For presentation at the International Society for Ecological Modelling, Global Conference 2016, Towson MD

The History and Generality of AQUATOX, a Robust Mechanistic Model

Richard Park[1], Jonathan Clough[2], Eldon Blancher[3],
Brenda Rashleigh*[4], Marjorie Wellman[5], and David Mauriello[5]
[1]Eco Modeling retired, [2]Warren Pinnacle, [3]Moffatt & Nichol,
*[4]Presenter, US EPA, [5] US EPA retired

In 1990 aquatic fate, toxicology, and ecosystem submodels were coupled to "close the loop," representing both direct and indirect effects; the model is also a platform to which other environmental stressors may be added for extensive analysis

1


2


3


4


5


5


AQUATOX Background and History

Consistent and deliberative development

- **Integrated ecosystem fate and effects model first envisioned 30 years ago**
- **Jon Clough, programmer, and Marge Wellman, EPA Project Manager, for 20 years**
- **QA/QC for every formulation and code, entire model peer-reviewed by 3 external EPA panels**
- **Specific applications reviewed by *ad hoc* panels**

Background:

- ***CLEAN***, *Lakes George & Wingra,* ***International Biological Program***, *1970-1974*
- ***CLEANER***, *6 European lakes, funded by* ***National Science Foundation*** *and* ***EPA Athens Lab***, *1975-1979*
- ***PEST***, *chemical fate and bioaccumulation model funded by* ***EPA Athens Lab*** *(Larry Burns), 1979-1980*

Early History:

- **EPA Off. Prevention, Pesticides, & Toxic Substances (**Dave Mauriello, Rufus Morison, Don Rodier)
  - Unfunded proposal, 1980
  - Workshop, Baltimore, ***specifications for model***, 1987
  - ***1st publication***, symposium proceedings, **EPA Athens Lab**, 1988
  - Initial development, **EPA OPPTS purchase order** through **Corvallis Lab** (Hal Kibby), 1989-1990
- Used in Environmental Risk Assessment class, **Indiana Univ. School Public & Environmental Affairs,** 1991-1992
- Potential use in assessment of corn pesticides, **Abt Associates,** 1993-1995

AQUATOX History continued

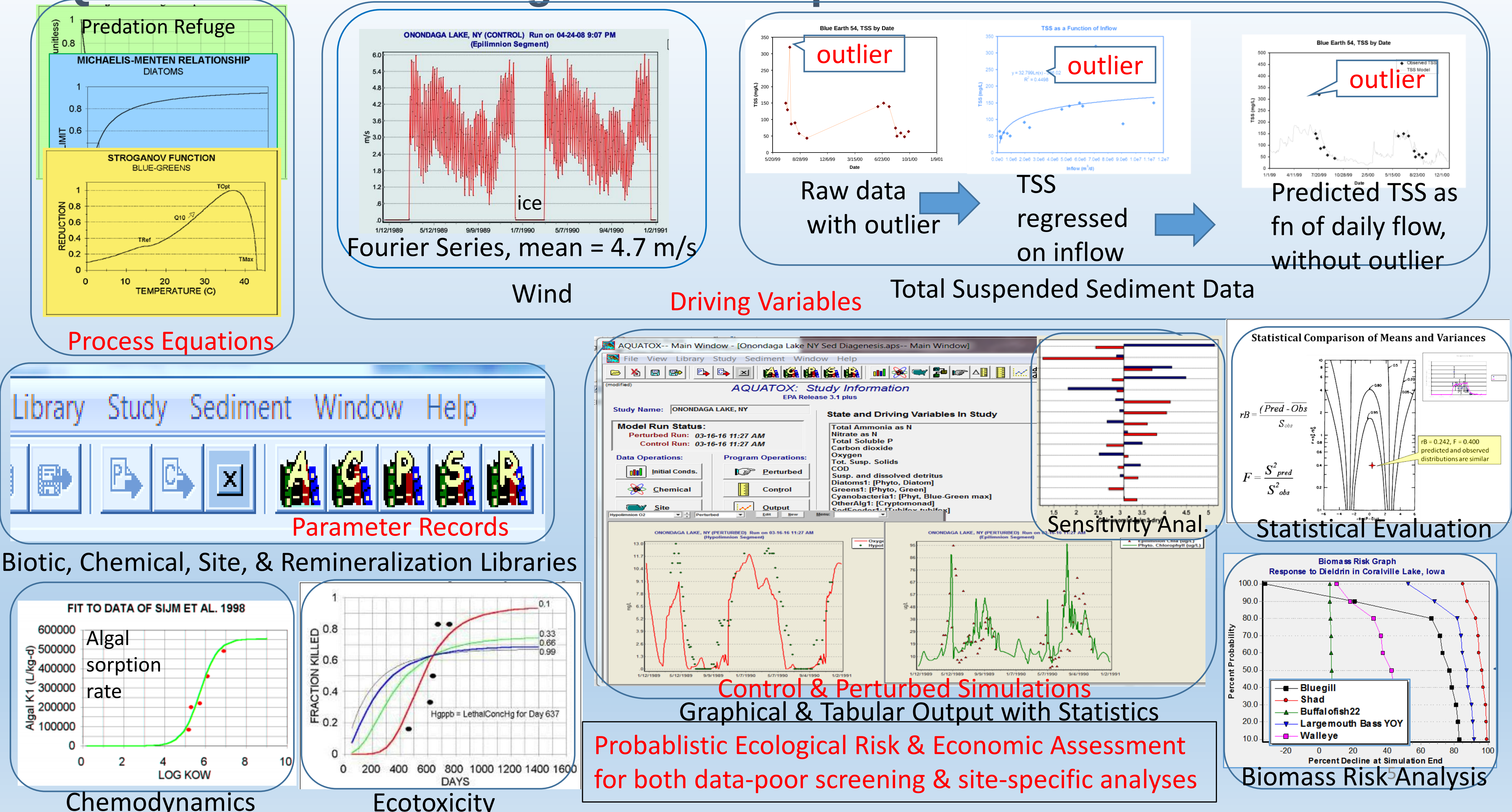
Development, **EPA Office of Water** (Russ Kinerson, **Marge Wellman**, Jim Carleton), 1995-2014

- Coded for Windows, 1995
- Verification, 1997:
  - Lake Onondaga NY, Coralville Res. Iowa, PCBs in Lake Ontario food web
- Linkage to BASINS (HSPF, SWAT) 2001
- Periphyton submodel, verification Walker Branch TN, 2001-2002
- Simultaneous calibration across nutrient gradient, 2004
  - Crow Wing, Rum, and Blue Earth Rivers MN
- Sediment diagenesis, sediment impacts, $CaCO_3$ pcpt and P sorption 2005
- Water quality criteria, Lower Boise River ID, Tenkiller Lake OK, 2005-2008
- Sensitivity and uncertainty analysis, 2009-2010
- Feasibility of modeling FL streams with minimal data, 2010
- Linkage to Web-based toxcity estimation database (ICE), 2010
- Water quality criteria, DeGray AR, Tenkiller OK Reservoirs, 2011
- CO2Sys linkage verified with Venice Lagoon data, 2011
- Bioacccumulation of PFOS in riverine foodweb, 2012
- Internal nutrients, 2014

AQUATOX History continued

- **Development, EPA Off. Prev., Pest., & Toxic Sub**. (**Dave Mauriello**, **Don Rodier**), 1996-2003
  - Validation: pesticides, nonylphenol, PCP in pond & stream mesocosms, 1996-1997
  - Wizard, enhanced graphics, context-sensitive Help file, 2001
  - Galveston Bay TX canonical environment for assessment of industrial chemicals, 2002
  - PFOS submodel, 2002-2003
  - Risk assessment of legacy contaminated sediments, Coralville IA, 2002
- Impact of surfactants on periphyton, **Procter & Gamble**, 1998-2000
- Assessment of remedial scenarios, PCBs in Housatonic River, **EPA Region I**, 1998-2001
- Periphyton-nutrient TMDL, Cahaba River, **Jefferson Co. AL** (**Don Blancher**), 2001-2002
- Comparison with other bioaccumulation models, **EPA Athens**, 2004
- Risk assessment of atrazine, **EPA Off. Pesticide Program** (**Frankenberry**), 2004-2006
- Biotic indices, impact of construction in watersheds, **Fort Benning GA, Army**, 2008-2011
- Anadromous fish submodel, **Columbia River Inter-Tribal Fish Commission**, 2011-2012
- Model support for TMDL of Lower Boise River, **Idaho Dept. Environ. Quality**, 2013-2014
- **Impacts of BP Oil on Natural Resources of MS and AL**, **MDEQ & ADEM** (USM, Berger **Don Blancher**), 2012-2015
  - Marsh-Edge, Oyster Reef, Sandy Open-water , Protected, Exposed, and Nourished Beach

