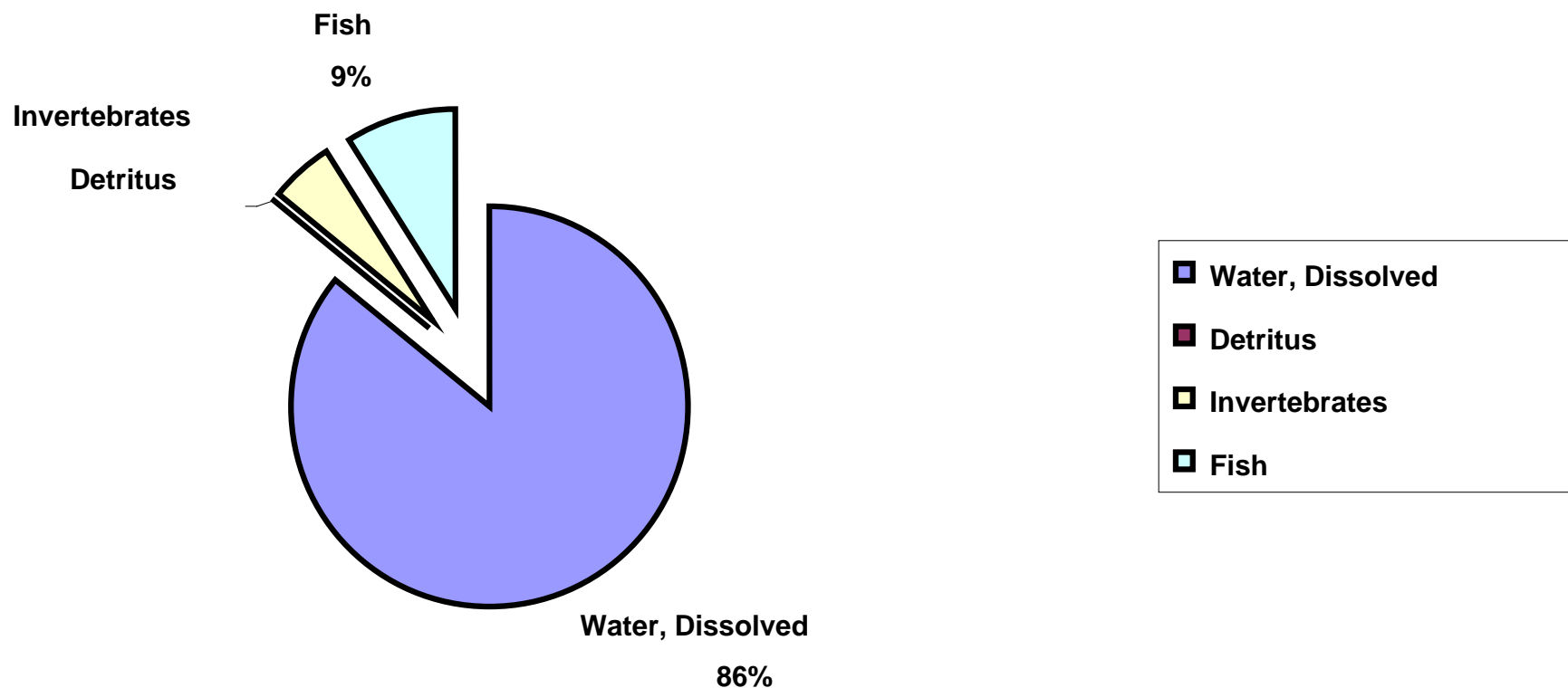
# Predicted rates for crabs (as % of biomass)

Galveston Bay TX (CONTROL) Run on 11-18-10 7:08 AM  
(Upper Segment)

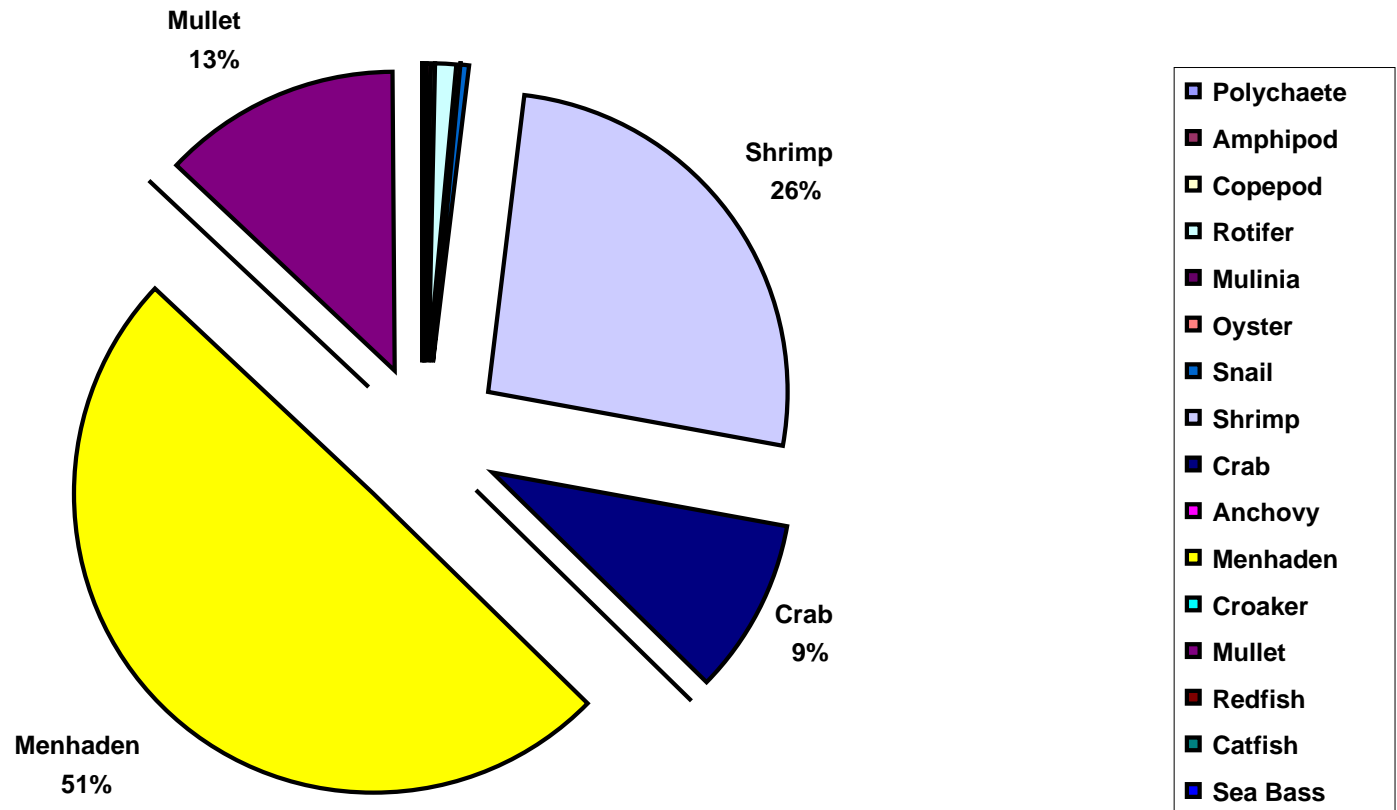


- Callinectes (Crab) Consumption (Percent)
- Callinectes (Crab) Defecation (Percent)
- Callinectes (Crab) Respiration (Percent)
- Callinectes (Crab) Excretion (Percent)
- Callinectes (Crab) Fishing (Percent)
- Callinectes (Crab) Predation (Percent)
- Callinectes (Crab) Mortality (Percent)

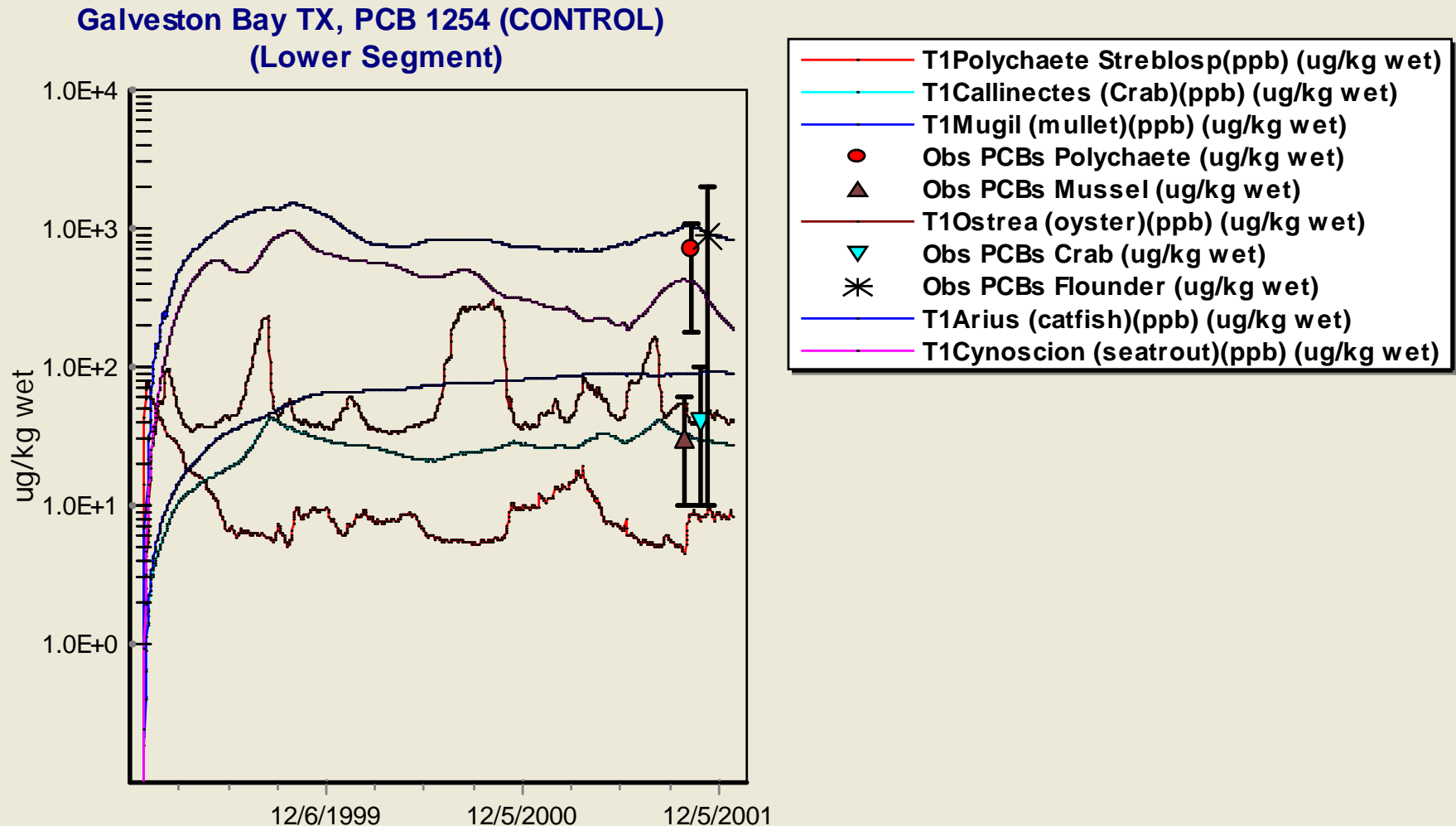
# Predicted distribution of PFOS among major compartments in Galveston Bay at end of year



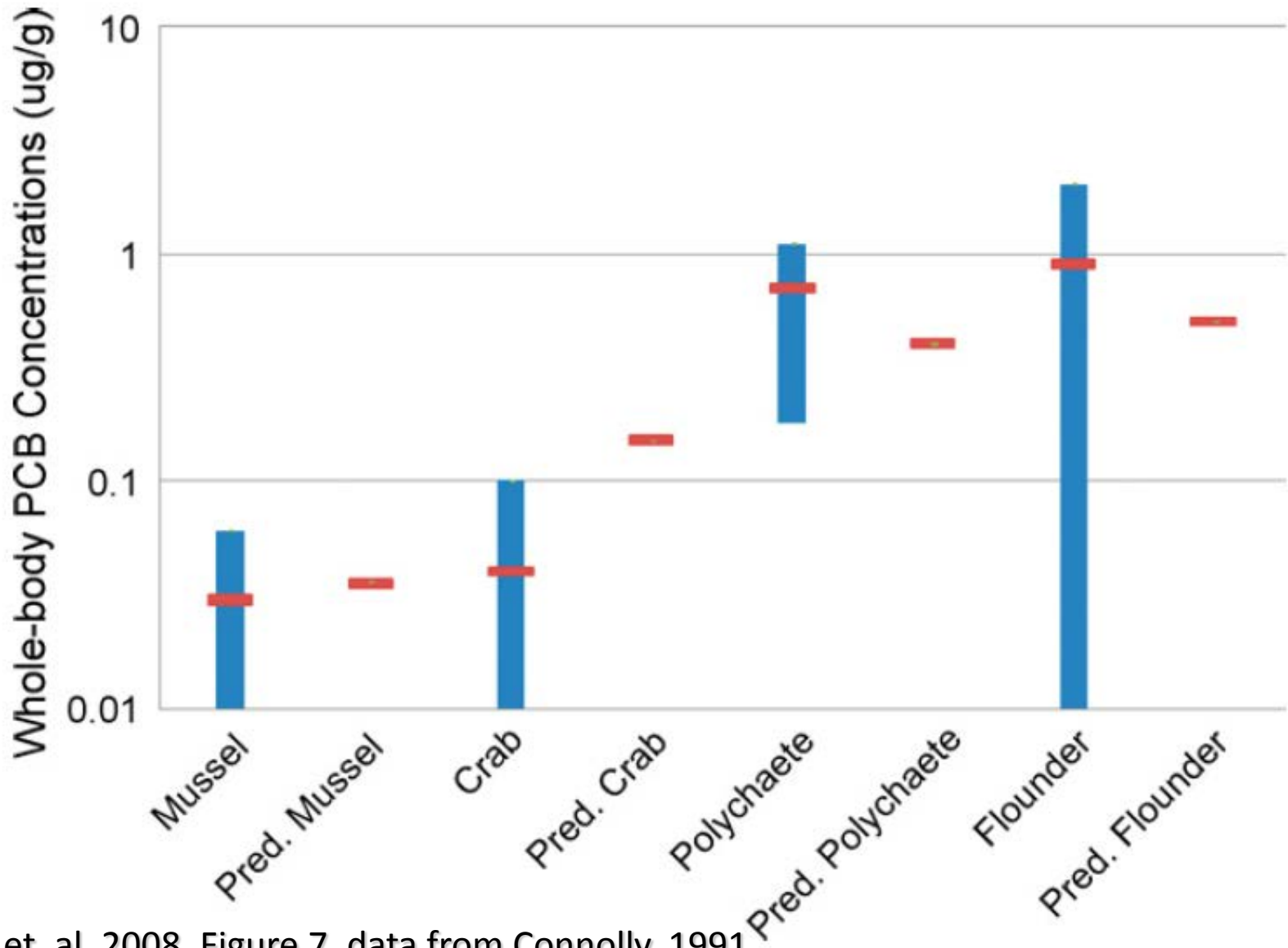
# Distribution of PFOS among biotic compartments at end of year



