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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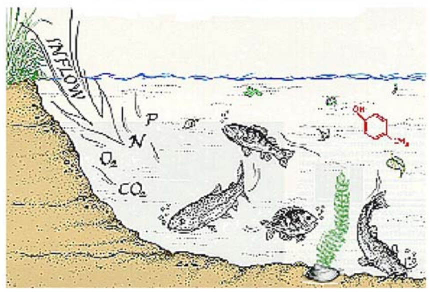


Modeling Estuarine Conditions

- Salt-balance submodel
- Estuarine species
- Shorebird bioaccumulation

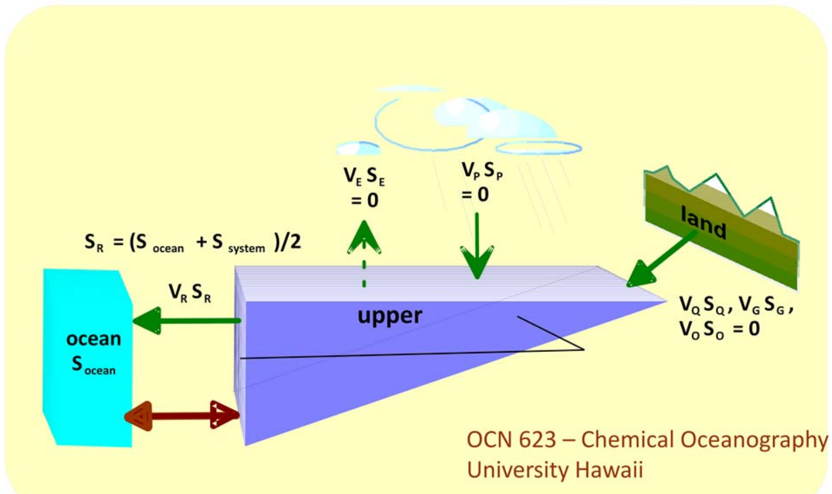
- Alternatively, salinity can be included in a linked-segment model; in that case water exchange is the responsibility of the user

The estuarine version of AQUATOX is intended to be an exploratory model for evaluating the possible fate and effects of toxic chemicals and other pollutants in estuarine ecosystems. It is not intended to represent detailed, spatially varying site-specific conditions, but rather to be used in representing the potential behavior of chemicals under average conditions. Therefore, it is best used as a screening-level model applicable to data-poor evaluations in estuarine ecosystems. However, it can be calibrated for different estuaries.

The AQUATOX Estuarine Submodel has the following Simplifying Assumptions:
• Estuary is a single segment that always has two well-mixed layers
• The estuary has freshwater inflow from upstream and saltwater inflow from the seaward end (salt-wedge)
• Water flows at the seaward end are estimated using the salt-balance approach
• Effects of salinity on sorption are minor and are not modeled
• Hourly tidal fluxes are not modeled
• Daily average volume of the estuary is assumed to remain constant over time
• The surface area of the lower layer is the same as the upper layer
• Nutrient concentrations in inflowing seawater are assumed to be constant
• Possible salinity effects on microbial degradation, hydrolysis, and photolysis are ignored.
The estuarine version is described in detail in Chapter 10 of the Technical Documentation.

Estuarine Features

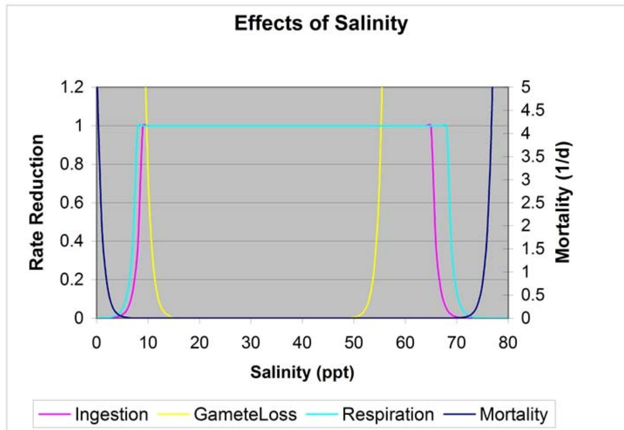
- Stratification – salt wedge
- Water Balance – salt balance approach
- Entrainment Process – lower to upper layers



- Estuaries are considered to be permanently stratified, though at times the extent of turbulent diffusion will essentially mean that they are well mixed.
- Salt balance approach: salt water inflow and outflow at the estuary mouth is a function of salinity and residual flow.
- Entrainment (i.e., water movement from the lower level to the upper level) transports suspended and dissolved substances from one layer to the next.

Estuarine Features

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



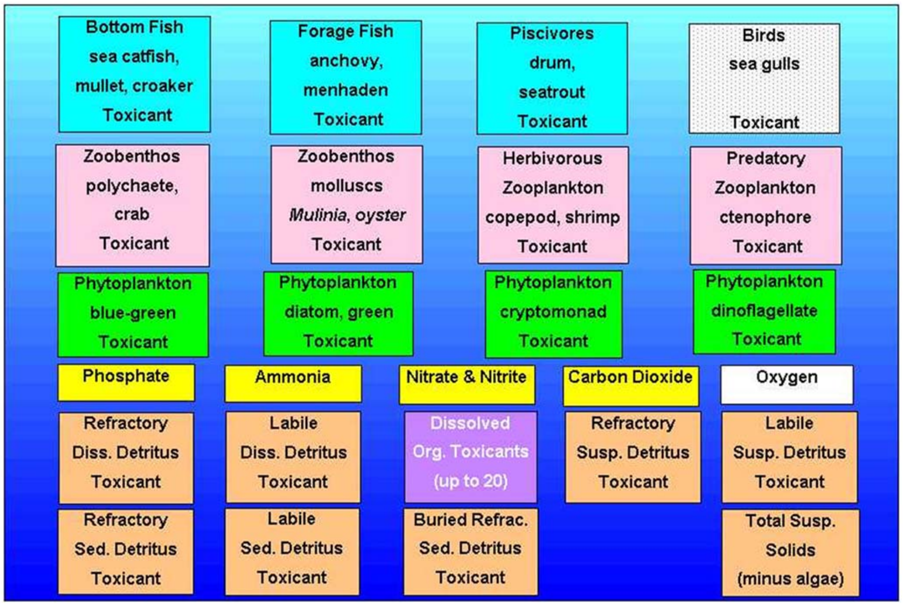
•Salinity that is less than or greater than threshold values increases mortality and gamete loss.
•Salinity beyond the range of tolerance for a particular process, including photosynthesis, ingestion, and respiration, will reduce the process
•Sinking of phytoplankton and suspended detritus also is affected by salinity
•Volatilization is affected by salinity, and can be represented by a linear increase in the Henry's Law constant
•Reaeration is affected by salinity, especially through calculation of the saturation level

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

Photo Courtesy NASA Johnson Space Center

Galveston Bay was simulated as a point model representing average conditions for this large bay.

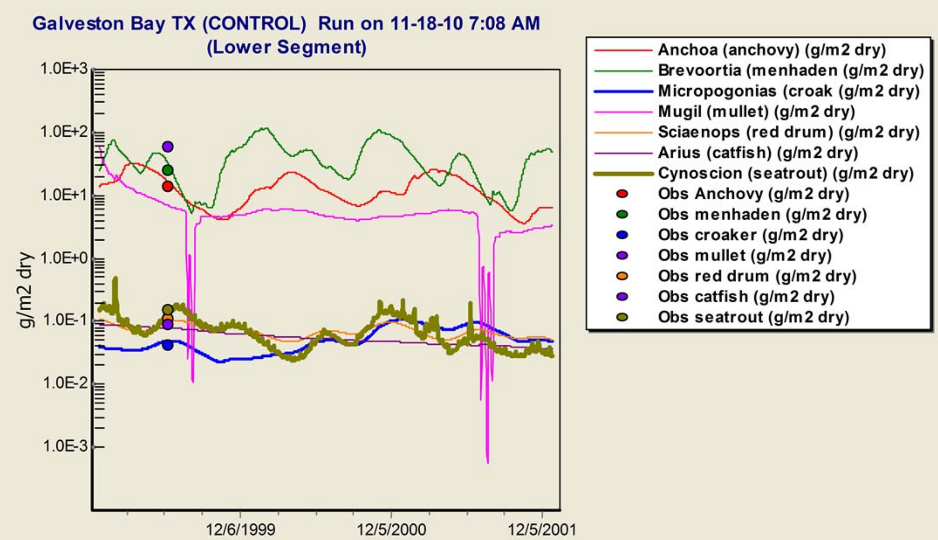
Galveston Bay, Texas, compartments



Many commercial species are represented, as well as other critical food web components. Birds are a bioaccumulative endpoint (i.e. their biomass is not simulated, only the tissue concentrations of the toxicant). The concentration of chemical in their tissues is a function of given Biomagnification Factors (BMFs) weighted by availability of preferred food.

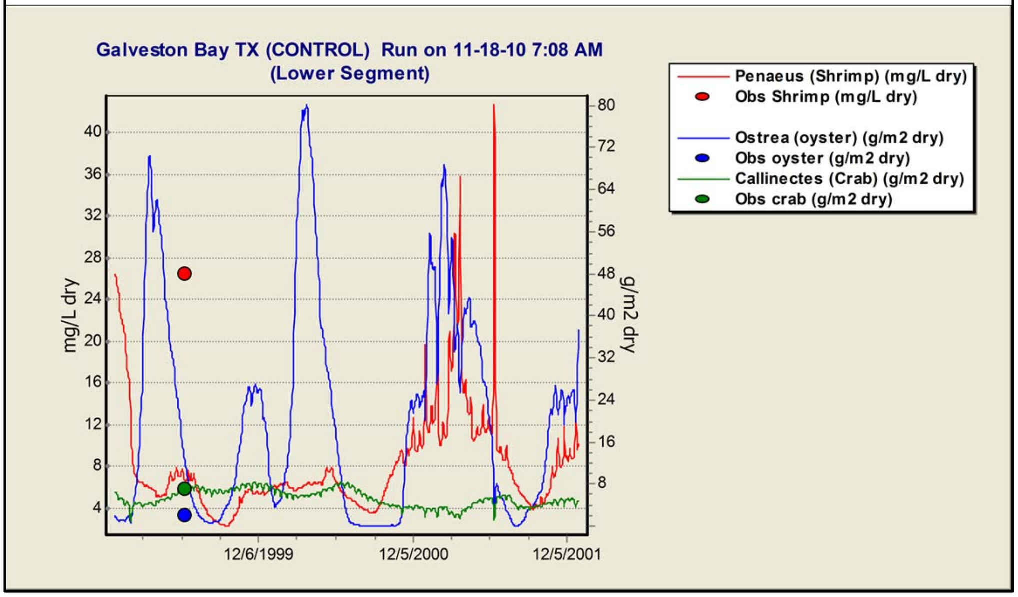
The Bioaccumulation Factor (BAF) is a measurement of how much toxicant an organism takes up through all routes of exposure compared to the concentration of toxicant in the water column.

Can model biomass of commercial and other species of fish



The ecosystem model has only been roughly calibrated for this highly productive system. The results have been compared to numerous data on the Bay, but only qualitatively. Data shown are converted from densities and averaged over time for particular habitats and are intended only as reality checks.