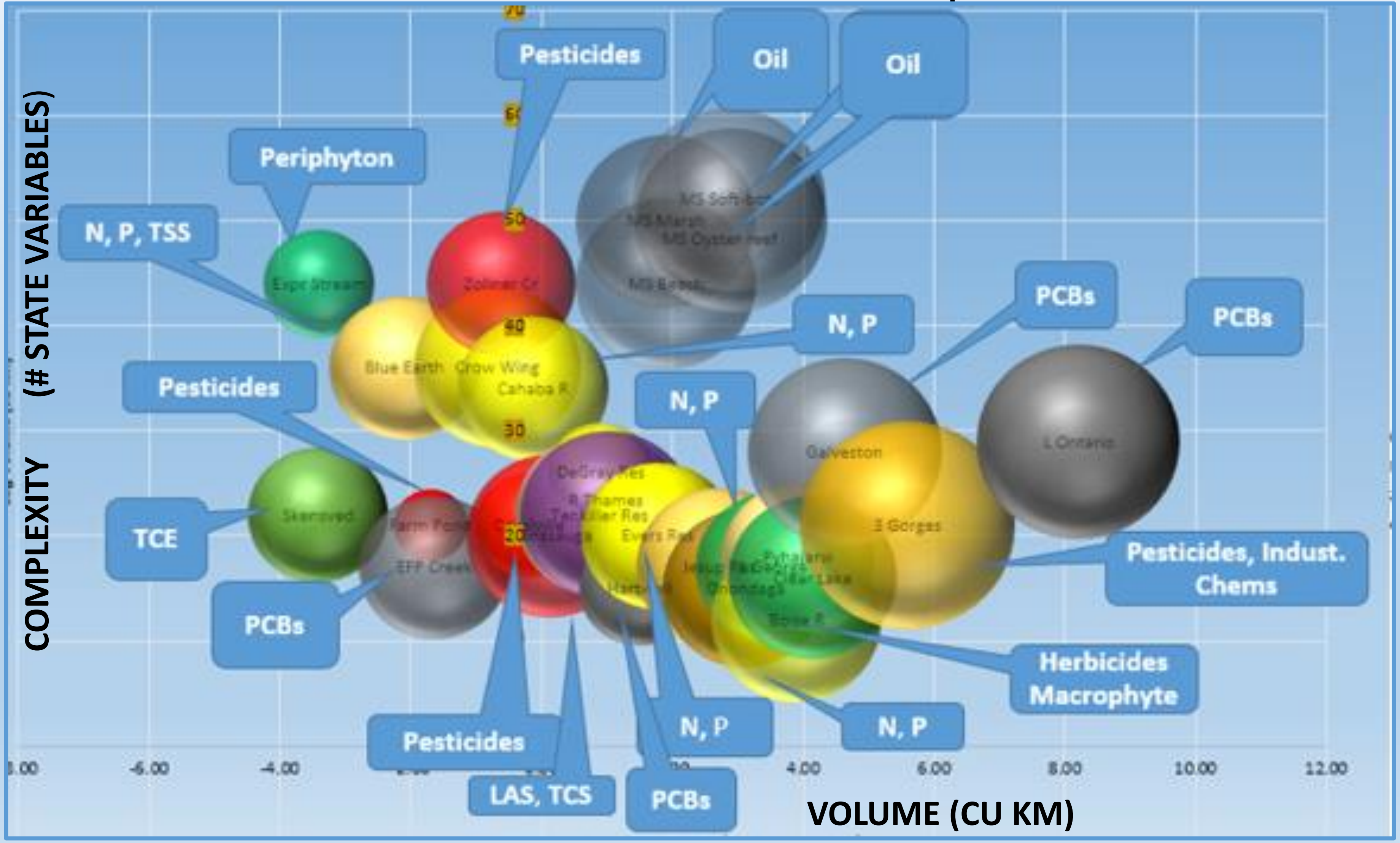
AQUATOX: Flexible Integration of Empirical & Mechanistic Constructs



Probablistic Ecological Risk & Economic Assessment for both data-poor screening & site-specific analyses

MODEL DOMAIN

AQUATOX spans a range of environmental conditions and applications from a simple aquarium with HCB and a macrophyte to the Three Gorges Reservoir in China with farm runoff and industrial pollution