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



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



# Estuarine Model Data Requirements

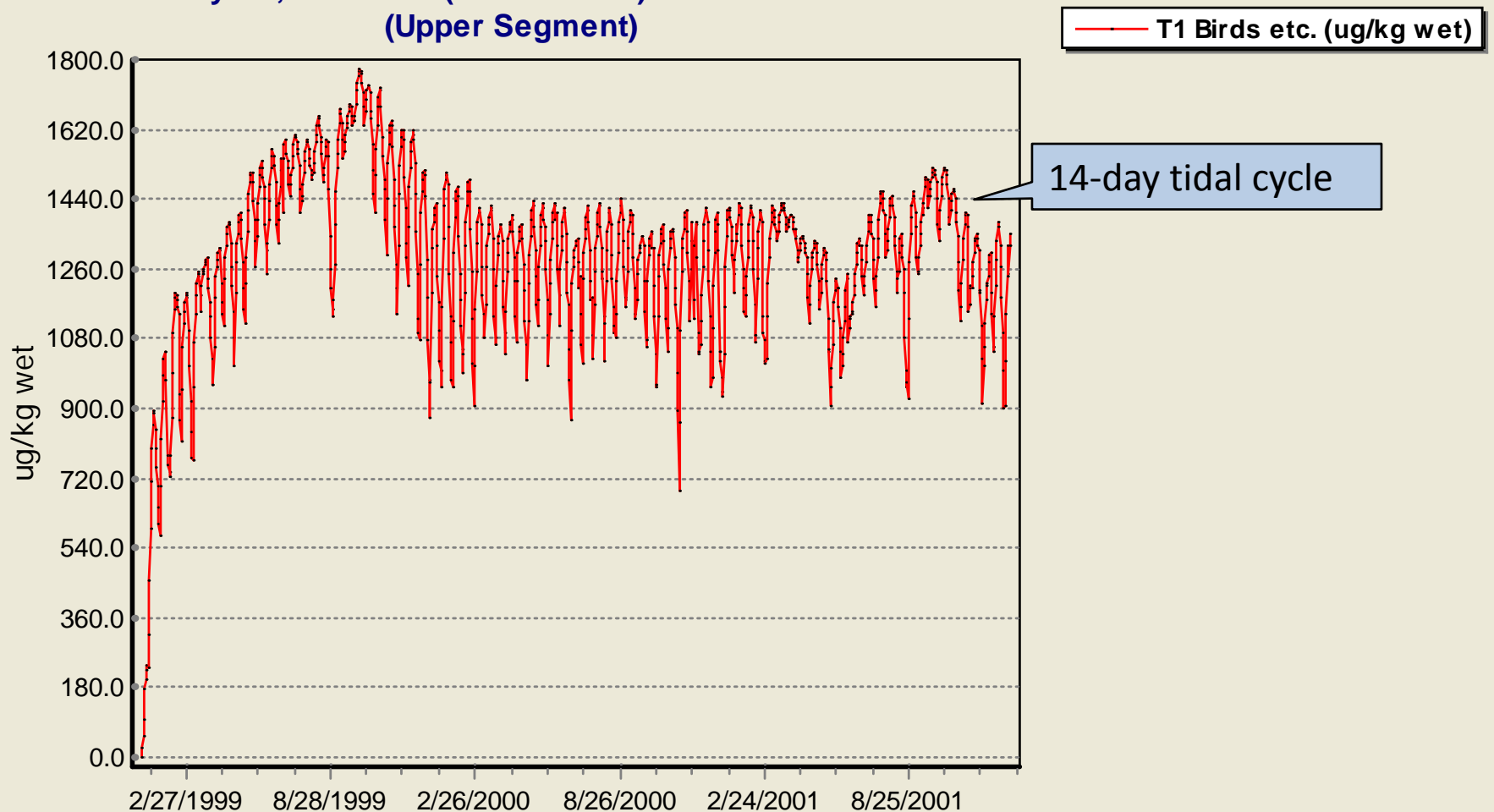
- Time Series of “Upper Layer” and “Lower Layer” Salinities for Salt Wedge Model
- Tidal Range Model Parameters
  - “harmonic constants”, often available from NOAA website
- Estuary Site Width
- Loadings of Freshwater Inflow

# 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

Galveston Bay TX, PCB 1254 (PERTURBED) Run on 01-4-10 9:07 AM  
(Upper Segment)





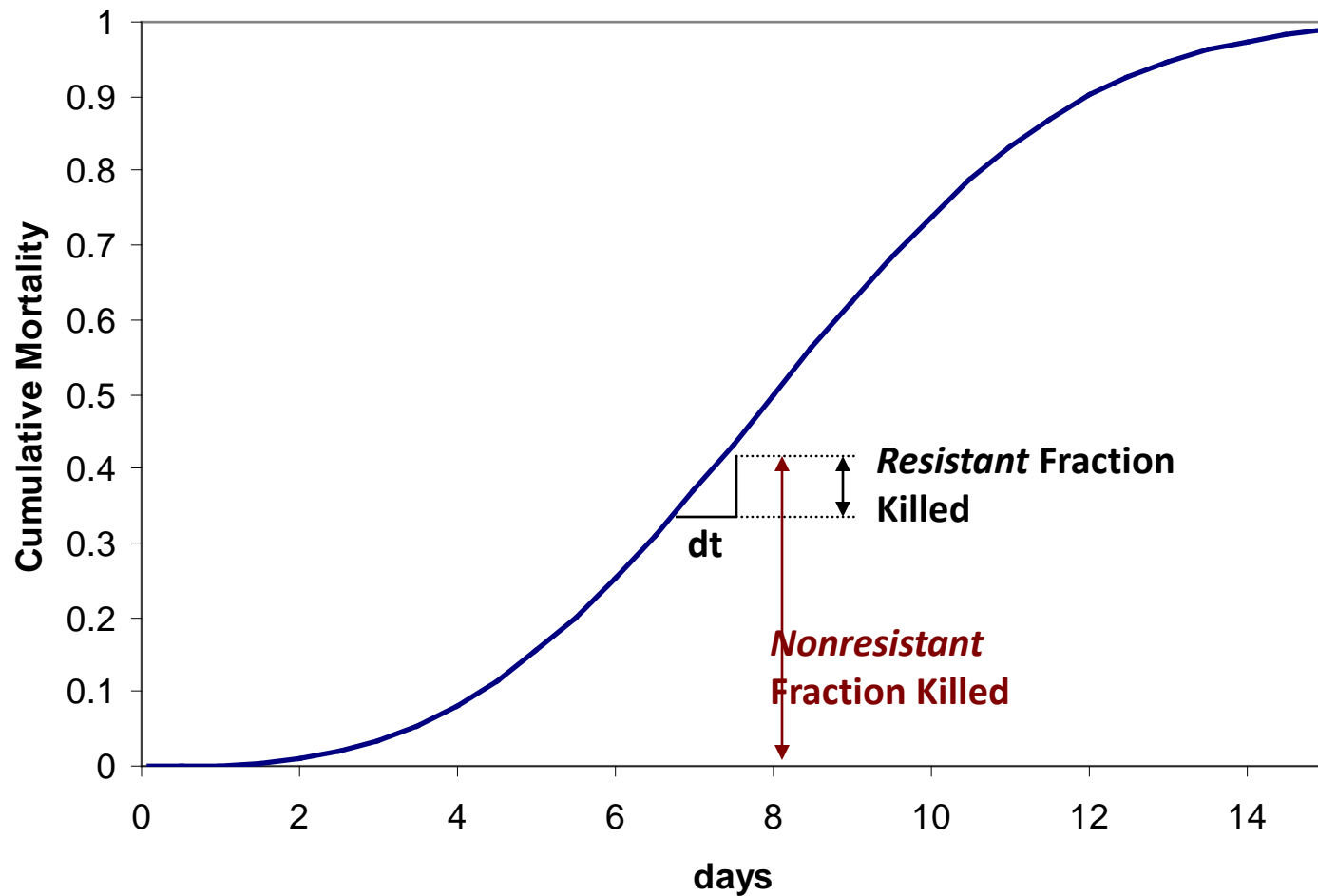
# Modeling Toxicity of Chemicals

- 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

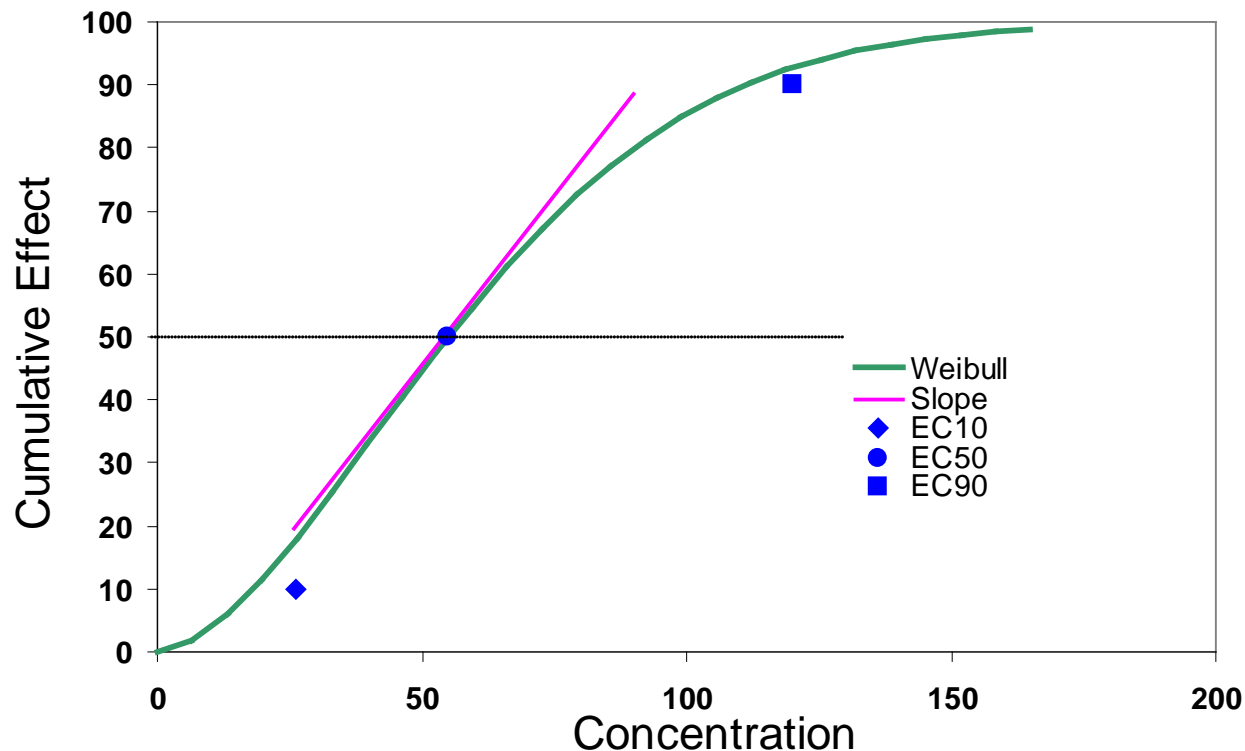
Two-parameter Weibull distribution as in Christensen and Nyholm (1984)

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

Two Required Parameters:

LC50 (or EC50)

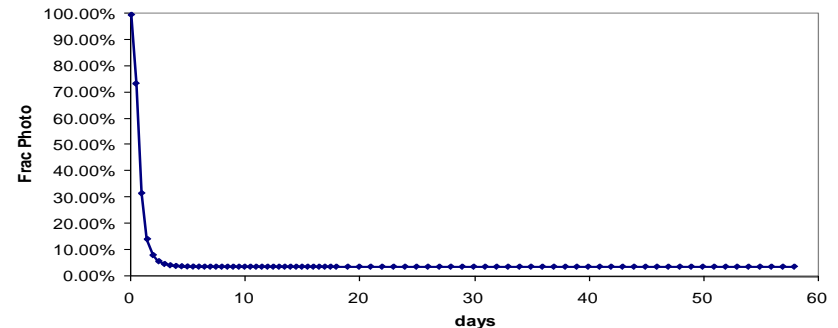
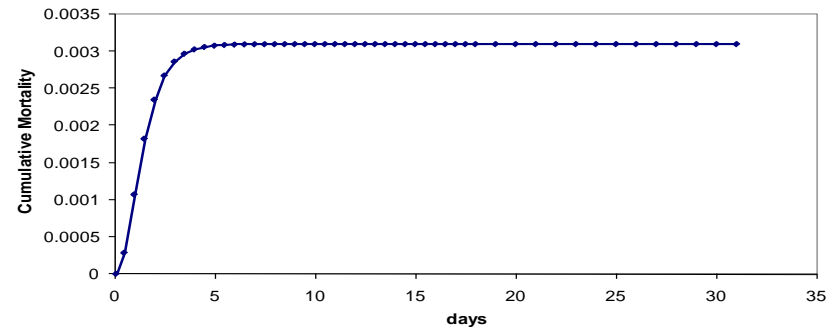
“Slope Factor” = Slope at LC50 multiplied by LC50



