

AQUATOX Training Workshop (Day 3)

Web Training Materials, August 2012

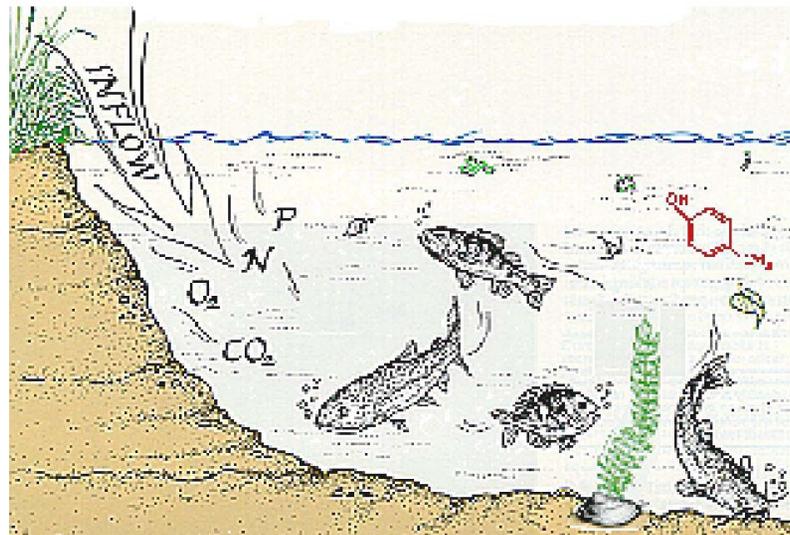
Based on Workshop Given for EPA Region 6, Dallas, Texas, December 2010
and Columbia River Intertribal Fish Commission, November 2011



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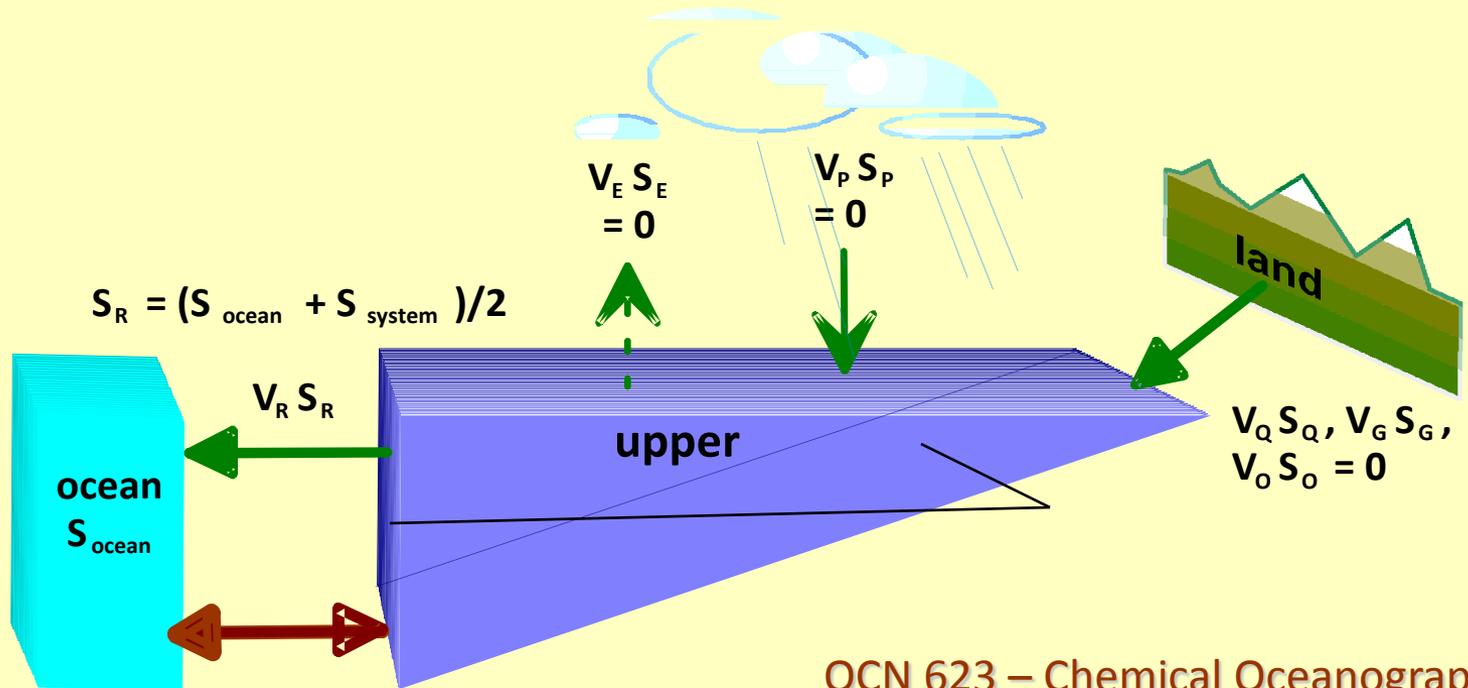
Modeling Estuarine Conditions

- 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

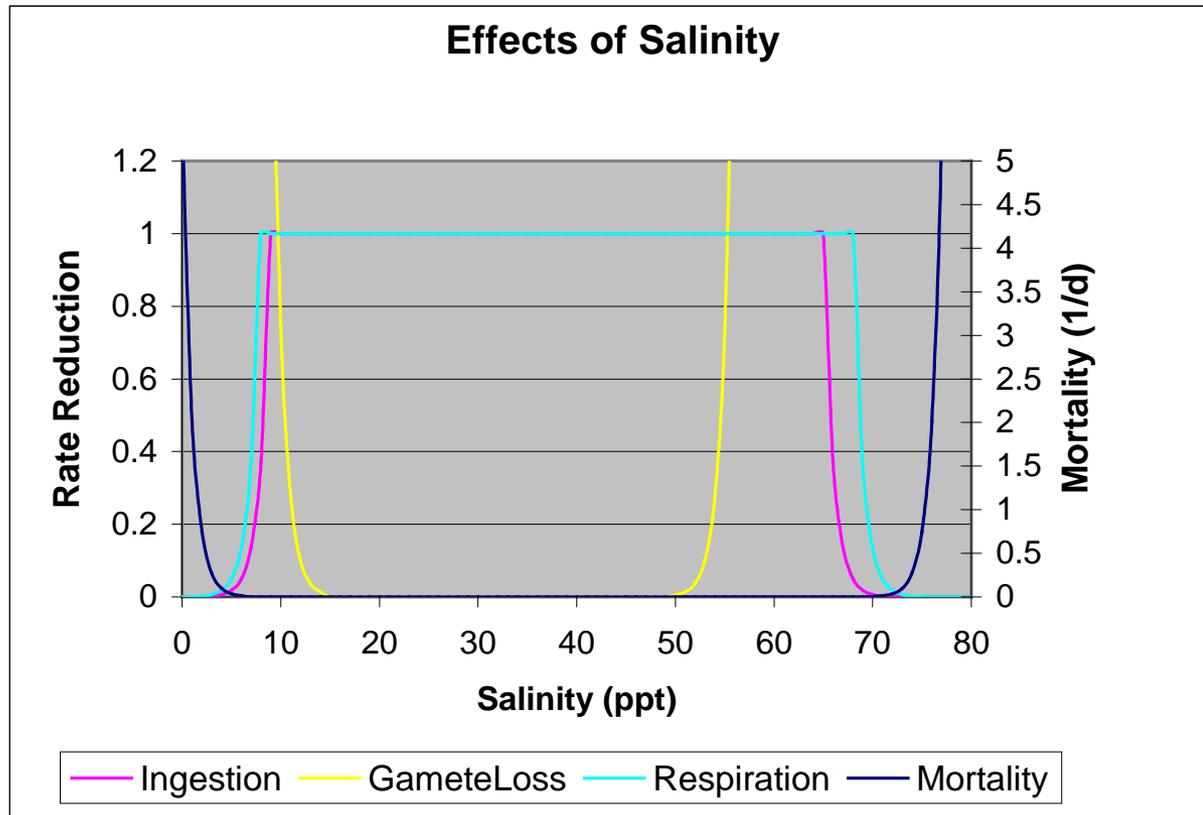
Estuarine Features

- 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

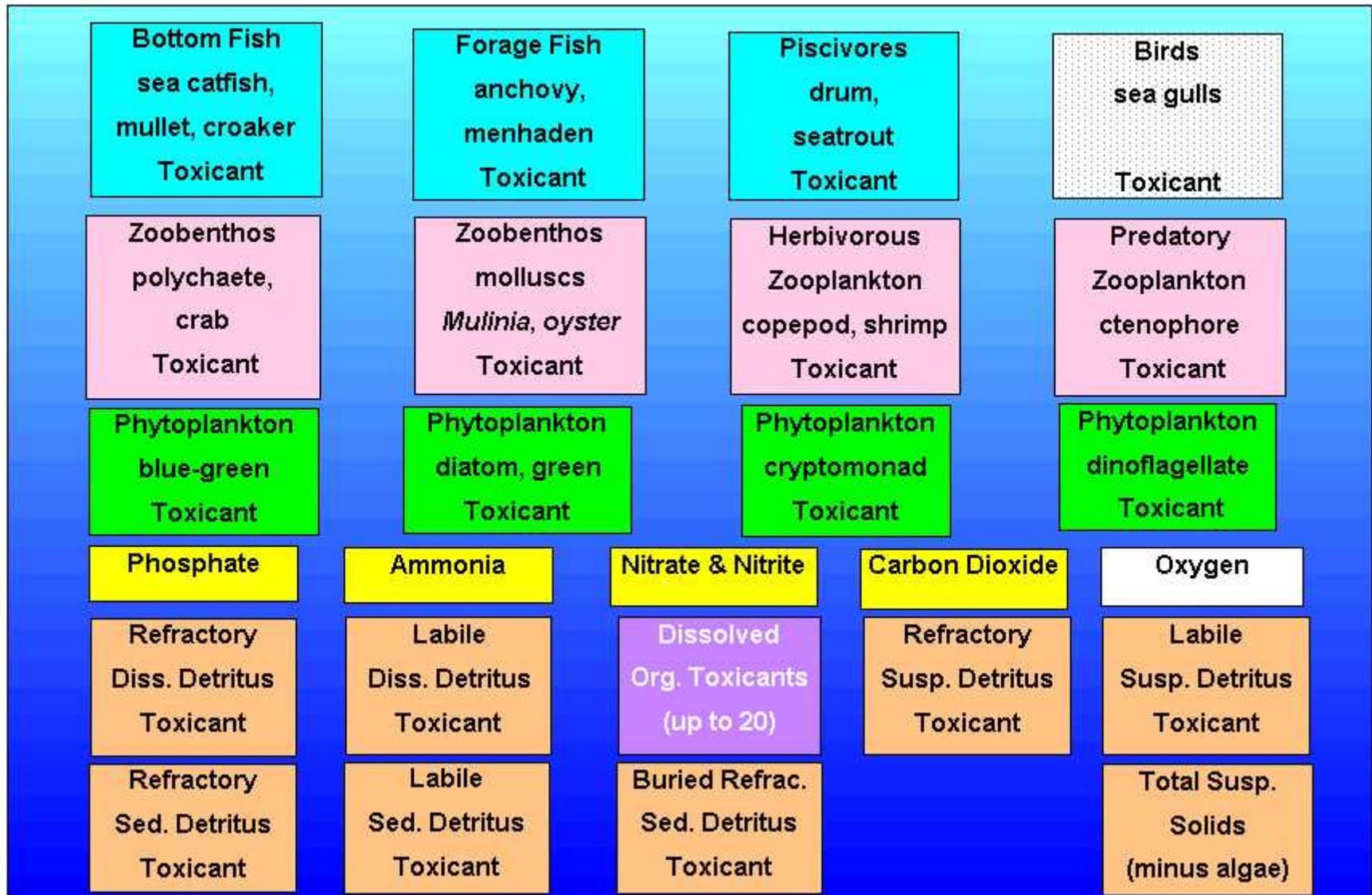


Estuarine version roughly calibrated for Galveston Bay, Texas, to evaluate toxicants



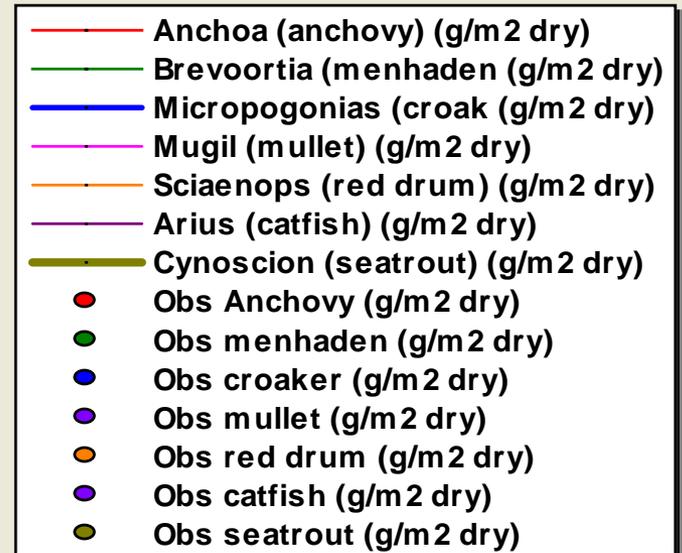
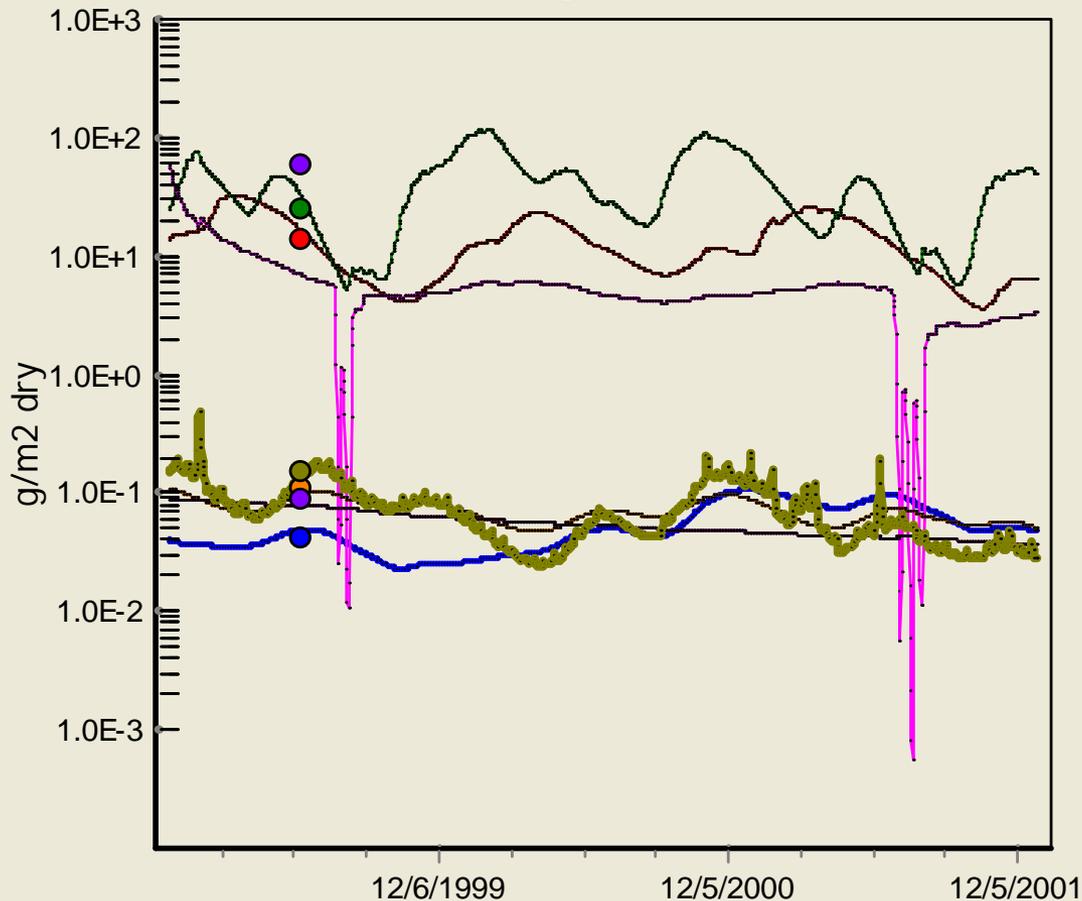
Photo Courtesy NASA Johnson Space Center