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



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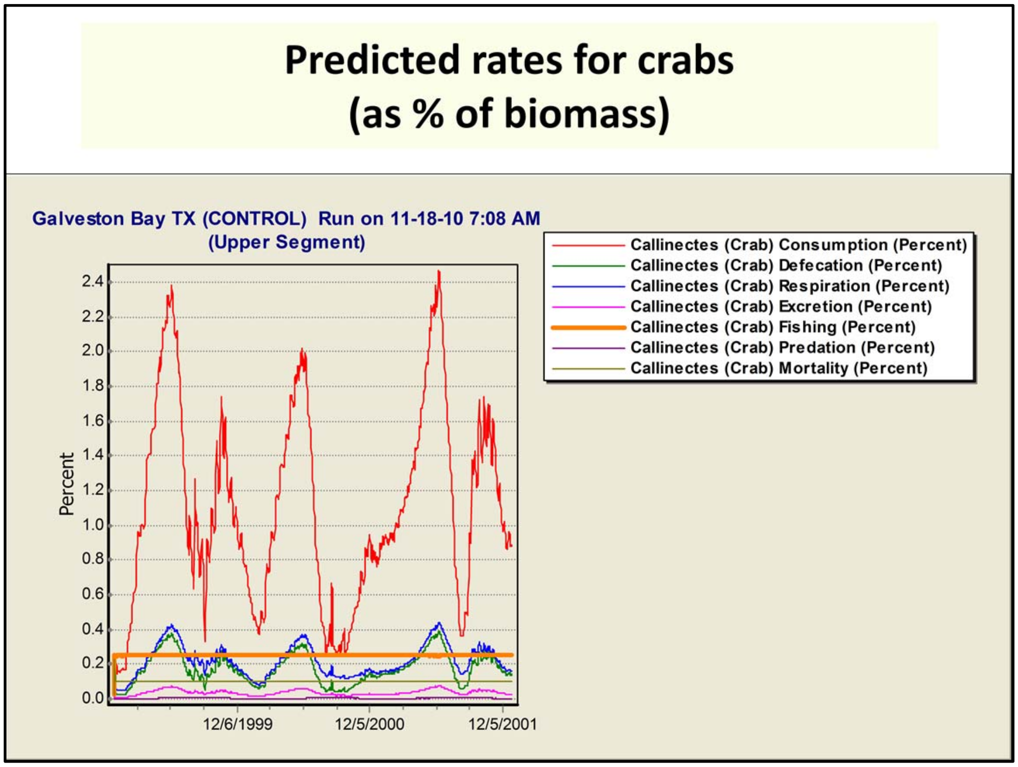
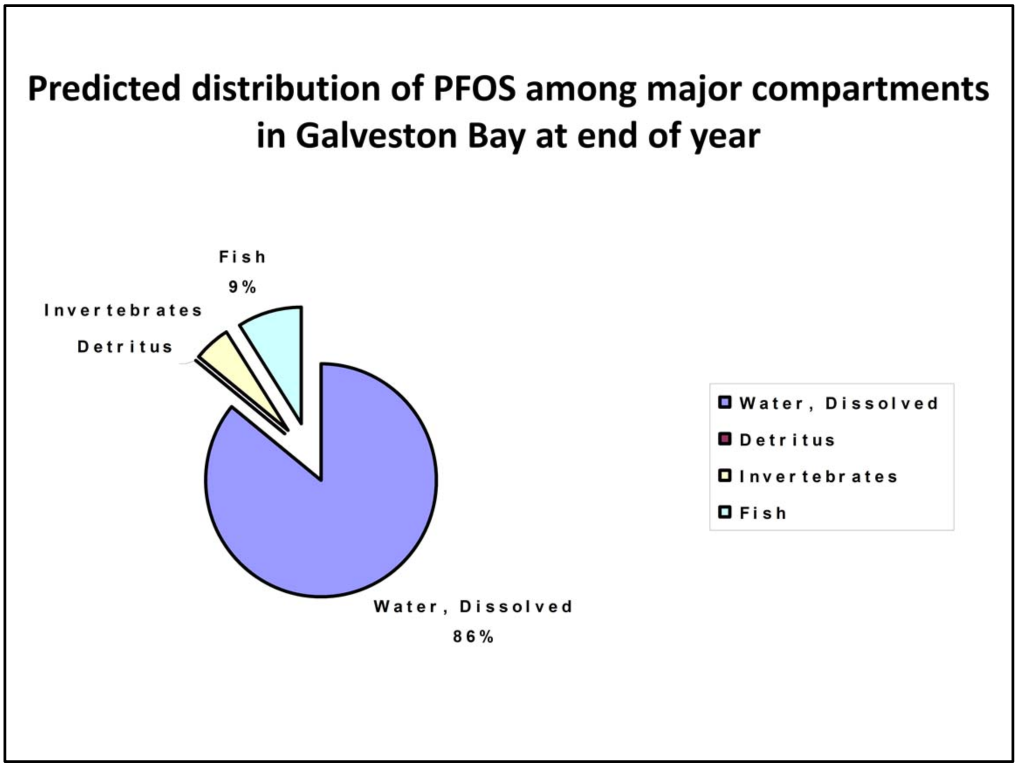
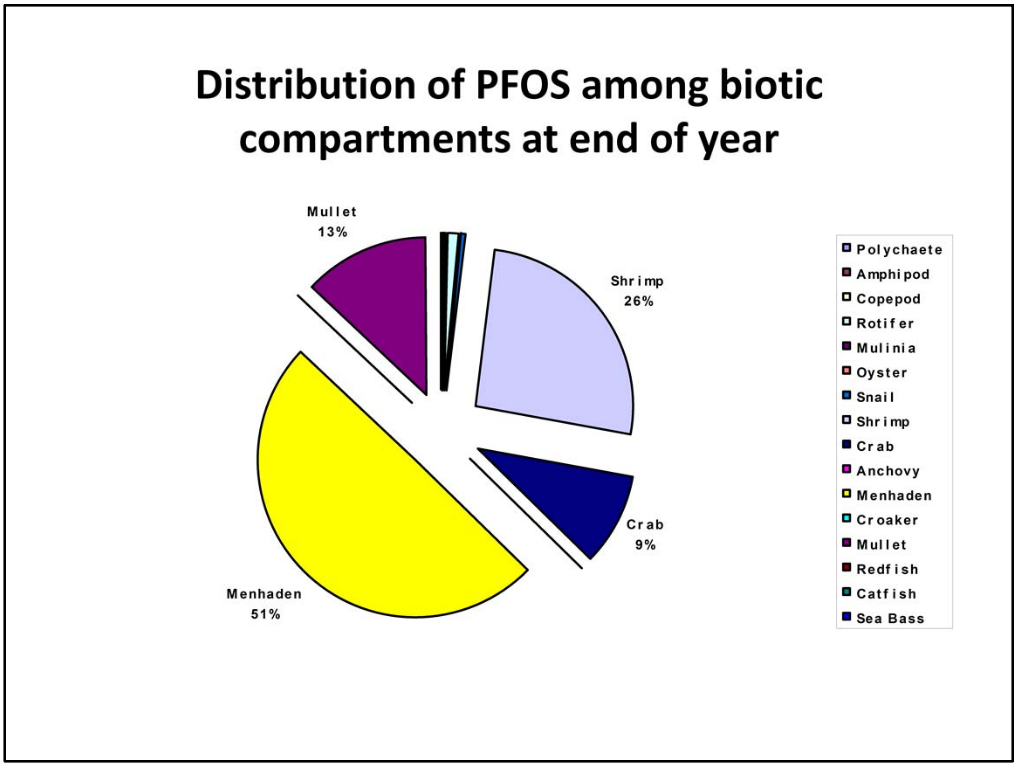


Loss rates for animals include constant fishing pressure.

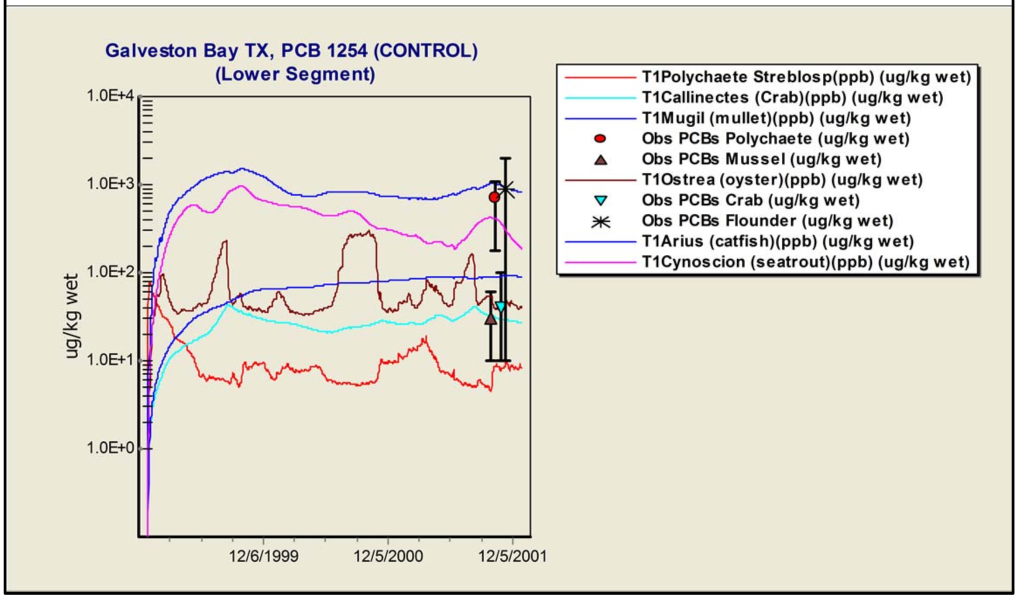


The estuarine version was used to predict the fate and bioaccumulation of Perfluoroctane sulfonate (PFOS) and other Perfluorooctanoic acids (PFOAs) in the nearshore environment. Because of the volume of water, most of the mass is predicted to reside in the dissolved phase.



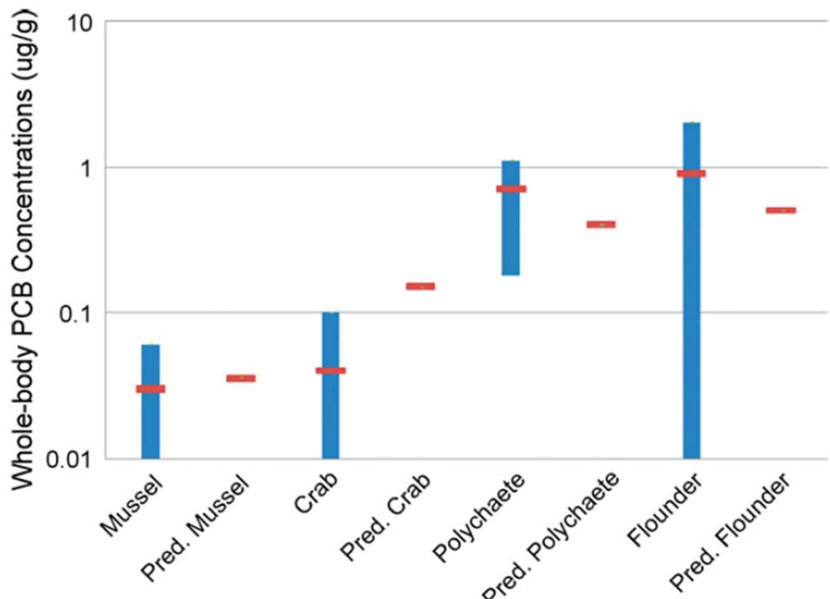
Of the Perfluoroctane sulfonate (PFOS) in the biota at the end of the simulated year, half was predicted to be in menhaden, which are harvested for fish meal.

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



In a partial validation, Polychlorinated biphenyl (PCB) concentrations in water and sediments in New Bedford Harbor, MA, were imported into the Galveston Bay TX simulation. The results were comparable between observed and predicted mean whole-body concentrations.

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



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

The ranges and means are shown for observed whole-body concentrations (Connolly 1991).

Connolly, J. P. 1991. Application of a food chain model to polychlorinated biphenyl contamination of the lobster and winter flounder food chains in New Bedford Harbor. *Environ. Sci. Technol.* **25**: 760-770.

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

The website to load tide prediction parameters (harmonic constants) within the United States is:

http://tidesandcurrents.noaa.gov/

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

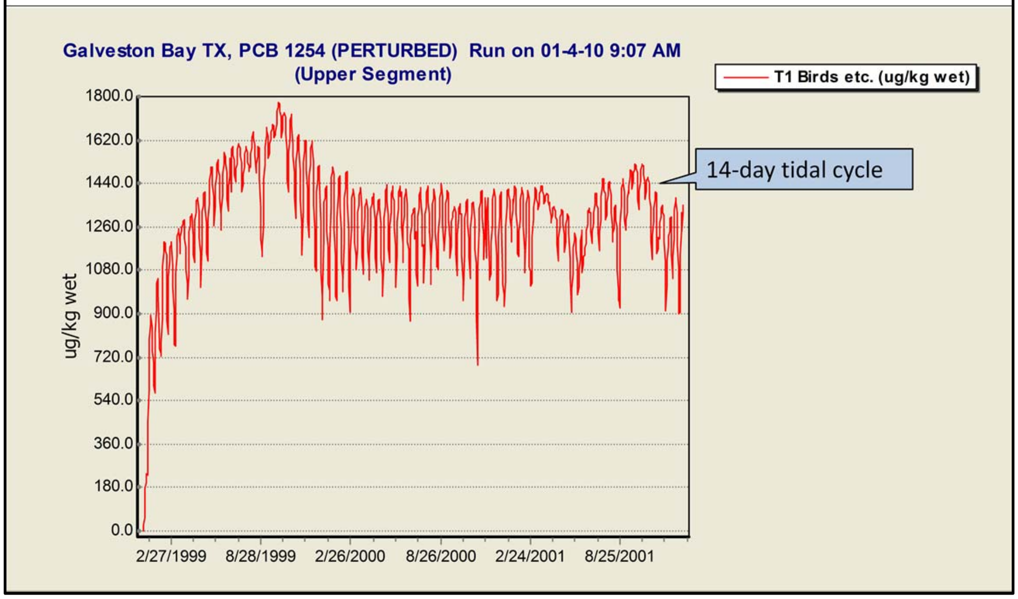
Aquatic-feeding vertebrates (previously just shorebirds) have been added as a bioaccumulative endpoint—not as a dynamic variable but as a post-processed variable reflecting dietary exposure to a contaminant.

This endpoint can be used for any animal that feeds primarily on aquatic organisms and for which there are biomagnification data. These could include bald eagles, mink, and otters.

The Biomagnification Factor (BMF) is the increase of a toxicant concentration in the tissue of an organism compared to the tissue concentrations of its prey.

The BMF should not be confused with the BCF – the Bioconcentration Factor – which is a measure of magnification based solely on exposure to the toxicant in water.

PCB Bioaccumulation in Shorebirds



Herring gulls and other shorebirds are included in AQUATOX as a bioaccumulative endpoint—not as a dynamic variable but as a post-processed variable reflecting dietary exposure to a contaminant. In fact, the endpoint can be used to simulate bioaccumulation for any aquatic feeding organism, such as bald eagles, mink, and dolphins, provided that the organism feeds exclusively on biotic compartments modeled within AQUATOX. The user can specify a Biomagnification Factor (BMF) and the preferences for various food sources so that alternate exposures can be computed. Dietary preferences are input as fraction of total food consumed by the modeled species and are normalized to 100% when the model is run.

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)

Sublethal effects include reduction in photosynthesis, ingestion, and reproduction, and increased egestion, drift, and sloughing of periphyton.