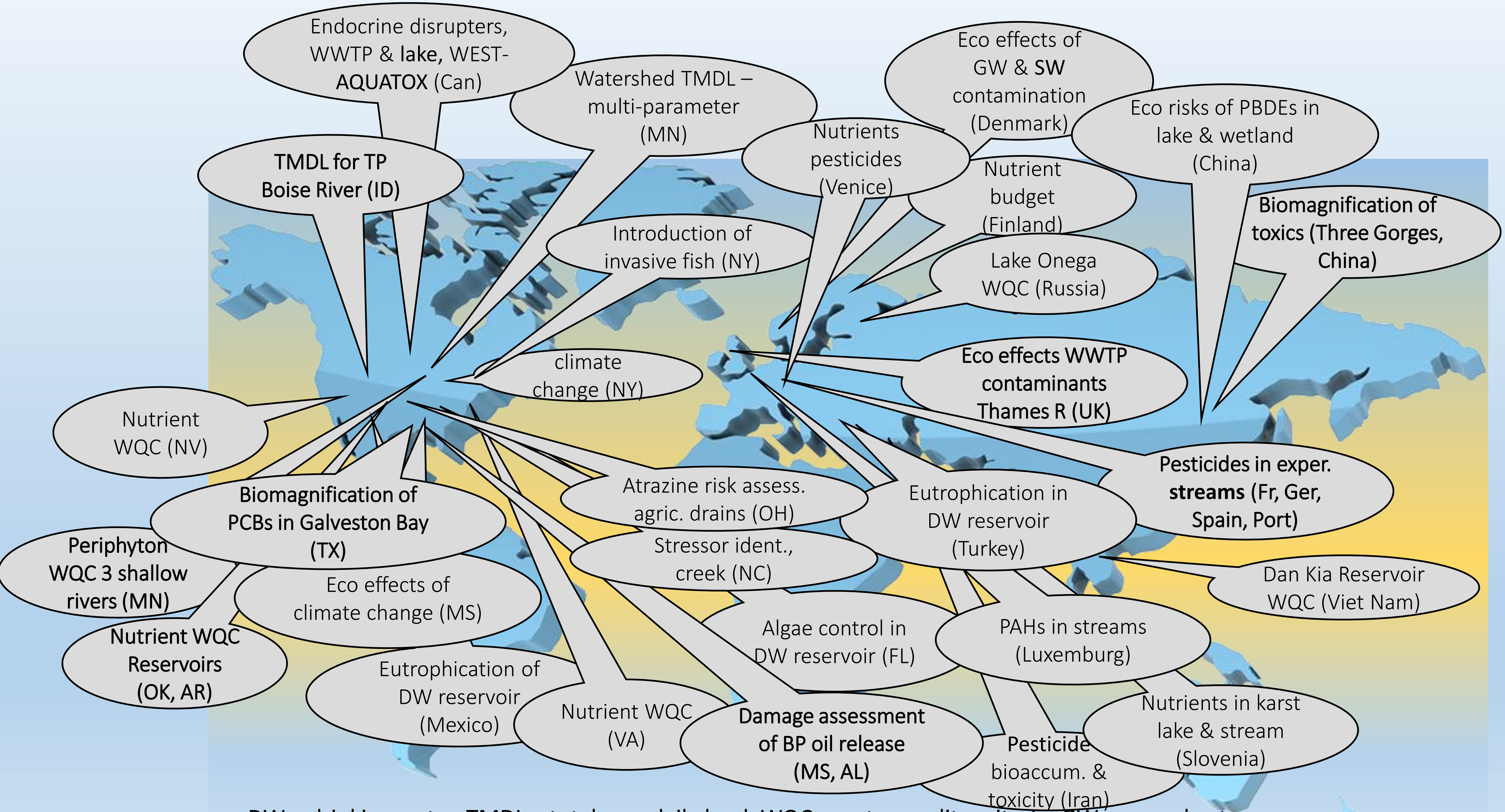


Discharge = 2.6 cu km/d

Discharge = 8.8 cu km/d

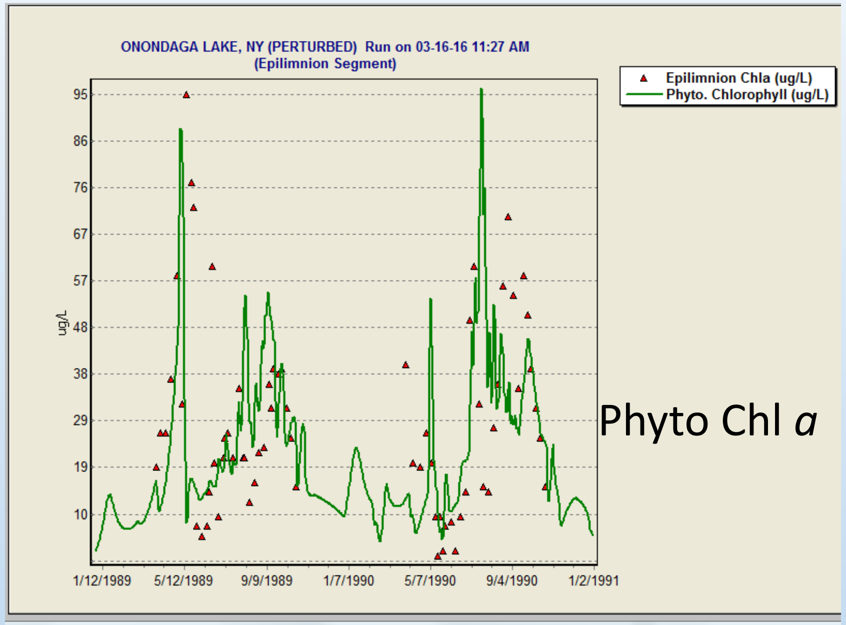
Colors denote model applications as indicated by call-outs; Aquarium has 0 discharge, therefore does not plot.

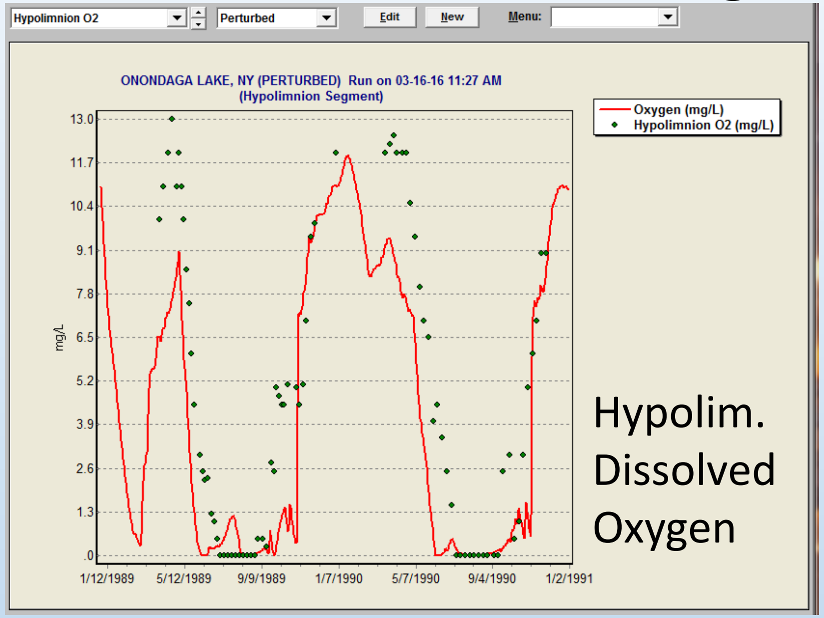
Worldwide applications of AQUATOX



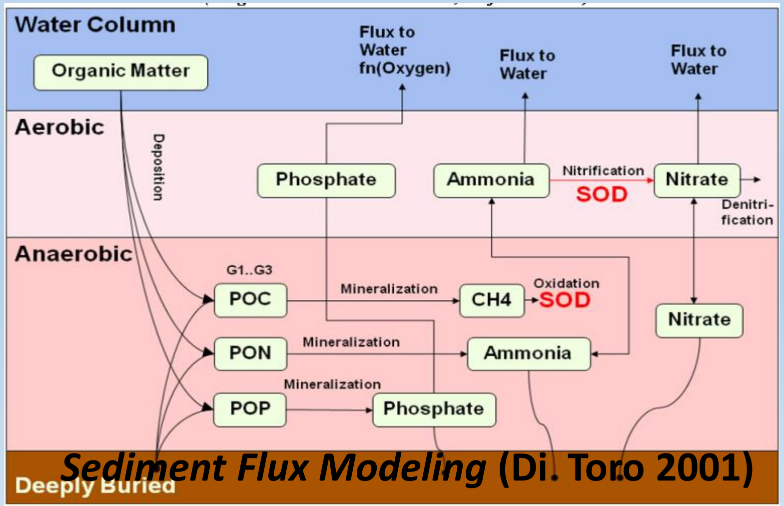
DW = drinking water, TMDL = total max daily load, WQC = water quality criteria, GW= groundwater

Calibration, sensitivity analysis, and verification/validation: Lake Onondaga NY is a well-studied hypereutrophic system that served as a test case for improvements to the model & forecasting impacts of wastewater diversion & climate change



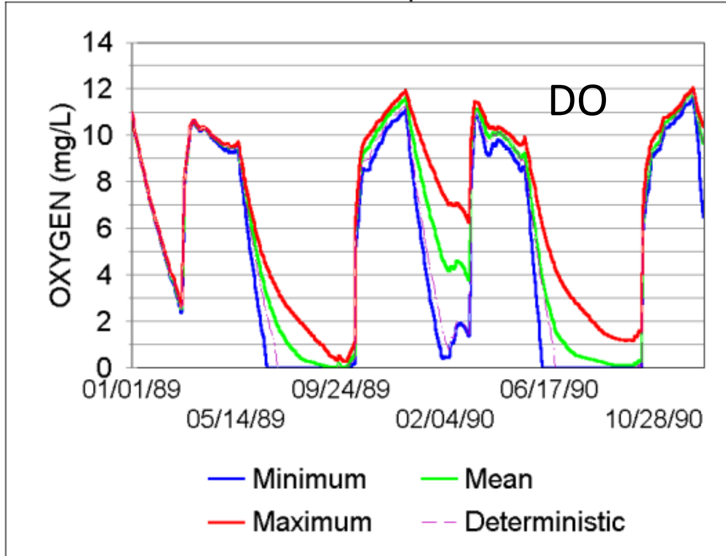


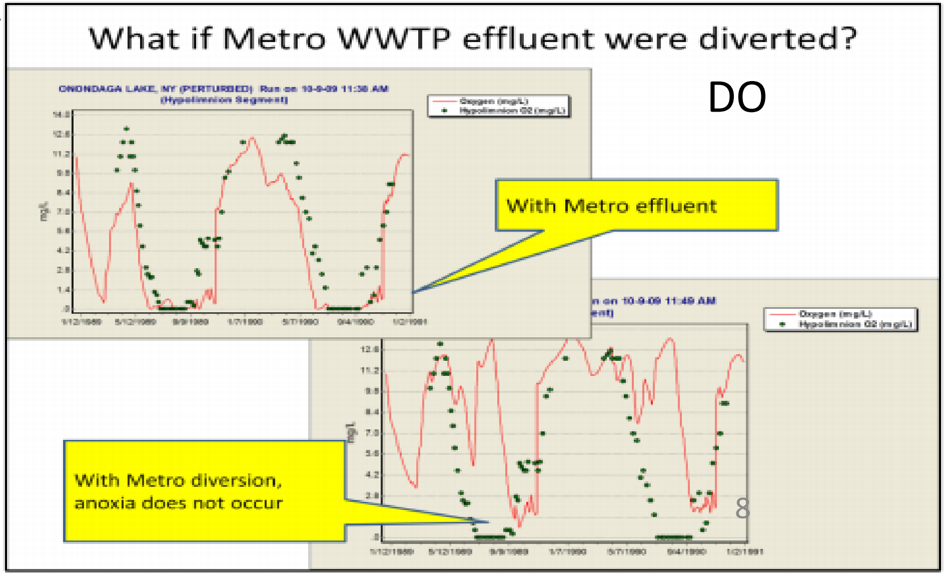
Formulations, such as remineralization from anaerobic sediments were incorporated