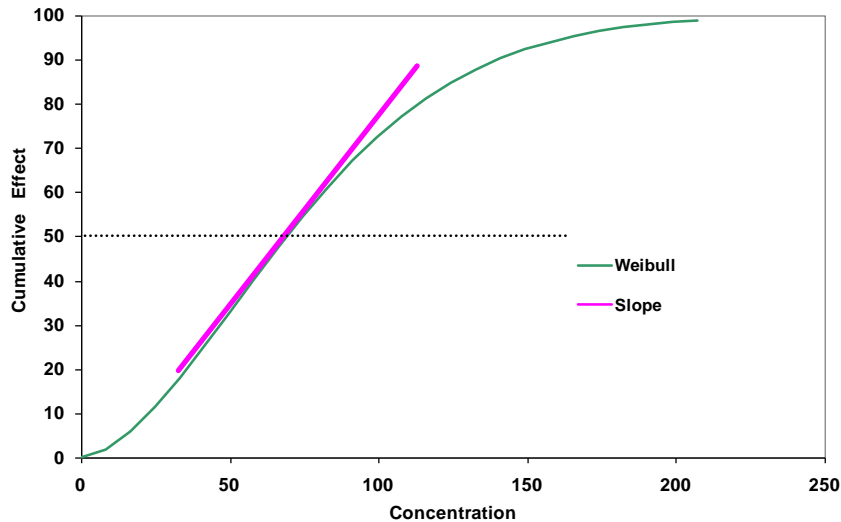
# Spreadsheet Demo

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

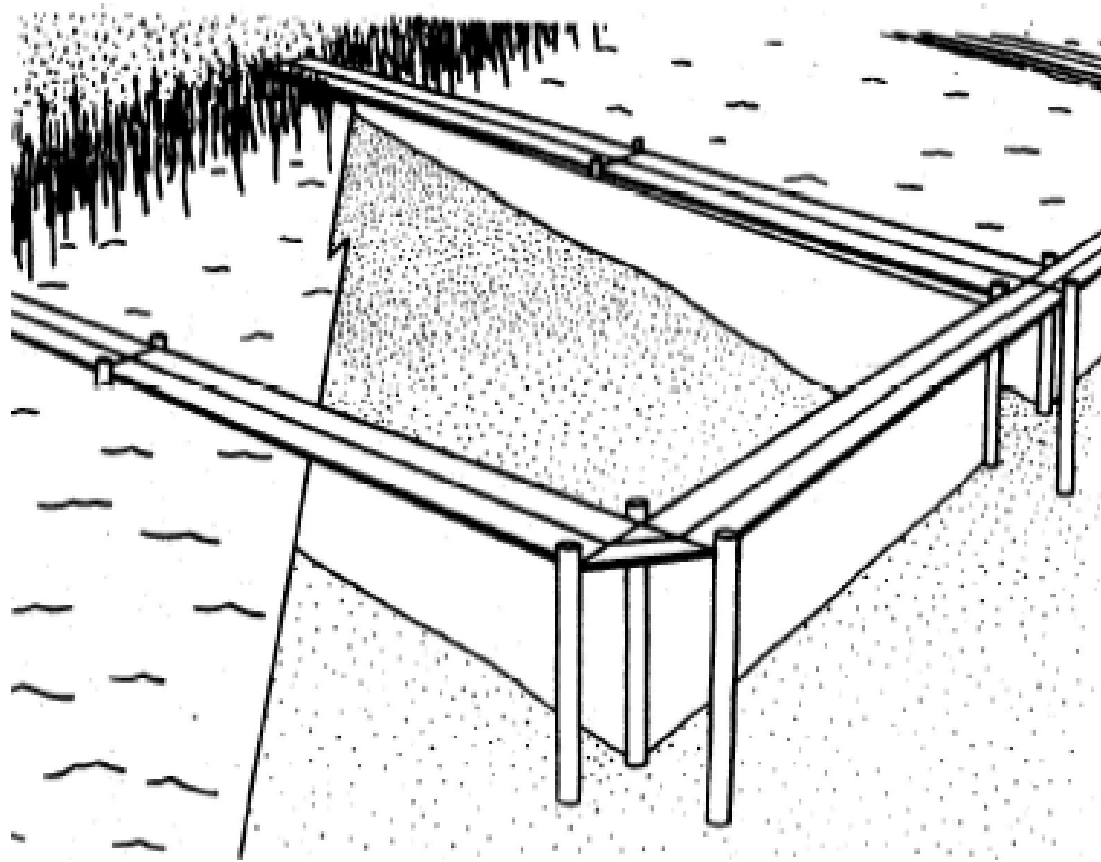
AQUATOX\_Internal\_Toxicity\_Model.xls



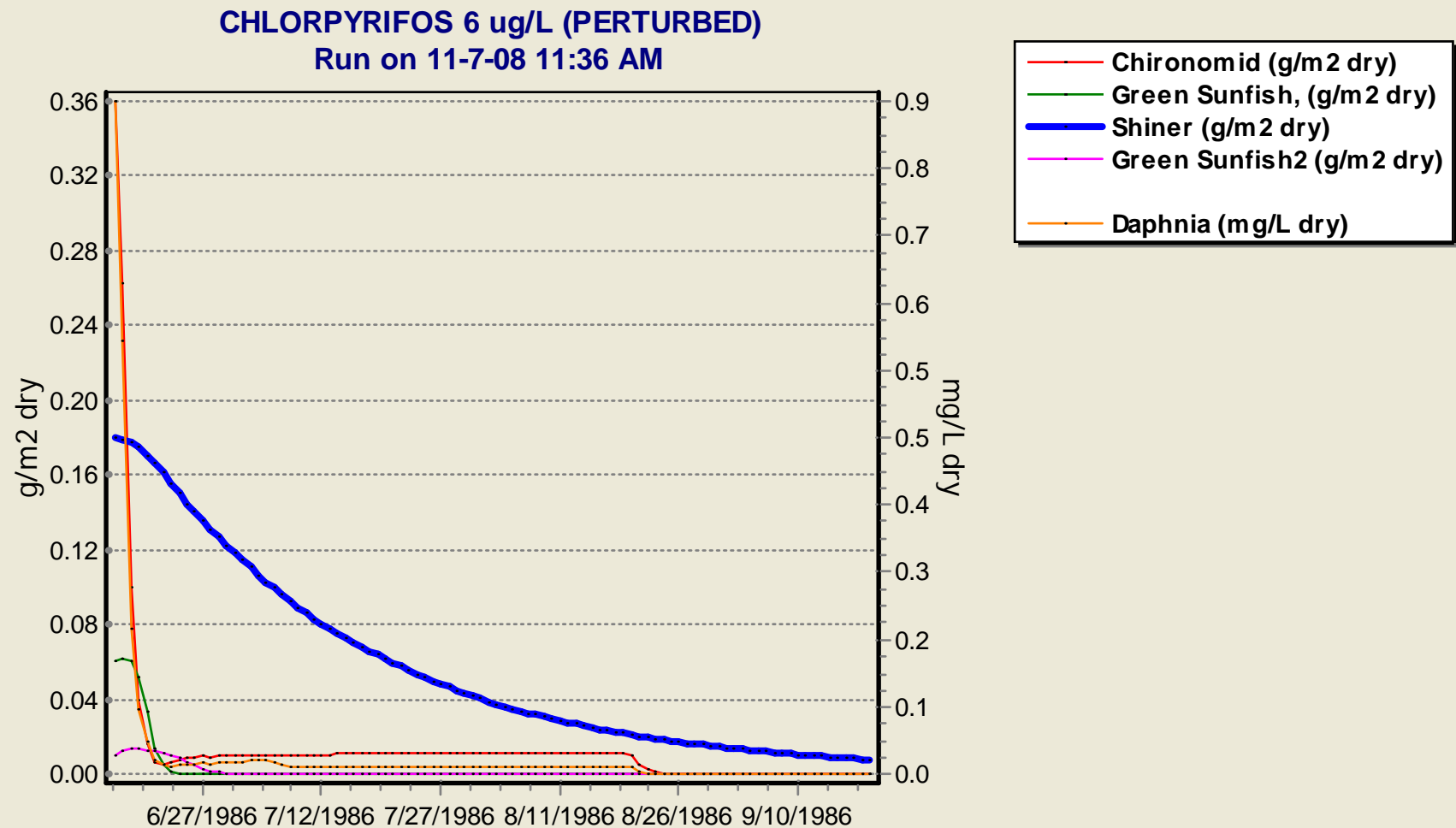
AQUATOX\_External\_Toxicity\_Model.xls



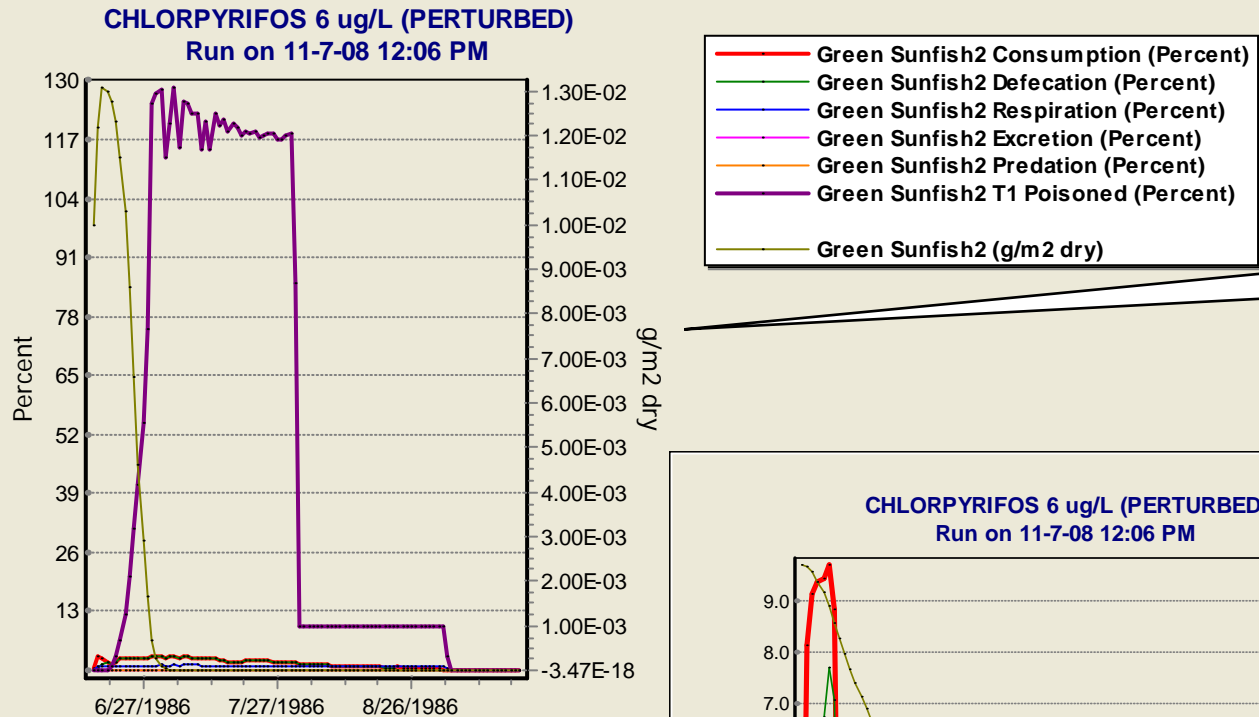
## Returning to the Enclosure in Duluth MN . . .