From Wikipedia, the free encyclopedia:
Chronic toxicity is a property of a substance that has toxic effects on a living organism, when that organism is exposed to the substance continuously or repeatedly.
Acute Toxicity is a property of a substance that has toxic effects on a living organism, when that organism is exposed to a lethal dose of a substance once. In other words, basically a short-term version of chronic toxicity.

AQUATOX models time-varying toxicity—both chronic and acute.

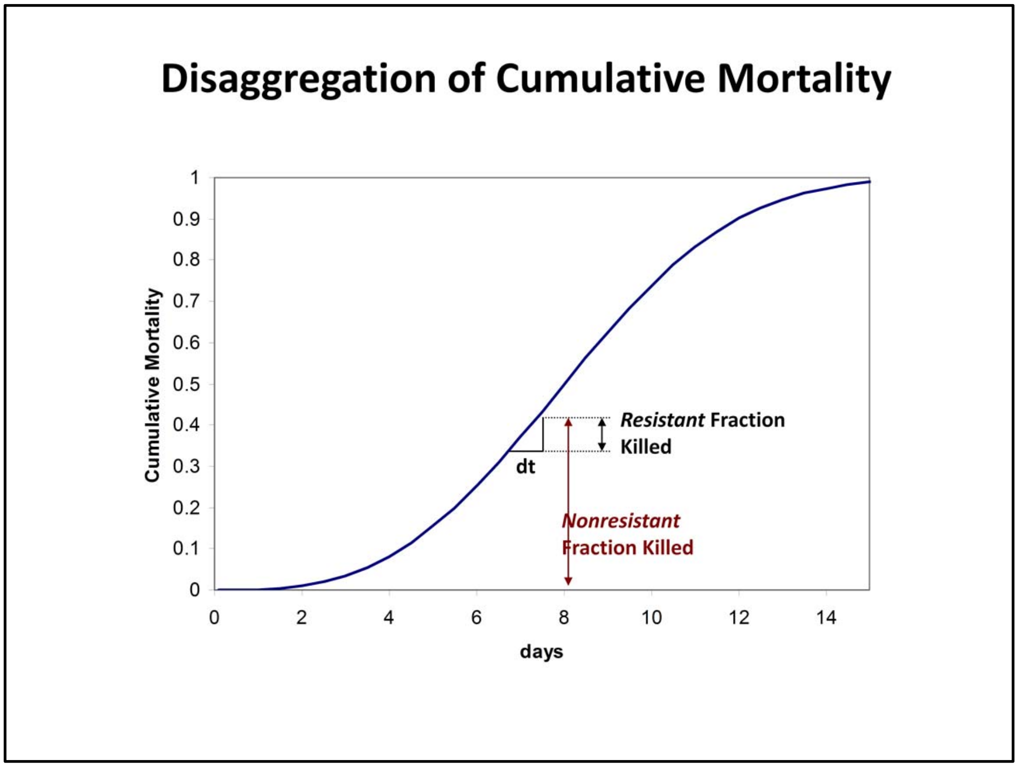
McCarty, L.S., G.W. Ozburn, A.D. Smith, and D.G. Dixon. 1992. Toxicokinetic Modeling of Mixtures of Organic Chemicals. *Environmental Toxicology and Chemistry*, 11:1037-1047.
Mackay, D., H. Puig, and L.S. McCarty. 1992. An Equation Describing the Time Course and Variability in Uptake and Toxicity of Narcotic Chemicals to Fish. *Environmental Toxicology and Chemistry*, 11:941-951.

Steps Taken to Estimate Toxicity

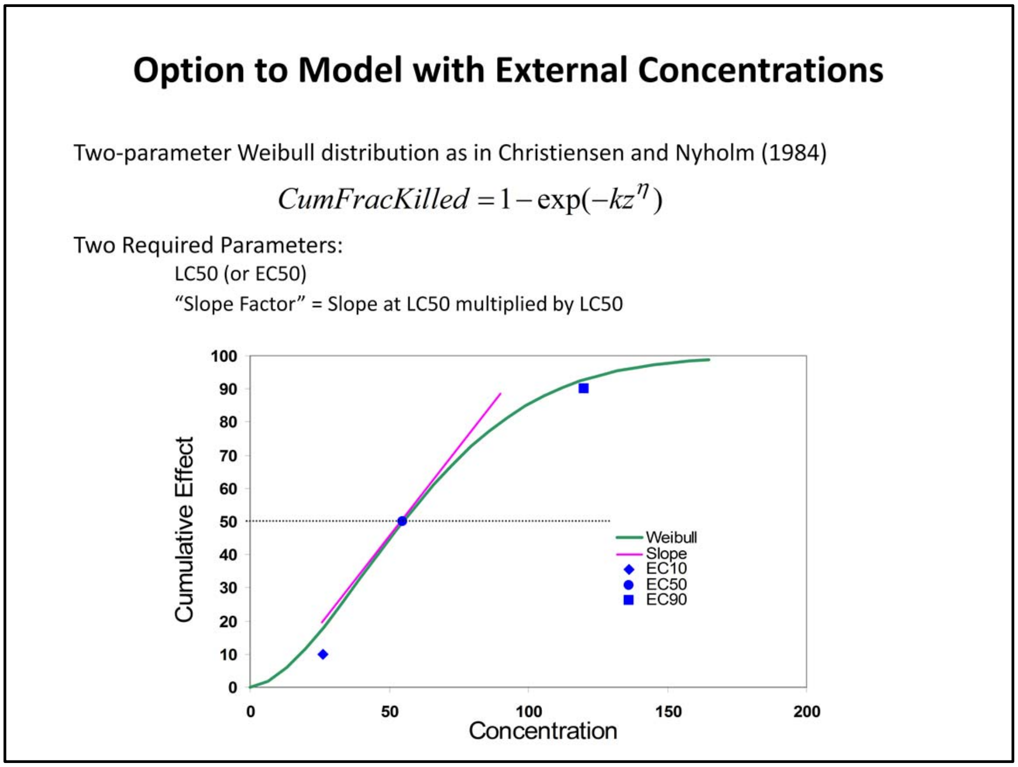
- Enter LC_{50} and EC_{50} values
  - LC_{50} estimators are available for species
- Compute internal LC_{50}
- Compute infinite LC_{50} (time-independent)
- Compute t-varying internal lethal concentration
- Compute cumulative mortality
- Compute biomass lost per day by disaggregating cumulative mortality
- Sublethal toxicity is related to lethal toxicity through an application factor
- Option has been added to use external concentration.

The modeling approach is complex; key elements are highlighted in red. The details are covered in Chapter 9 of the *Technical Documentation*.

By entering both LC_{50} and EC_{50} values for a species the application factor can be computed.



The biomass killed per day is computed by disaggregating the cumulative mortality. Think of the biomass at any given time as consisting of two types: biomass that has already been exposed to the toxicant previously, which is called *Resistant* because it represents the fraction that was not killed; and new biomass that has formed through growth, reproduction, and migration and has not been exposed to a given level of toxicant and therefore is referred to as *Nonresistant*.



Chemicals that are taken up very rapidly and those that have an external mode of toxicity, such as affecting the gills directly, are best simulated with an external toxicity construct. Rather than require the user to fit toxicological bioassay data to determine the parameters for $\boldsymbol{k}$ and $\boldsymbol{\eta}$, these parameters are derived to fit the LC50 and the slope of the cumulative mortality curve at the LC50 (in the manner of the RAMAS Ecotoxicology model, Spencer and Ferson, 1997). (See section 9.3 in the *Technical Documentation*)

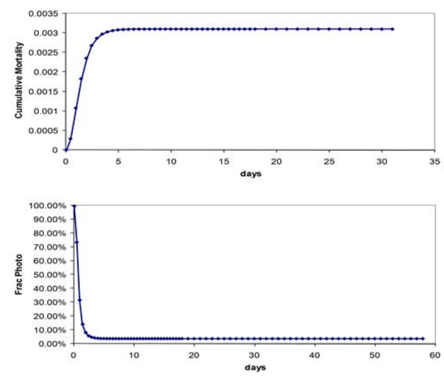
AQUATOX assumes that each chemical's dose response curve has a distinct shape, relevant to all organisms modeled. In this manner, a single parameter describing the shape of the Weibull parameter can be entered in the chemical record rather than requiring the user to derive slope parameters for each organism modeled. However, as shown in the slide above, the slope of the curve at the LC50 is both a function of the shape of the Weibull distribution and also the magnitude of the LC50 in question. For this reason, rather than have a user enter "the slope at LC50" into the chemical record, AQUATOX asks that the user enter a "slope factor" defined as "the slope at LC50 multiplied by LC50." In the above example, the user would enter a slope factor of 1.0 and then, given an LC50 of 1 or an LC50 of 100, the above curve would be generated.

When modeling toxicity based on external concentrations, organisms are assumed to come to equilibrium with external concentrations (or the toxicity is assumed to be based on external effects to the organism).

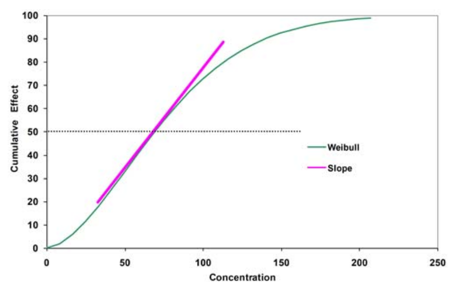
Spreadsheet Demo

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

AQUATOX_Internal_Toxicity_Model.xls



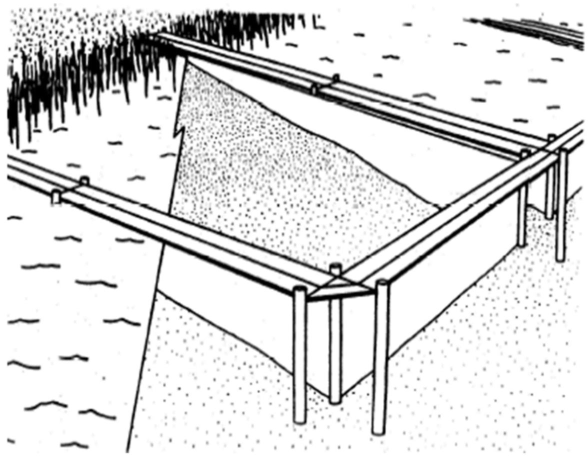
AQUATOX_External_Toxicity_Model.xls



These spreadsheets are simplifications of AQUATOX, in that they represent a constant toxicant water concentration, rather than being subject to the various fate processes normally simulated.

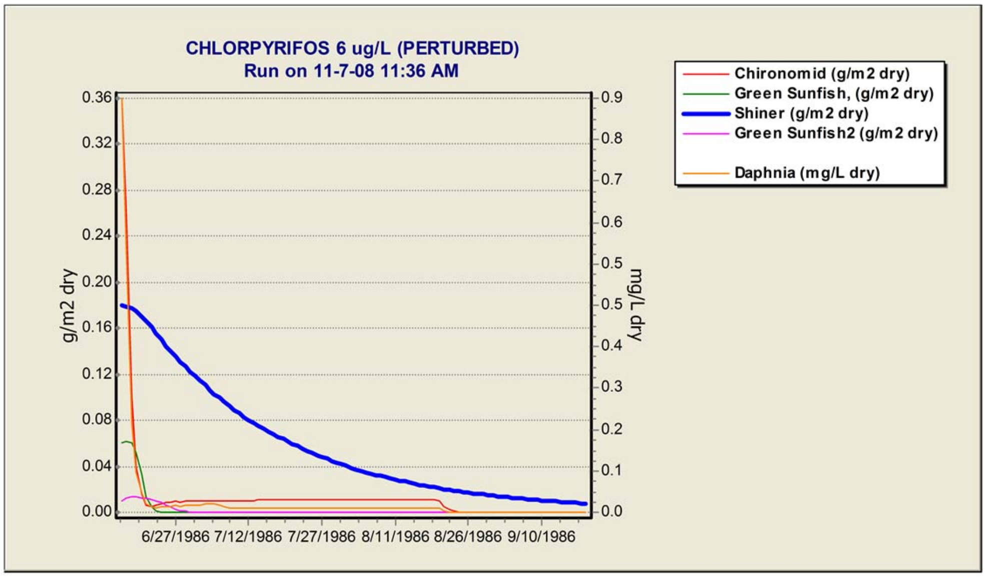
These Excel spreadsheets are located in the DATA directory of your short-course CD.

Returning to the Enclosure in Duluth MN . . .