Galveston Bay, Texas, compartments



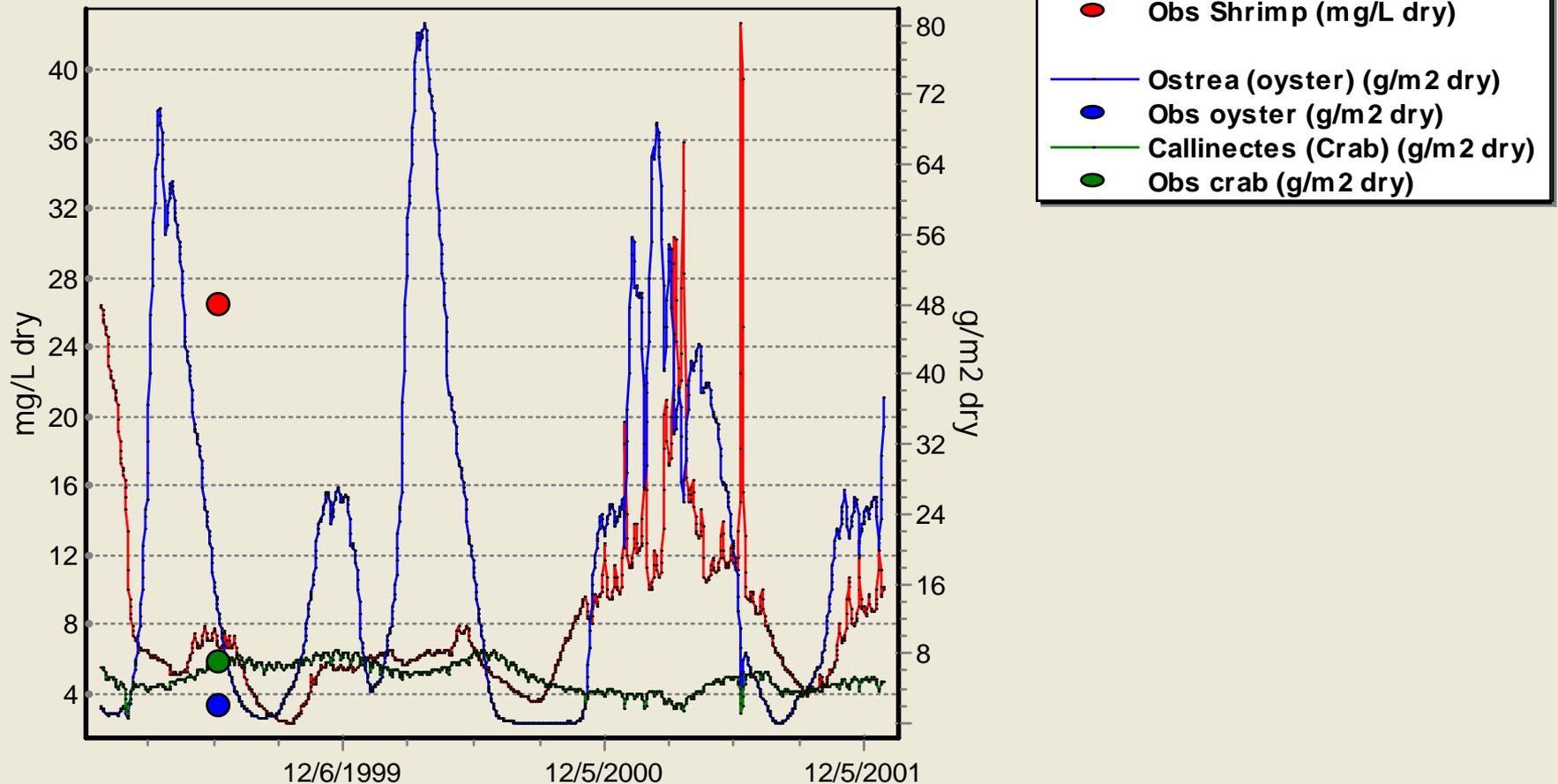
Can model biomass of commercial and other species of fish

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



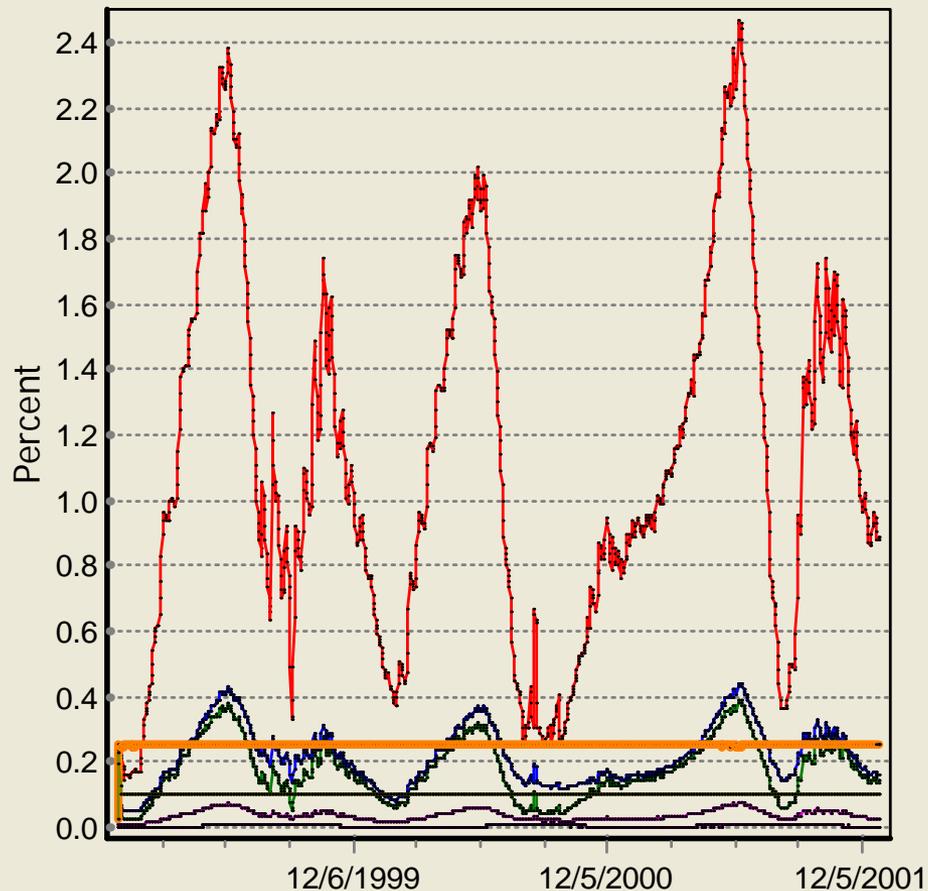
Can also model biomass of shrimp, oysters, and other invertebrates

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



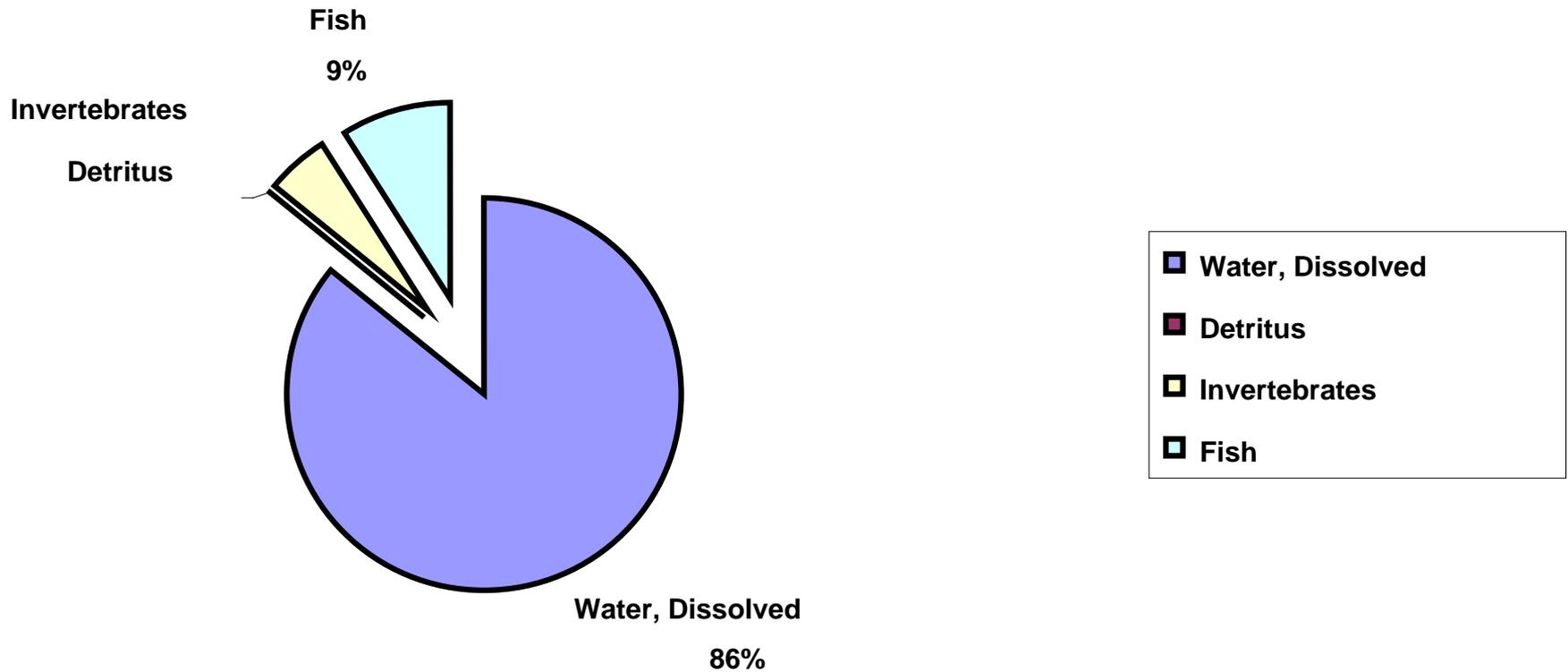
Predicted rates for crabs (as % of biomass)

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

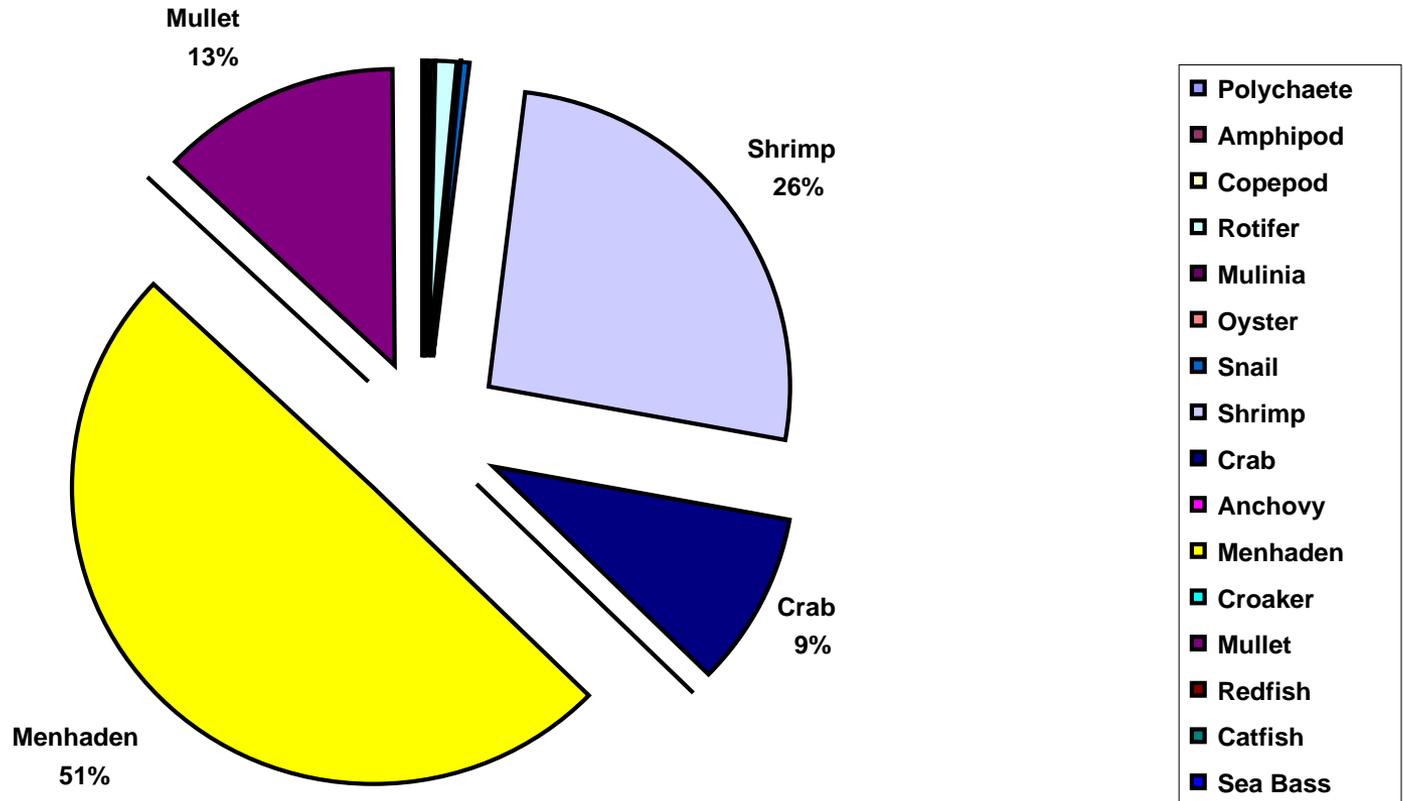


- Callinectes (Crab) Consumption (Percent)
- Callinectes (Crab) Defecation (Percent)
- Callinectes (Crab) Respiration (Percent)
- Callinectes (Crab) Excretion (Percent)
- Callinectes (Crab) Fishing (Percent)
- Callinectes (Crab) Predation (Percent)
- Callinectes (Crab) Mortality (Percent)

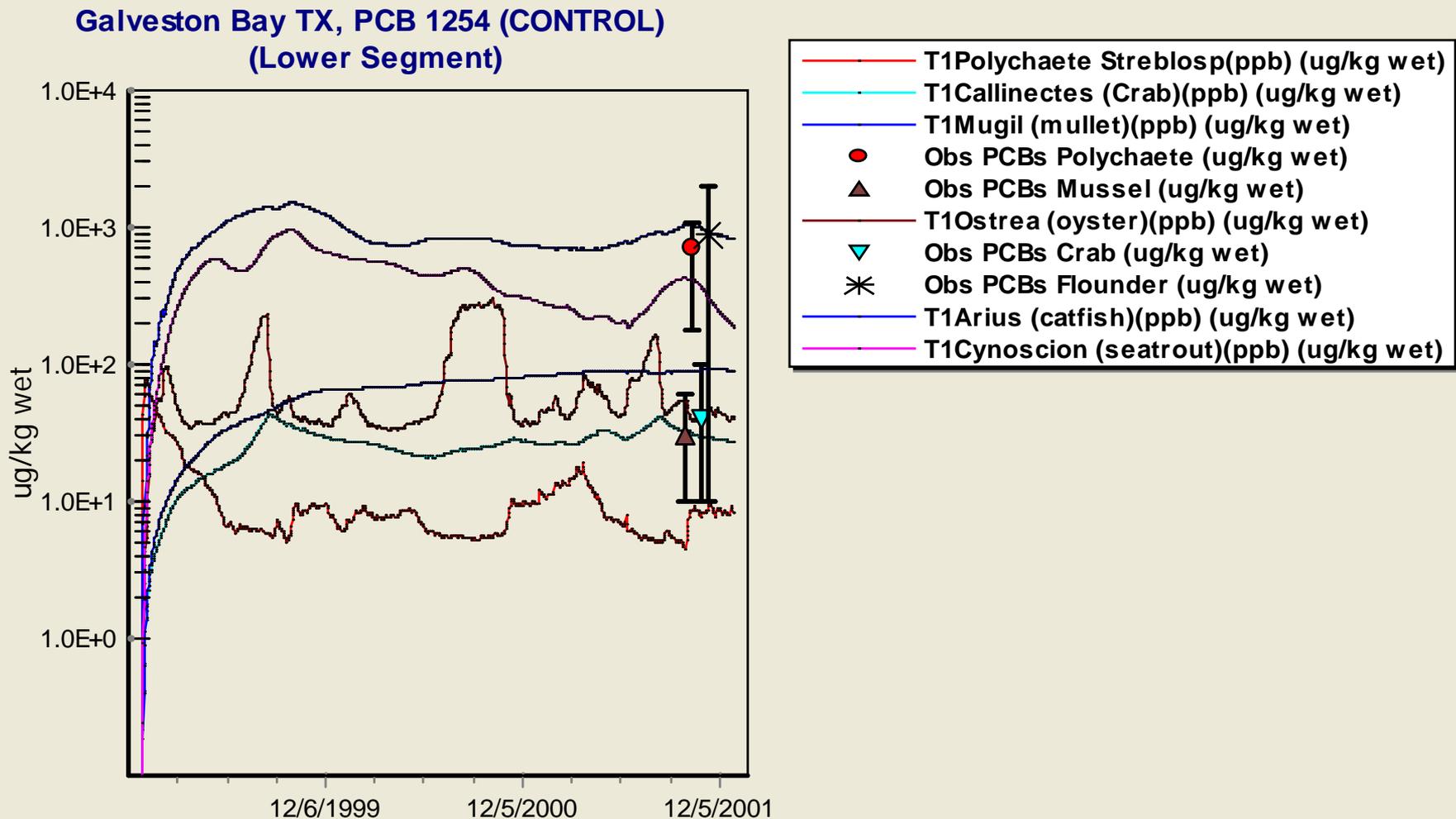
Predicted distribution of PFOS among major compartments in Galveston Bay at end of year



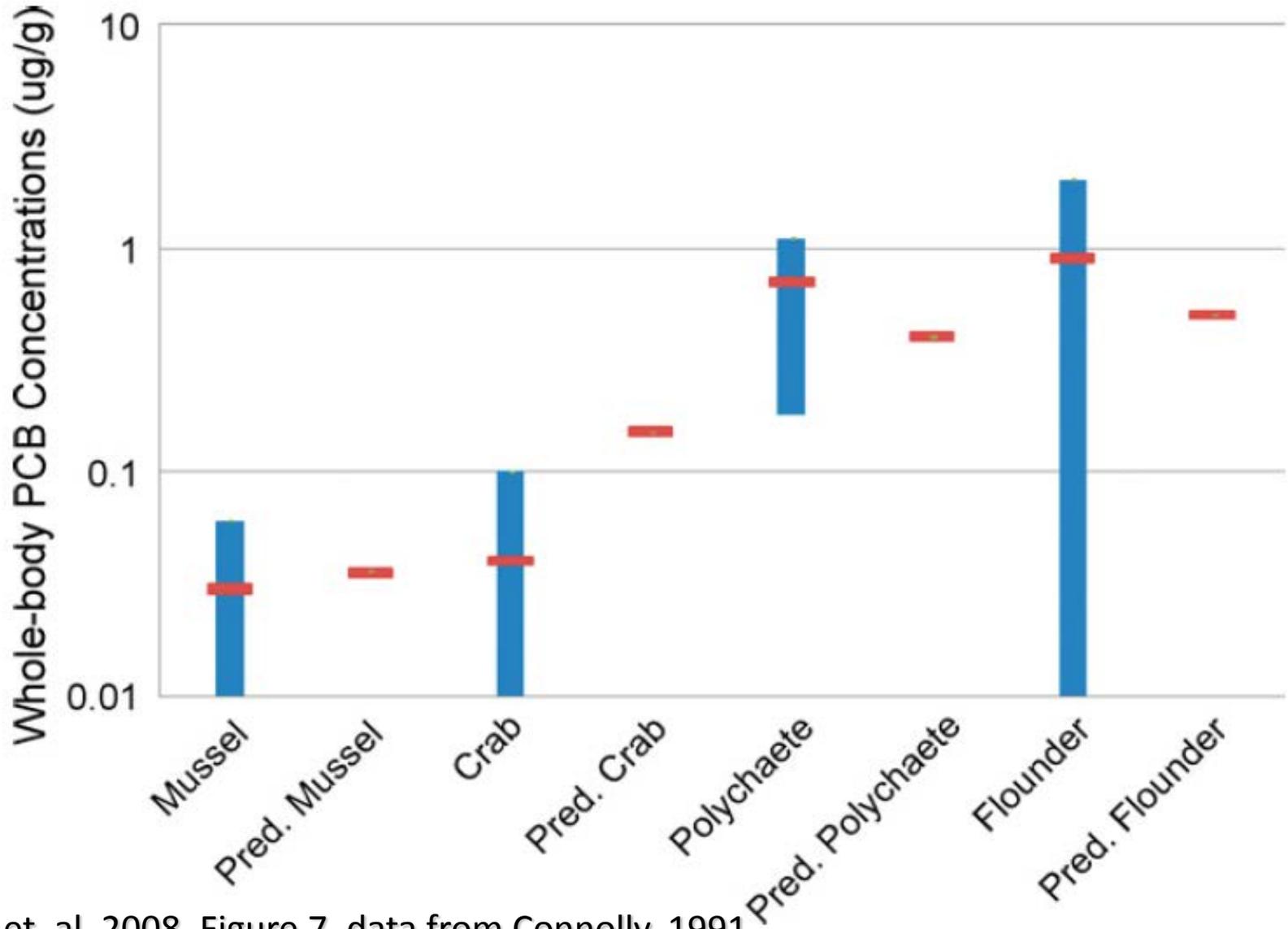
Distribution of PFOS among biotic compartments at end of year