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

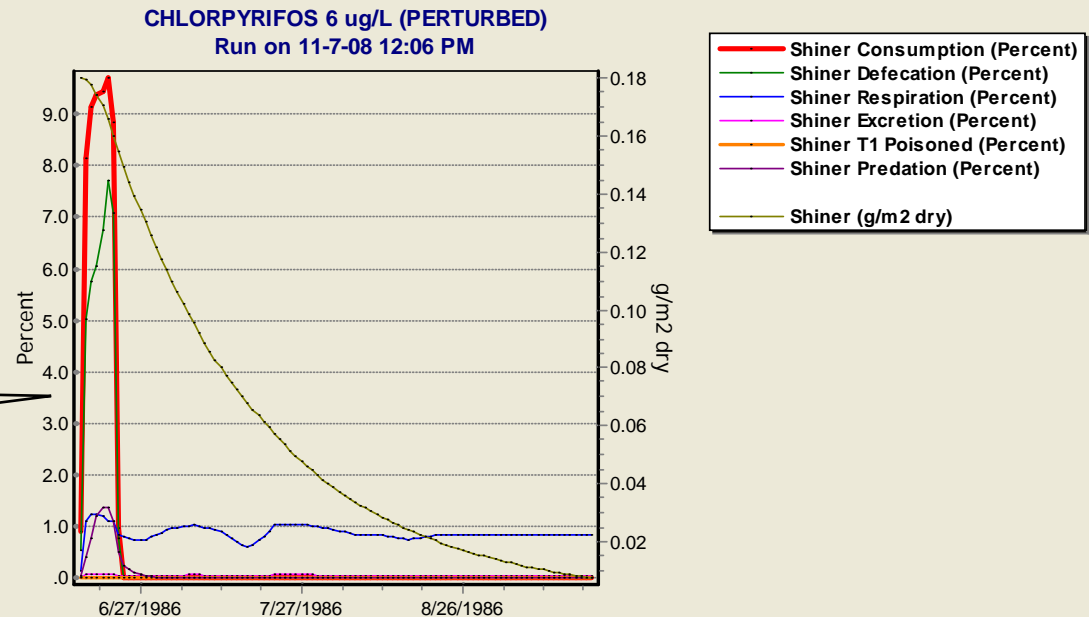


# Sunfish have lethal effects, shiners have sublethal effects from chlorpyrifos



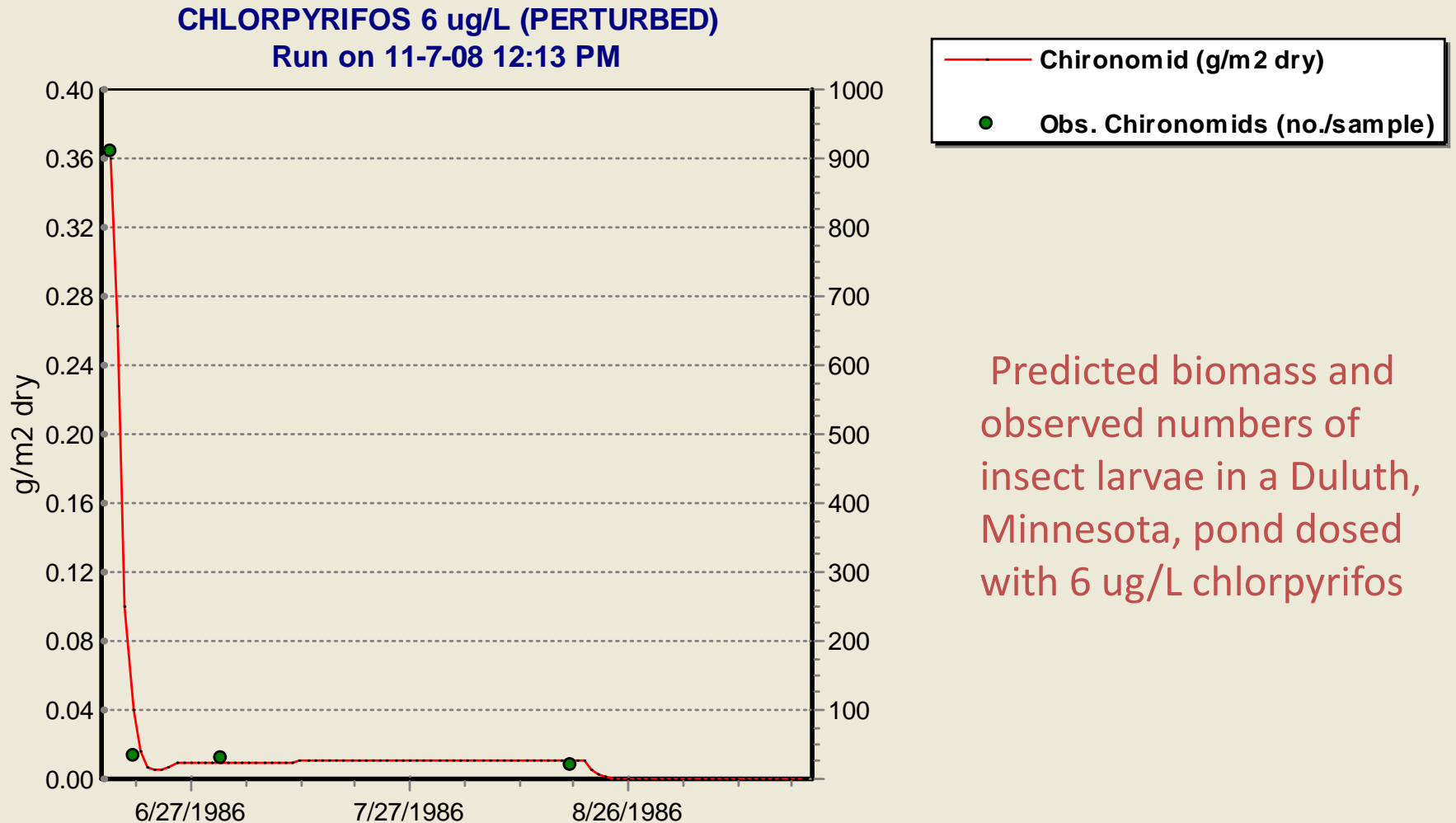
Sunfish with lethal effects

Shiner with sublethal effects only

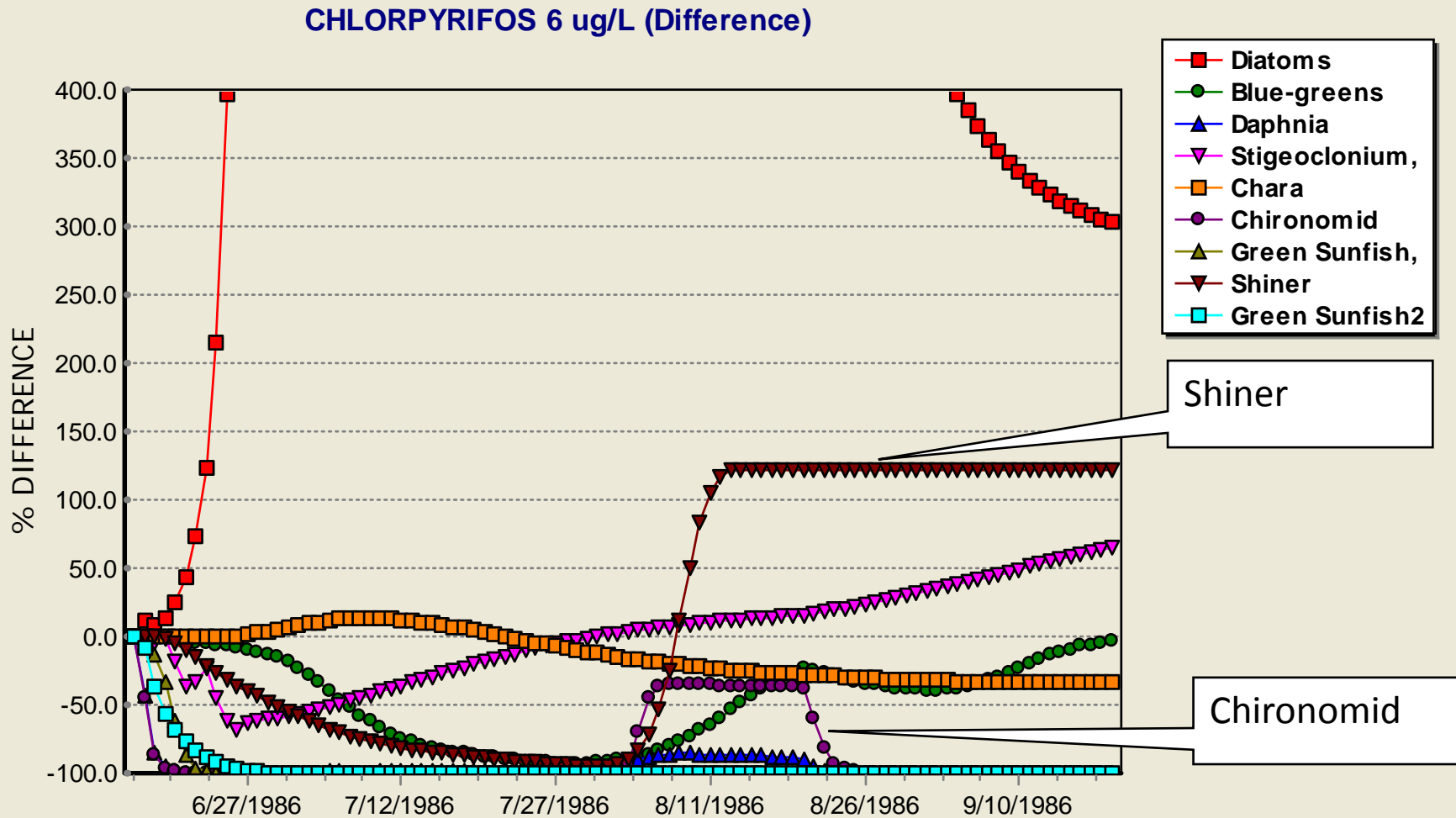




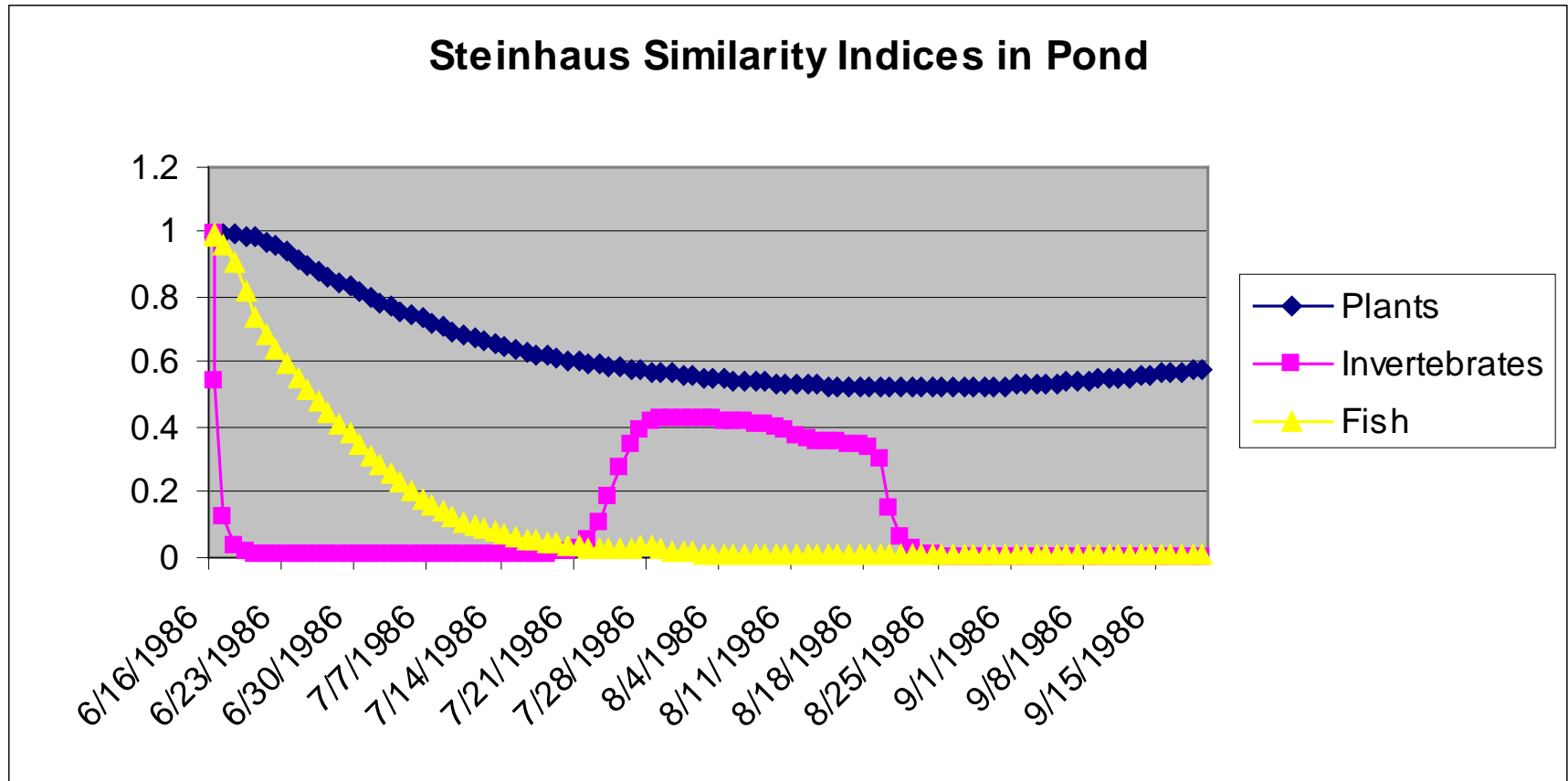
# Toxic effects of Chlorpyrifos in Duluth pond



# % Difference Graph shows differences in species response to toxicant



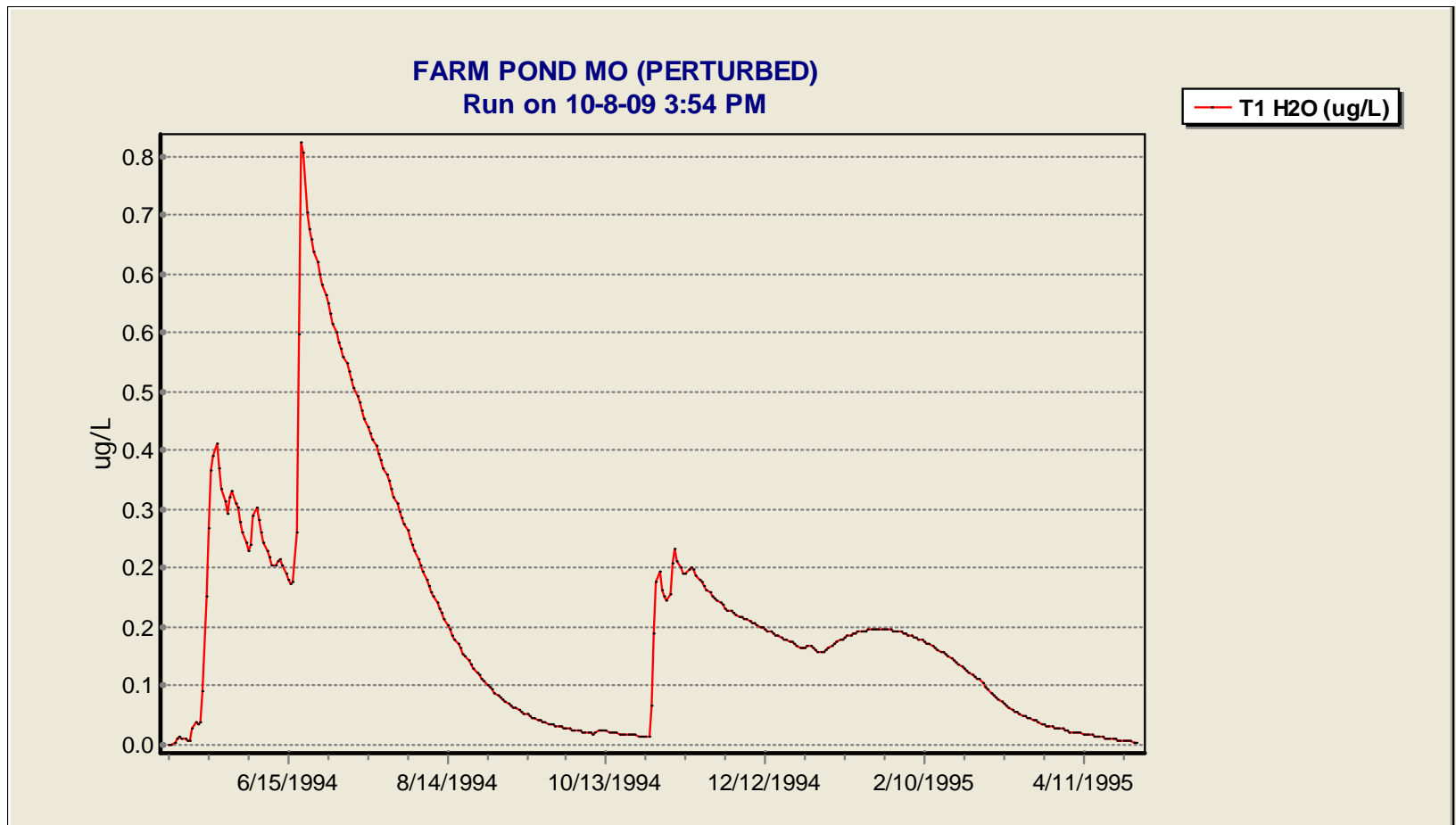
# Steinhaus Indices show ecosystem impacts predicted by the model