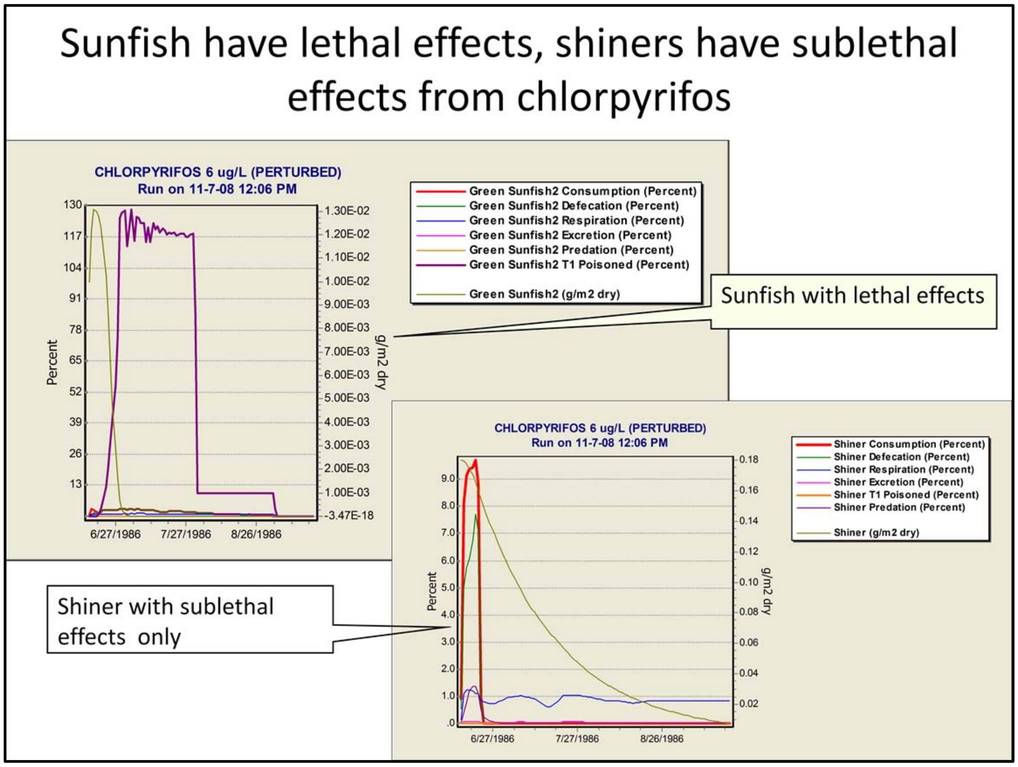


In the day two lectures we saw the simulated chemical fate and bioaccumulation of chlorpyrifos in the mesocosm, now we'll look at the simulated toxic effects.

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



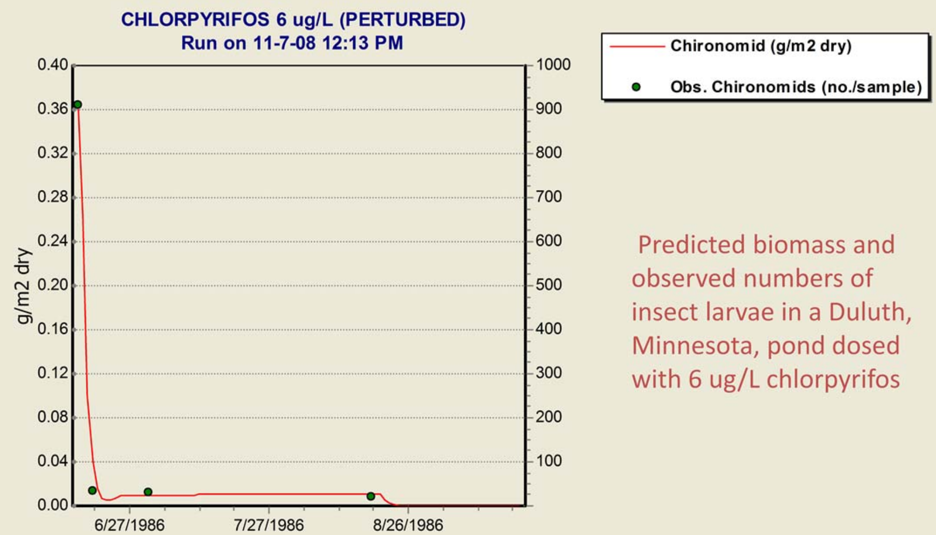
Shiners are most tolerant to chlorpyrifos according to toxicity data. Chironomids and *Daphnia* are most sensitive.



Sunfish have a low tolerance to chlorpyrifos (LC50 = 2.4 ug/L), so bioaccumulation is followed by significant mortality with gradual recovery.

Shiners are tolerant of chlorpyrifos (LC50 =203 ug/L) and exhibit no mortality with an initial dose of 6 ug/L chlorpyrifos; they do exhibit sublethal toxicity in the form of decreased consumption and assimilation; loss of forage is a predicted indirect effect. Predicted recovery of sunfish eventually leads to high predation on shiners.

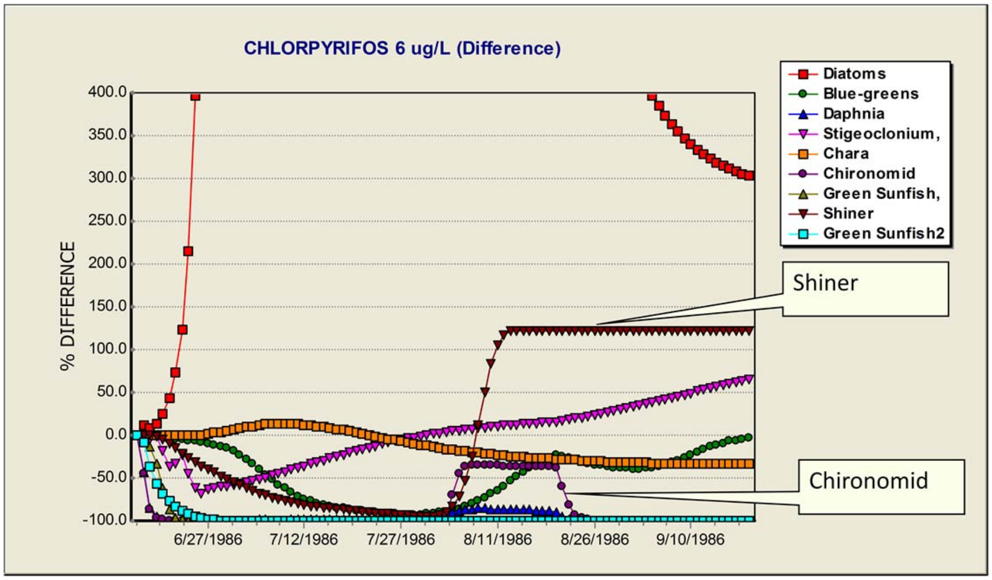
Toxic effects of Chlorpyrifos in Duluth pond



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

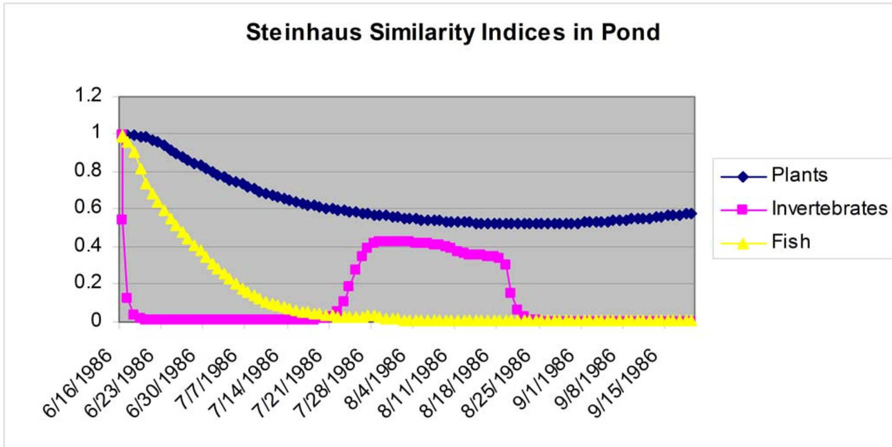
In a validation study 6 ug/L initial dose of chlorpyrifos in a pond resulted in a decline in predicted insect biomass, which compared favorably to decline in observed numbers of insects.

% Difference Graph shows differences in species response to toxicant



An initial 6 ug/L chlorpyrifos in the pond has an immediate impact on the invertebrates and sunfish. Removal of predation causes an explosive increase in diatoms; shiners recover, partly in response to chironomid recovery half way through the simulation period.

Steinhaus Indices show ecosystem impacts predicted by the model



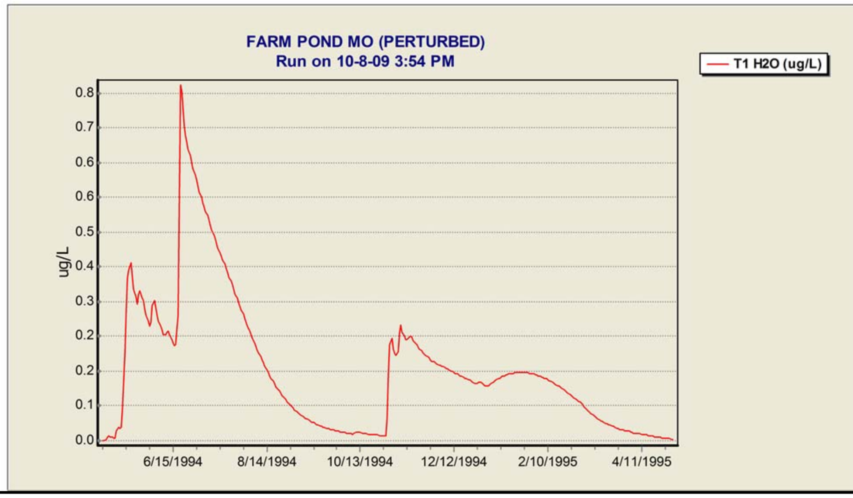
$$S = \frac{2 * \sum_{k=1}^{n} Min(a_{1,k}, a_{2,k})}{\sum_{k=1}^{n} a_{1,k} + \sum_{k=1}^{n} a_{2,k}}$$

Coefficients of similarity are used to determine whether the composition of two communities is similar. The Steinhaus coefficient or similarity index (S) is based on the species abundances (in this case indicated by the species specific daily biomass) common to two communities, where $a_{i,k}$ is abundance of species k in sample I.

The Steinhaus coefficient may be calculated from the Graph Menu; the values will export to EXCEL. You can then graph the Steinhaus values over time.

Farm Pond MO, Esfenvalerate

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

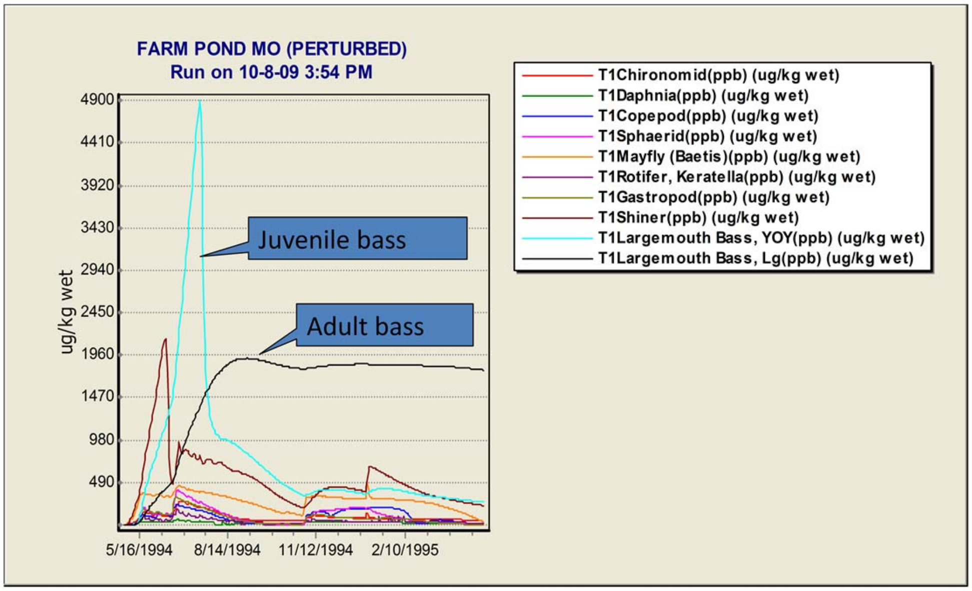


The assumptions in setting up this hypothetical case is that it is a typical farm pond located adjacent to and receiving runoff from a corn field in Missouri. The Pesticide Root Zone Model (PRZM) was run to obtain loadings for AQUATOX using the worst-case scenario out of 20 years (rain with runoff immediately after pesticide applications).

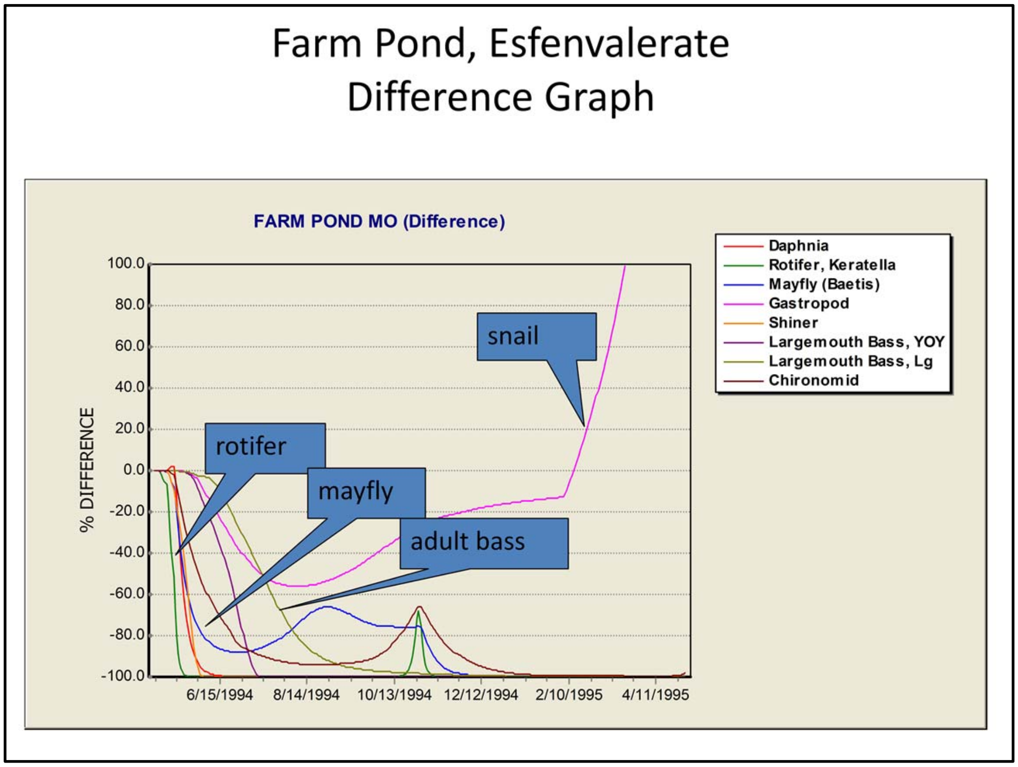
From http://extoxnet.orst.edu/pips/esfenval.htm: " Esfenvalerate is a synthetic pyrethroid insecticide which is used on a wide range of pests such as moths, flies, beetles, and other insects. It is used on vegetable crops, tree fruit, and nut crops."