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

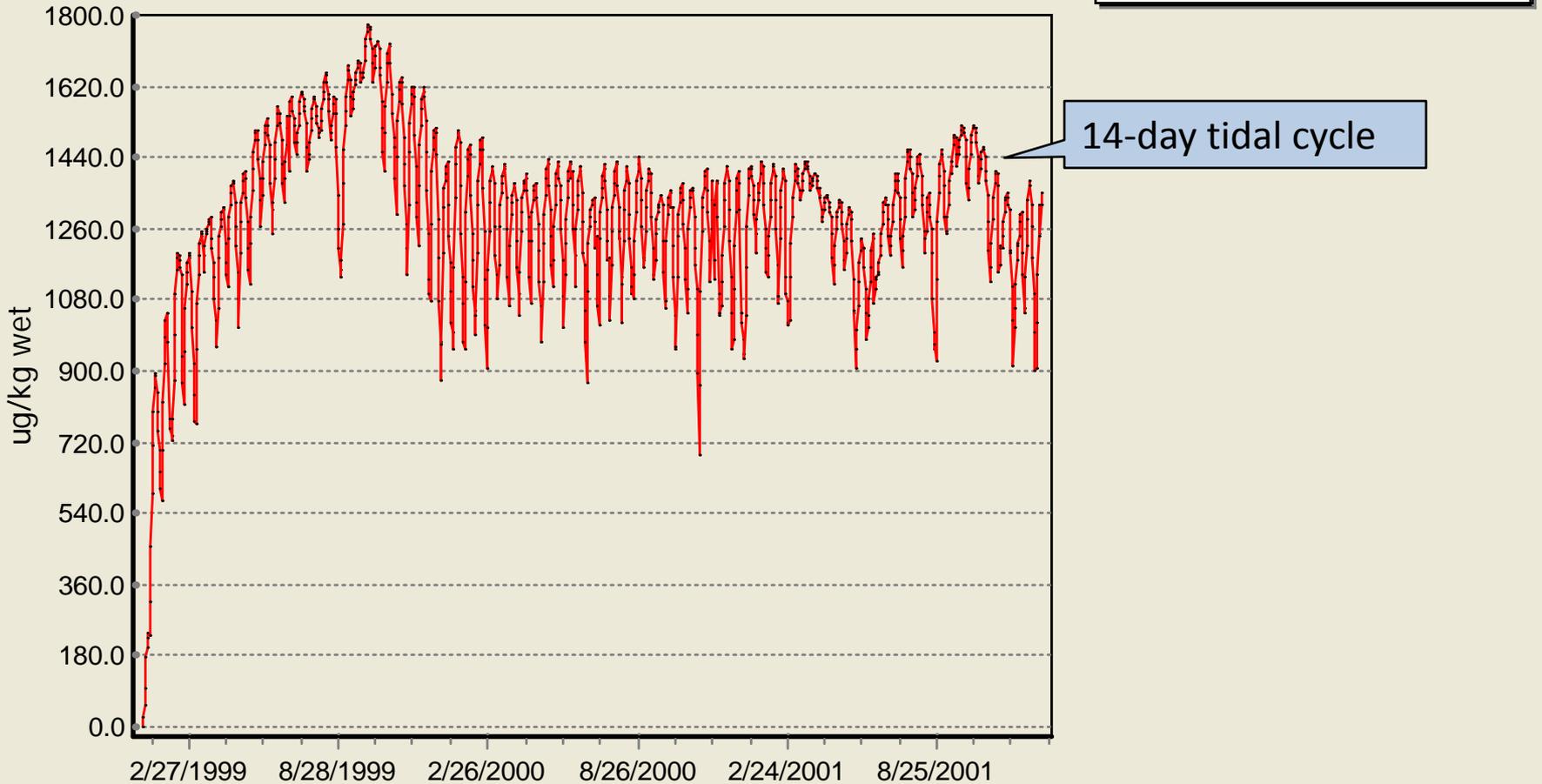
- Time Series of “Upper Layer” and “Lower Layer” Salinities for Salt Wedge Model
- Tidal Range Model Parameters
 - “harmonic constants”, often available from NOAA website
- Estuary Site Width
- Loadings of Freshwater Inflow

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)



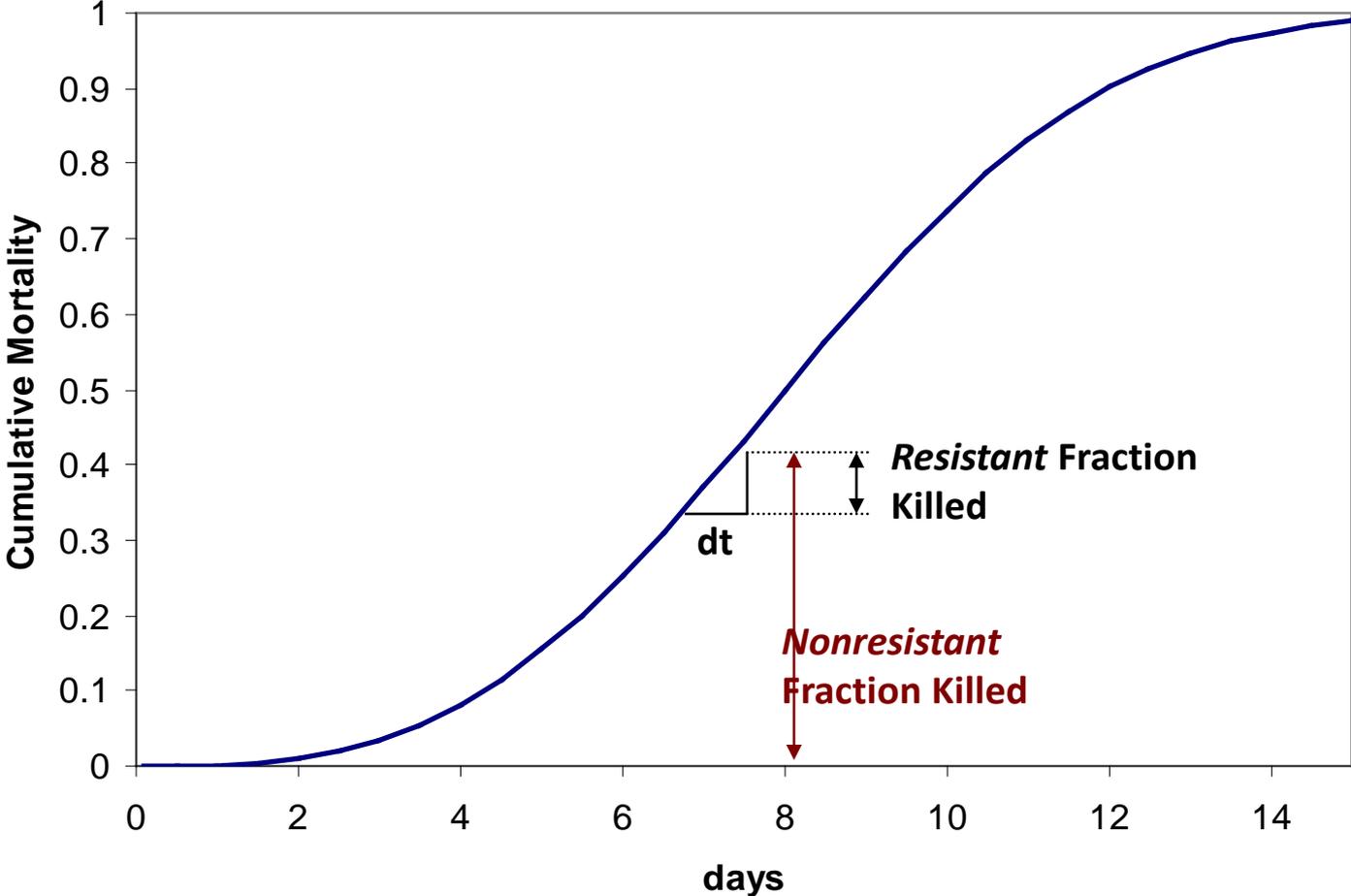
Modeling Toxicity of Chemicals

- 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

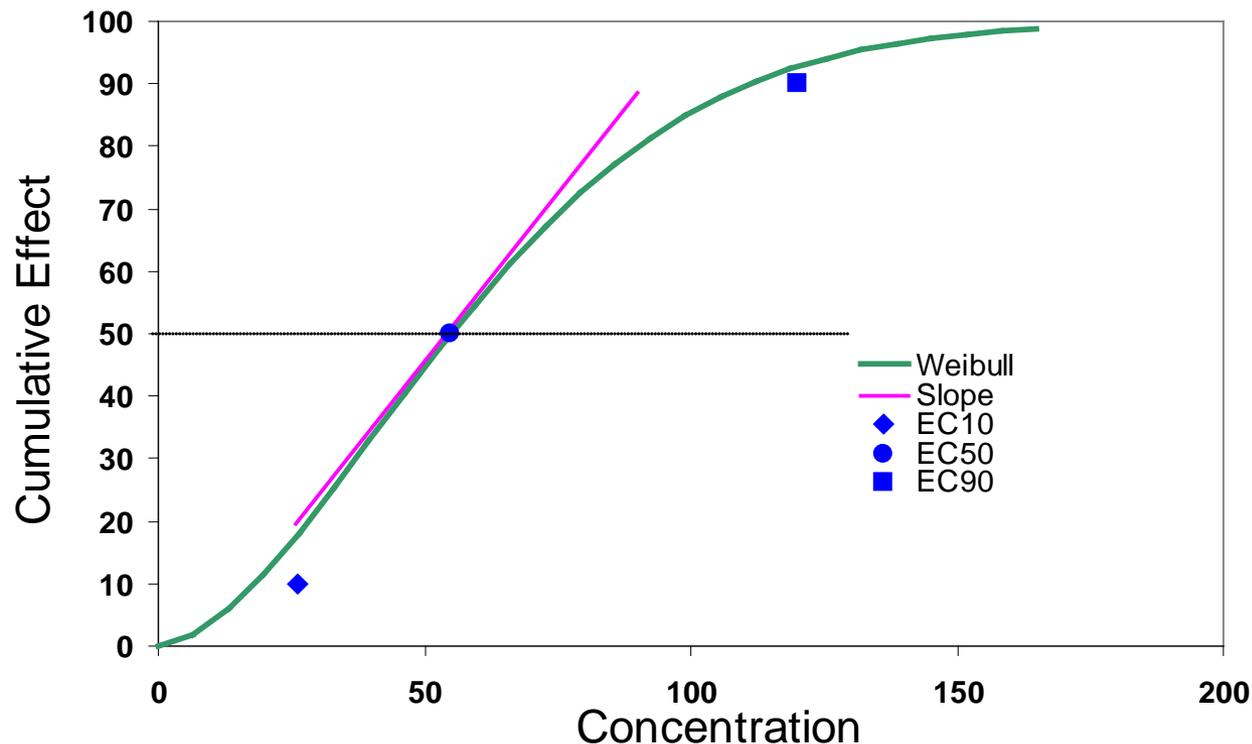
Two-parameter Weibull distribution as in Christensen and Nyholm (1984)

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

Two Required Parameters:

LC50 (or EC50)

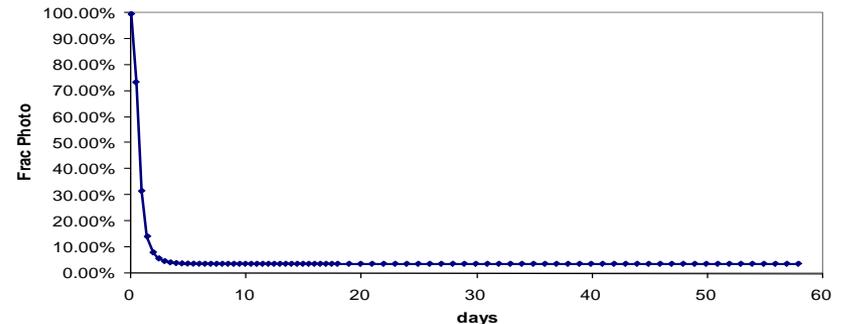
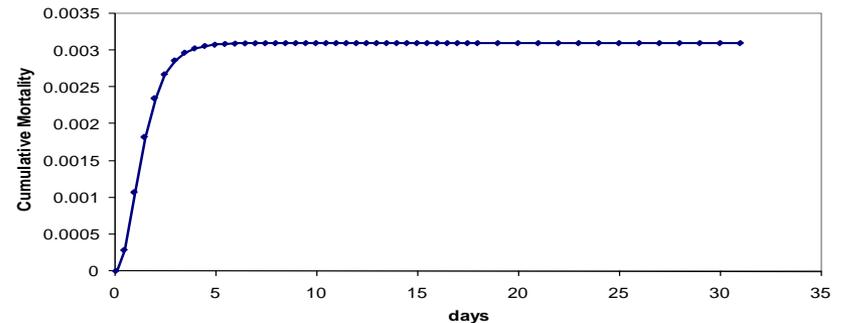
“Slope Factor” = Slope at LC50 multiplied by LC50