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

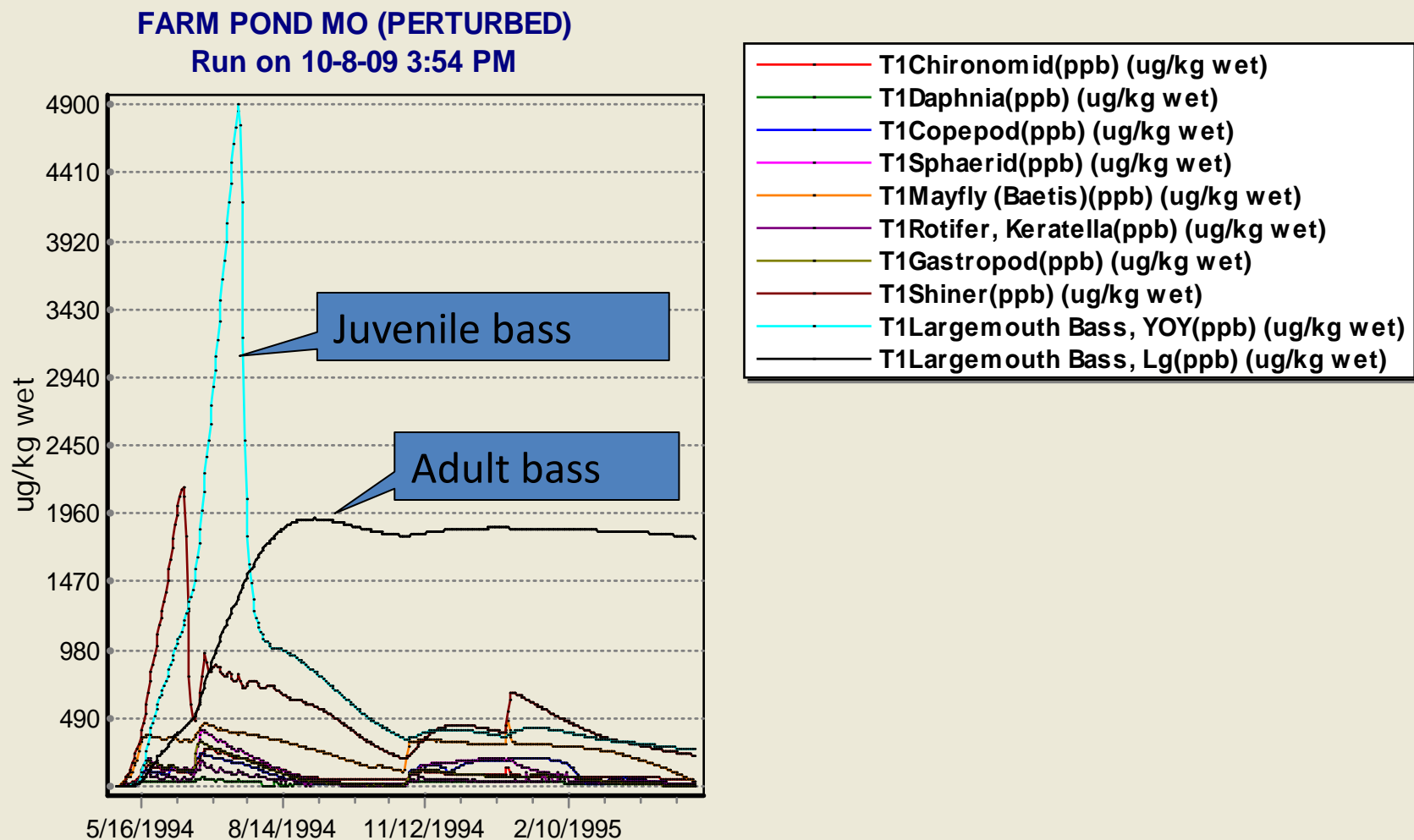
# Farm Pond MO, Esfenvalerate

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

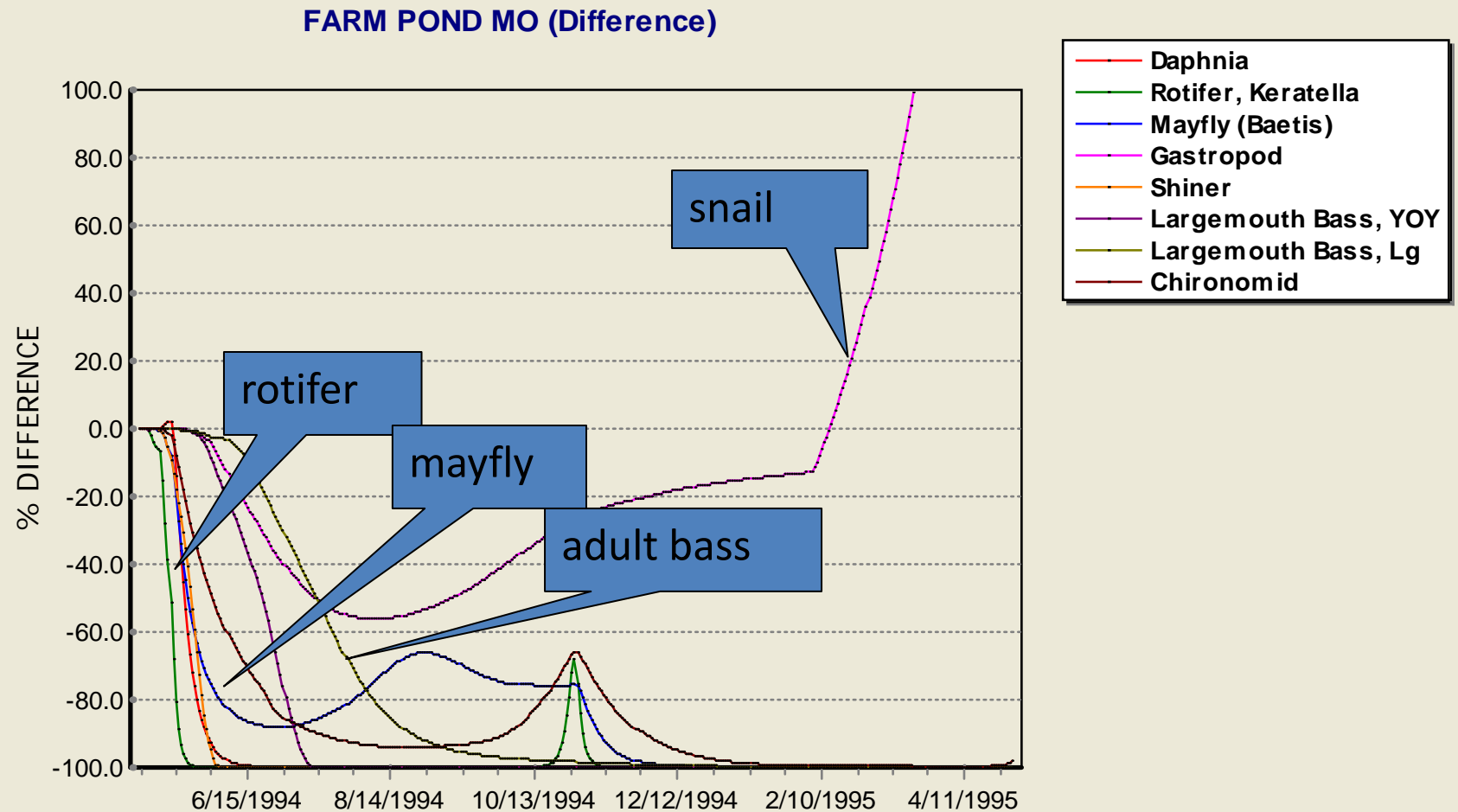


# Farm Pond, Esfenvalerate

## Chemical Uptake in animals



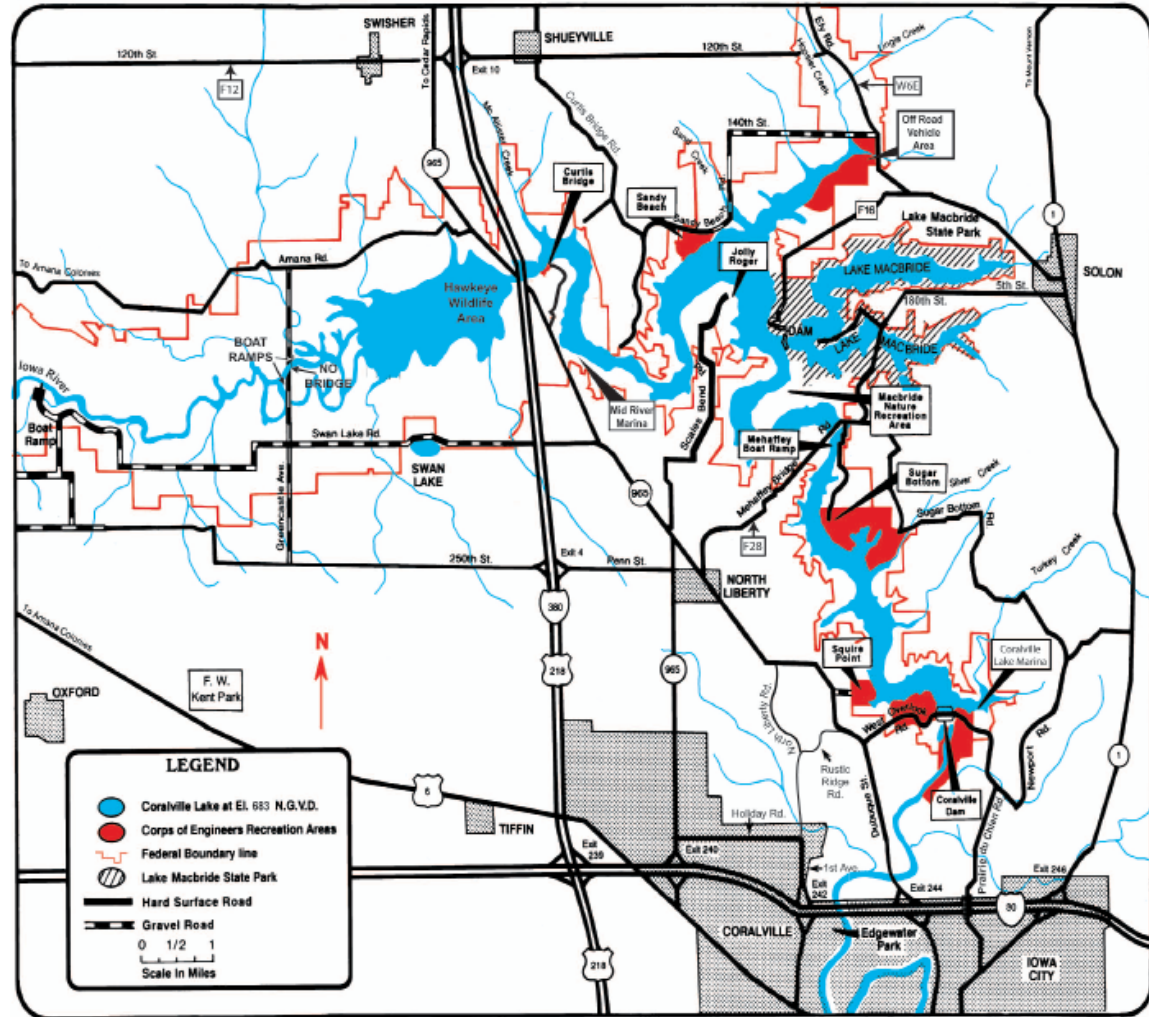
# Farm Pond, Esfenvalerate Difference Graph



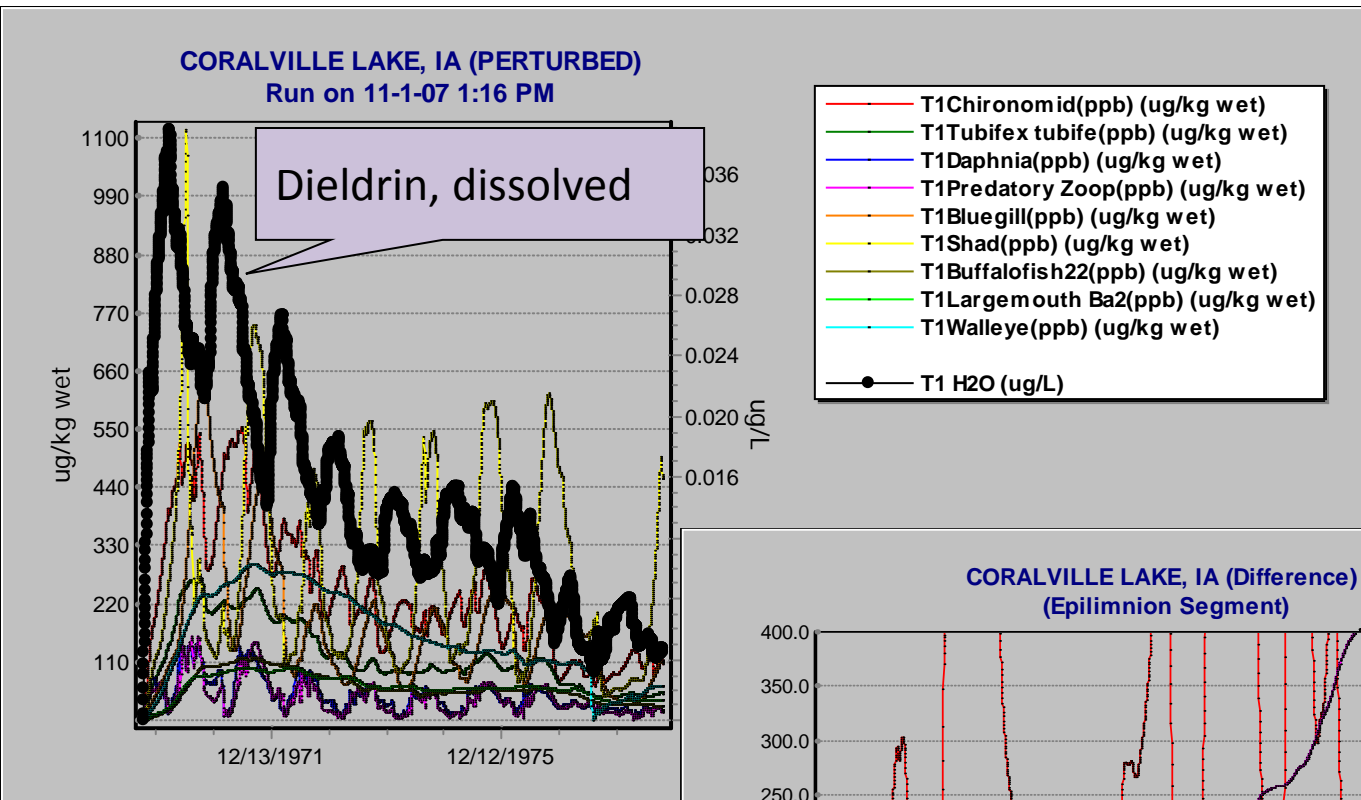
# Coralville Reservoir Iowa

## long-term contamination with dieldrin

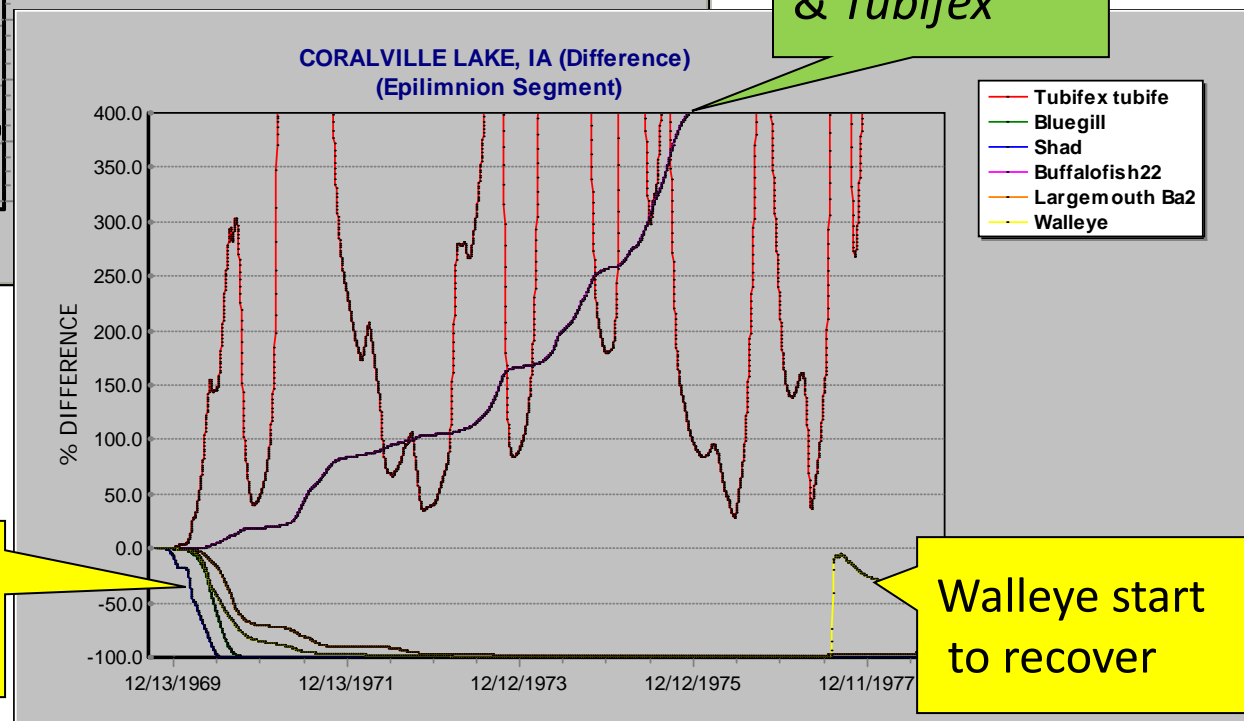
- Run-of-river
- Flood control
- 90% of basin in agriculture
  - Nutrients
  - Pesticides
  - Sediment



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



Buffalofish  
& *Tubifex*

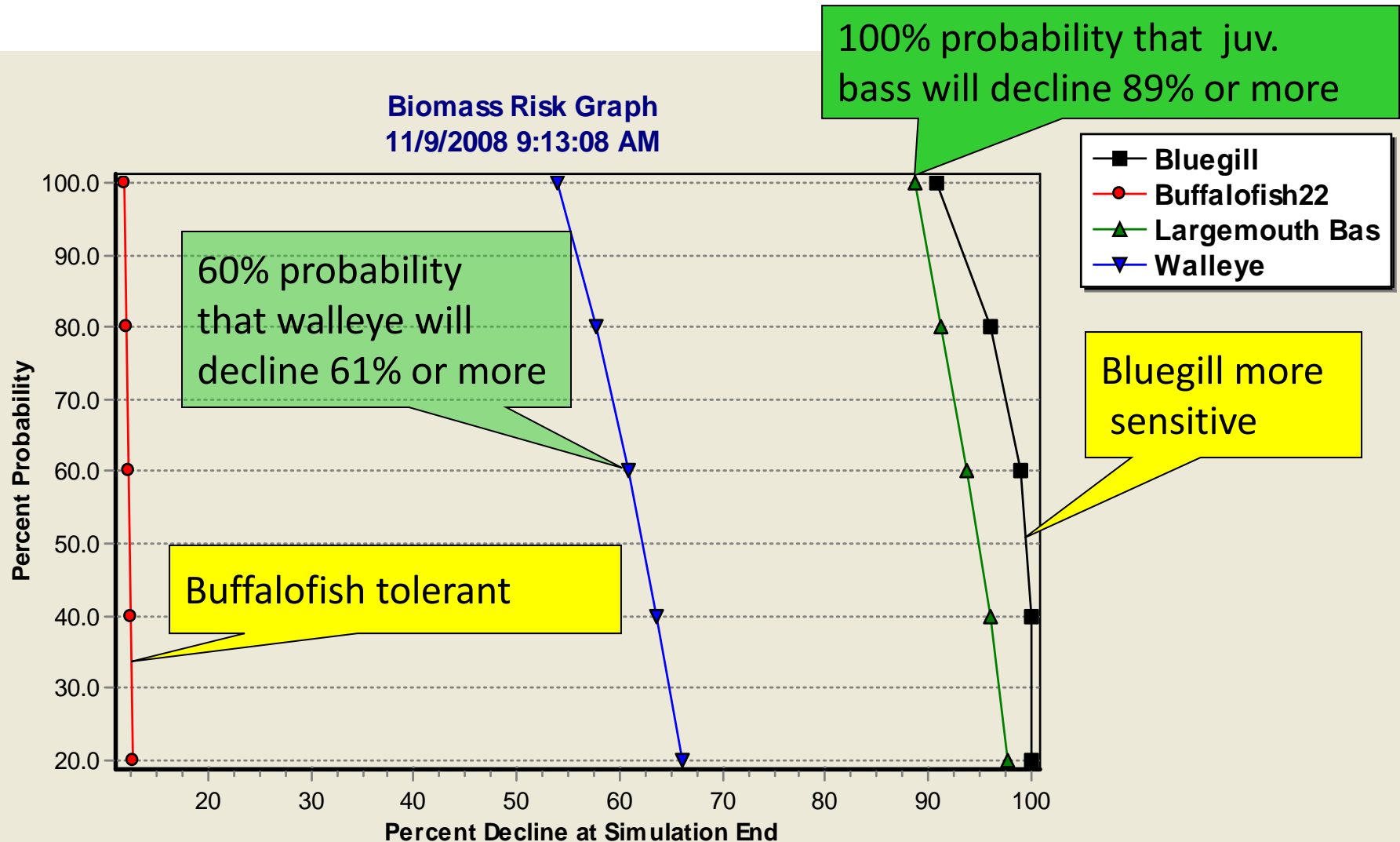


Shad, bluegill, walleye,  
bass die off

Walleye start  
to recover



# Probability of decline in biomass (end of 1<sup>st</sup> year) can be estimated based on uncertainty



# Toxicant Parameters and Loadings are 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**

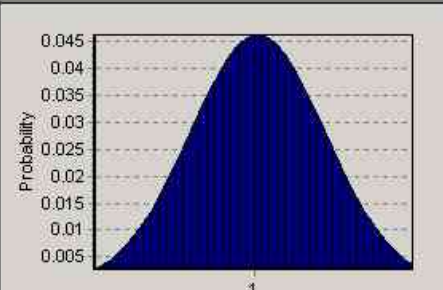
- T1: Molecular Weight
- T1: Dissociation Constant (pKa)
- T1: Solubility (ppm)
- T1: Henry's Law Const. (atm. m<sup>3</sup>/mol)
- T1: Vapor Pressure (mm Hg)
- T1: Octanol-Water Partition Coeff (Log Kow)
- T1: Sed/Detr-Water Partition Coeff (mg/L)
- T1: Activation Energy for Temp (cal/mol)
- T1: Anaerobic Microbial Degrdn. (L/d)
- T1: Aerobic Microbial Degrdn. (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    ☐ 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

# 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)	Biotnsfm. 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	
Minnnow	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)	Biotnsfm. rate (1/d)
▶ 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

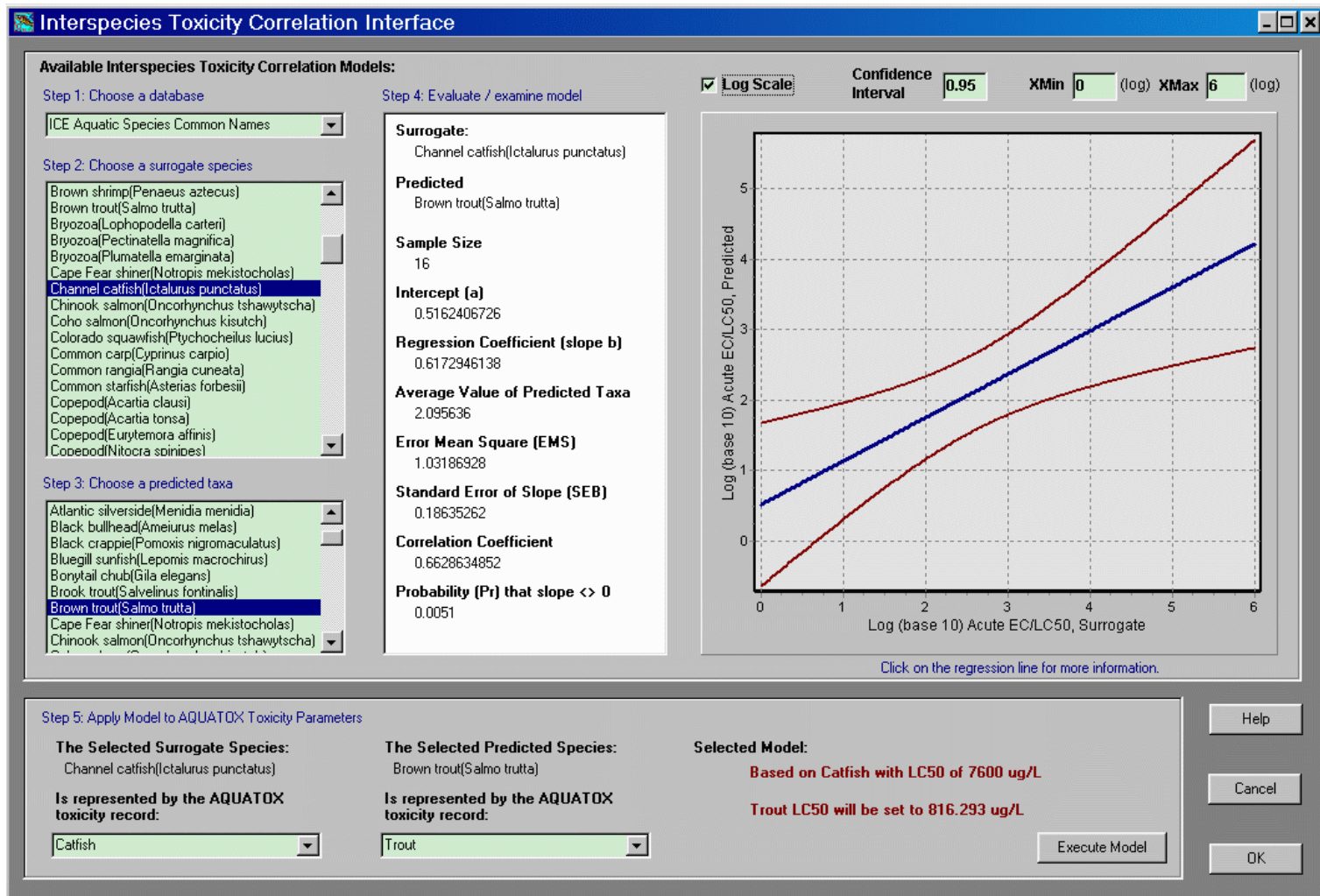
✓ O.K.