Esfenvalerate is listed as very highly toxic to aquatic animals., and this was reflected in the toxicity data used in the model.

Farm Pond, Esfenvalerate
Chemical Uptake in animals



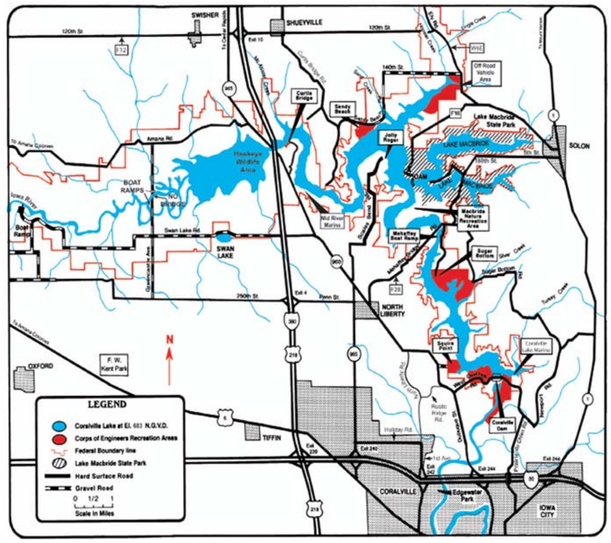
Juvenile bass are predicted to bioaccumulate esfenvalerate quickly because of bioenergetics (i.e they respire and consume more food per body weight); adult bass are predicted to bioaccumulate more slowly but to retain the pesticide due to lower clearance rate.



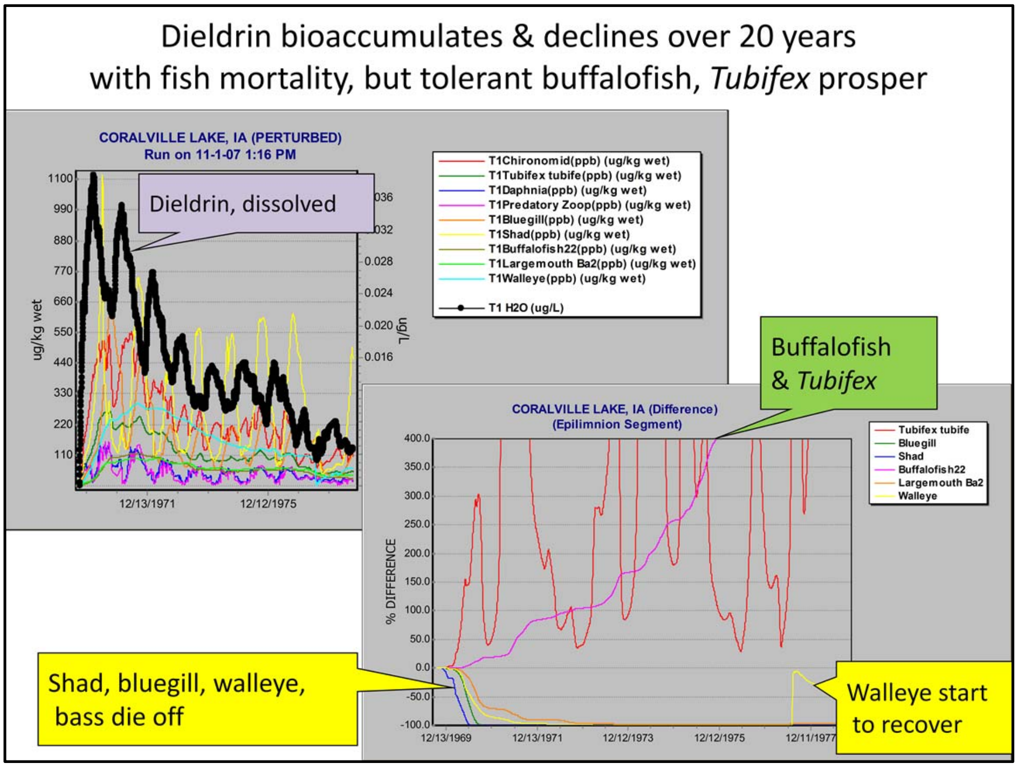
A difference graph shows the rapid decline and almost total extinction of all smaller animals except snails, which are tolerant and benefit from reduced competition for periphyton. Adult bass decline slowly because of slower bioaccumulation.

Coralville Reservoir Iowa
long-term contamination with dieldrin

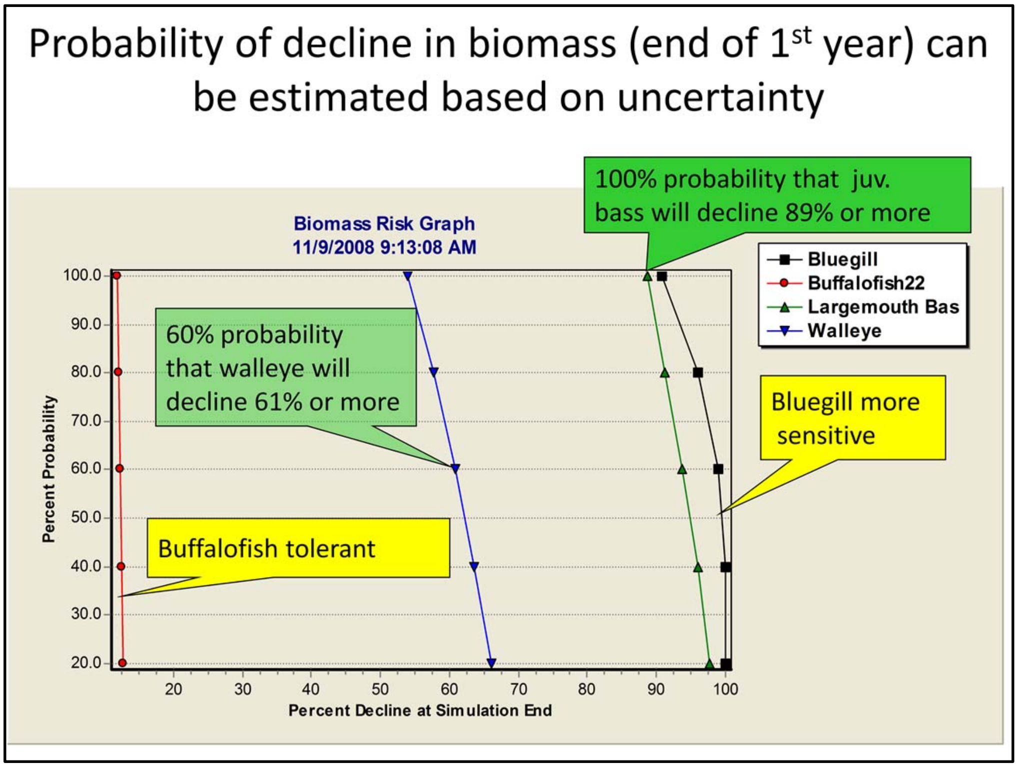
- Run-of-river
- Flood control
- 90% of basin in agriculture
  - Nutrients
  - Pesticides
  - Sediment



Coralville is a shallow, run-of-the river reservoir built in 1958 for flood control. It captures large quantities of agricultural runoff. Most dangerous is dieldrin, a chlorinated hydrocarbon insecticide, which is also a degradation product of the pesticide aldrin. It was widely used from 1950 to 1974 and was banned for most uses in 1985.

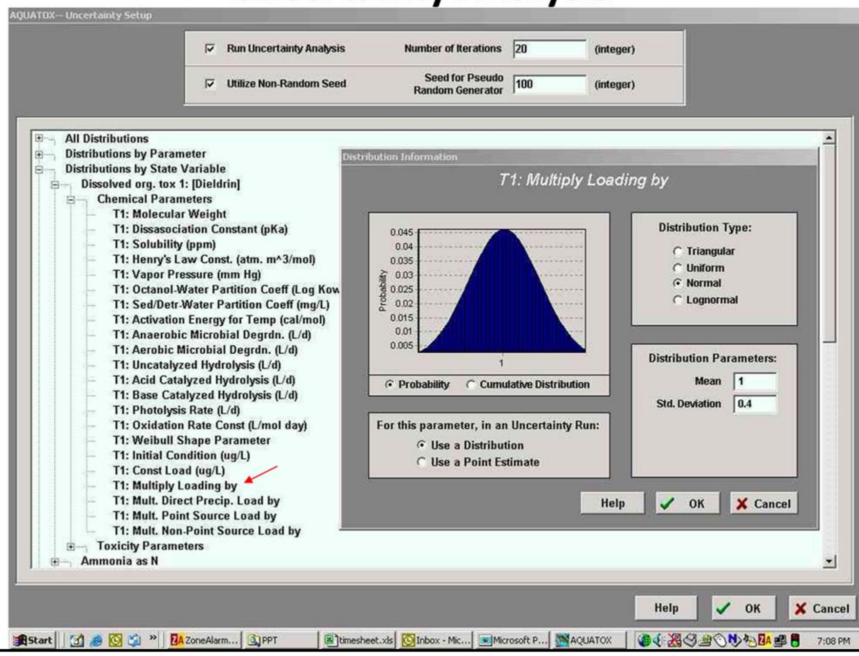


Buffalofish are tolerant of dieldrin and prospered—so much so that there was a commercial fishery on Coralville until it was realized that the levels of dieldrin in the tissue was quite high! The model predicted the eventual recovery of bass; and, in fact, Coralville is known for the best bass fishing in Iowa!



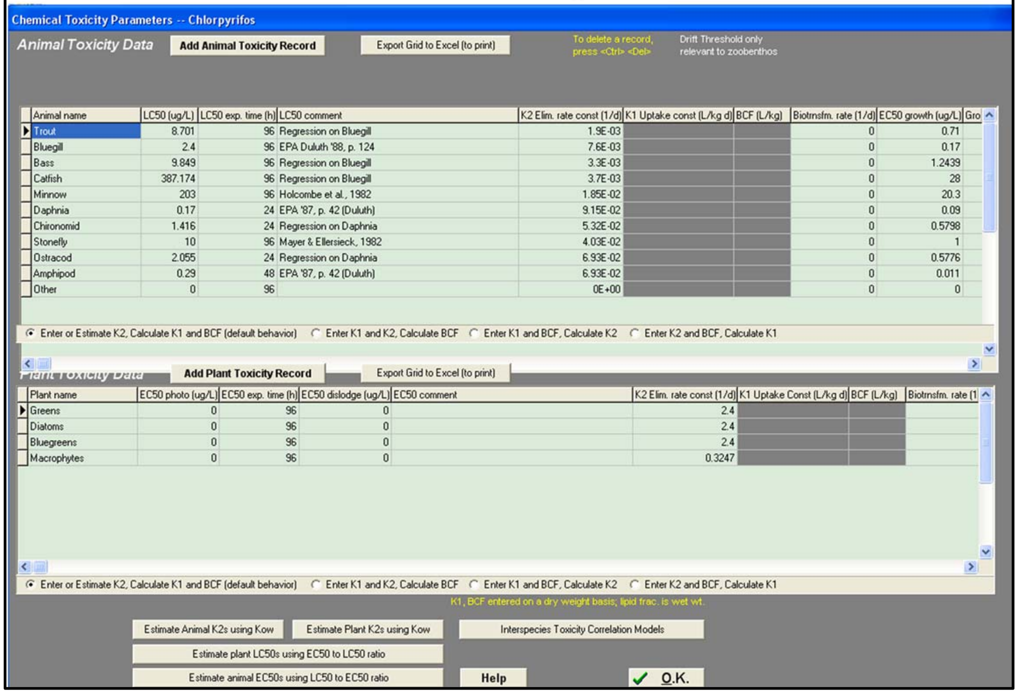
AQUATOX can estimate probability of decline, which is a powerful tool for risk assessment. In this example, using a distribution of loadings of dieldrin, we see that bluegill are the most sensitive to dieldrin and buffalofish are the least sensitive. Walleye are of intermediate sensitivity, as suggested by their recovery shown in the previous slide.

Toxicant Parameters and Loadings are Subject to Uncertainty Analysis



By running uncertainty analysis with a normal distribution of multiplicative loadings of dieldrin we can easily see the probabilistic response to dieldrin. Let's reexamine this tool and its application to toxic response.

Chemical Toxicity Screen



This screen is where all of the important chemical toxicity parameters are located. To get to this screen go to Chemical Underlying Data and select the “Toxicity Data” button.

There are multiple options for entering uptake rate constant (k1), the elimination rate constant (k2) and the Bioconcentration Factor (BCF) or allowing the model to calculate these parameters (BCF=k1/k2).

Additionally, elimination rates may be estimated using the octanol water partition coefficient (Kow).