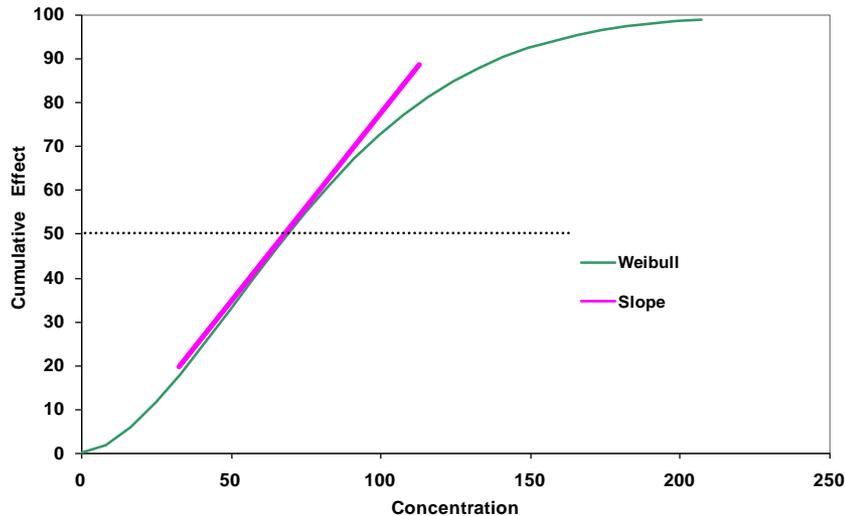
Spreadsheet Demo

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

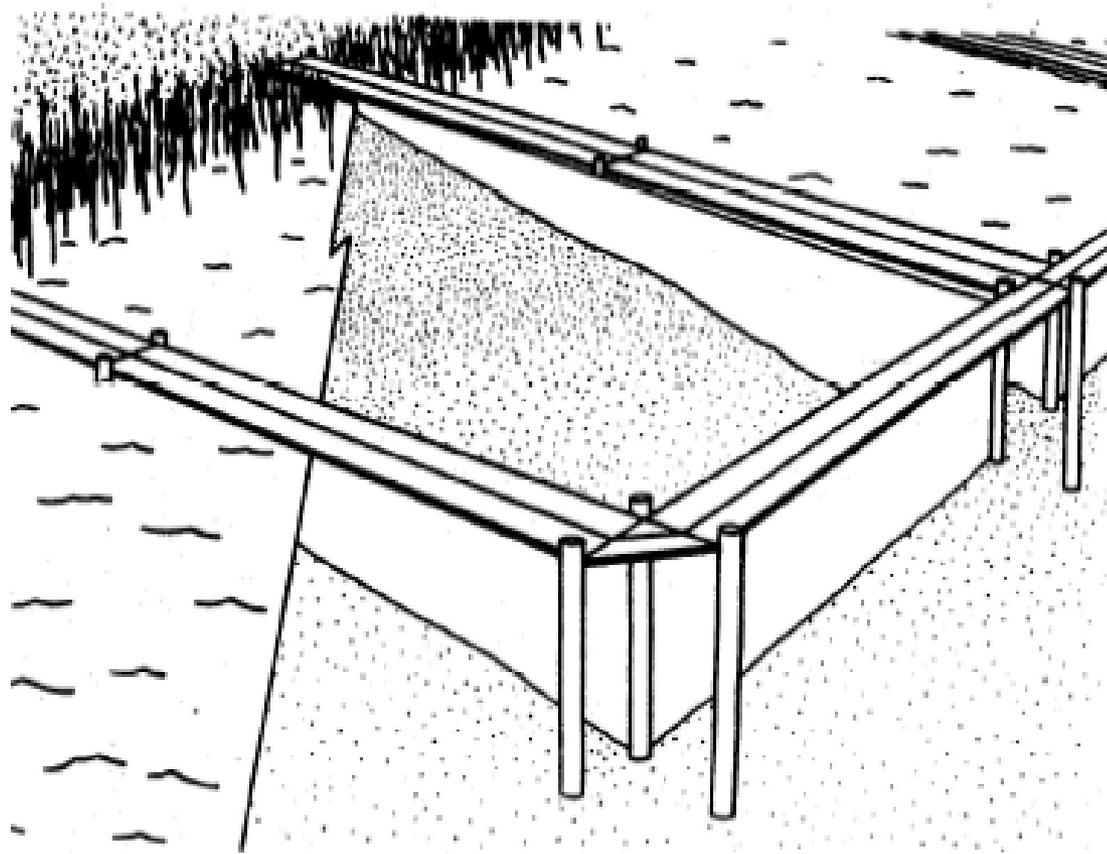
AQUATOX_Internal_Toxicity_Model.xls



AQUATOX_External_Toxicity_Model.xls

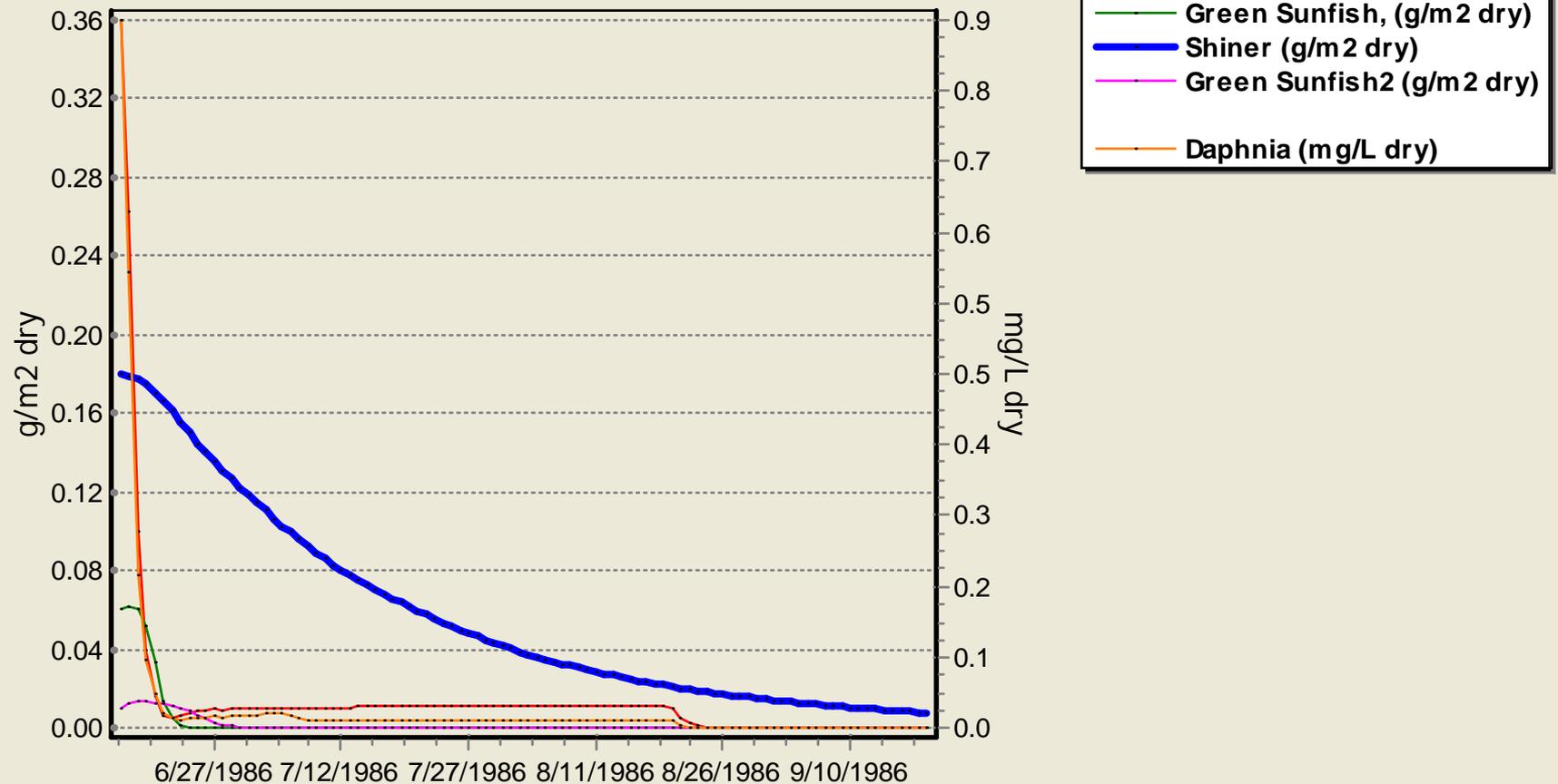


Returning to the Enclosure in Duluth MN . . .

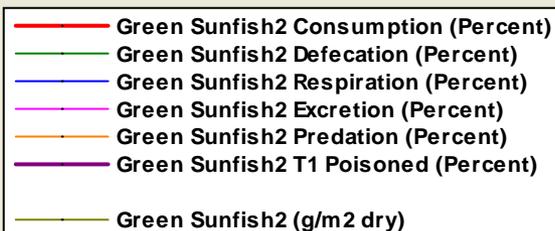
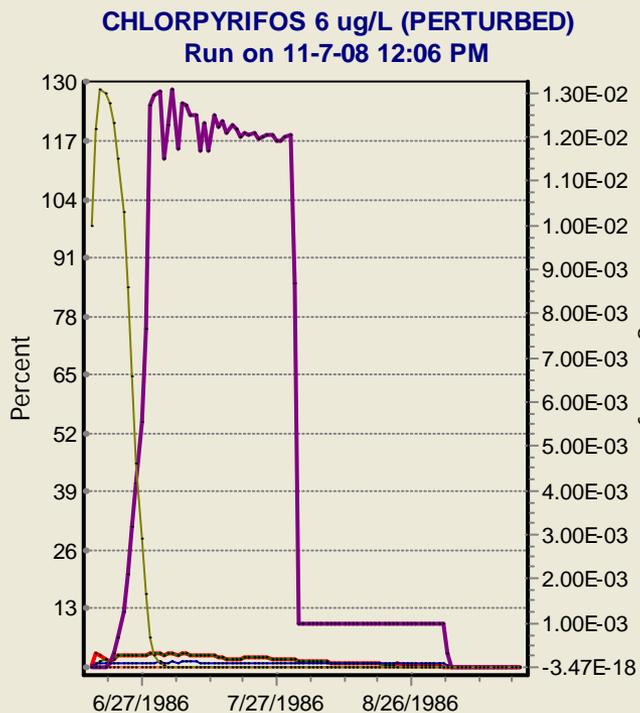


Animals all decline at varying rates following a single initial dose of chlorpyrifos

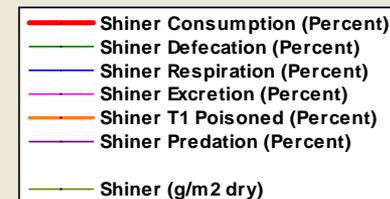
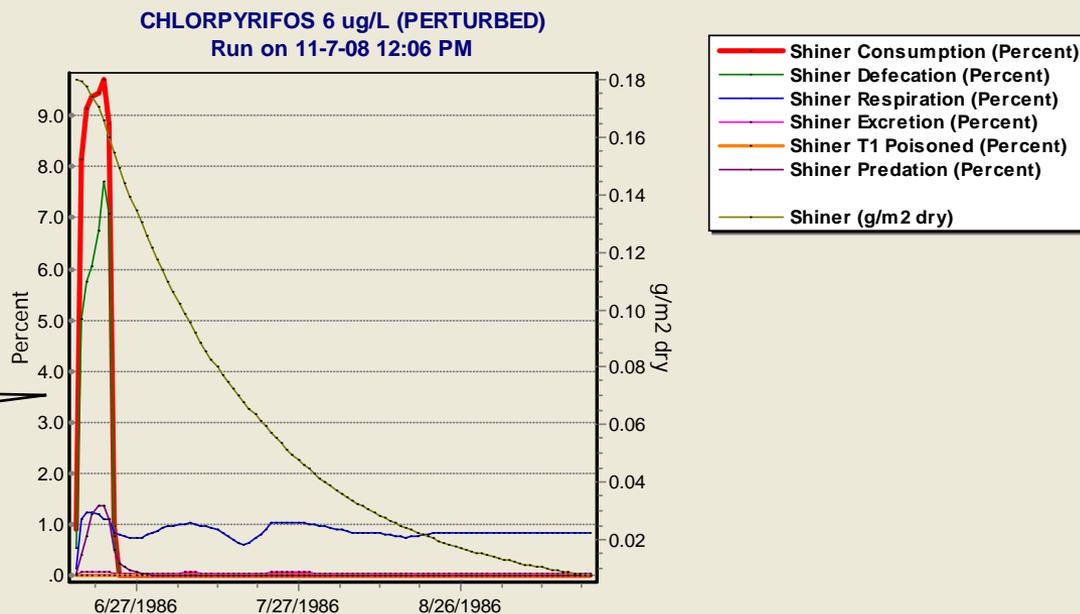
CHLORPYRIFOS 6 ug/L (PERTURBED)
Run on 11-7-08 11:36 AM