# **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



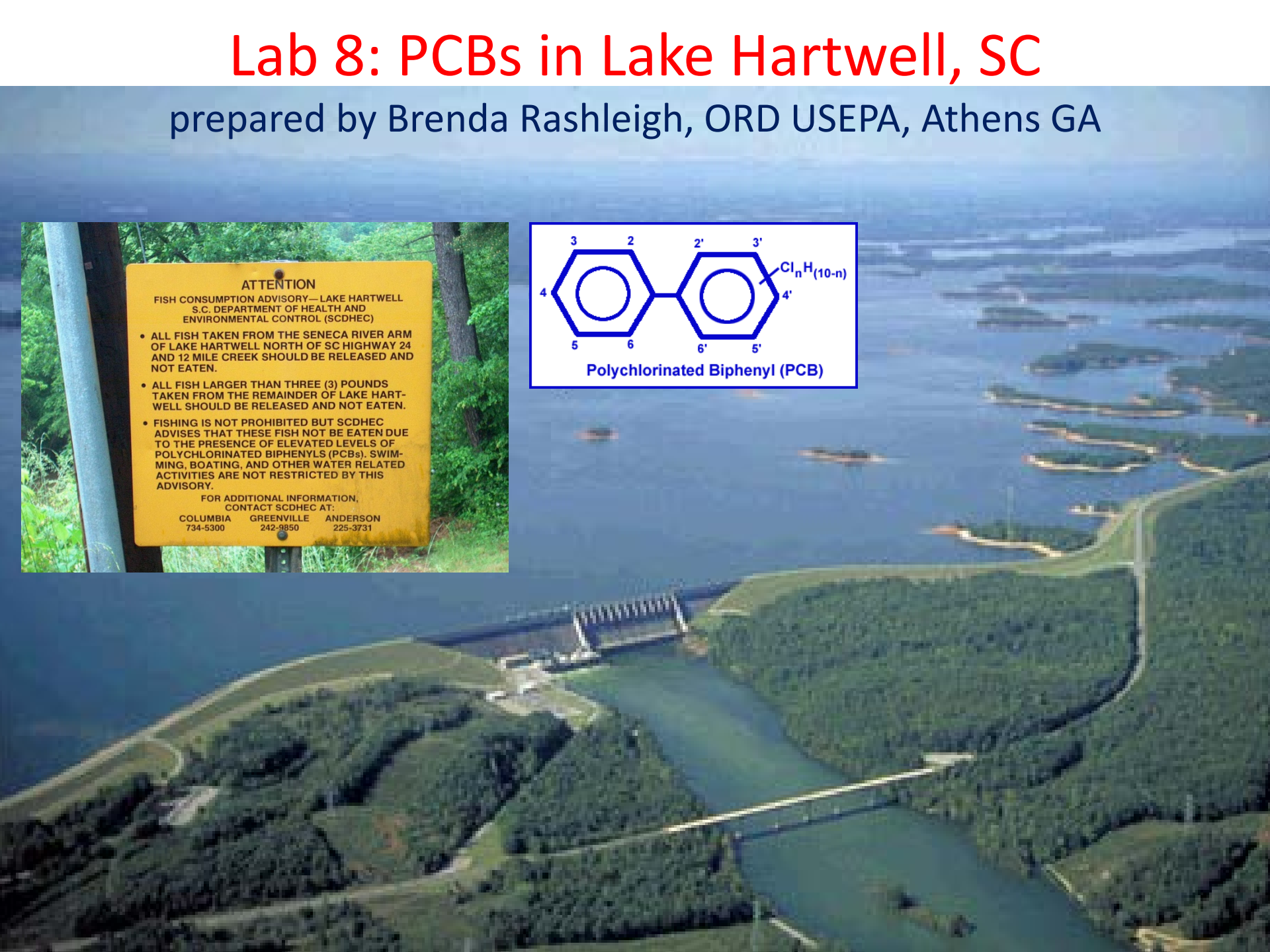
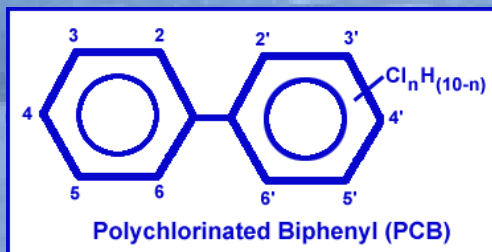
# Lab 8: PCBs in Lake Hartwell, SC

prepared by Brenda Rashleigh, ORD USEPA, Athens GA

**ATTENTION**  
FISH CONSUMPTION ADVISORY—LAKE HARTWELL  
S.C. DEPARTMENT OF HEALTH AND  
ENVIRONMENTAL CONTROL (SCDHEC)

- ALL FISH TAKEN FROM THE SENECA RIVER ARM OF LAKE HARTWELL NORTH OF SC HIGHWAY 24 AND 12 MILE CREEK SHOULD BE RELEASED AND NOT EATEN.
- ALL FISH LARGER THAN THREE (3) POUNDS TAKEN FROM THE REMAINDER OF LAKE HARTWELL SHOULD BE RELEASED AND NOT EATEN.
- FISHING IS NOT PROHIBITED BUT SCDHEC ADVISES THAT THESE FISH NOT BE EATEN DUE TO THE PRESENCE OF ELEVATED LEVELS OF POLYCHLORINATED BIPHENYLS (PCBs). SWIMMING, BOATING, AND OTHER WATER RELATED ACTIVITIES ARE NOT RESTRICTED BY THIS ADVISORY.

FOR ADDITIONAL INFORMATION,  
CONTACT SCDHEC AT:  
COLUMBIA 734-5300    GREENVILLE 242-9850    ANDERSON 225-3731



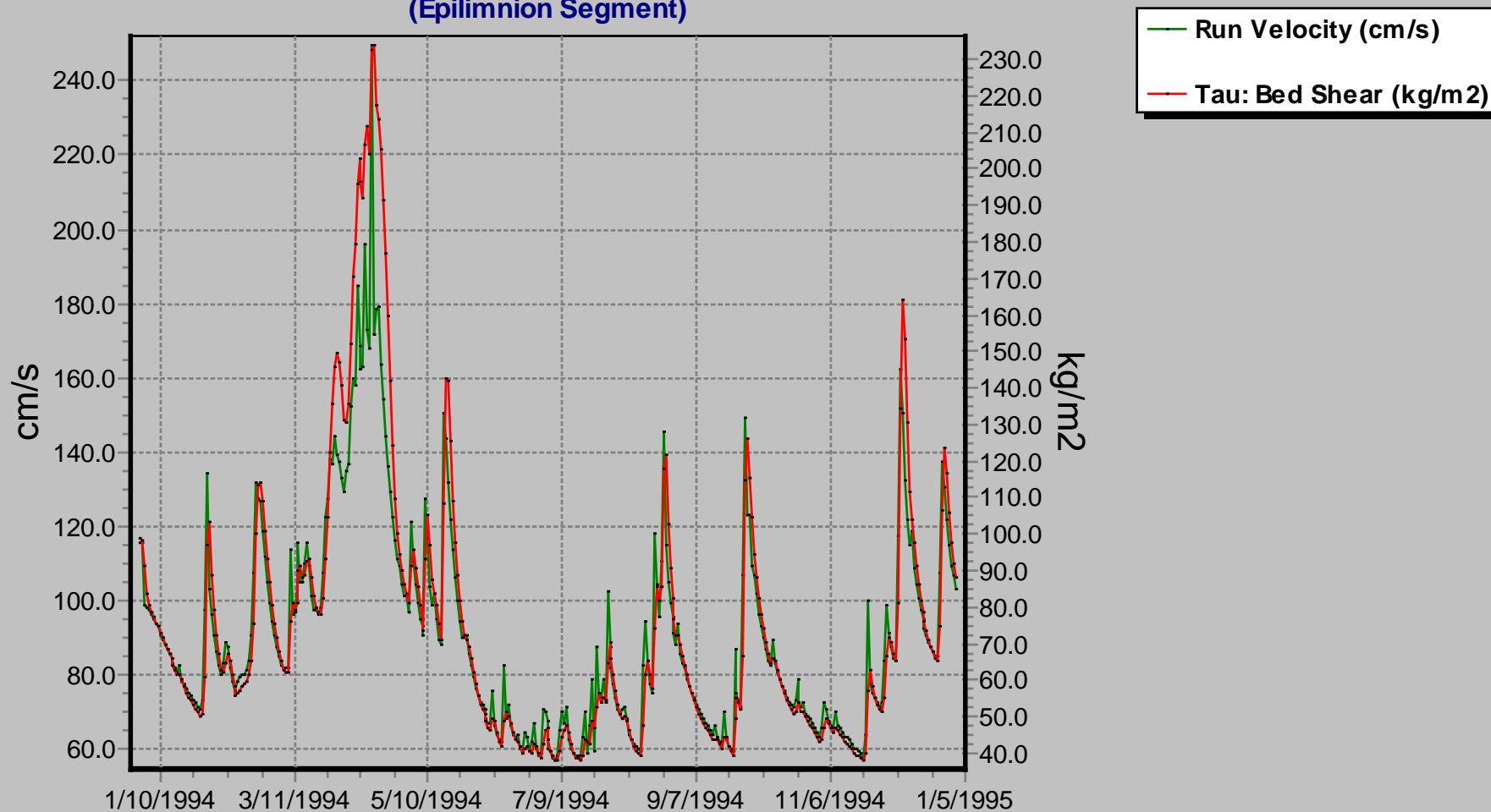
# Modeling Inorganic Sediments (sand, silt, and clay)

- 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

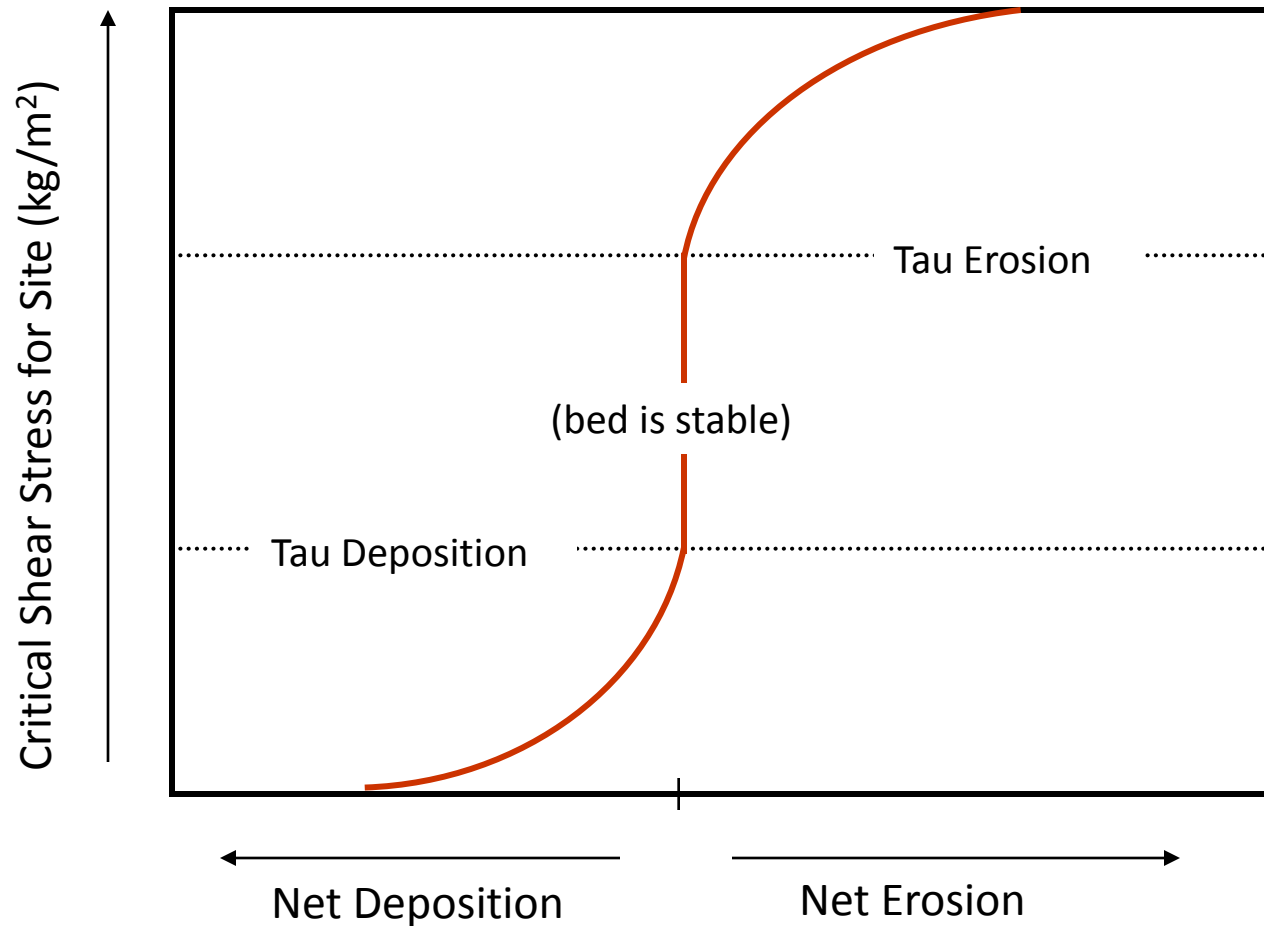


# Bed Shear Stress (Tau) Closely Related to Water Velocity

Housatonic Test Rch. (PERTURBED) 10/13/2004 12:30:06 PM  
(Epilimnion Segment)



# Critical Shear Stress for Erosion and Deposition Key Parameters



# Sediment Model Parameters


## Silt Parameters

		References:
Critical Shear Stress for Scour	<input type="text" value="0.7"/> kg/m <sup>2</sup>	<input type="text" value="default"/>
Critical Shear Stress for Deposition	<input type="text" value="0.1"/> kg/m <sup>2</sup>	<input type="text" value="default"/>
Fall Velocity	<input type="text" value="8.89E-5"/> m/s	<input type="text" value="default"/>

## Clay Parameters

		References:
Critical Shear Stress for Scour	<input type="text" value="0.6"/> kg/m <sup>2</sup>	<input type="text" value="default"/>
Critical Shear Stress for Deposition	<input type="text" value="0.07"/> kg/m <sup>2</sup>	<input type="text" value="default"/>
Fall Velocity	<input type="text" value="1.02E-5"/> m/s	<input type="text" value="default"/>