Fish and invertebrate regressions (i.e. estimating toxicity from one species to another) are available for many organisms using the ICE database (see next slide).

As explained previously, by entering both LC_{50} and EC_{50} values for a species the application factor can be computed. The user has the option of applying that same ratio to the rest of the species in the animal or plant toxicity screen using the buttons **Estimate animal LC50s**... and **Estimate plant EC50s...**.

Interspecies Correlation Estimates (ICE Version 3.1, January 2010)

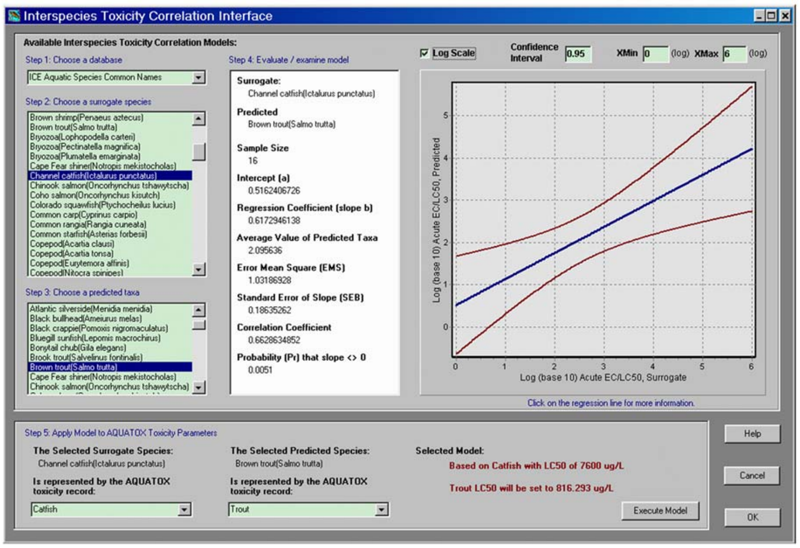
- Developed by EPA ORD
- Estimates the acute toxicity of a chemical to a species with no test data
- 1440 regression models derived
  - 180 species and 1258 chemicals
- Regressions on species, families, genus
- Goodness of fit information for regressions

Predictive toxicological models are integral to ecological risk assessment because data for most species are limited. Web-based Interspecies Correlation Estimation (Web-ICE) models are least square regressions that predict acute toxicity (LC50/LD50) of a chemical to a species, genus, or family based on estimates of relative sensitivity between the taxon of interest and that of a surrogate species. Web-ICE 3.0 includes a total 1440 models for aquatic taxa and 852 models for wildlife taxa. For aquatic species within the same family, Web-ICE models predict within 5-fold and 10- fold of the actual value with 91 and 96% certainty, respectively. For two species within the same order, aquatic models predict within 5-fold and 10-fold of the actual value with 86 and 96% certainty, respectively. Overall for wildlife species, Web-ICE predicts toxicity within 5-fold of the actual value with 85% certainty and within 10-fold of the actual value with 95% certainty. Models predict within 5-fold and 10-fold of the actual value with 90 and 97% certainty for wildlife surrogate and predicted taxa within the same order. For both aquatic and wildlife taxa, model certainty increases with decreasing taxonomic distance. Web-ICE 3.0 improves on earlier versions with the inclusion of an endangered species module, improved functionality of the SSD module, and more rigorous standardization of toxicity data.

Raimondo, S., D.N. Vivian, and M.G. Barron. 2010. Web-based Interspecies Correlation Estimation (Web-ICE) for Acute Toxicity: User Manual. Version 3.1. EPA/600/R-10/004. Office of Research and Development, U. S. Environmental Protection Agency. Gulf Breeze, FL.

Release 3: Additional Toxicity Features

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



http://www.epa.gov/ceampubl/fchain/webice/index.htm

This site is not compatible with all browsers (currently does not work with Google Chrome, for example)

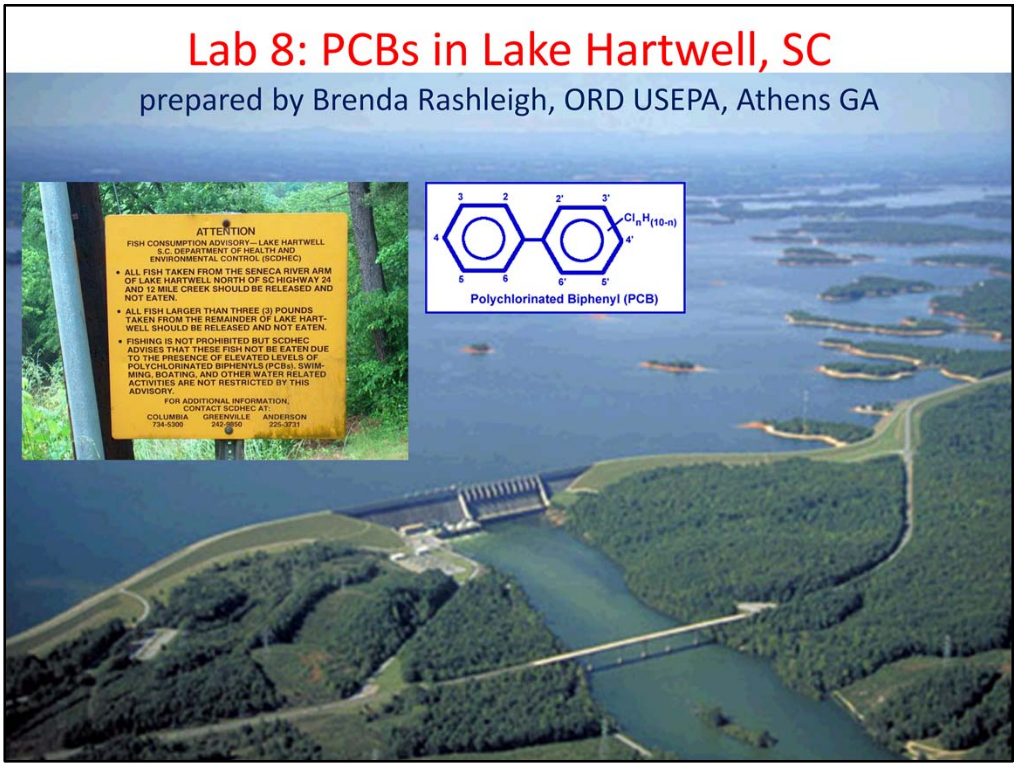
Lab 7: Risk Assessment of Insecticide in Ohio Stream

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

We will use a constant level of 0.4 ug/L chlorpyrifos in a generic small stream for purposes of risk assessment. This concentration is based on the worst-case value chosen by US EPA for risk assessment of chlorpyrifos. We will start the simulation on May 1, the start of the growing season.

The second simulation will compare a constant dose against a single, initial dose of the same magnitude.



We will use **Lab8_Lake_Hartwell_PCBs.aps** in the Data directory.

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

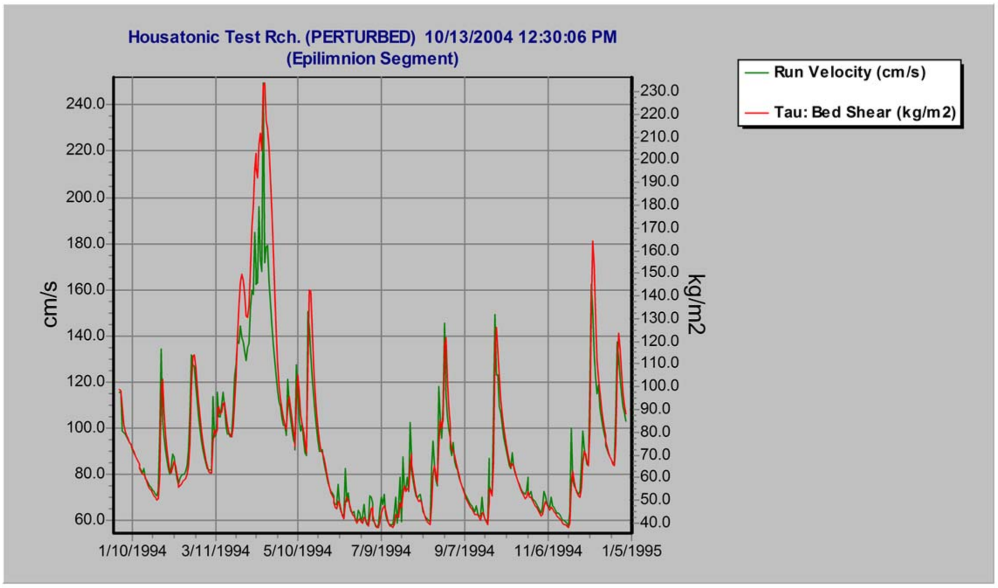
Inorganic sediments are important to the functioning of natural and perturbed ecosystems for several reasons. When suspended, they increase light extinction and decrease photosynthesis. When sedimented, they can temporarily or permanently remove toxicants from the active ecosystem through deep burial. Scour can adversely affect periphyton and zoobenthos. All these processes are represented to a certain degree in AQUATOX, particularly with the addition of explicit suspended and bedded sediment effects discussed in Day 2.

In addition, rapid sedimentation also can adversely affect periphyton and some zoobenthos; and the ratio of inorganic to organic sediments can be used as an indicator of aerobic or anaerobic conditions in the bottom sediments. These are not simulated in the model at this time.

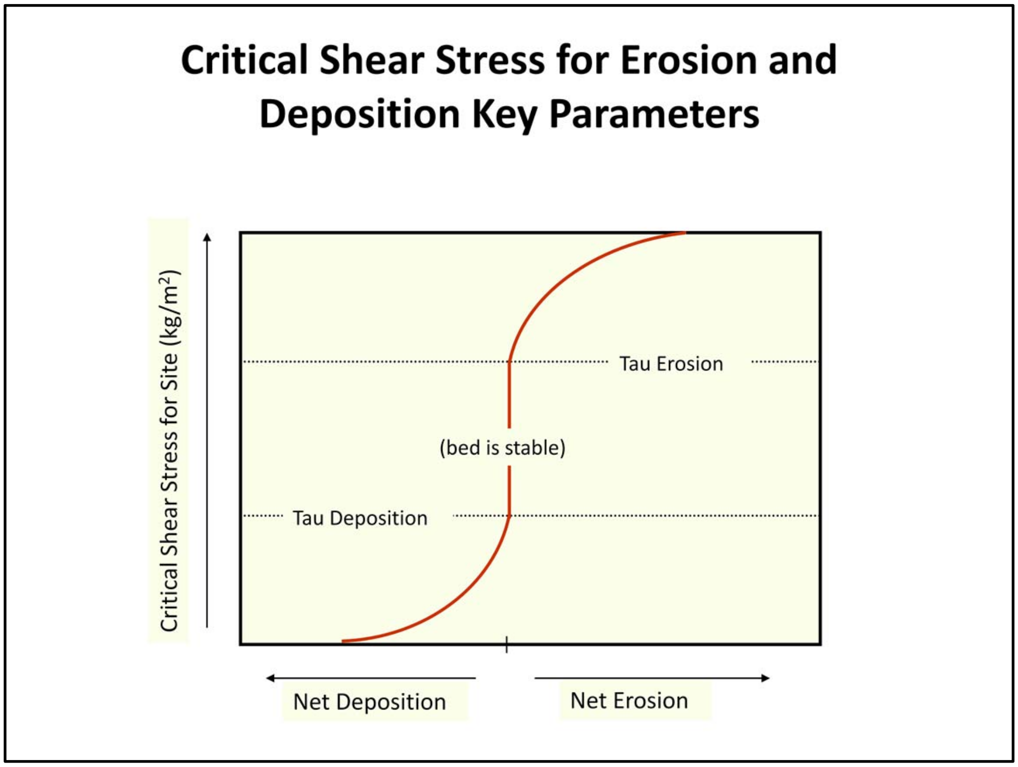
The sediment transport component of AQUATOX simulates scour, deposition and transport of sediments and calculates the concentration of sediments in the water column and sediment bed within a river reach. For running waters, the sediment is divided into three categories according to the particle size: 1) sand, with particle sizes between 0.062 to 2.0 millimeters (mm), 2) silt (0.004 to 0.062 mm), and 3) clay (0.00024 to 0.004 mm). Wash load (primarily clay and silt) is deposited or eroded within the channel reach depending on the daily flow regime. Sand transport is also computed within the channel reach. At present, inorganic sediments in standing water are computed based on total suspended solids loadings.

Output variables resulting from the inclusion of sand/silt/clay include suspended sand, silt and clay, bed sheer, and bed depth.
Sand/silt/clay modeling is discussed in more detail in Section 6.1 of the Technical Documentation.

Bed Shear Stress (Tau) Closely Related to Water Velocity



Tau is calculated as a function of channel slope and channel depth and width (hydraulic radius). This shear stress indicates whether deposition or erosion is taking place for silt and clay.