Sunfish have lethal effects, shiners have sublethal effects from chlorpyrifos

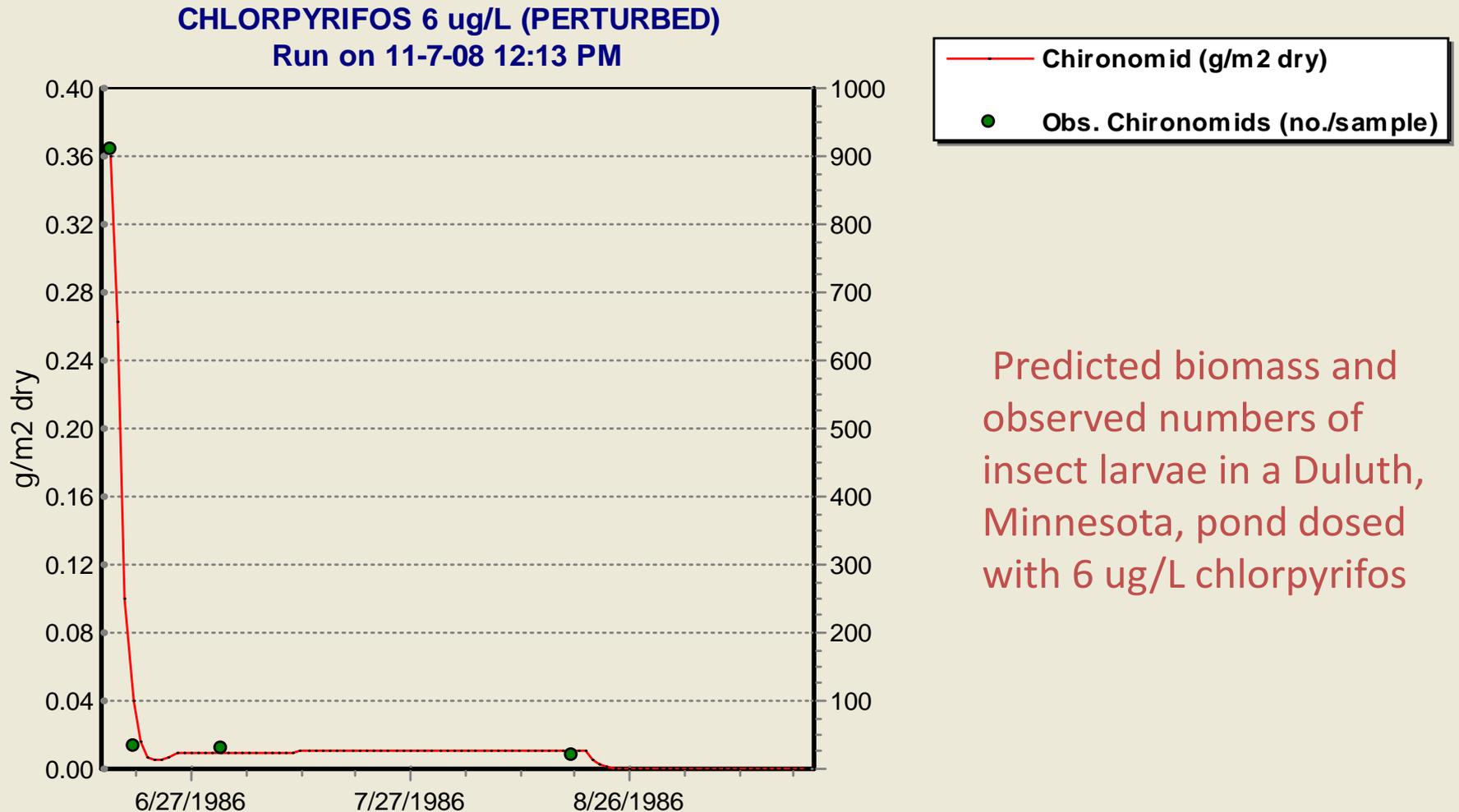


Sunfish with lethal effects



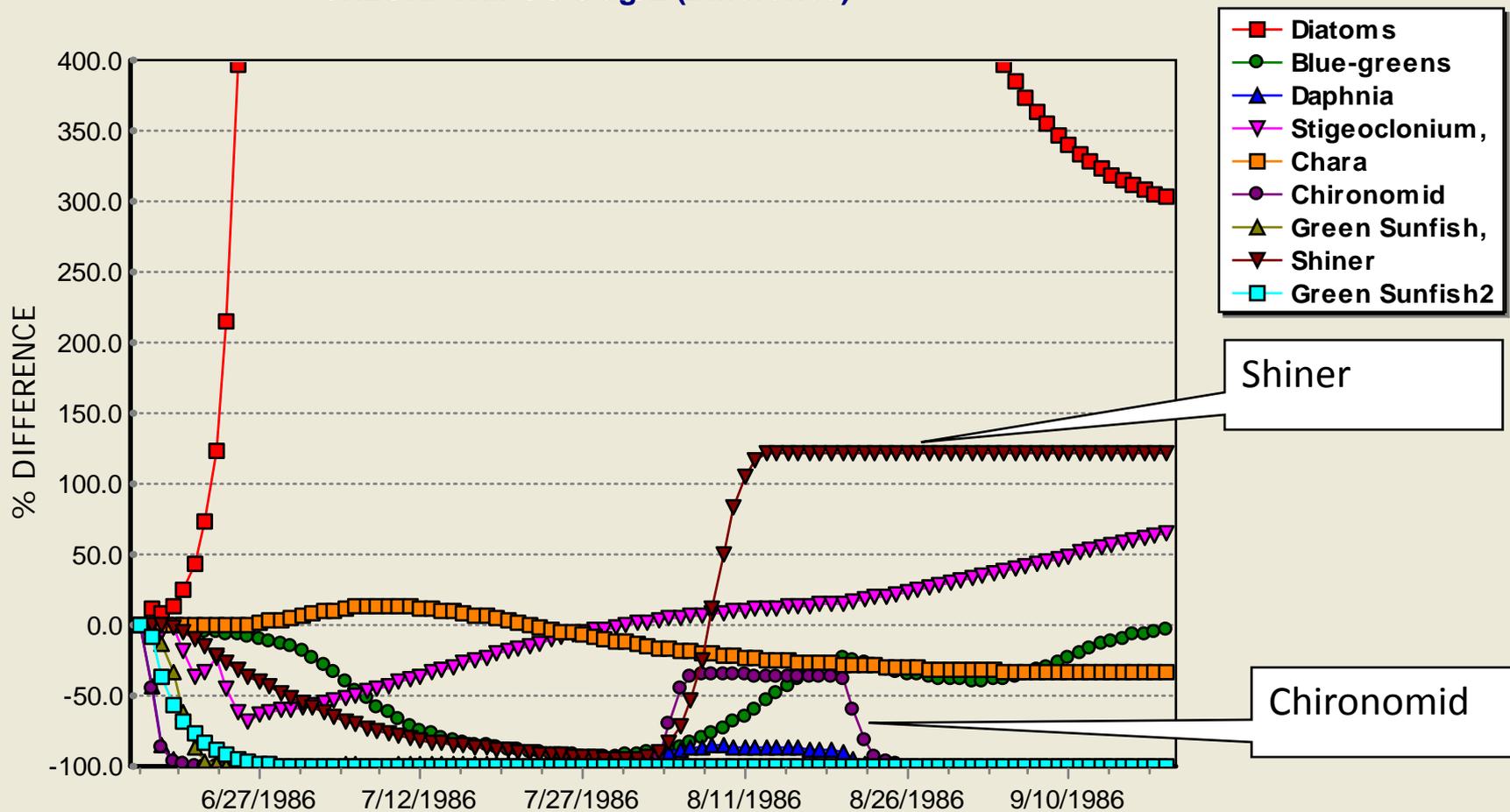
Shiner with sublethal effects only

Toxic effects of Chlorpyrifos in Duluth pond

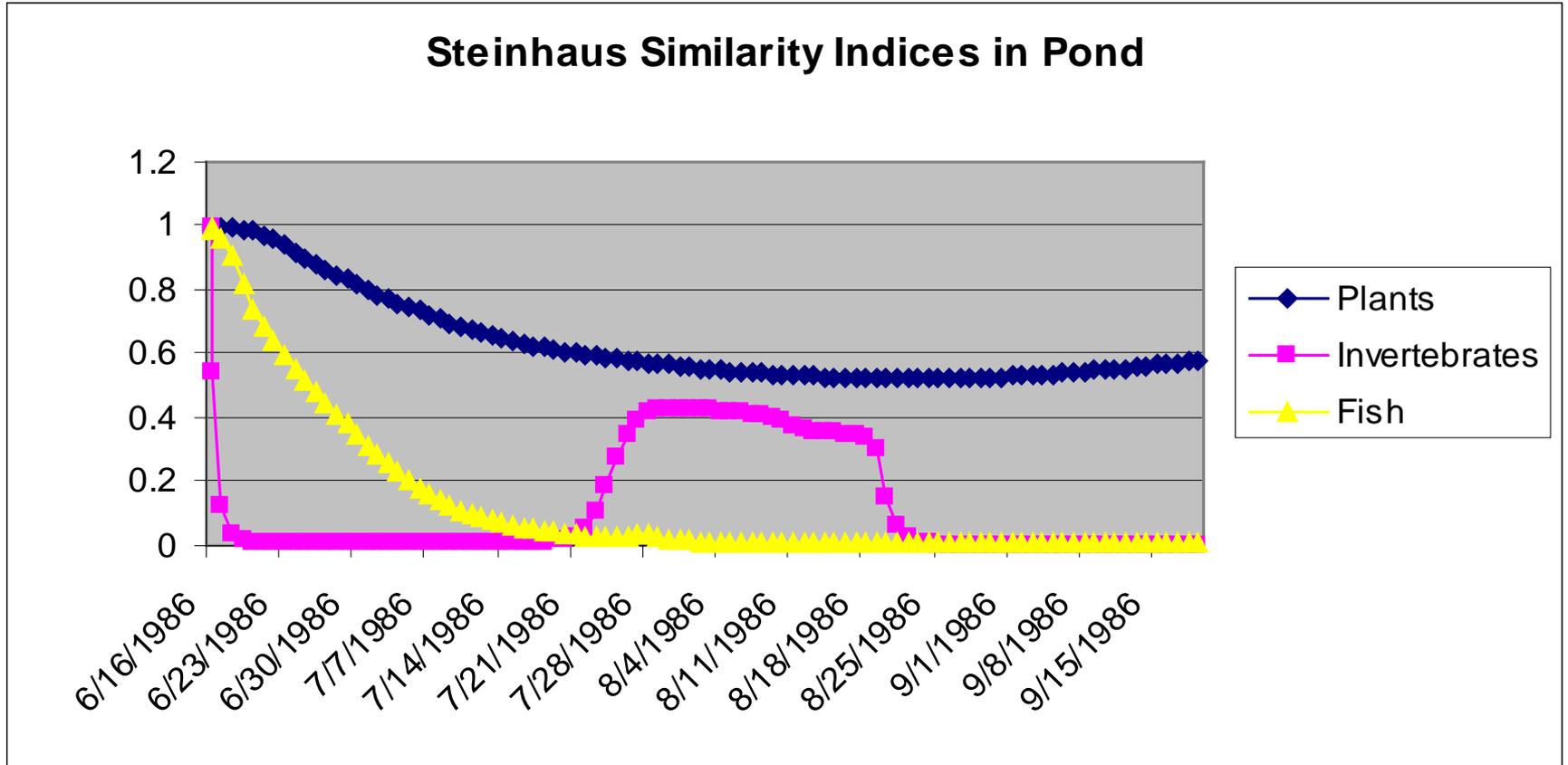


% Difference Graph shows differences in species response to toxicant

CHLORPYRIFOS 6 ug/L (Difference)



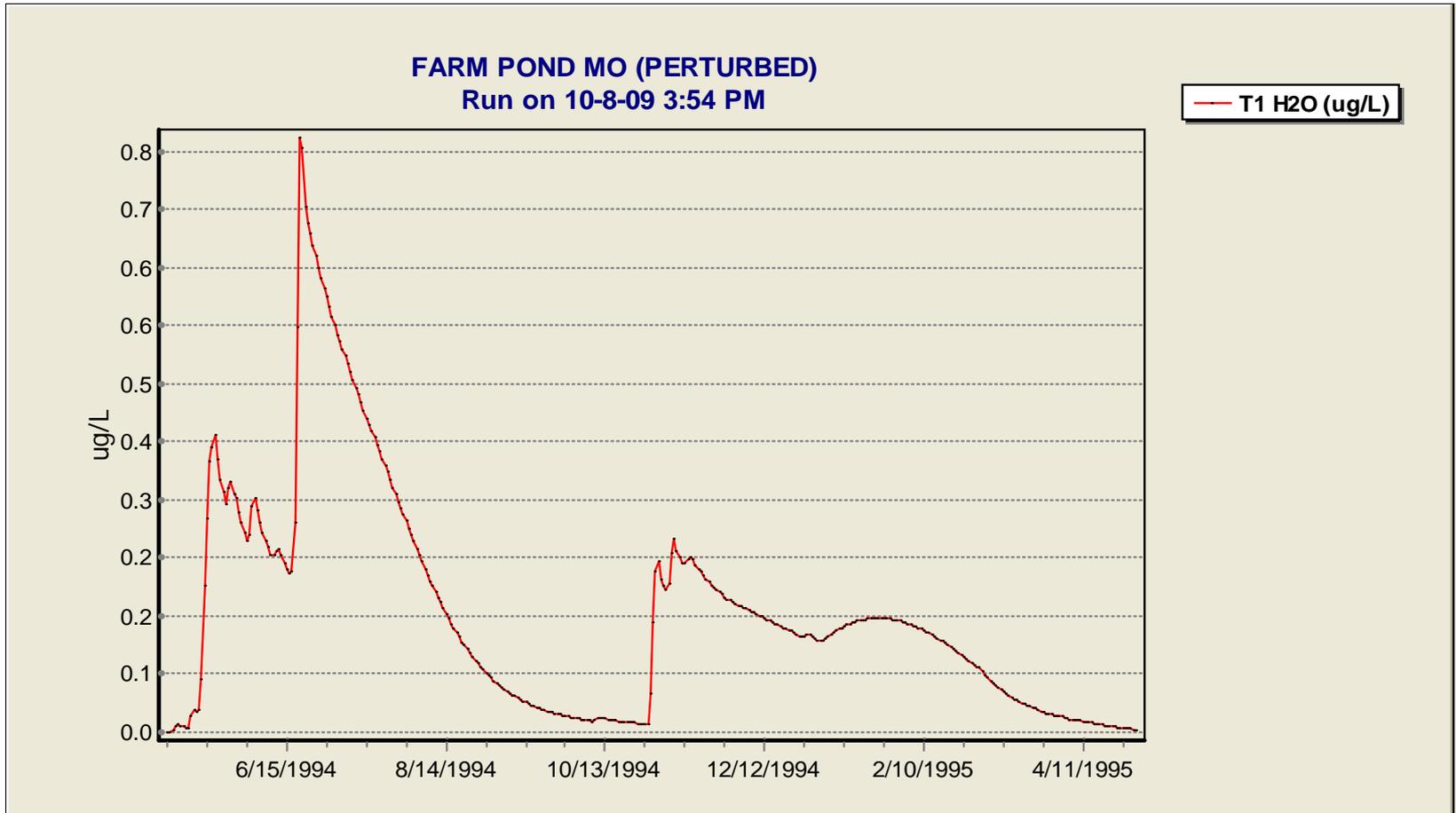
Steinhaus Indices show ecosystem impacts predicted by the model



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

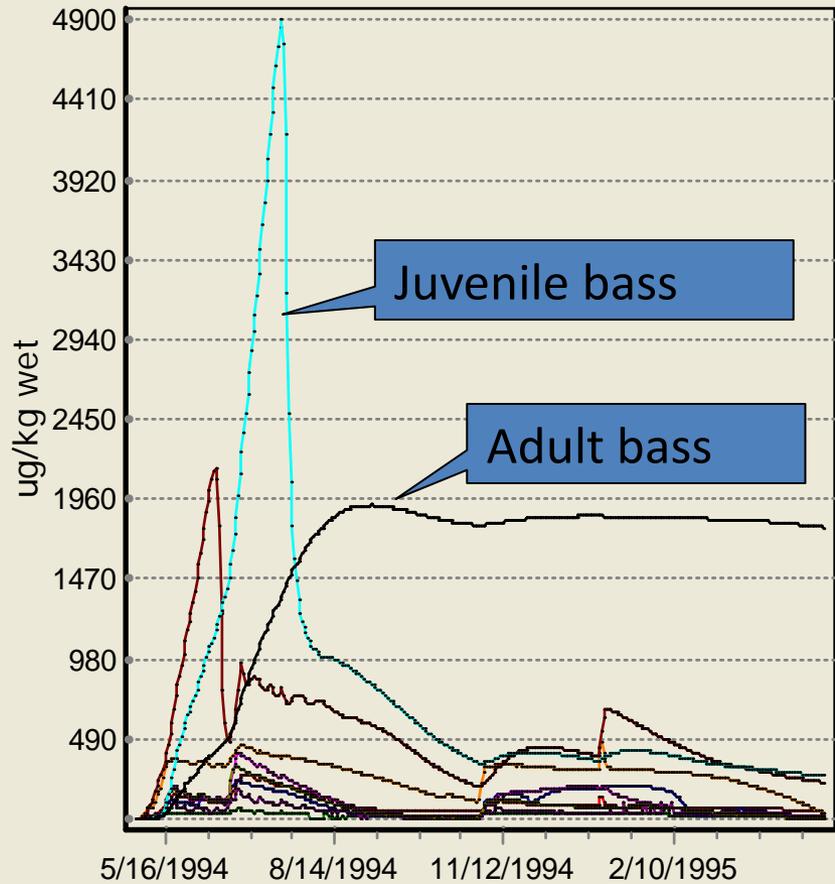
Farm Pond MO, Esfenvalerate

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



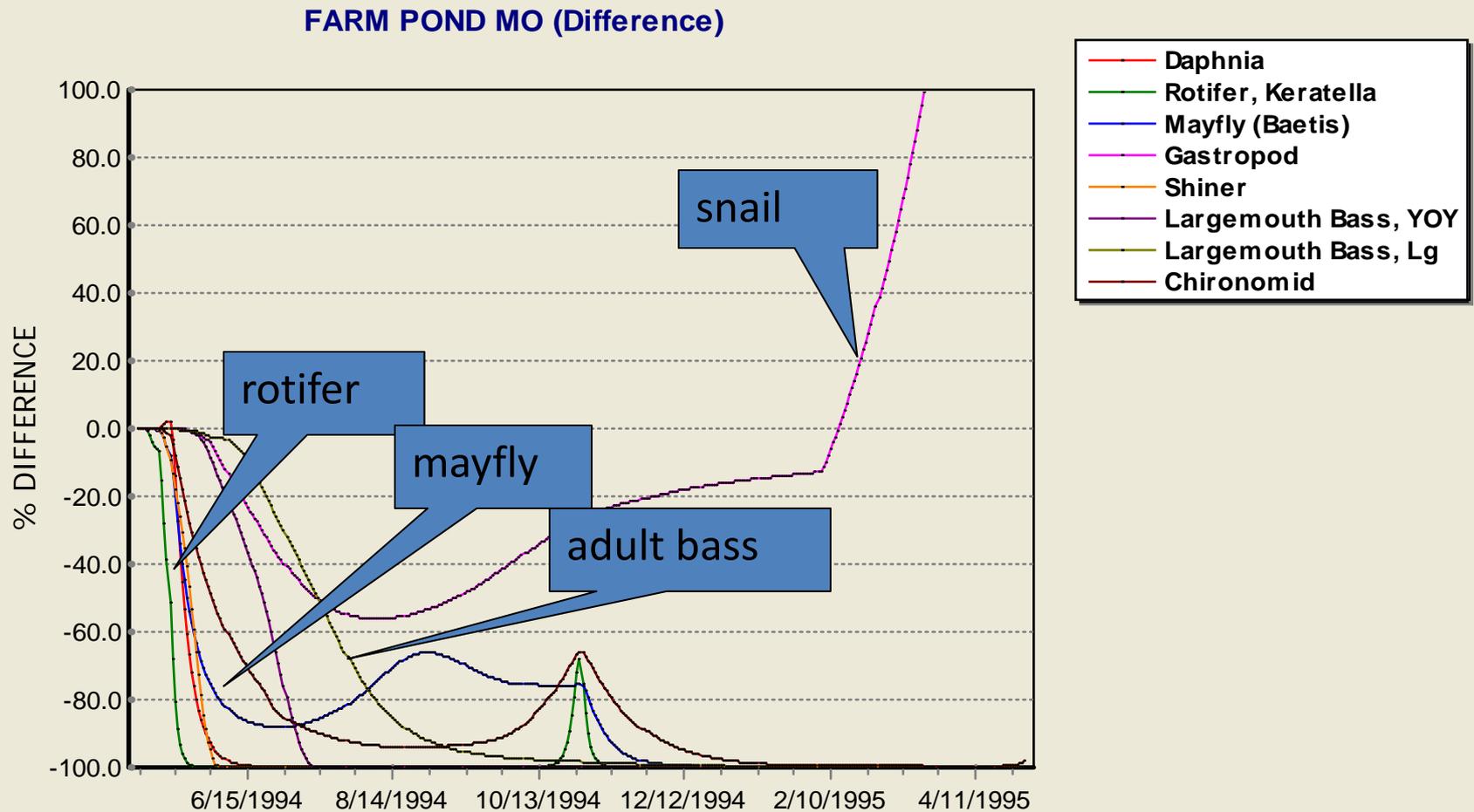
Farm Pond, Esfenvalerate Chemical Uptake in animals

FARM POND MO (PERTURBED)
Run on 10-8-09 3:54 PM



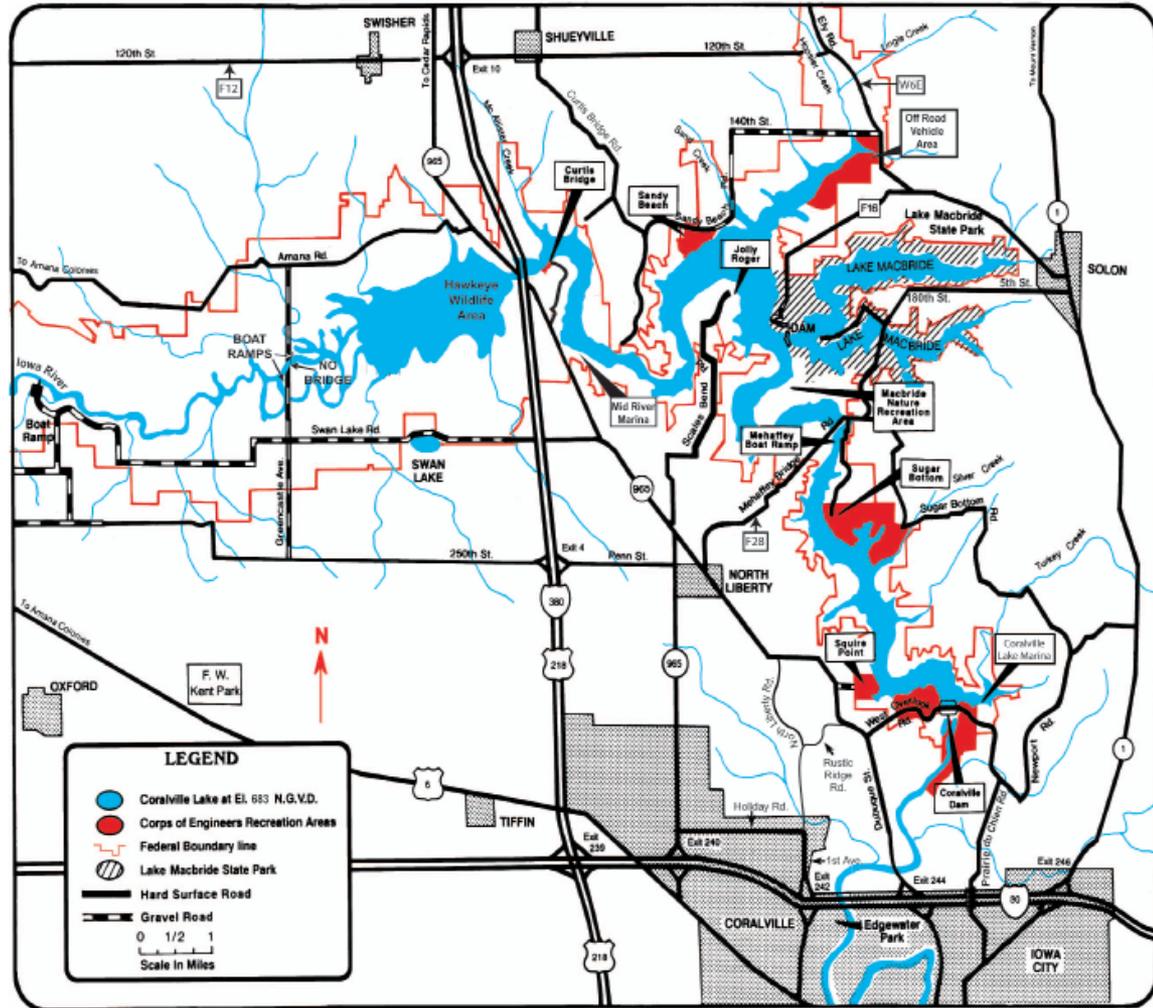
- T1Chironomid(ppb) (ug/kg wet)
- T1Daphnia(ppb) (ug/kg wet)
- T1Copepod(ppb) (ug/kg wet)
- T1Sphaerid(ppb) (ug/kg wet)
- T1Mayfly (Baetis)(ppb) (ug/kg wet)
- T1Rotifer, Keratella(ppb) (ug/kg wet)
- T1Gastropod(ppb) (ug/kg wet)
- T1Shiner(ppb) (ug/kg wet)
- T1Largemouth Bass, YOY(ppb) (ug/kg wet)
- T1Largemouth Bass, Lg(ppb) (ug/kg wet)