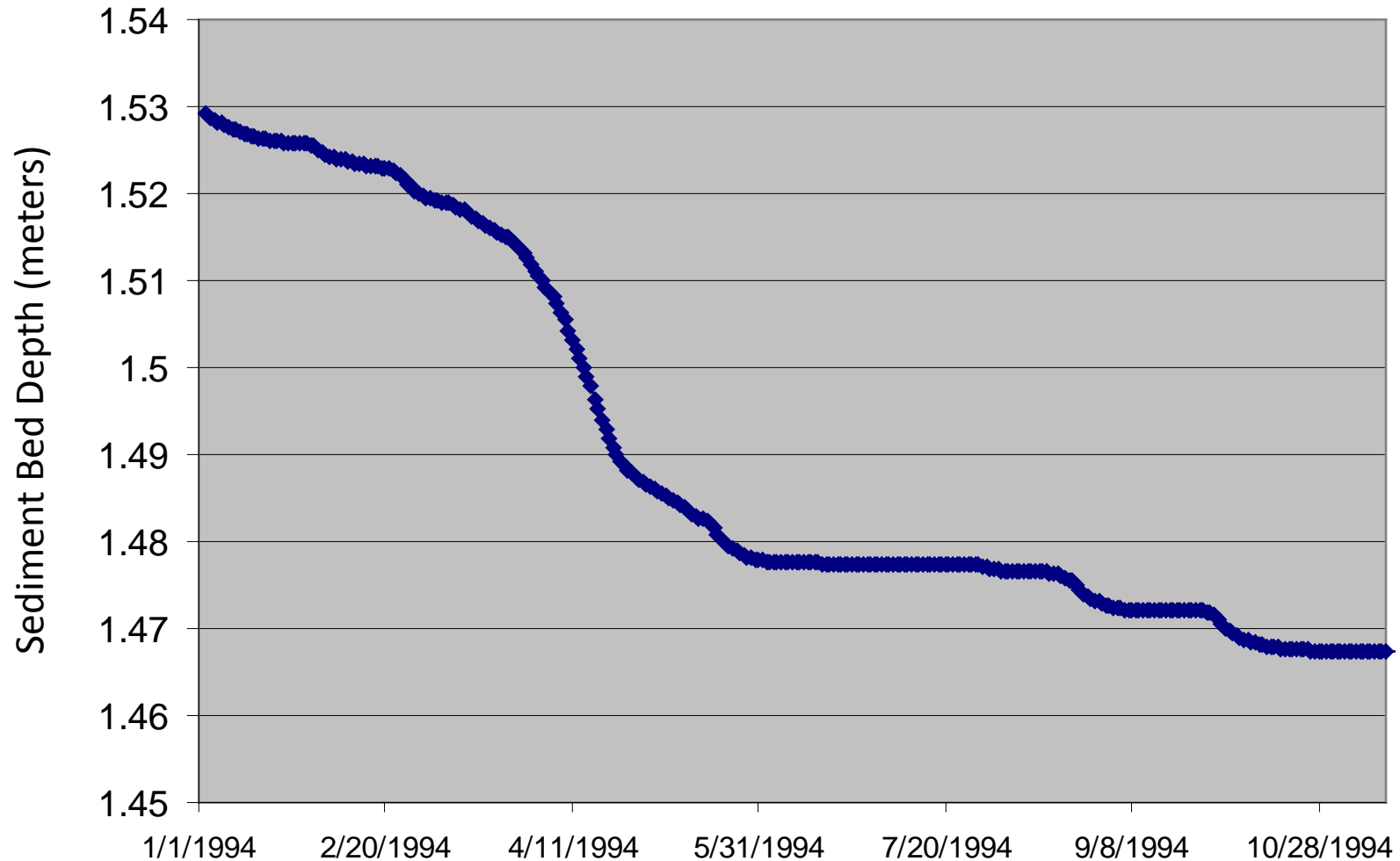
Help

 **OK**

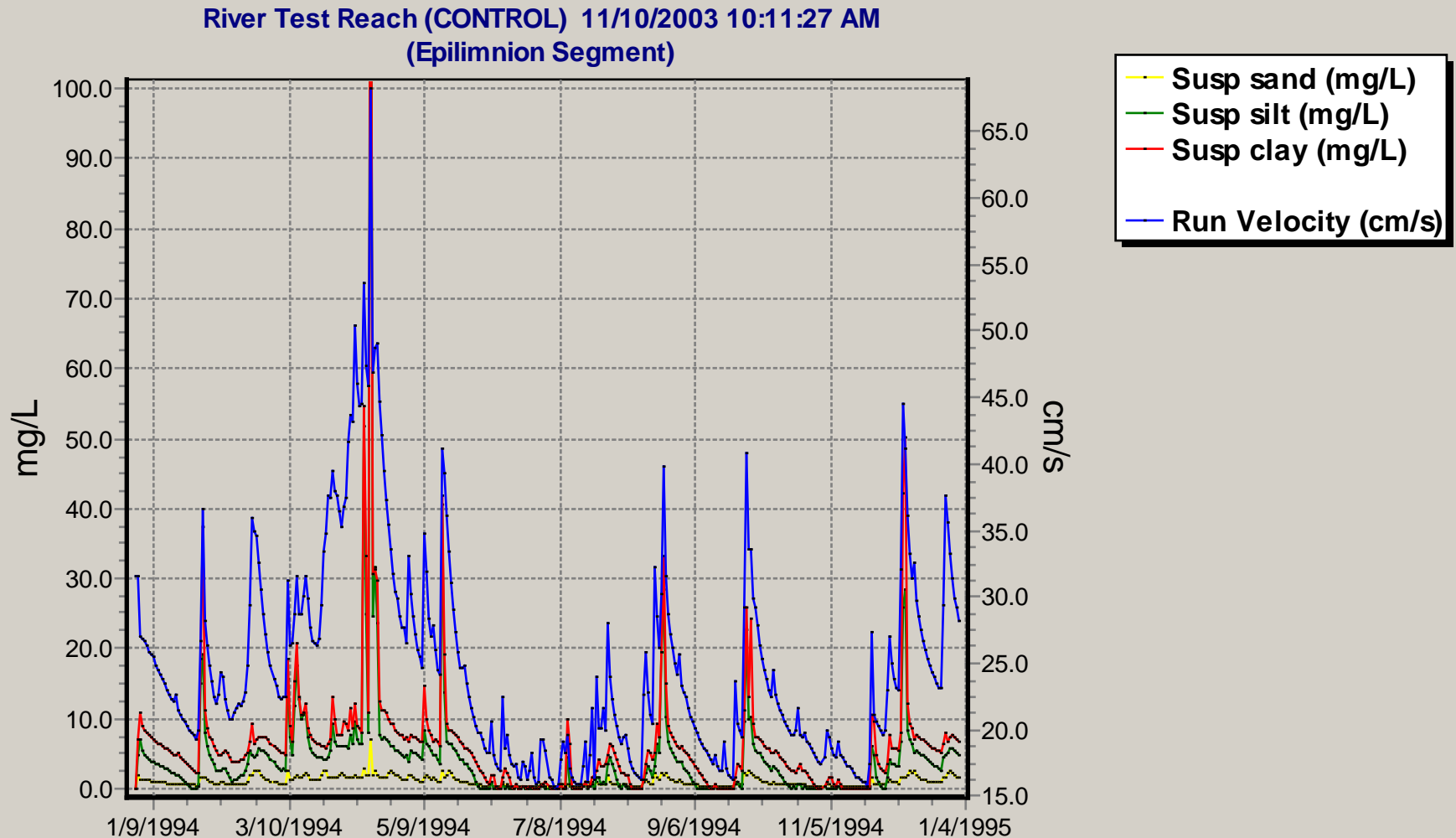
# Sand Model

- 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

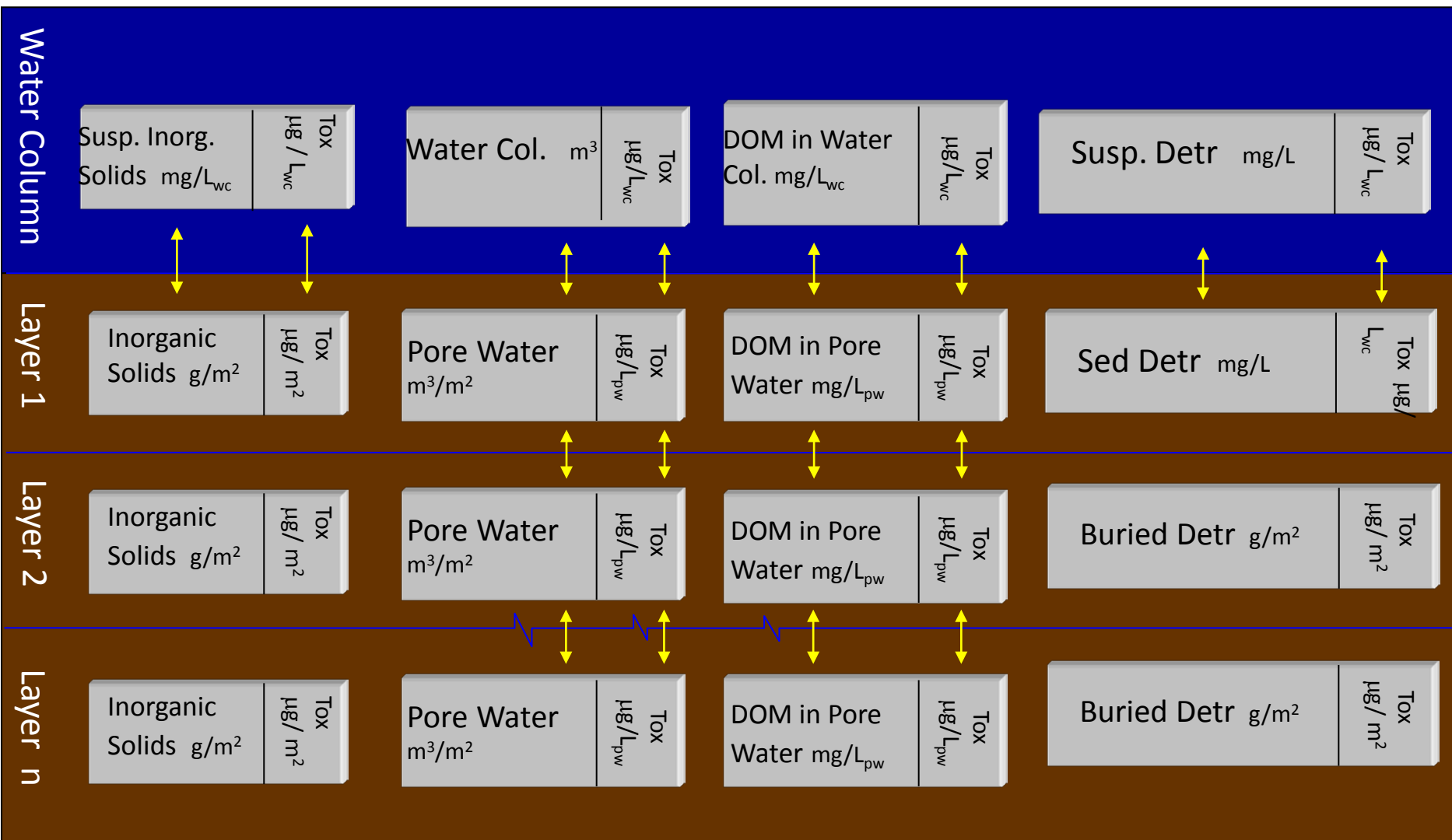


# **AQUATOX Multi-Layer Sediment Model**

- **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  $\mu\text{m}$   
(clay)
- **Non-Cohesives:** particle size from 63 to 250  $\mu\text{m}$   
(silt)
- **Non-Cohesives2:** particle size greater than 250  $\mu\text{m}$   
(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

Change Graph Variables

☐ Show All Results

☒ Filter By Substring:  ☐ Exclude Substring

**Selected Set of Results:**

- N Load as Detritus (kg)
- N Load as Biota (kg)
- N Root Uptake (kg)
- N Fixation (kg)
- N Exposure (kg)
- N Net Layer Sink (kg)
- N Net TurbDiff (kg)
- N Net Layer Migr. (kg)
- N Total Net Layer (kg)
- P Tot. Mass (kg)
- P Mass Dissolved (kg)
- P Mass Detritus (kg)
- P Mass Animals (kg)
- P Mass Plants (kg)
- P Tot. Loss (kg)
- P Tot. Washout (kg)
- P Wash, Dissolved (kg)
- P Wash, Animals (kg)
- P Wash, Detritus (kg)
- P Wash, Plants (kg)
- P Loss Emergel (kg)
- P Burial (kg)
- P Tot. Load (kg)
- P Load, Dissolved (kg)
- P Load as Detritus (kg)
- P Load as Biota (kg)
- P Root Uptake (kg)
- P Exposure (kg)