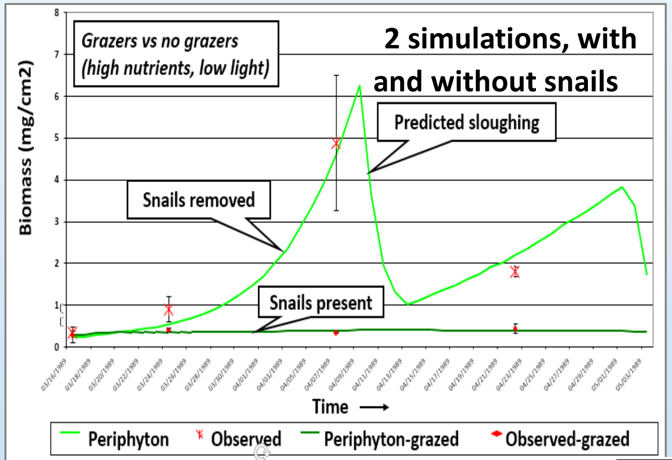
Sediment Flux Modeling **(Di. Toro 2001)**

Figure 15. Sensitivity of hypolimnetic oxygen in Lake Onondaga to variations in maximum consumption rates of detritivores.



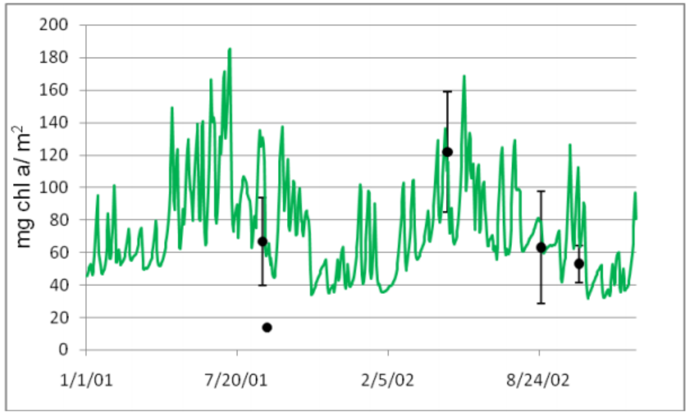


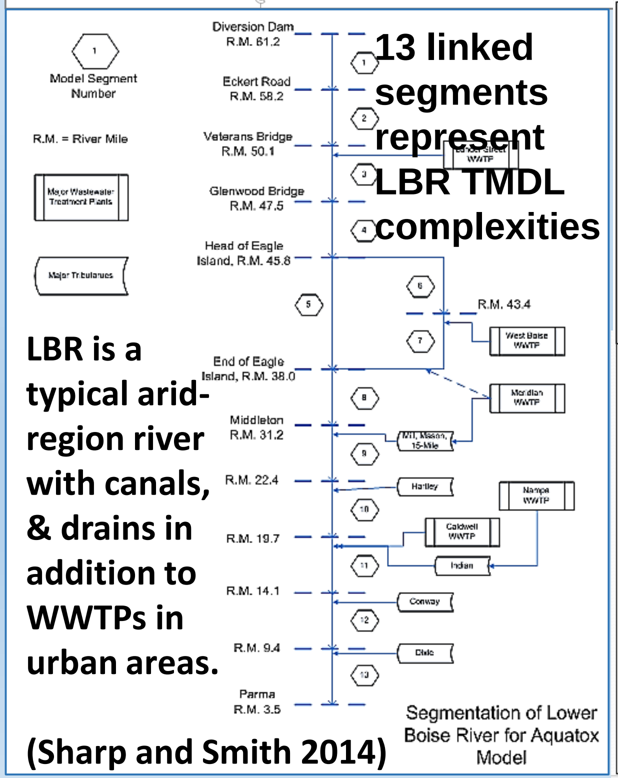
Periphyton model has proven to be robust, with numerous applications ranging from screening model, with little or no site calibration, to detailed TMDL model



Initial calibration and verification of periphyton model was based on a series of experiments that manipulated nutrient levels, ambient light and grazing pressure by snails in **Walker Branch TN**, and in adjacent experimental stream (Rosemond, 1993).

Figure 22. Predicted and observed benthic chlorophyll a in Cahaba River, Alabama; bars indicate one standard deviation in observed data.



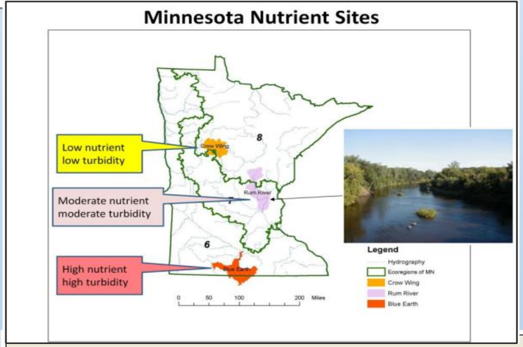


13 linked segments represent LBR TMDL complexities

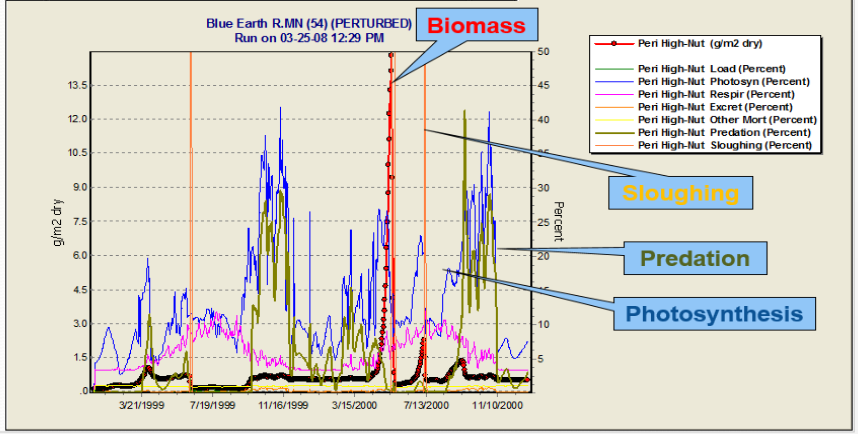
LBR is a typical arid-region river with canals, & drains in addition to WWTPs in urban areas.