Farm Pond, Esfenvalerate Difference Graph

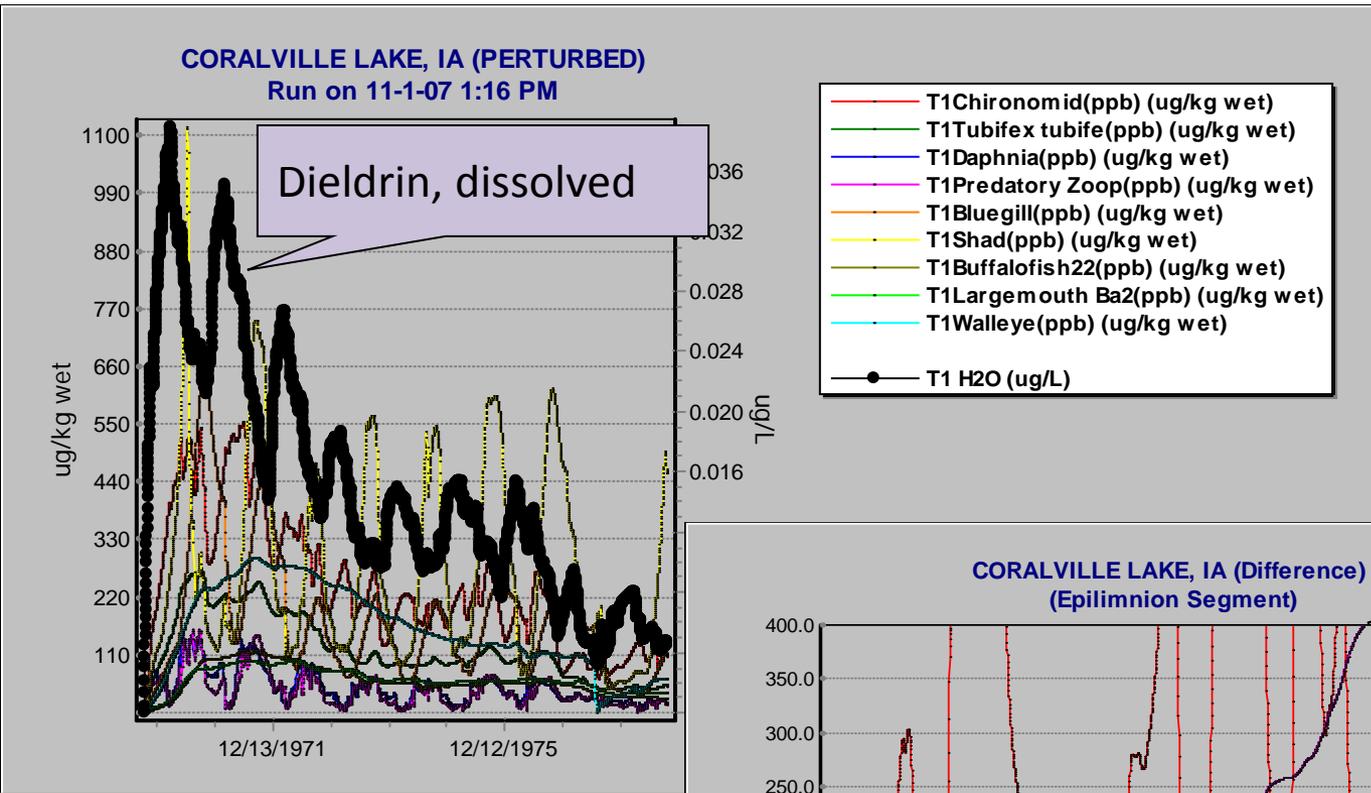


Coralville Reservoir Iowa long-term contamination with dieldrin

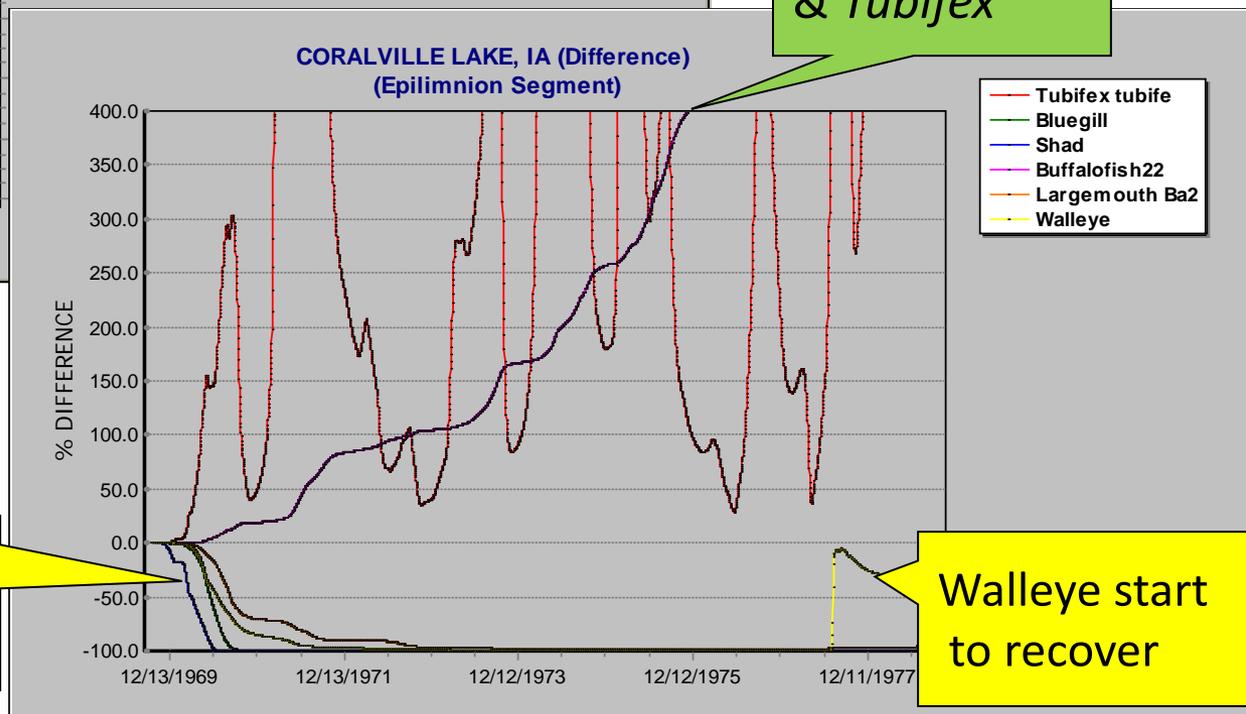
- Run-of-river
- Flood control
- 90% of basin in agriculture
 - Nutrients
 - Pesticides
 - Sediment



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



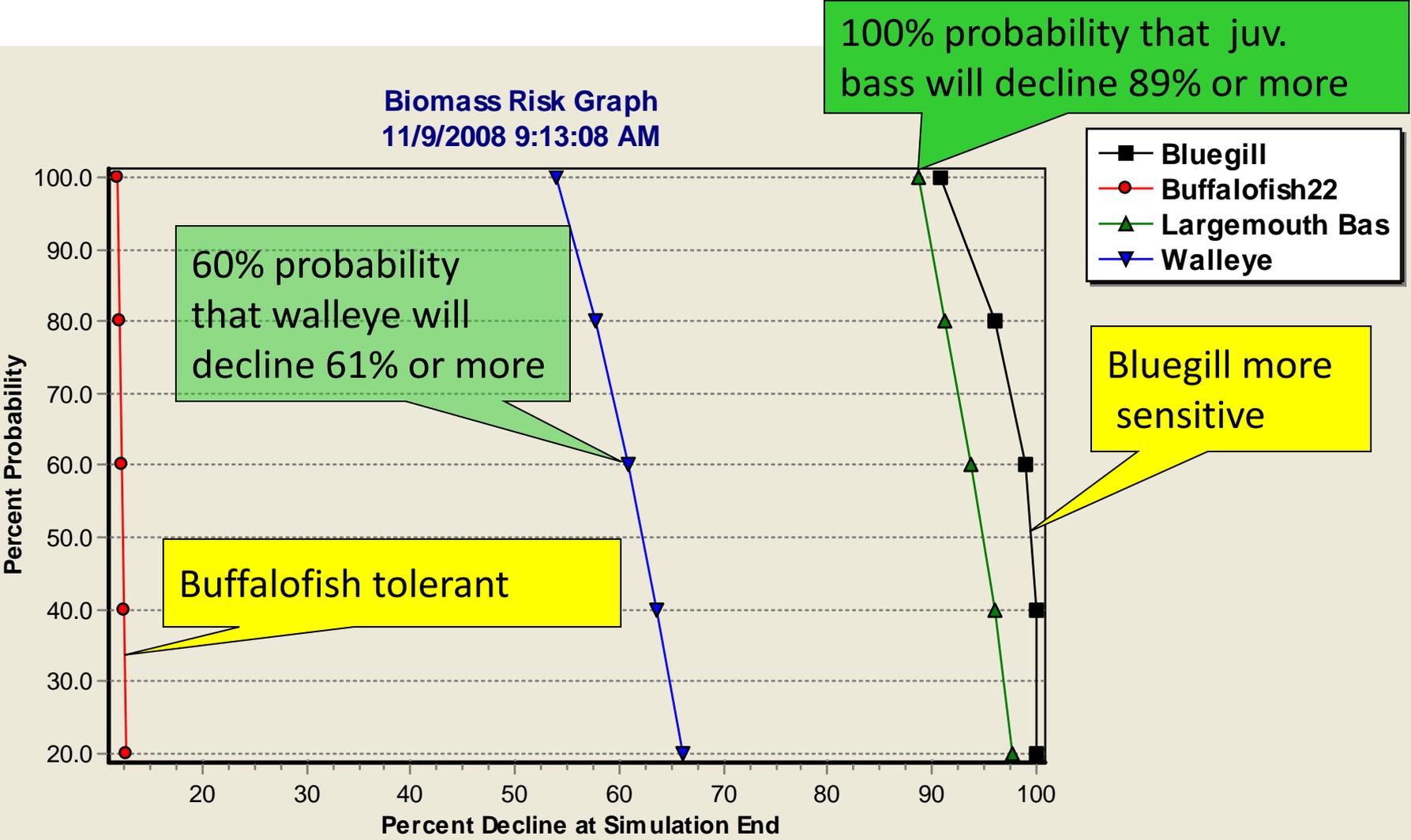
Buffalofish & *Tubifex*



Shad, bluegill, walleye, bass die off

Walleye start to recover

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



Toxicant Parameters and Loadings are Subject to Uncertainty Analysis

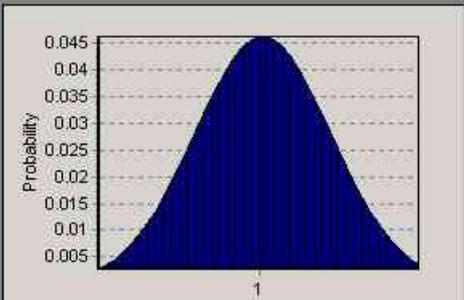
AQUATOX – Uncertainty Setup

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. 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 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

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

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>

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)	Biotransf. 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)	Biotransf. 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

Interspecies Toxicity Correlation Interface

Available Interspecies Toxicity Correlation Models:

Step 1: Choose a database
ICE Aquatic Species Common Names

Step 2: Choose a surrogate species
Brown shrimp(Penaeus aztecus)
Brown trout(Salmo trutta)
Bryozoa(Lophopodella carteri)
Bryozoa(Pectinatella magnifica)
Bryozoa(Plumatella emarginata)
Cape Fear shiner(Notropis mekistocholas)
Channel catfish(Ictalurus punctatus)
Chinook salmon(Oncorhynchus tshawytscha)
Coho salmon(Oncorhynchus kisutch)
Colorado squawfish(Ptychocheilus lucius)
Common carp(Cyprinus carpio)
Common ranga(Rangia cuneata)
Common starfish(Asterias forbesii)
Copepod(Acartia clausi)
Copepod(Acartia tonsa)
Copepod(Eurytemora affinis)
Copepod(Nitocra spinipes)

Step 3: Choose a predicted taxa
Atlantic silverside(Menidia menidia)
Black bullhead(Ameiurus melas)
Black crappie(Pomoxis nigromaculatus)
Bluegill sunfish(Lepomis macrochirus)
Bonytail chub(Gila elegans)
Brook trout(Salvelinus fontinalis)
Brown trout(Salmo trutta)
Cape Fear shiner(Notropis mekistocholas)
Chinook salmon(Oncorhynchus tshawytscha)

Step 4: Evaluate / examine model

Surrogate:
Channel catfish(Ictalurus punctatus)

Predicted:
Brown trout(Salmo trutta)

Sample Size:
16

Intercept (a):
0.5162406726

Regression Coefficient (slope b):
0.6172946138

Average Value of Predicted Taxa:
2.095636

Error Mean Square (EMS):
1.03186928

Standard Error of Slope (SEB):
0.18635262

Correlation Coefficient:
0.6628634852

Probability (Pr) that slope <> 0:
0.0051

Log Scale: Confidence Interval **0.95** XMin **0** (log) XMax **6** (log)

Click on the regression line for more information.

Step 5: Apply Model to AQUATOX Toxicity Parameters

The Selected Surrogate Species:
Channel catfish(Ictalurus punctatus)

The Selected Predicted Species:
Brown trout(Salmo trutta)

Selected Model:
Based on Catfish with LC50 of 7600 ug/L
Trout LC50 will be set to 816.293 ug/L

Is represented by the AQUATOX toxicity record:
Catfish

Is represented by the AQUATOX toxicity record:
Trout

Execute Model

Help
Cancel
OK

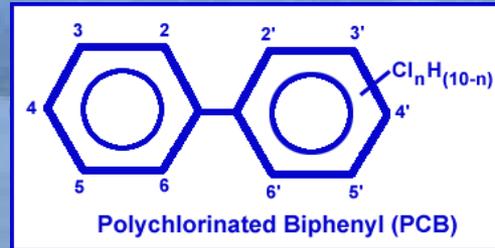
Lab 7: Risk Assessment of Insecticide in Ohio Stream

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

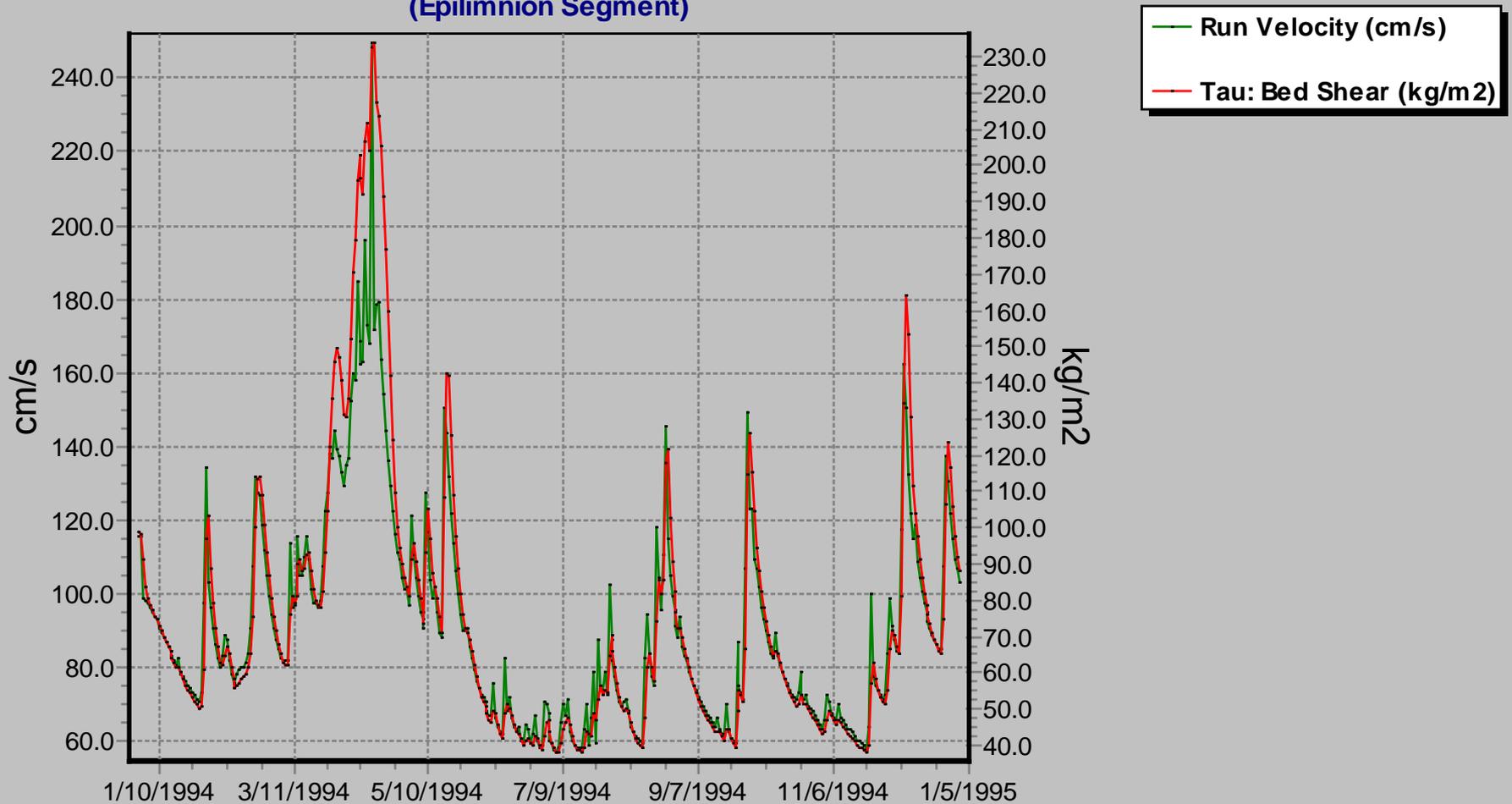


Modeling Inorganic Sediments (sand, silt, and clay)