**Results on Y1 Axis (kg):**

P MB Test

**Results on Y2 Axis (kg):**

N MB Test

**Y1 Axis Scale**

☒ Use Automatic Scaling

☐ Use Below Values

Min

Max

**Y2 Axis Scale**

☒ Use Automatic Scaling

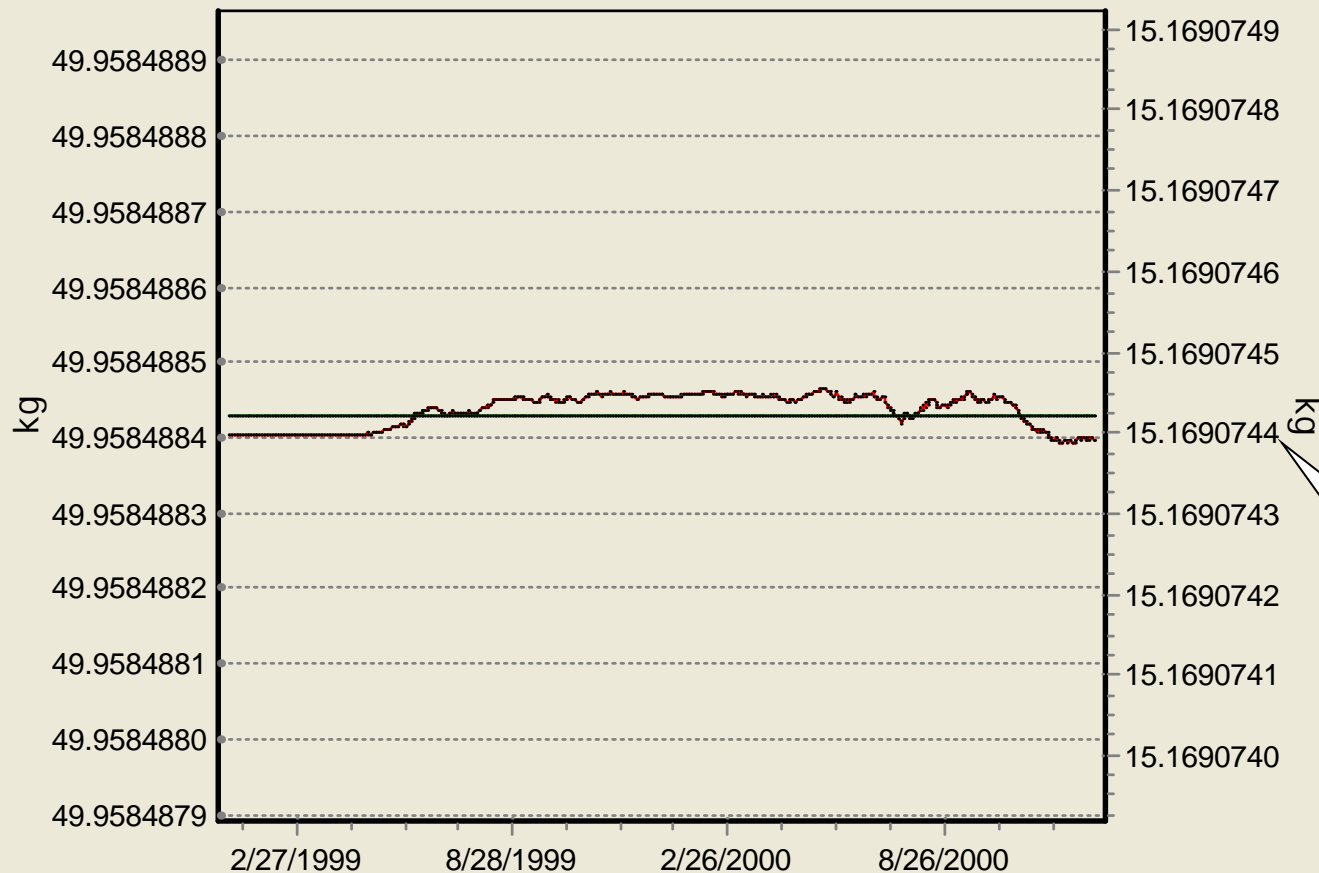
☐ Use Below Values

Min

Max

# Mass is Balancing

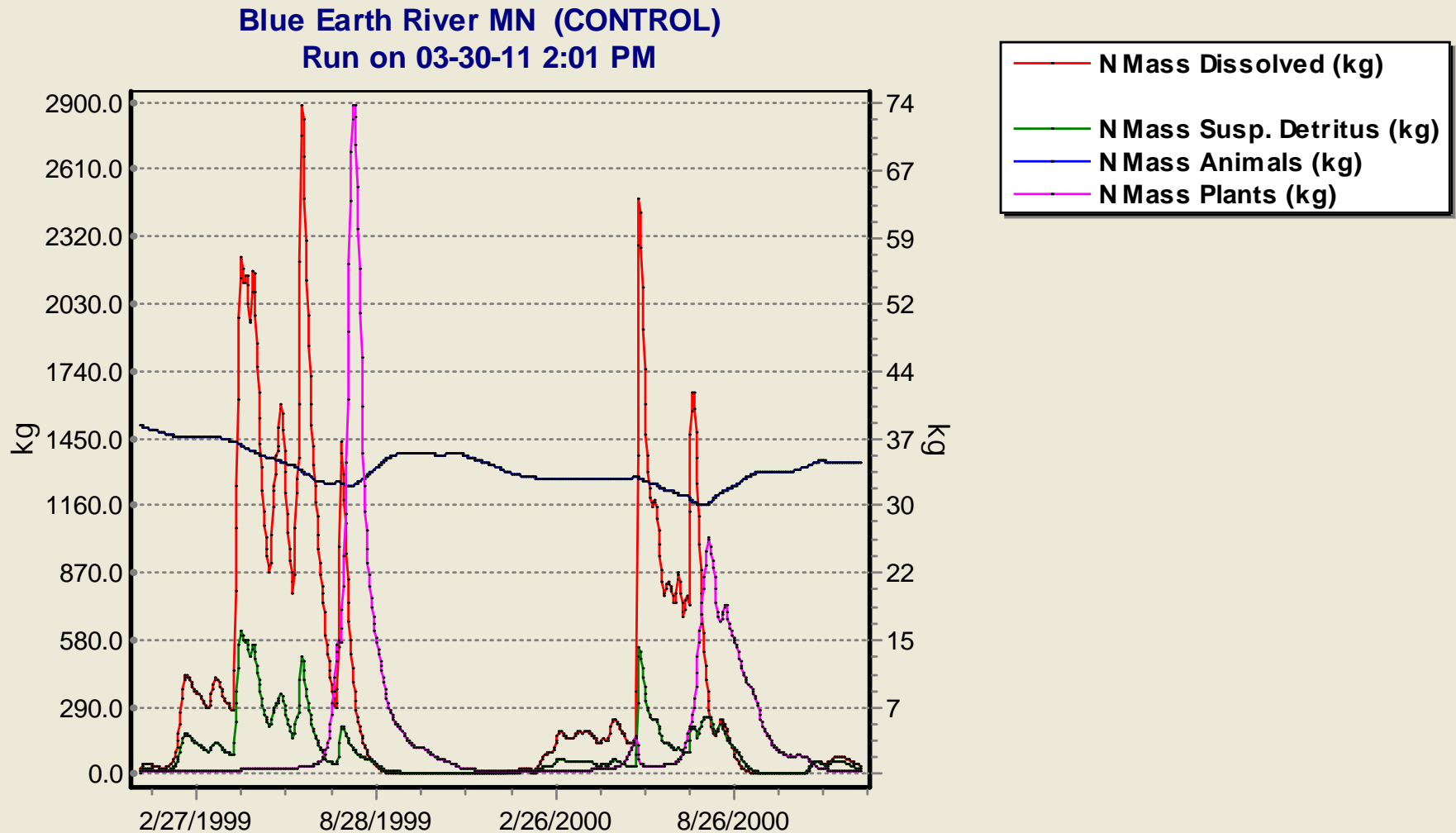
Blue Earth River MN (CONTROL)  
Run on 03-30-11 2:01 PM



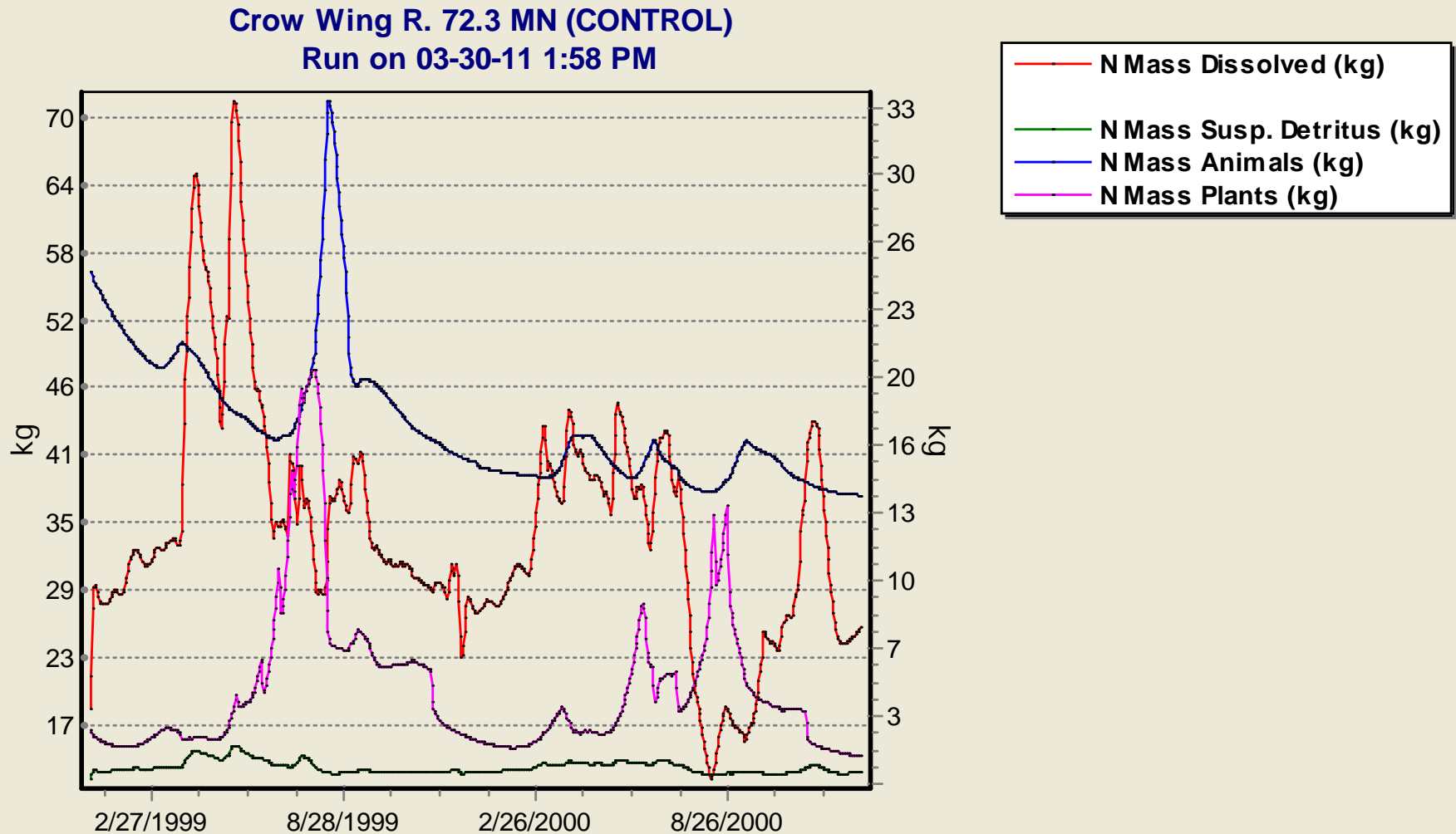
NMB Test (kg)  
PMB Test (kg)

Axes reflect a  
very narrow  
range

# Where are the Nutrients within the System?

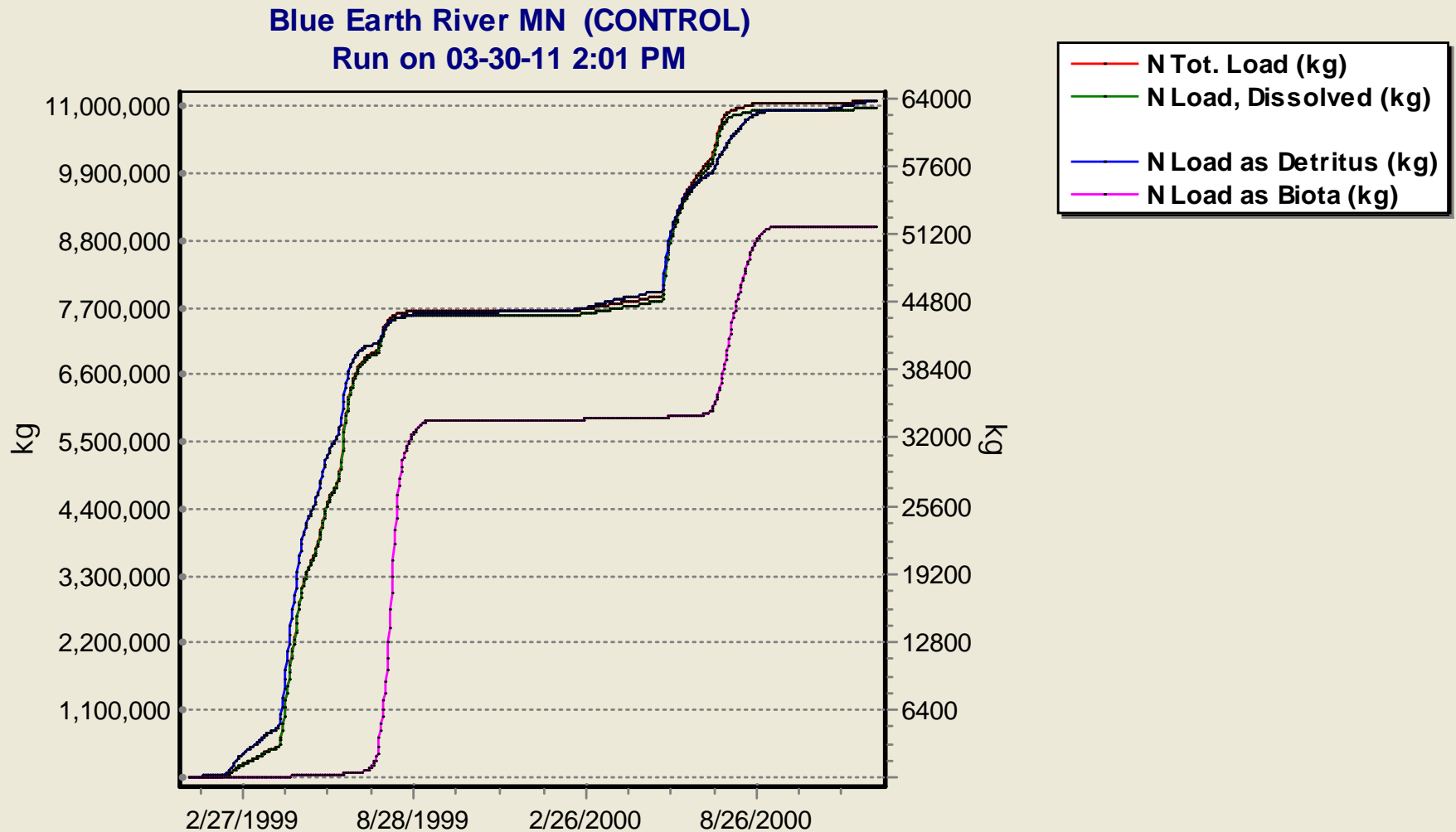


# Contrast Blue Earth with the Crow Wing River

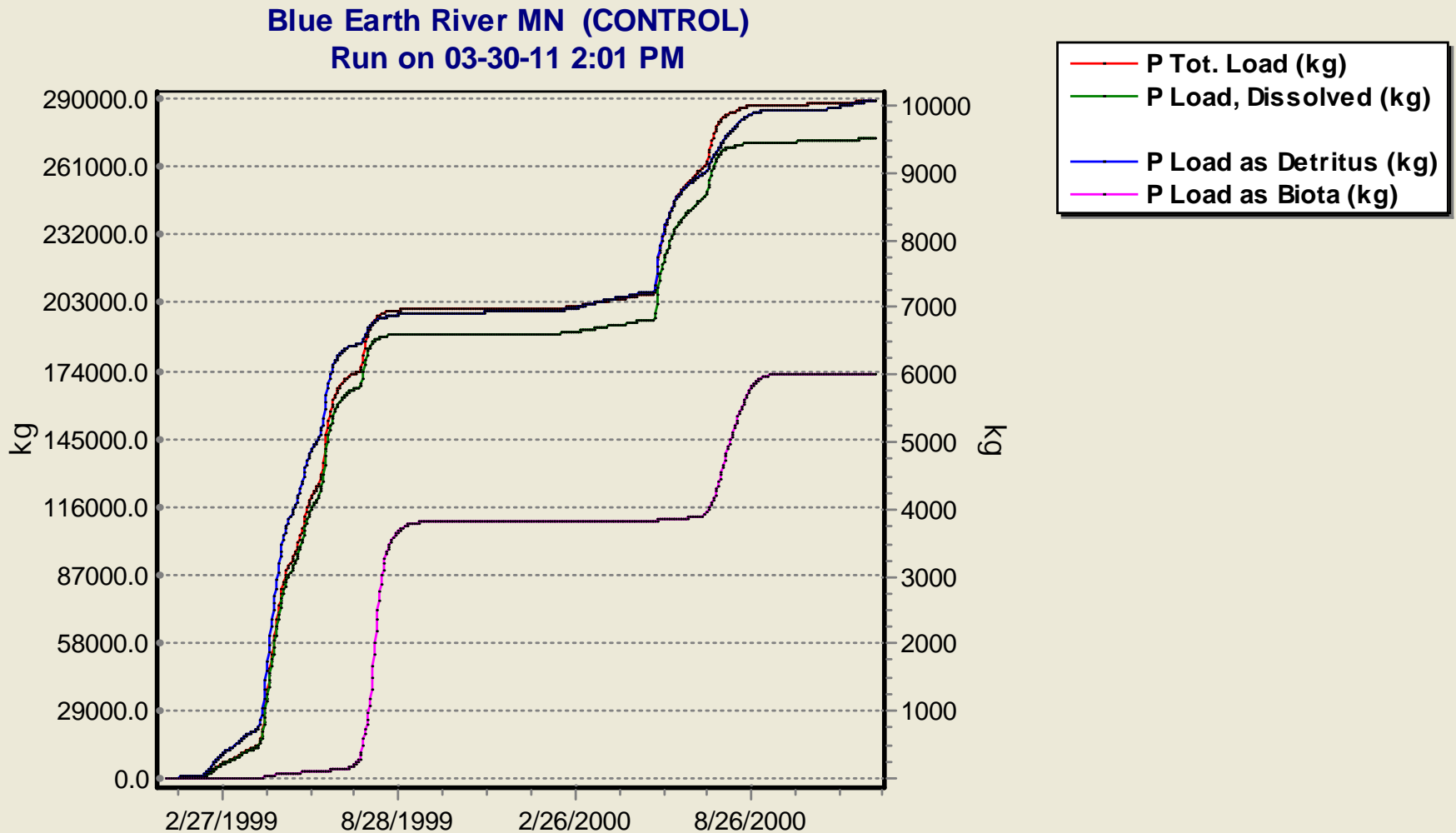




# Nitrogen Loadings, Blue Earth River



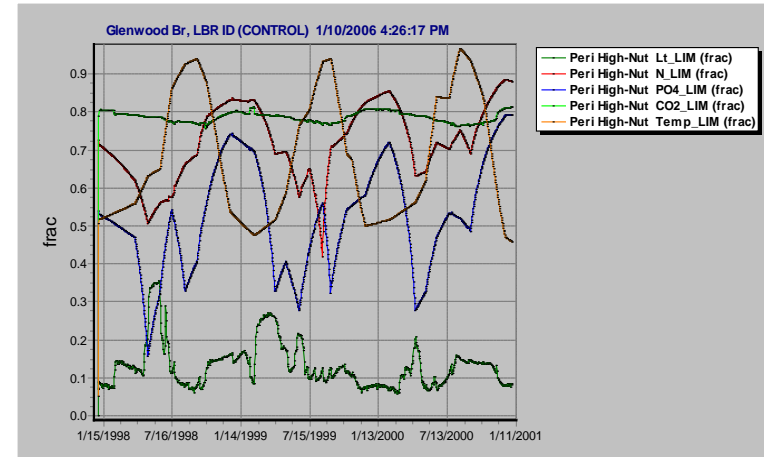
# Phosphorus Loadings, Blue Earth River



# 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](http://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