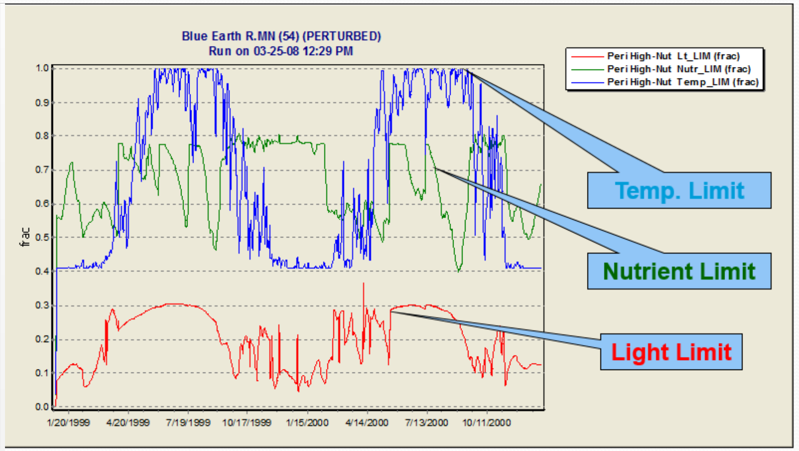
Segmentation of Lower Boise River for Aquatox Model

(Sharp and Smith 2014)



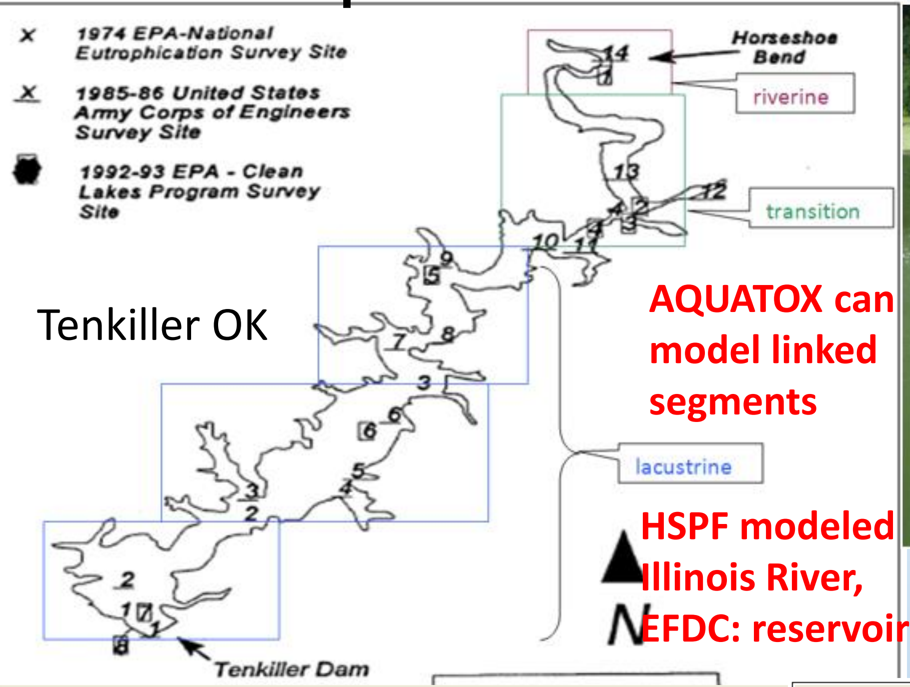
The model was also calibrated with data from **the Cahaba River**, AL. The model seems to give a reasonable fit to the observed data, considering the spread in the observations as indicated by the error bars (+/- 1 standard deviation). Furthermore, **it was calibrated with data from 3 MN rivers with very different N, P, TSS.** More recently it was used by IDEQ in the 60-mi **Lower Boise R TMDL**. **Model application is transparent; can "drill down" to see process dynamics, such as algal rates and photosynthesis limitations.**



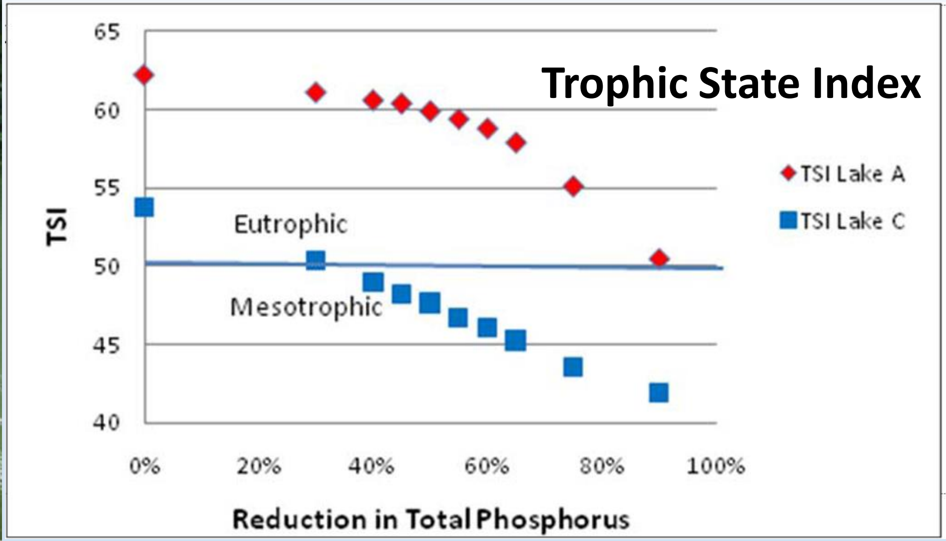


WERF used model *without calibration* as a screening-level model

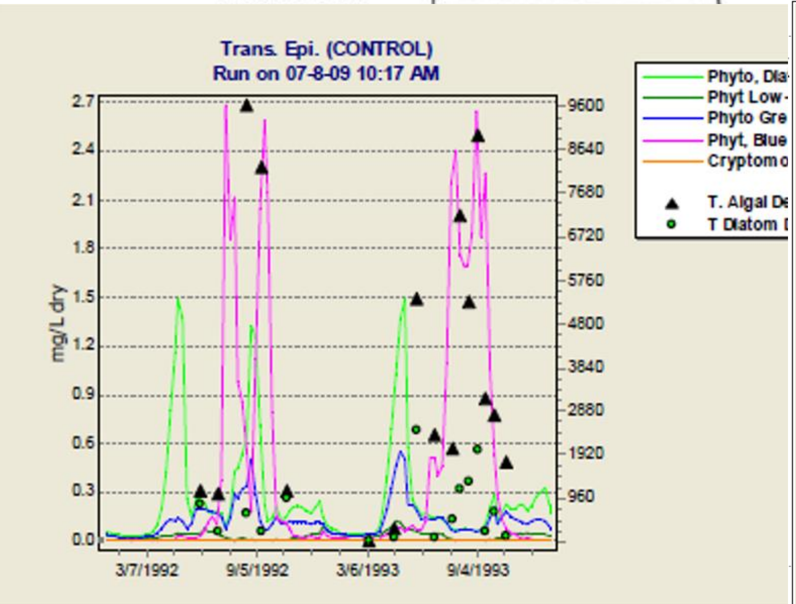
AQUATOX has been linked to watershed and hydrodynamic models and used to analyze eutrophication and contamination in stratified reservoirs such as Tenkiller Oklahoma



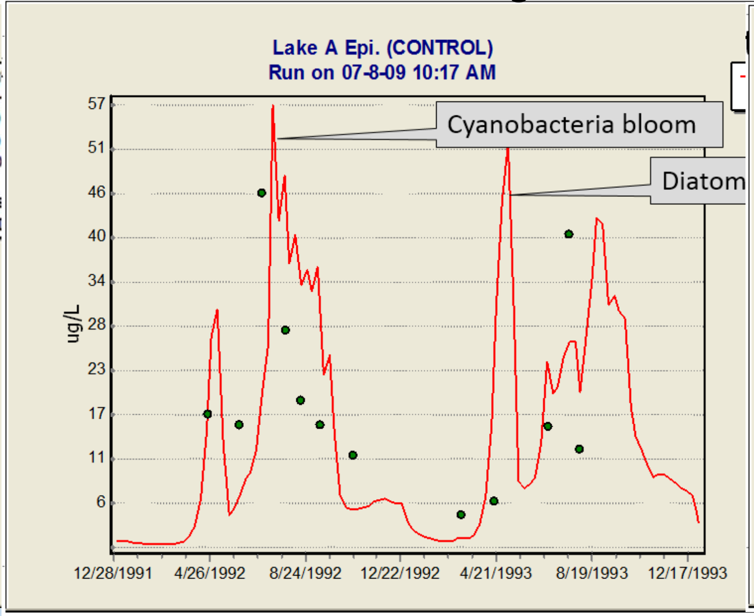
Denser storm runoff with duckweed in Illinois River flows under Tenkiller transition water with algae to the left