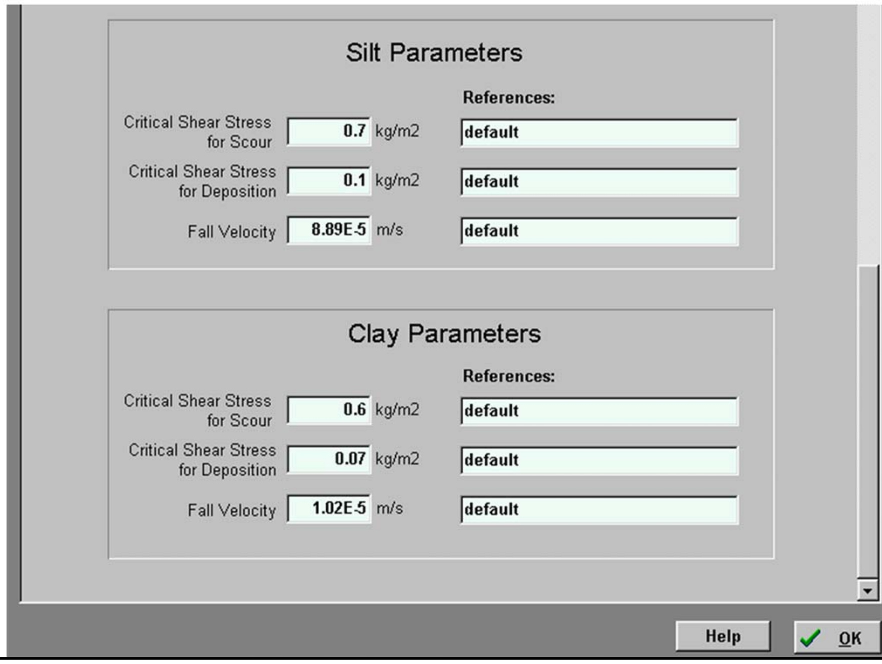


These two parameters are specified for silt and clay and can be found in the Stream section of the Site underlying data. This section of model is identical to the Hydrologic Simulation Program Fortran (HSPF) model. These parameters can be highly site specific and are usually used as calibration parameters when calibrating the HSPF inorganic sediment model.

The river reach is assumed to be short and well mixed so that concentration does not vary longitudinally. Flow routing is not performed within the river reach. The daily average flow regime determines the amount of scour, deposition and transport of sediment. Scour, deposition and transport quantities are also limited by the amount of solids available in the bed sediments and the water column.

When the inorganic sediments model is included in a stream simulation, particulate detritus moves to and from the bed to and from the water column along with the deposition and resuspension of the Cohesives compartment.

Sediment Model Parameters



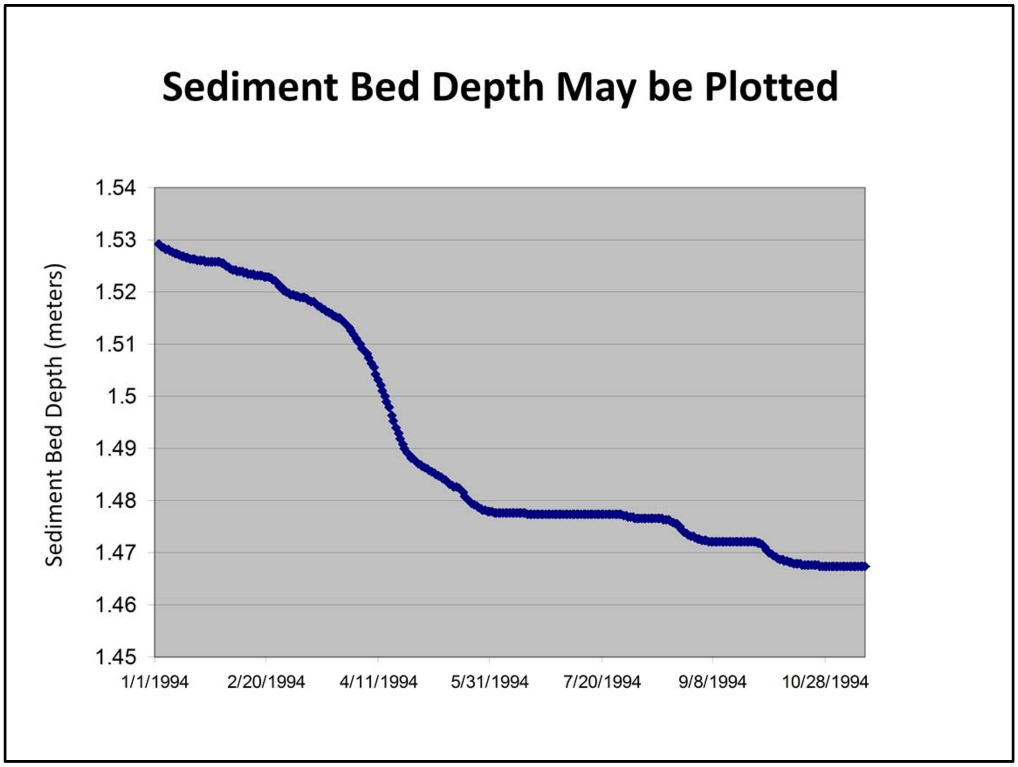
Also important are channel slope and sediment depth that occur up higher on the “stream” screen. (Within Site Underlying Data)

The fall velocity affects the rate of deposition for silt and clay.

Sand Model

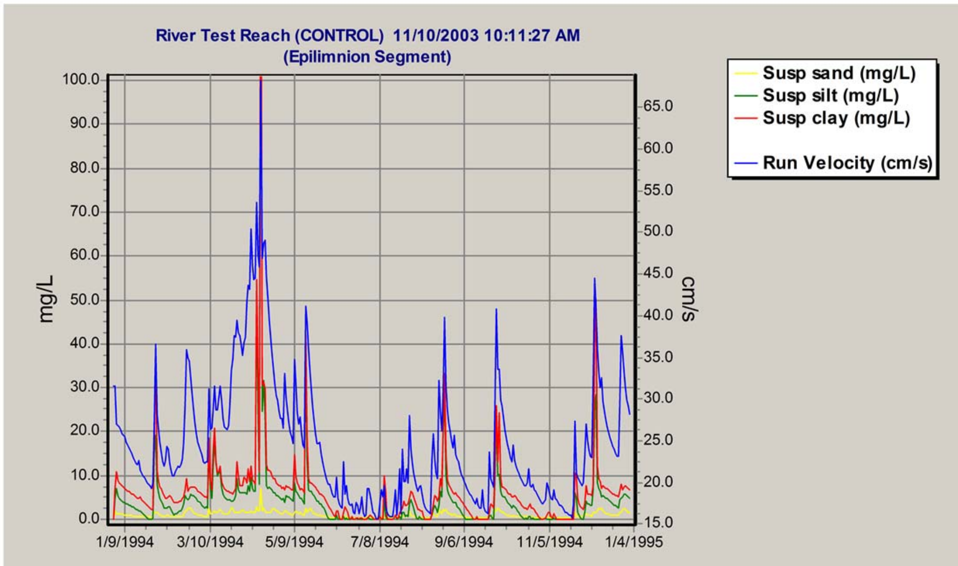
- No additional parameters / calibration required
- Potential concentration of sand in the water column is calculated as a function of water velocity and slope
- Uses Engelund and Hansen (1967) sediment transport relationships as presented by Brownlie (1981).

Scour, deposition and transport of sand are simulated using the Engelund and Hansen (1967) sediment transport relationships as presented by Brownlie (1981). This relationship was selected because of its simplicity and accuracy. Brownlie (1981) shows that this relationship gives good results when compared to 13 others using a field and laboratory data set of about 7,000 records.



The sediment bed is assumed to be uniformly mixed and is composed of the three inorganic sediments, sedimented detritus, and toxins in sedimented detritus. Initial condition fractions of sand silt and clay in the sediment bed must be supplied by the user under the sand, silt, and clay state variable screens.

Suspended Sand, Silt, Clay may be Plotted



As was the case with the TSS inputs that we saw earlier, getting an appropriate accounting for inflows of sand / silt / and clay is vital for calculating appropriate concentrations in the water column.

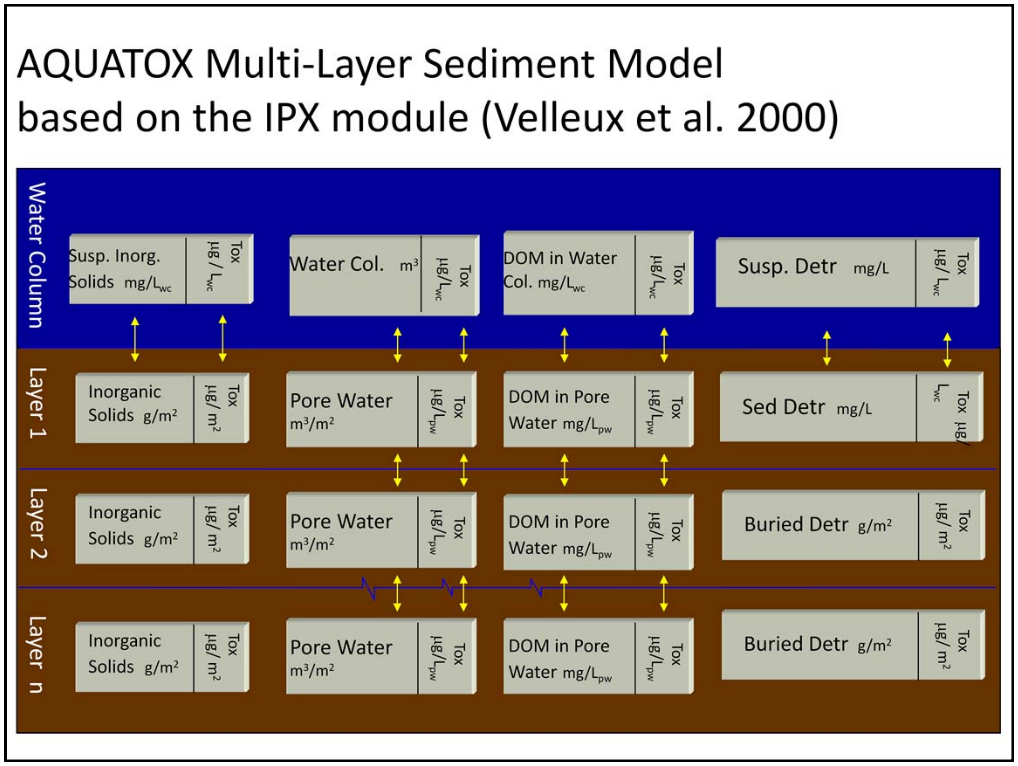
AQUATOX Multi-Layer Sediment Model

- **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**.

- For those who don't immediately recognize what "Pez" is, it's a candy composed of little tablets. When you take the top tablet from the Pez dispenser the other tablets all move up.
- We cannot allow the layers to be defined by depth from the top and keep the active layer a constant thickness because this, combined with the assumption of perfect mixing in each layer, results in advection of chemicals in inappropriate ways.

Velleux, M., S. Westenbroek, J. Ruppel, M. Settles, and D. Endicott. 2000. A User's Guide to IPX, The In-Place Pollutant Export Water Quality Modeling Framework, Version 2.7.4. Pages 179. US Environmental Protection Agency, Grosse Ile, MI.

The multi-layer sediment model is discussed in more detail in Section 6.2 of the Technical Documentation.



- From left to right each sediment layer is composed of inorganic solids, water, dissolved organic matter, and organic solids. Each category can have toxicant sorbed to it, or in the case of water, dissolved within it.
- In this case the top layer (Layer 1) is the active layer and interacts with the water column through scour, deposition and diffusion. This layer changes height and if it gets too big it is split into two layers; if it gets too small it is joined with the layer below it.
- Lower layers only interact through pore-water diffusion.

Velleux, M., S. Westenbroek, J. Ruppel, M. Settles, and D. Endicott. 2000. A User's Guide to IPX, The In-Place Pollutant Export Water Quality Modeling Framework, Version 2.7.4. US Environmental Protection Agency, Grosse Ile, MI.

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)

There are additional data requirements for this complex sediment model, but note that the simple "HSPF-like" sand-silt-clay model may also be run.

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

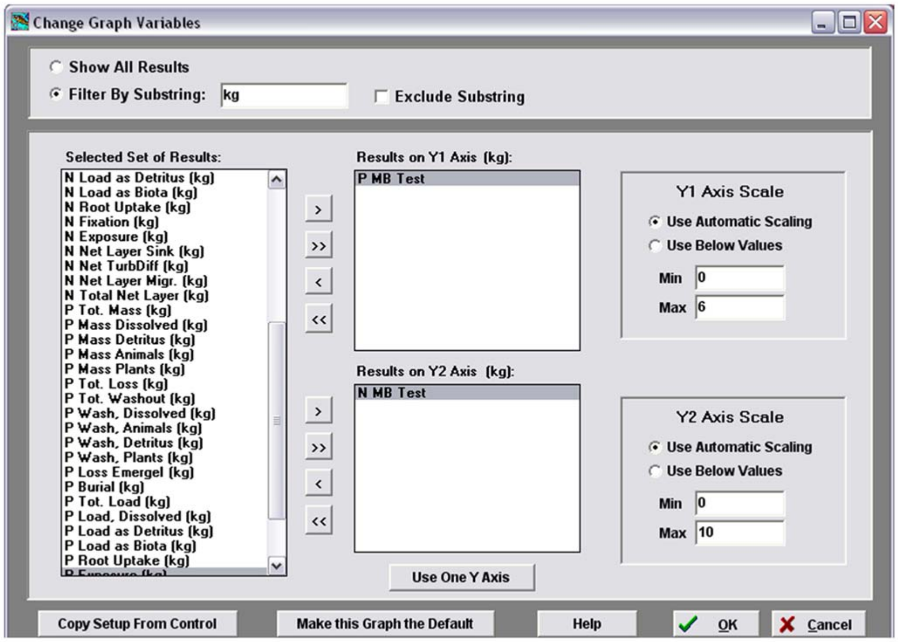
Densities of inorganic and organic sediments are not assumed to change between layers.