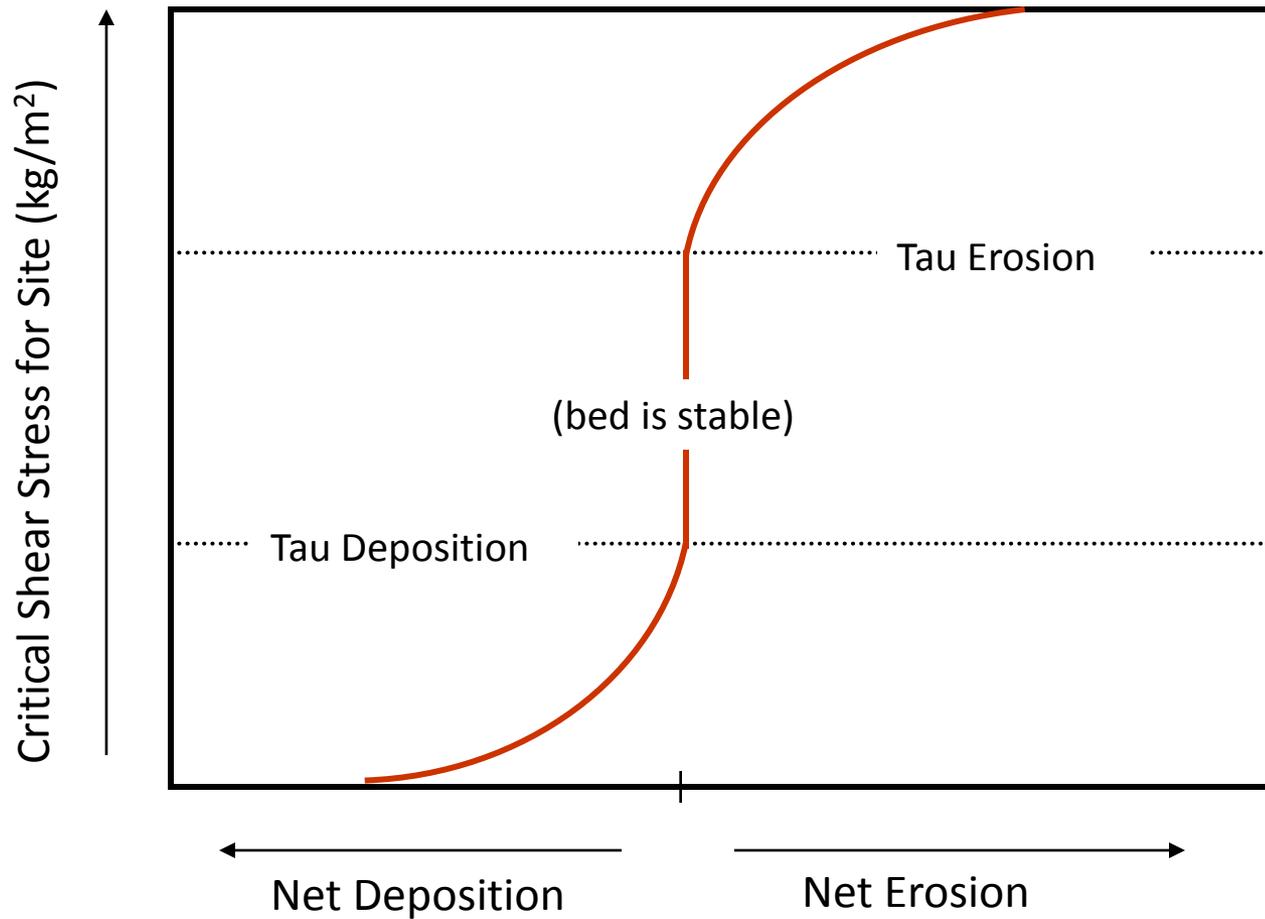
- Stream simulations only
- Scour, deposition and transport of sediments
- River reach assumed short and well mixed
- Daily average flow regime determines shear stresses
- Feedback to biota through light limitation, sequestration of chemicals, and now direct sediment effects

Bed Shear Stress (Tau) Closely Related to Water Velocity

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

Critical Shear Stress
for Scour kg/m²

References:

Critical Shear Stress
for Deposition kg/m²

Fall Velocity m/s

Clay Parameters

Critical Shear Stress
for Scour kg/m²

References:

Critical Shear Stress
for Deposition kg/m²

Fall Velocity m/s

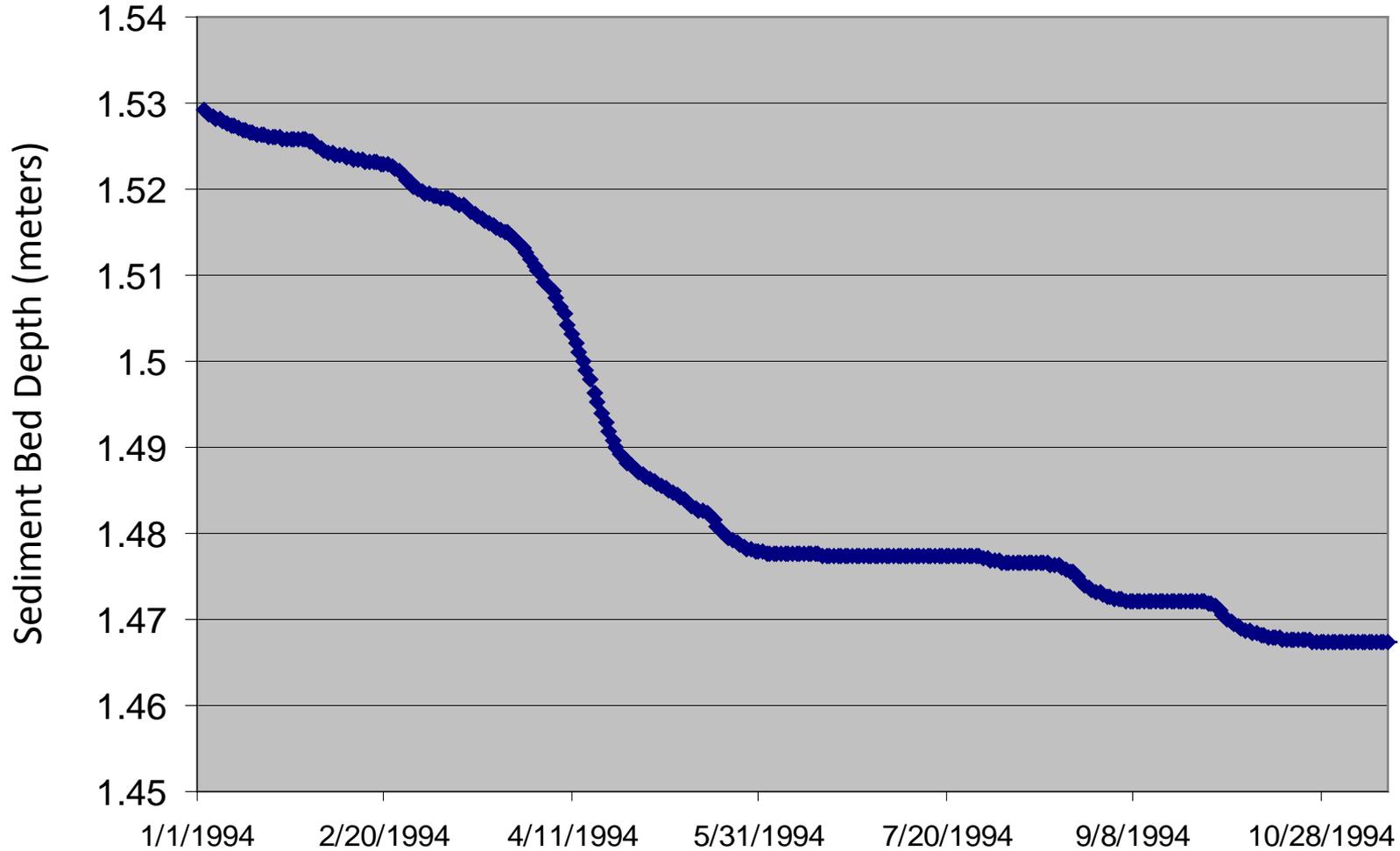
Help

 OK

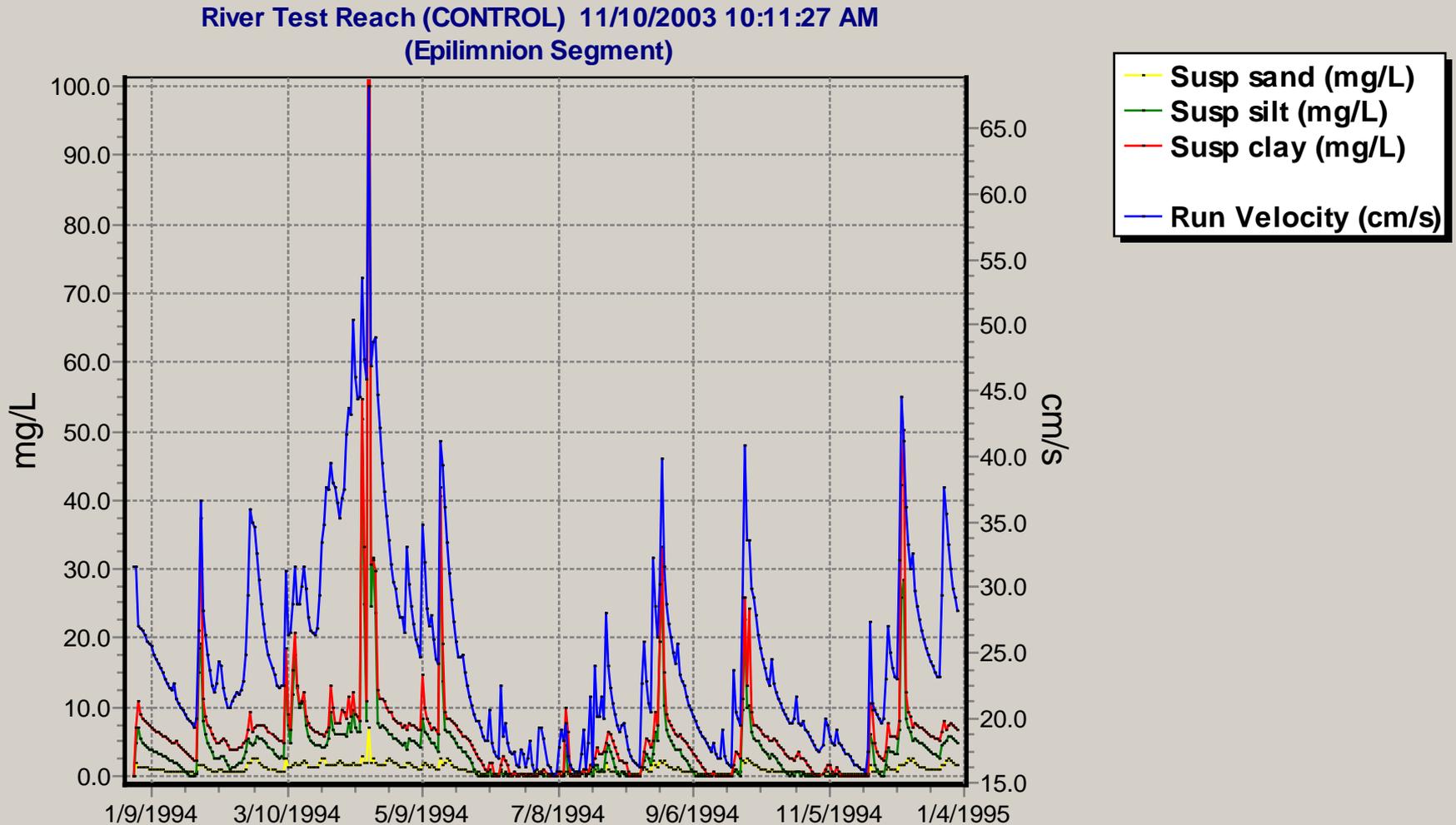
Sand Model

- 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

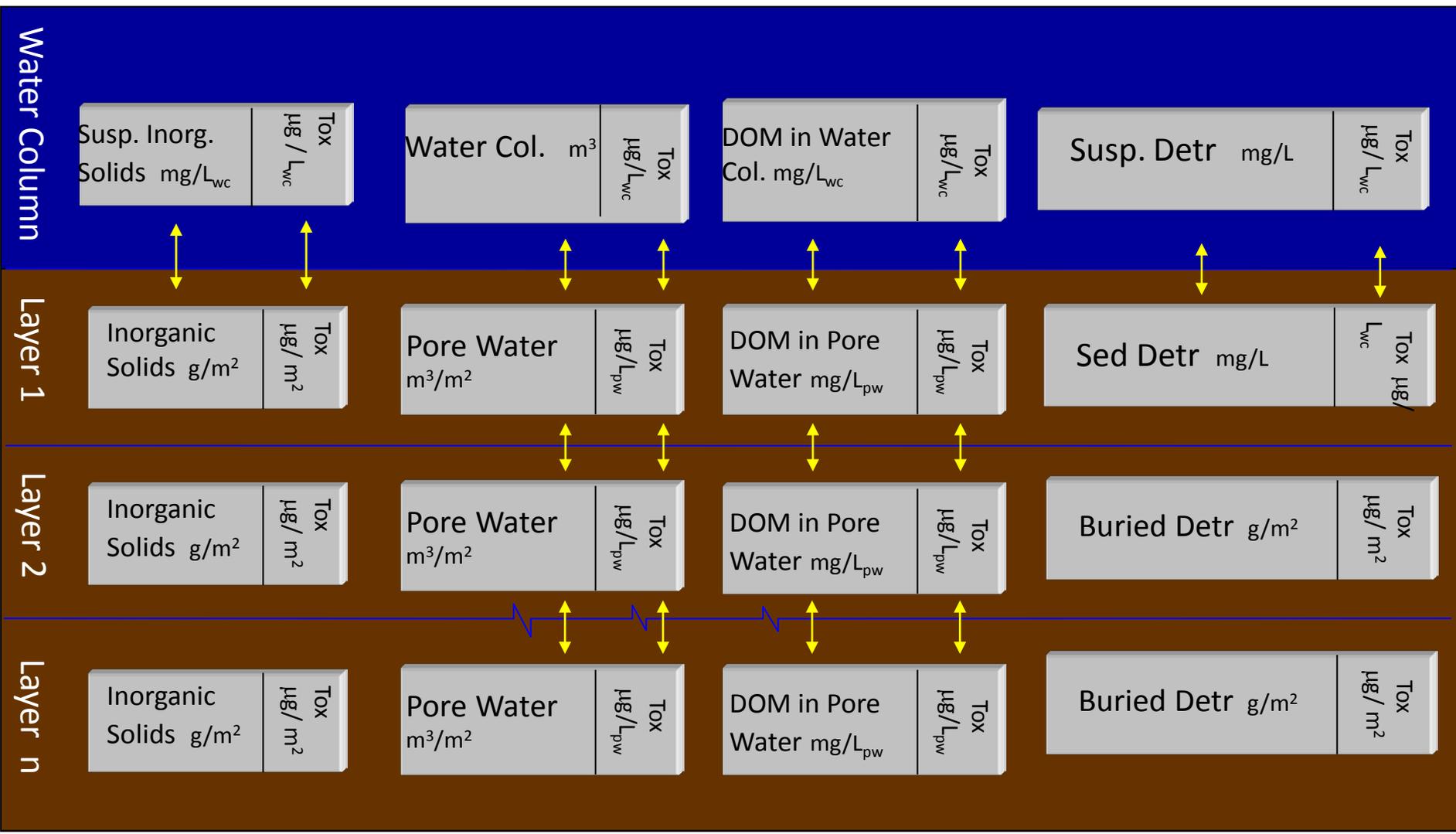


AQUATOX Multi-Layer Sediment Model

- **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 μm
(clay)
- **Non-Cohesives:** particle size from 63 to 250 μm
(silt)
- **Non-Cohesives2:** particle size greater than 250 μm
(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