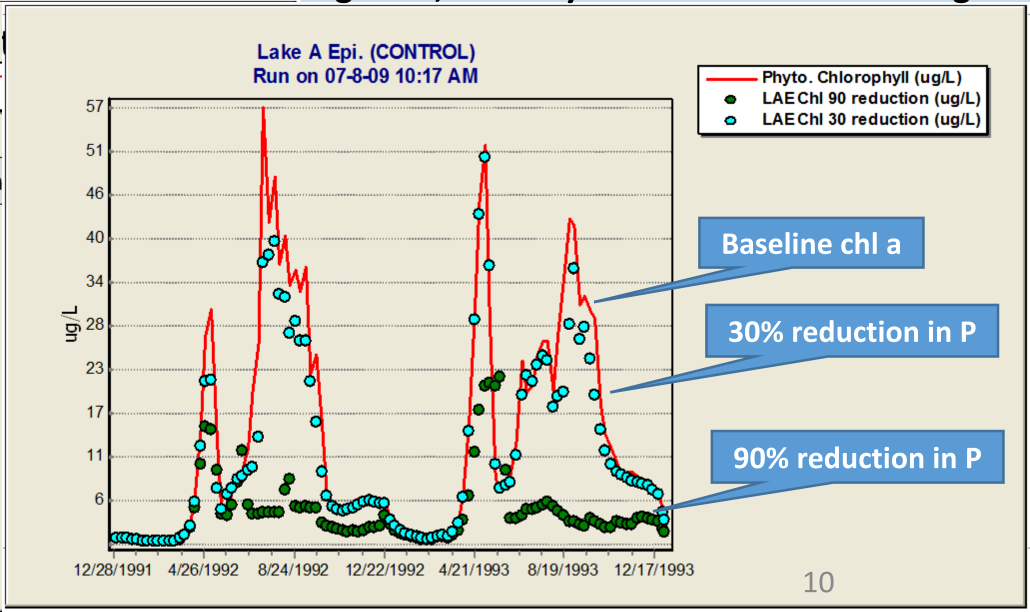
Simulation suggests that 90% reduction in P will be required to achieve mesotrophic status for upstream lacustrine segment, but only 30% for downstream seg.



Calibrated phytoplankton in transition epilimnion



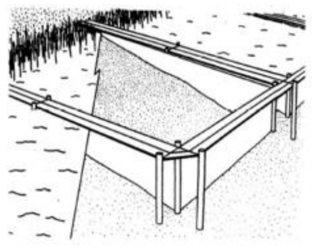
Calibrated phytoplankton in lacustrine epi.



Calibrated baseline phytoplankton compared to predicted

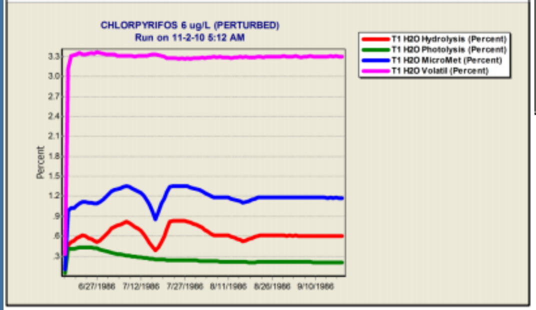
Ecotoxicity is a function of internal concentrations of toxicants; external submodel is available if required for mode of action or if uptake and clearance are rapid

Chlorpyrifos-dosed pond enclosures at Duluth MN used to validate fate and effects model

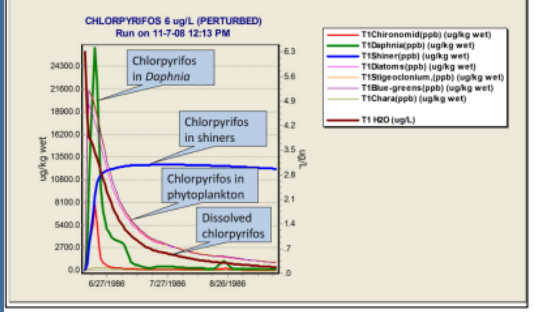


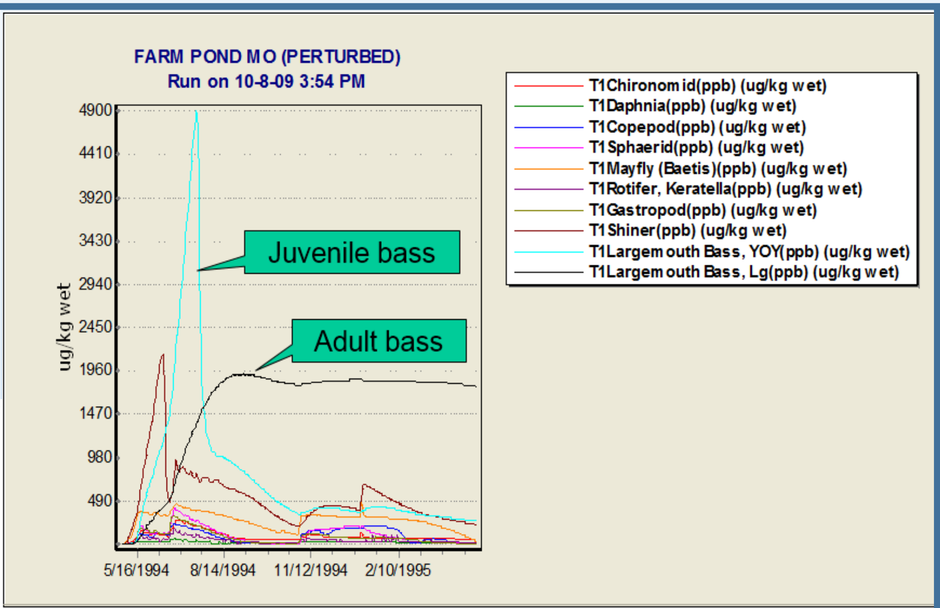
Chemical rates may be tracked

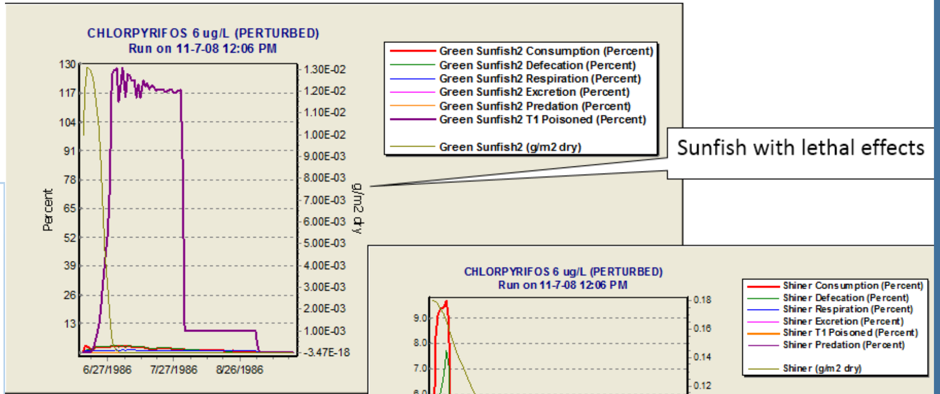
Predicted In-situ Degradation Rates for Chlorpyrifos in Pond