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)

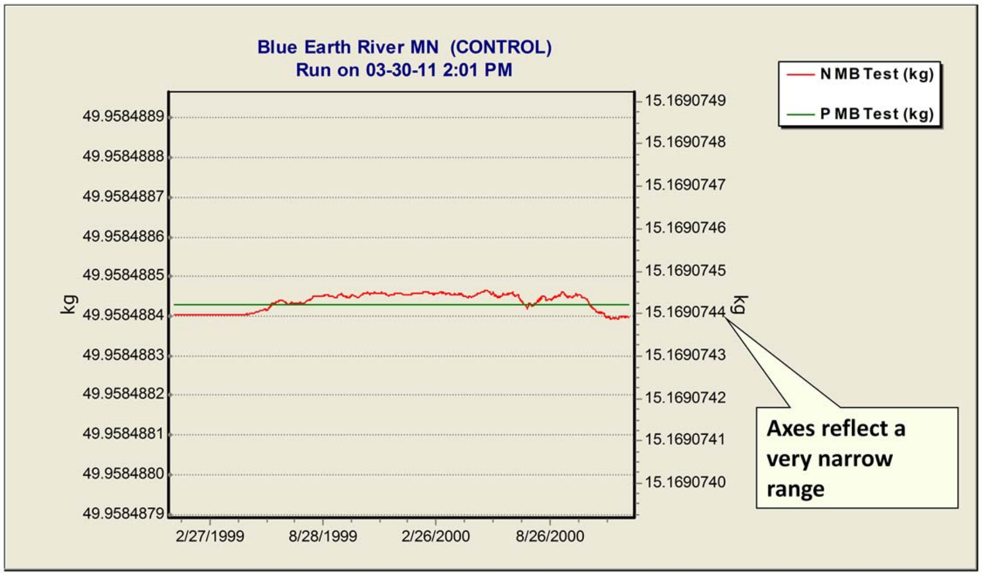
If you'd like to follow along within AQUATOX, load **BlueEarth54 Results.aps** that should still have results intact. We will now look at some of these results through the output screen.

Nutrient Mass Balance Results Grouped



Using the change variables button and filtering on “kg”, the nutrient mass balance results are all grouped together. Units are all in terms of kilograms of nitrate and kilograms of phosphate. As a demonstration, I will select the nitrogen mass balance test and phosphate mass balance test for interest. Select Automatic Scaling if it’s not already selected.

Mass is Balancing



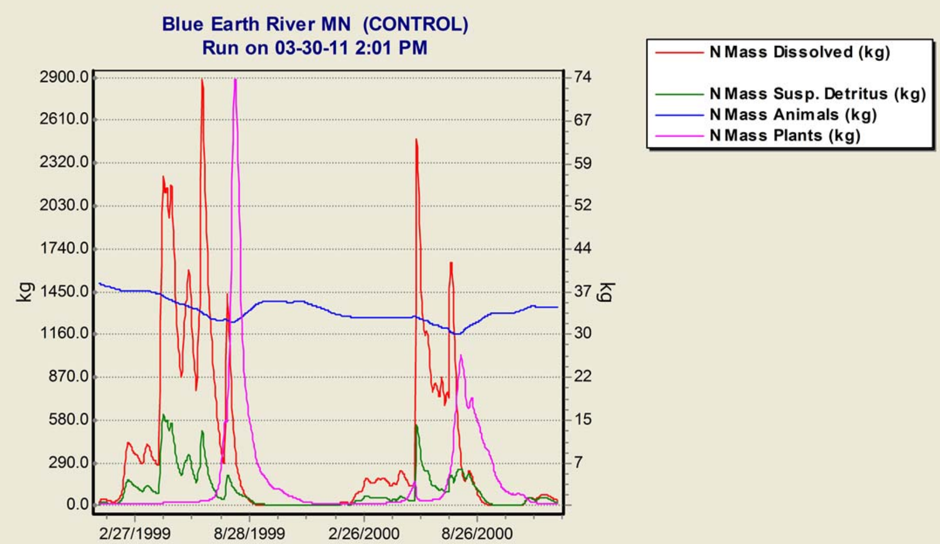
There are very small changes in mass because of machine error (also called machine epsilon http://en.wikipedia.org/wiki/Machine_epsilon).

If you export these mass balance results they are accurate to 4e-8 kg or 40ug of nitrate over the two year simulation.

This machine error is not the same as the error produced by the differential equations solver for which you can set the relative error within the setup screen.

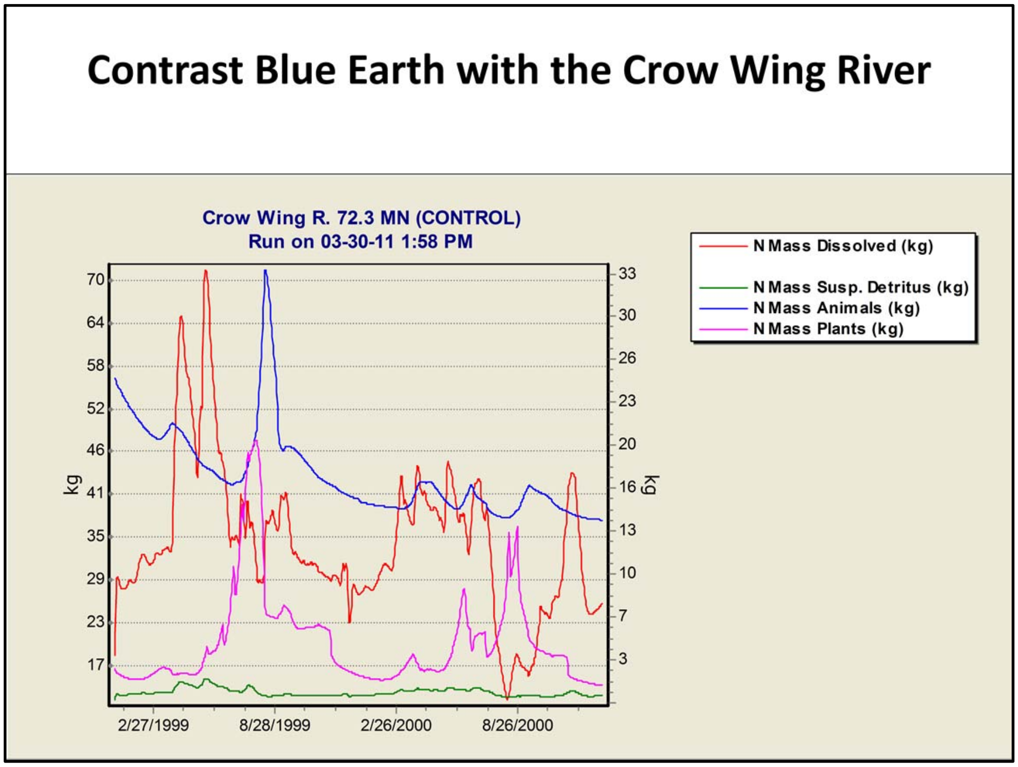
Occasionally when there are no nutrients left in the system the mass will not balance perfectly. This is a result of interactions within the food-chain that require uptake of nutrients from water to balance mass.

Where are the Nutrients within the System?



To examine where the nutrient mass is within the system at any given time, go to the Change Variables screen again and select N Mass Dissolved for Y axis 1 and N Mass Susp. Detritus, Animals, and Plants for Y axis 2.
(Filter "N Mass")

Note the different units on the Y axes. There is a significant inflow of nitrogen into the system during May and lasting through July . Within Biota you can see that there are algal blooms that trap some of this nitrogen. Detritus matches dissolved inflow closely as the detritus category includes dissolved organic matter flows into the system. Finally, the nitrogen within animals remains fairly consistent throughout the simulation.



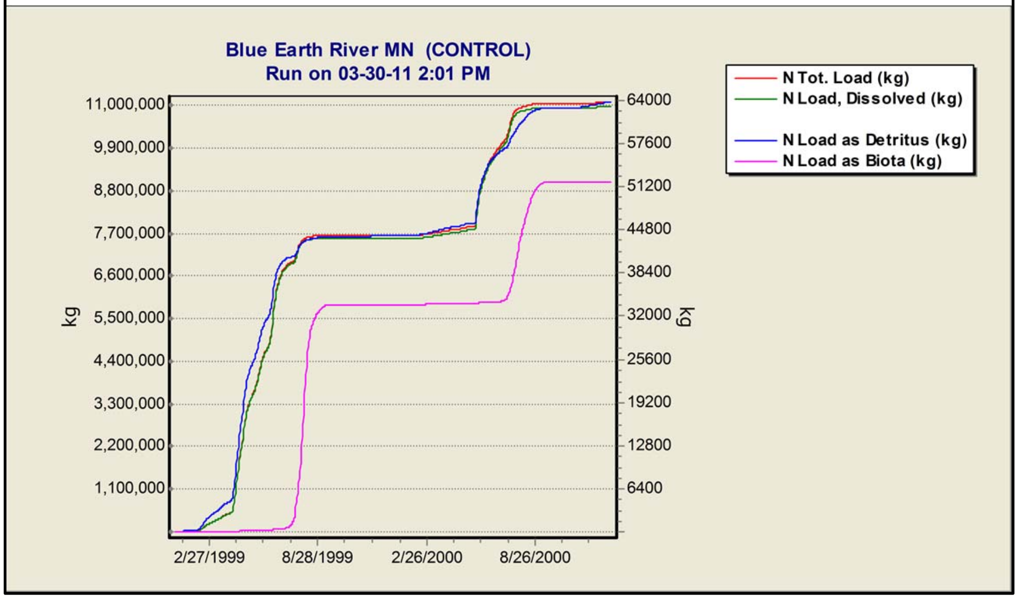
To look at a different system, load in **CrowWing72 Results.aps** and select N Mass Dissolved for Y axis 1 and N Mass Susp. Detritus, Animals, and Plants for Y axis 2.

This time there is far less nitrogen washing through the system and far less nitrogen in the water column. Roughly two orders of magnitude less. N sequestered in detritus is also significantly lower.

Note, it's important to compare two sites of the same size when making such a comparison as the units are in a total mass basis.

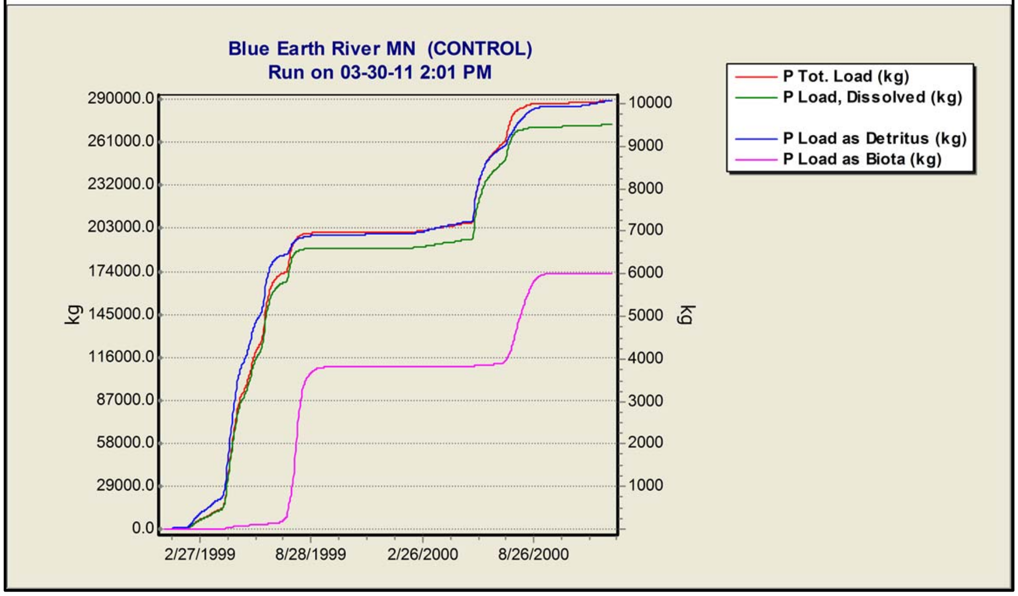
As an additional demonstration, we will also examine inflow loadings of nutrients with the graphic interface.

Nitrogen Loadings, Blue Earth River



Most of the nitrogen loading in Blue Earth River is dissolved, although that is tracked closely by detrital loadings (note difference in scale), much of which is also dissolved. Loadings are calculated as cumulative; 1999 was a wet year so that there was a much larger cumulative loading.

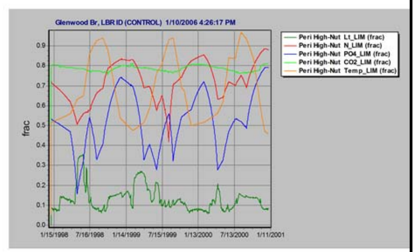
Phosphorus Loadings, Blue Earth River



Most of the phosphorus loading in Blue Earth River is dissolved, although that is tracked closely by detrital loadings (note difference in scale), much of which is also dissolved. Loadings are calculated as cumulative; 1999 was a wet year so that there was a much larger cumulative loading.

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



- Current version available at EPA AQUATOX website.

Significant testing initially ensured that the functionality of Release 2.2 and Release 3.0 (single-segment mode) were initially identical.

However, as we have continued to refine Release 3.0 and Release 3.1, we have not upgraded Release 2.2.

For example, low oxygen and ammonia toxicity effects may make a Release 3.0 simulation behave differently if those effects are not turned off in Release 3.0.

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

Listserver URL: **http://water.epa.gov/scitech/datait/models/aquatox/listserv.cfm**