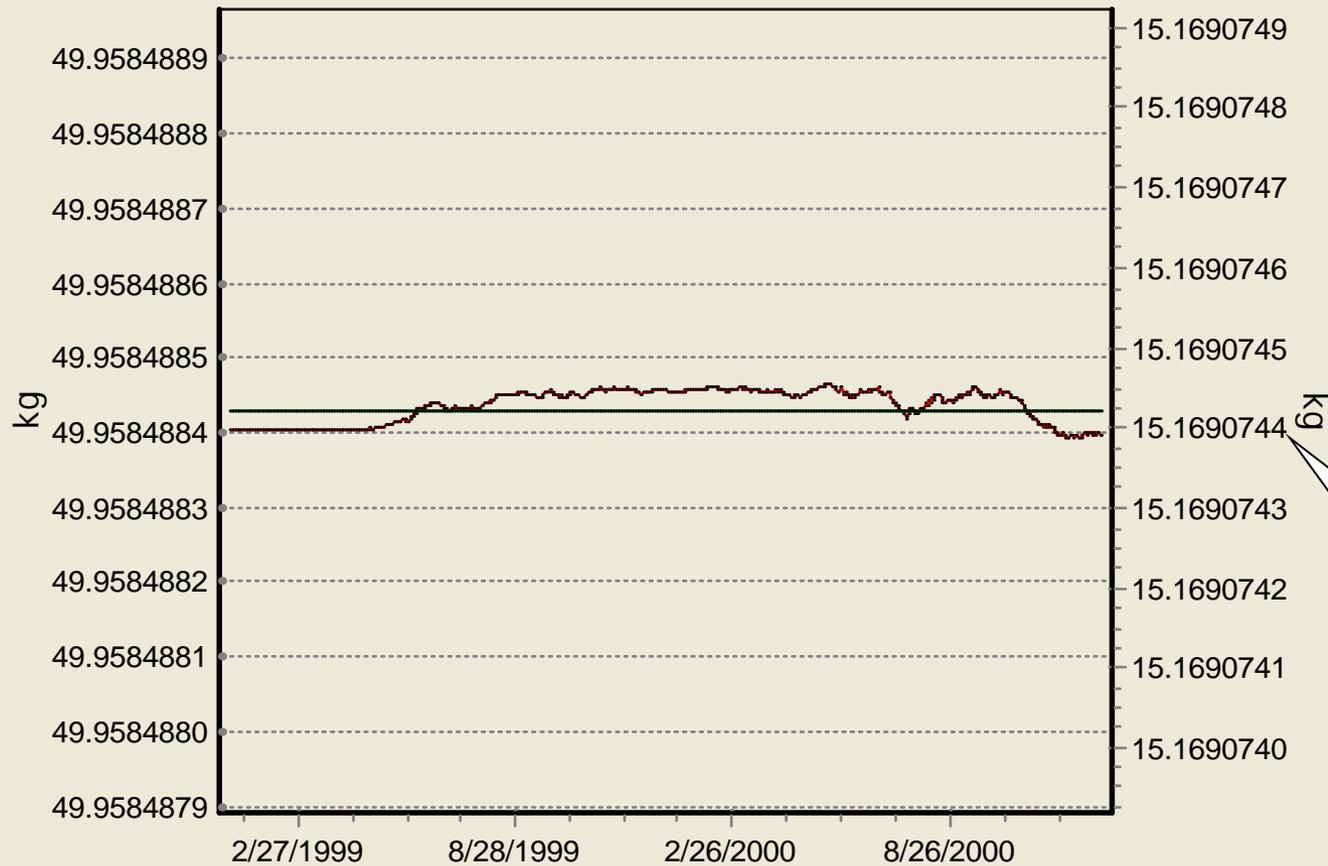
Y2 Axis Scale

Use Automatic Scaling
 Use Below Values

Min
Max

Mass is Balancing

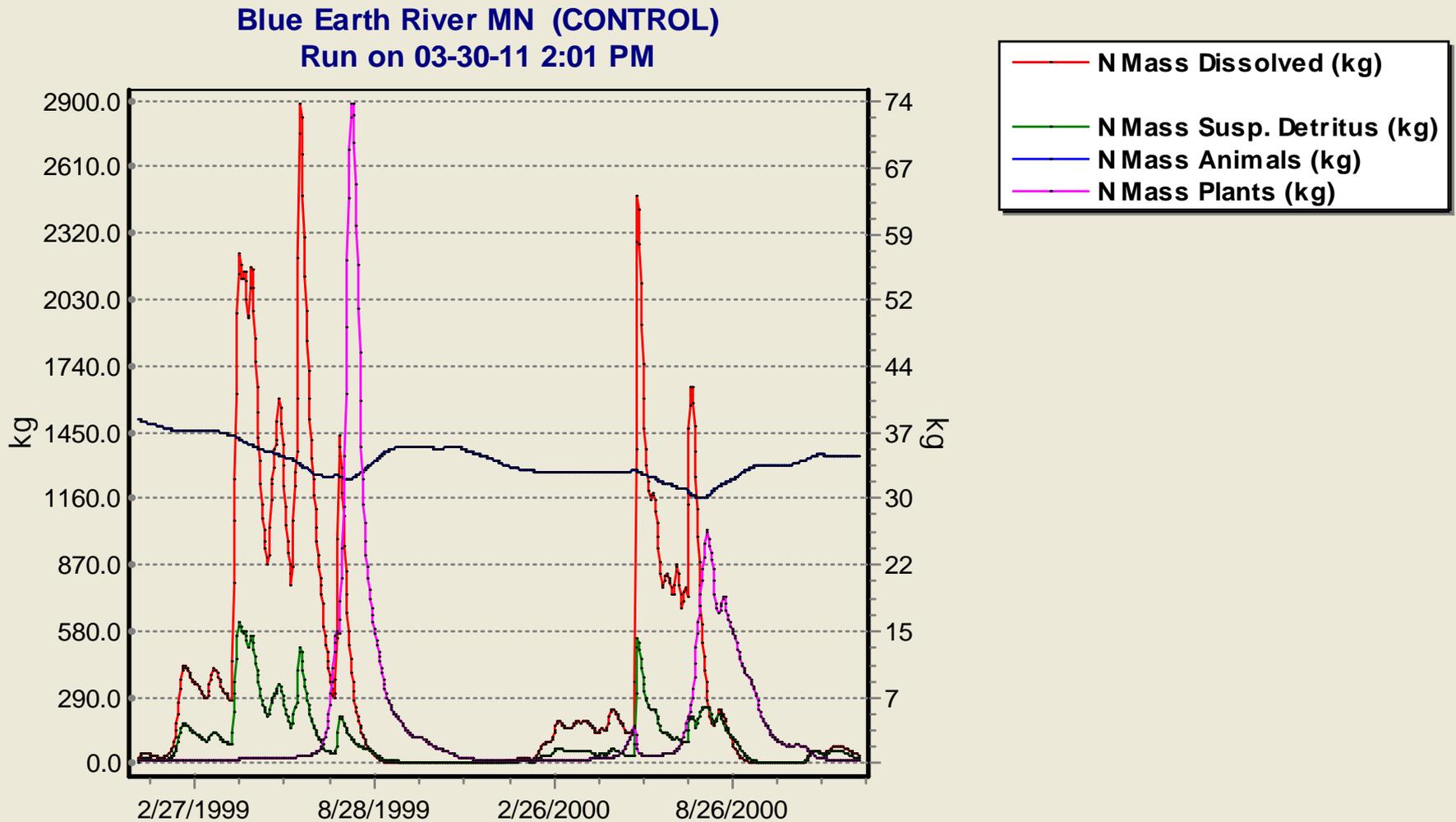
Blue Earth River MN (CONTROL)
Run on 03-30-11 2:01 PM



— NMB Test (kg)
— P MB Test (kg)

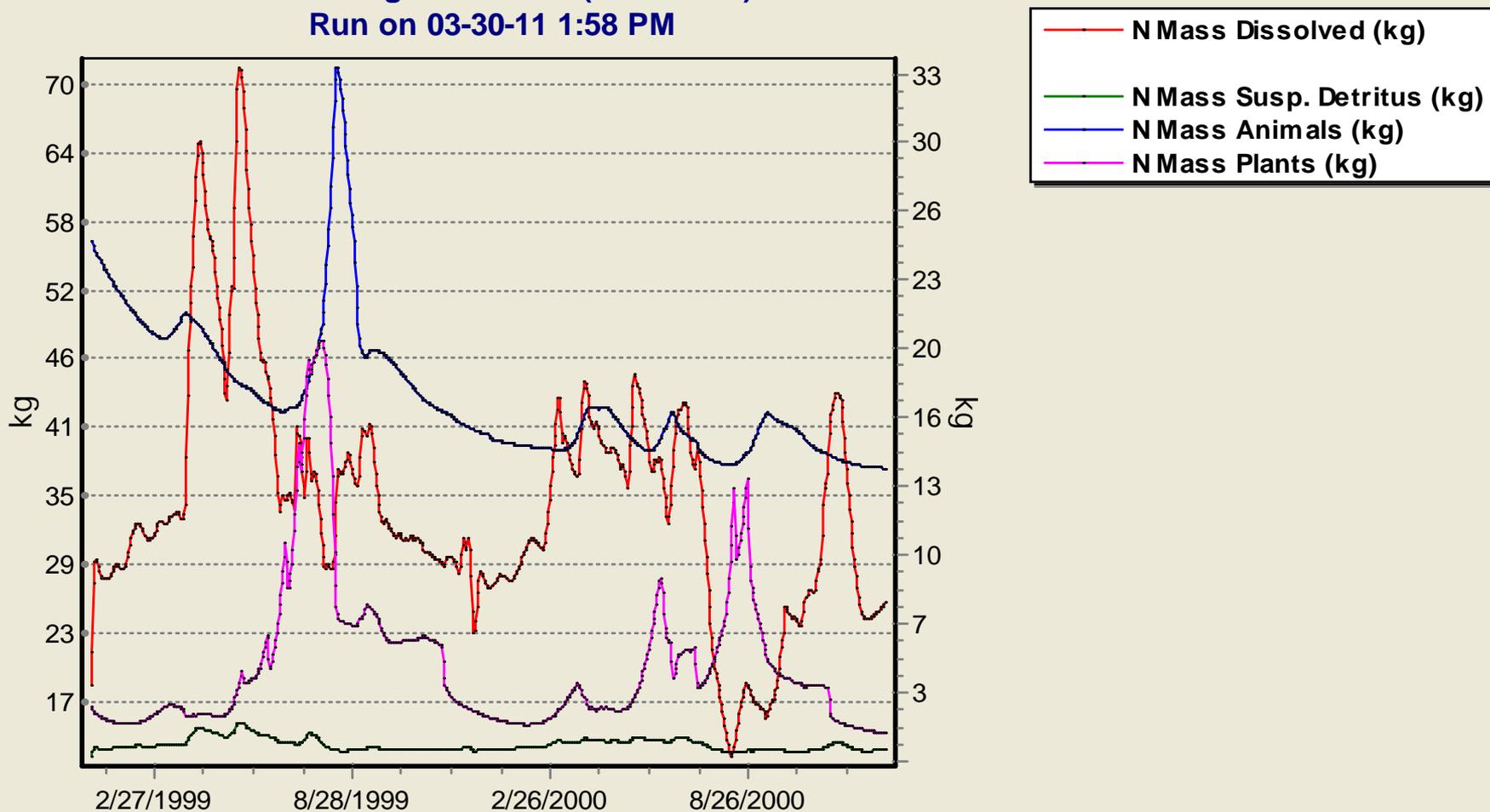
Axes reflect a very narrow range

Where are the Nutrients within the System?



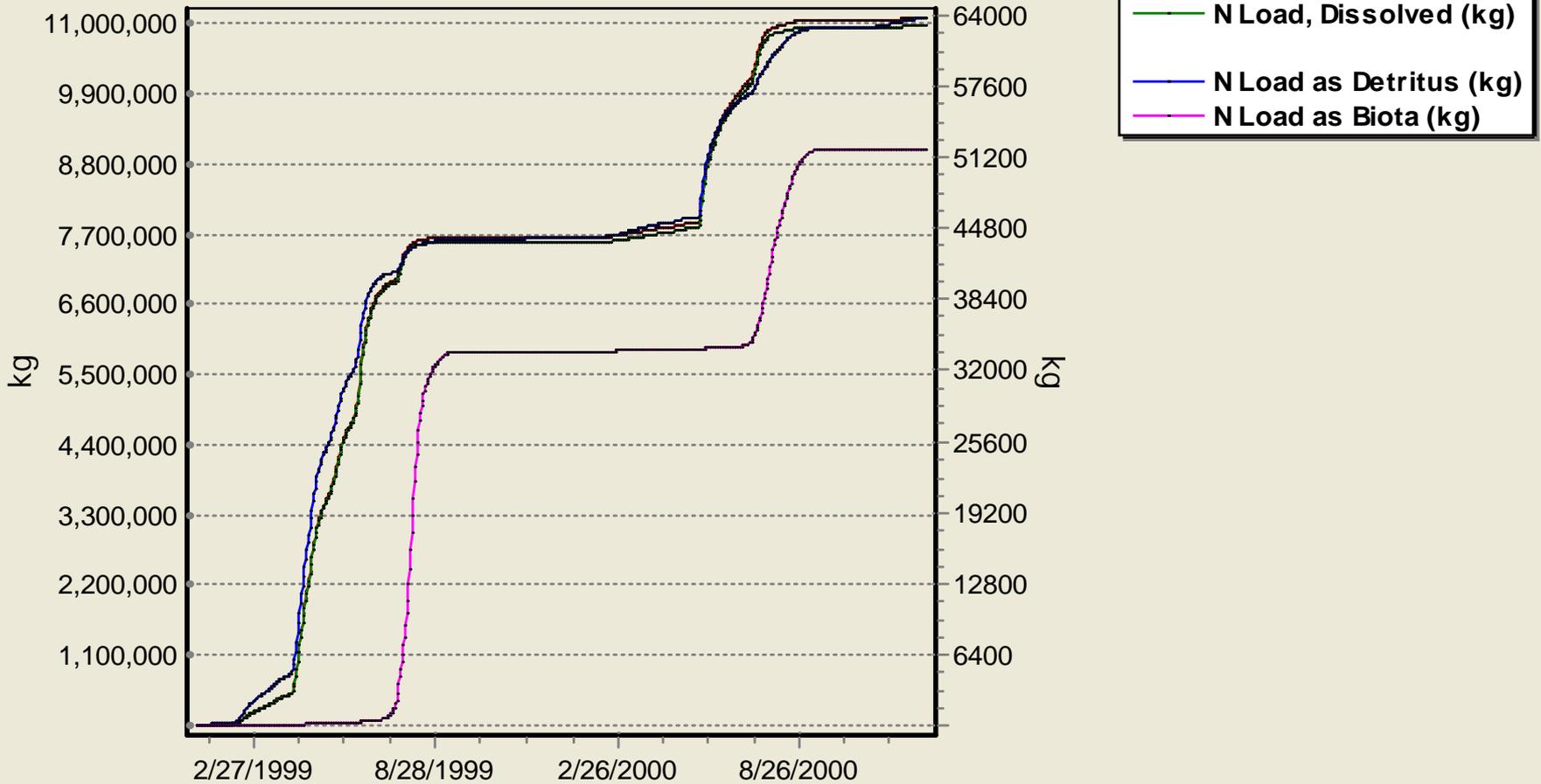
Contrast Blue Earth with the Crow Wing River

Crow Wing R. 72.3 MN (CONTROL)
Run on 03-30-11 1:58 PM



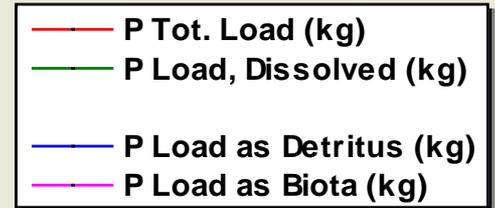
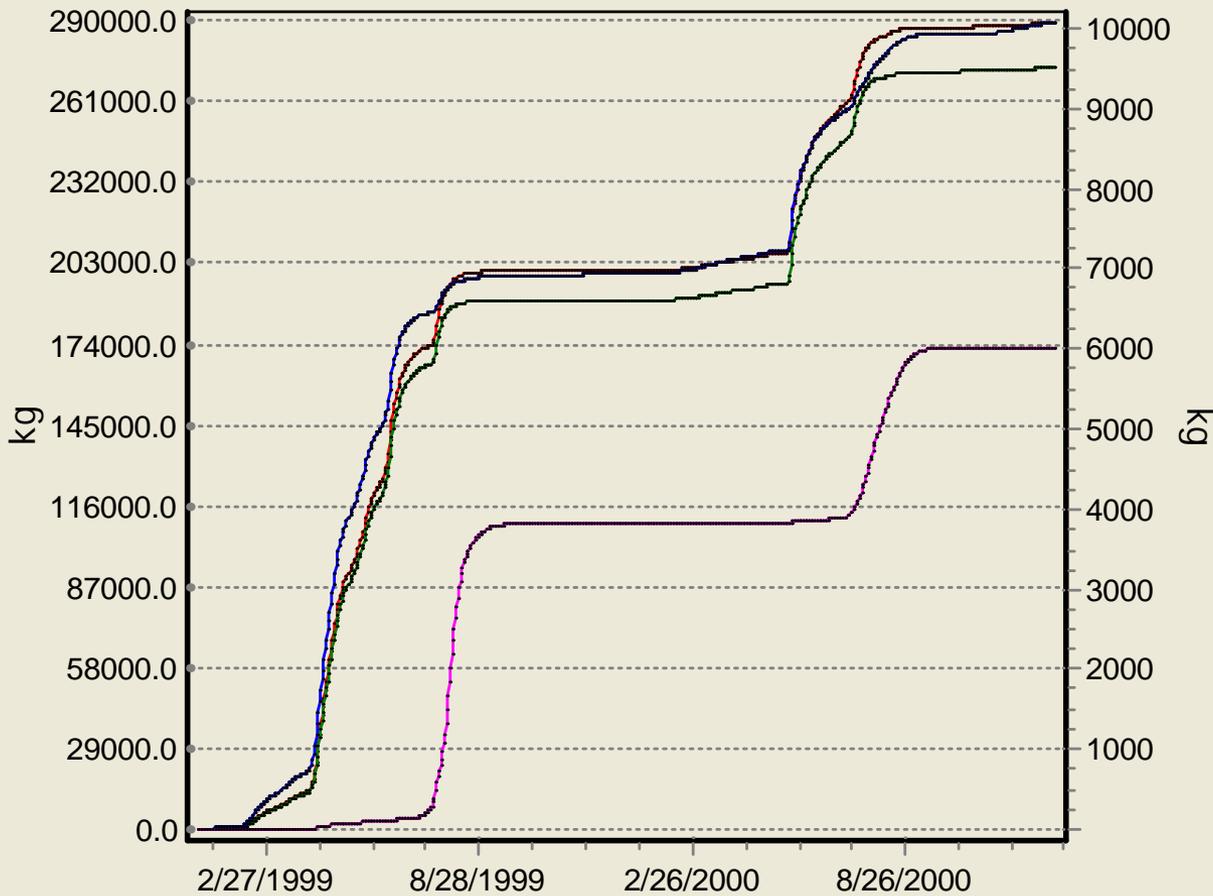
Nitrogen Loadings, Blue Earth River

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



Phosphorus Loadings, Blue Earth River

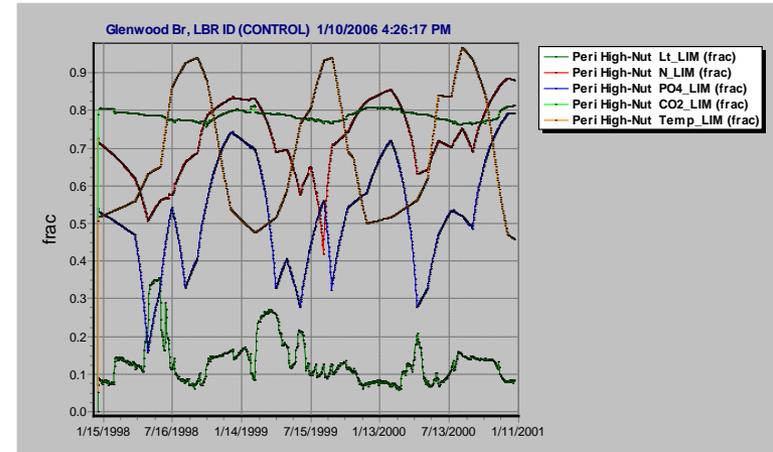
Blue Earth River MN (CONTROL)
Run on 03-30-11 2:01 PM



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