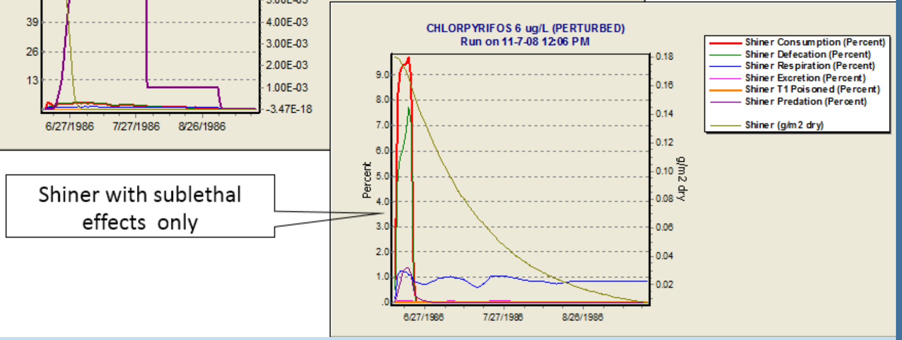


Model can trace how the toxicant is partitioned in the biota



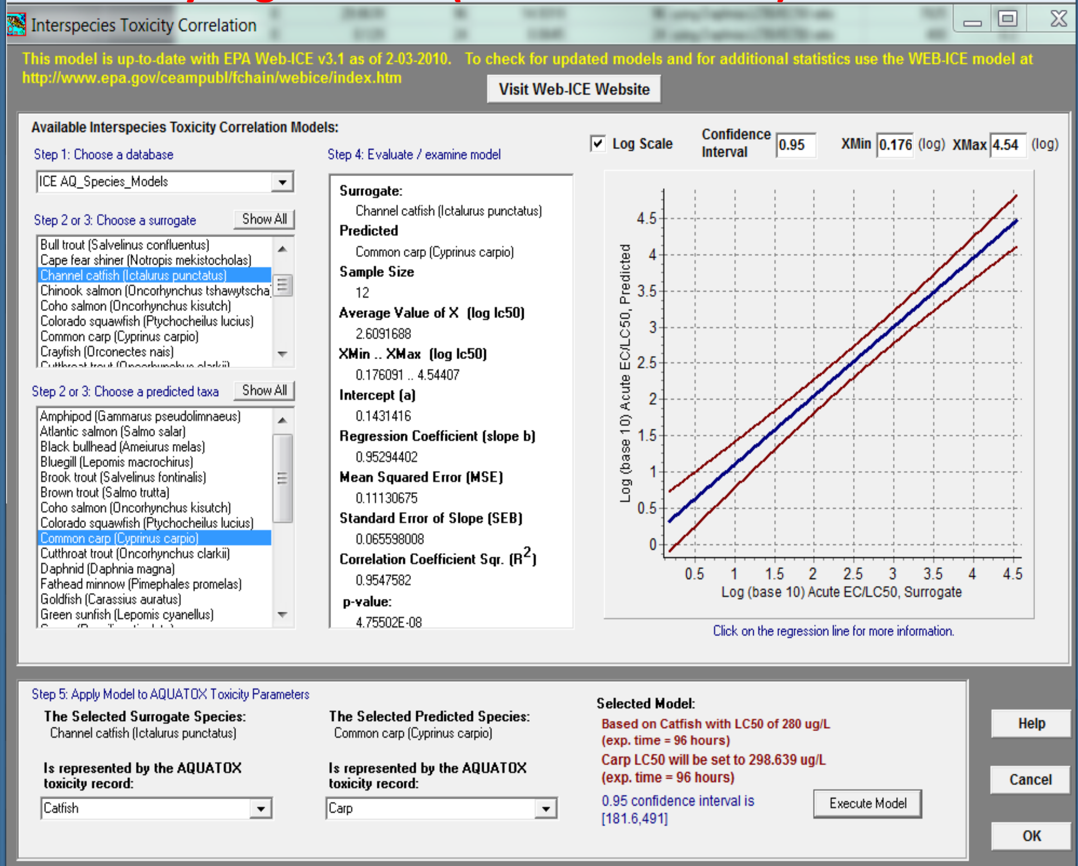






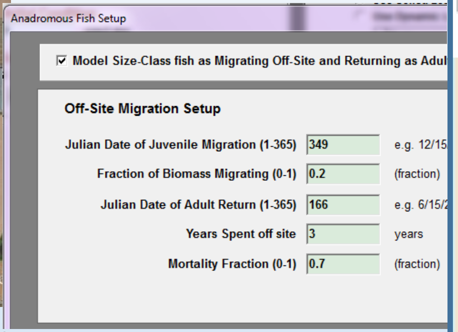
Initial Verification with Data from EPA MN and F&WS MO mesocosms

Integration with Web-ICE, a large EPA database of toxicity regressions (Raimondo 2013)



Challenge is to obtain the large number of toxicity parameters required in a typical AQUATOX run. ICE regressions are linked to the model and can be used to populate the toxicity record if data are not available in ECOTOX and elsewhere.

In addition to ecotoxicity, AQUATOX provides a quantitative platform to evaluate multiple environmental stressors acting singly or together

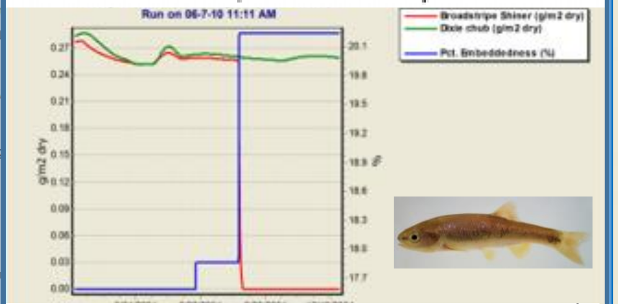


Zollner Creek OR, a TMDL site, exemplifies the action of **multiple stressors from ag runoff: sediments, nutrients, and pesticides (including legacy in soil, dieldrin, and one exceeding state criterion, for concentration in water, chlorpyrifos);** these affect growth and mortality of fish, including **anadromous lamprey and salmon**; in addition, tissue concentrations exceed action levels, resulting in fishery advisories.

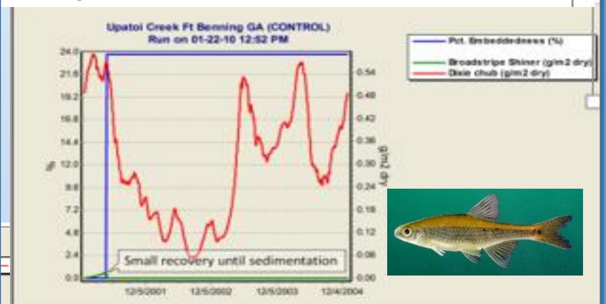
Case study developed as demonstration by Dr. Richard Park, Eco Modeling, for Columbia River Inter-Tribal Fish Commission (CRITFC), Workshop held Nov 29-Dec 1, 2011.

Anadromous fish (salmon & lamprey) submodel developed by J. Clough For CRITFC workshop

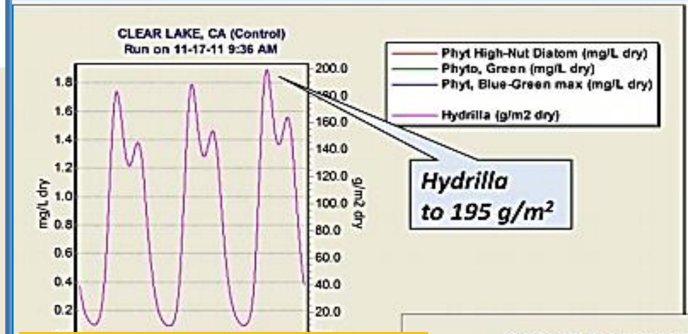
Broadstripe shiner is sensitive to embeddedness; Dixie chub is not; otherwise they are similar



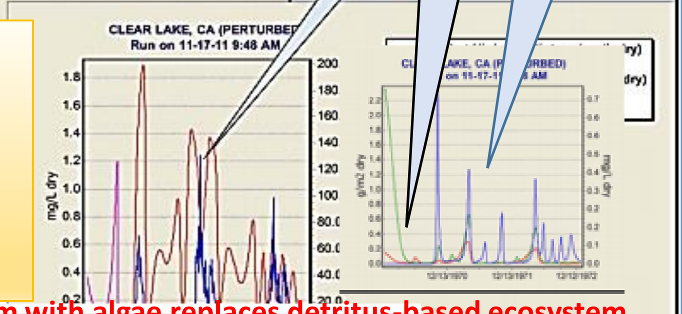
Broadstripe shiner is excluded from another creek due to embeddedness



Siltation may destroy habitat, as in some small watersheds in Fort Benning GA

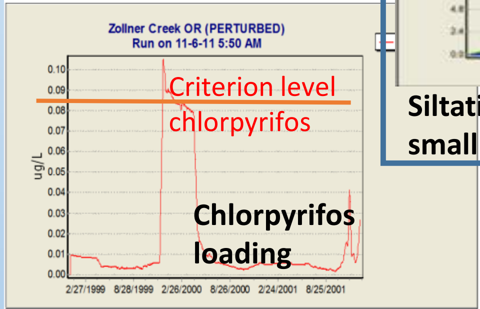


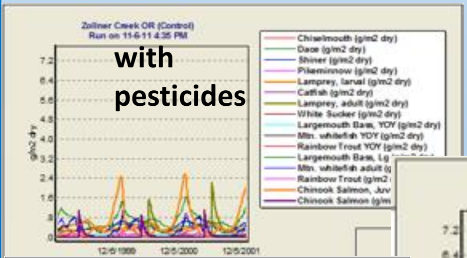
Clear Lake CA Invasive species

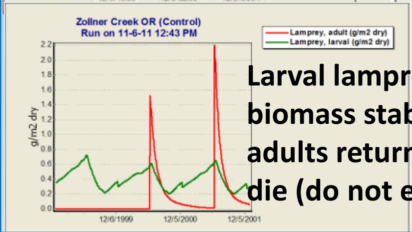


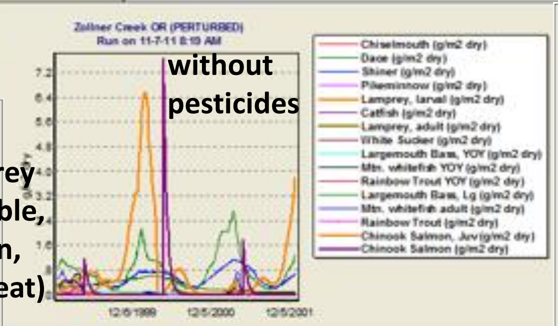
Addition of Fluridone in model causes crash of *Hydrilla* and change to pelagic ecosystem; "nutrient pumping" from sediments stops; benthic detritivores are replaced by herbivorous zooplankton; silversides and bass are favored.

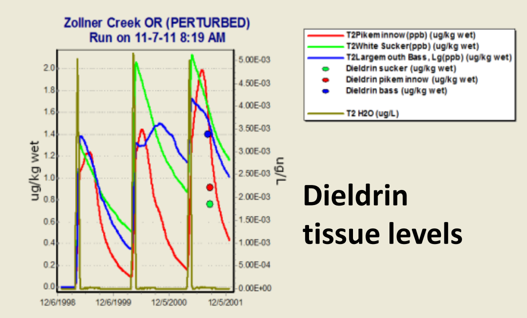
Pelagic ecosystem with algae replaces detritus-based ecosystem

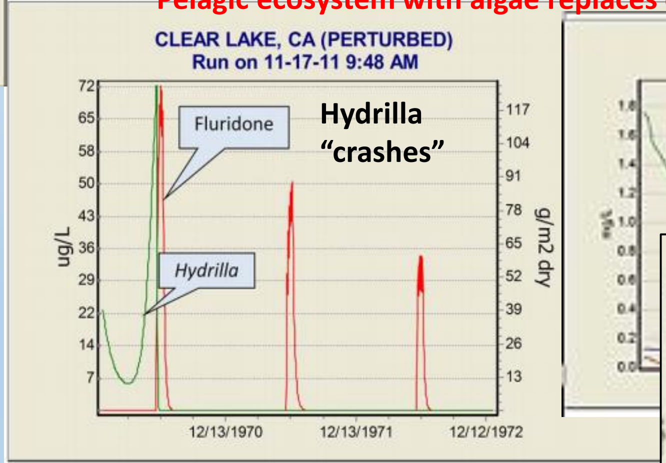


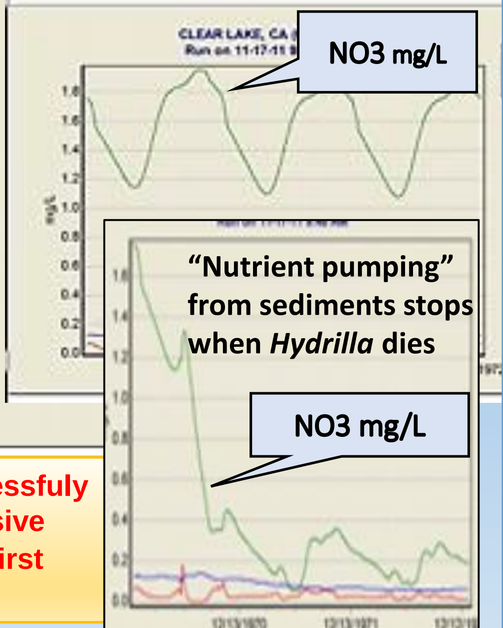












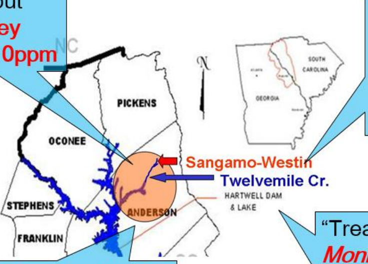
Sonar (fluridone) has been used successfully in Clear Lake CA to eradicate the invasive macrophyte *Hydrilla*, which actually first appeared in 1994.

Chemical fate, bioaccumulation, and ecotoxicological processes are fully integrated in aquatic ecosystem model for analyzing both direct and indirect effects

Background

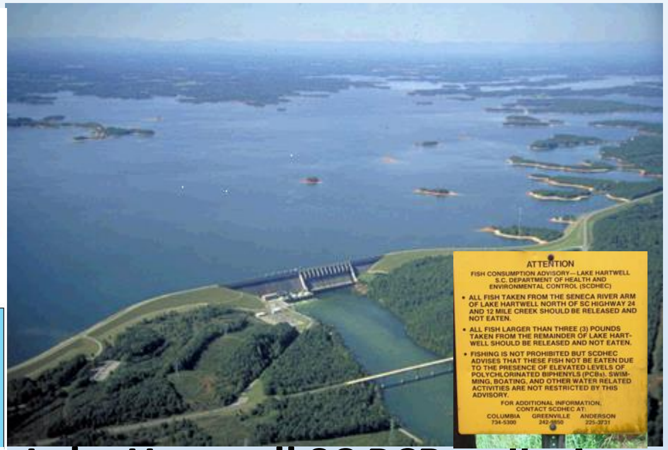
PCBs declined since 1995 in sediment but in bass, they remain 5-10ppm

Discharged 400,000 lbs of PCBs into creek from 1955-1990s



"Treated" through *Monitored Natural Recovery* (allow clean sediment to cover PCBs)

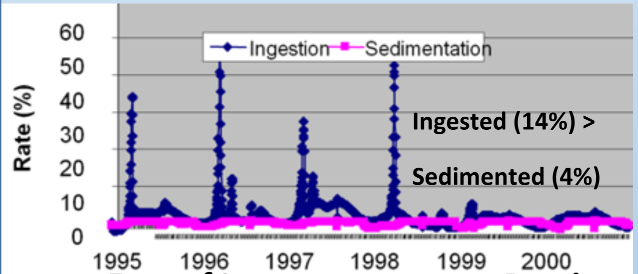
Modeled 20km from USGS gage to confluence:
Mean depth 4.3m
Max depth 14.7m



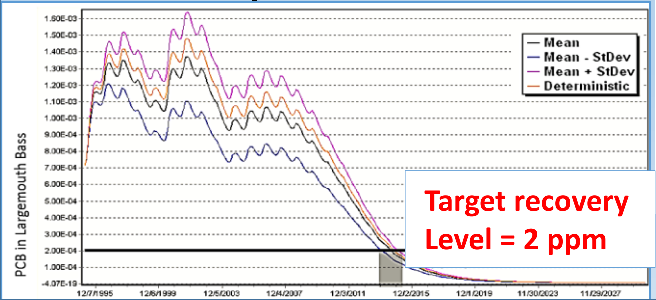
Lake Hartwell SC PCB pollution

Why are bass still contaminated while sediment is recovering? When will fish recover?

Due to contaminated input detritus, 2013



Fate of Input Detritus



Target recovery Level = 2 ppm

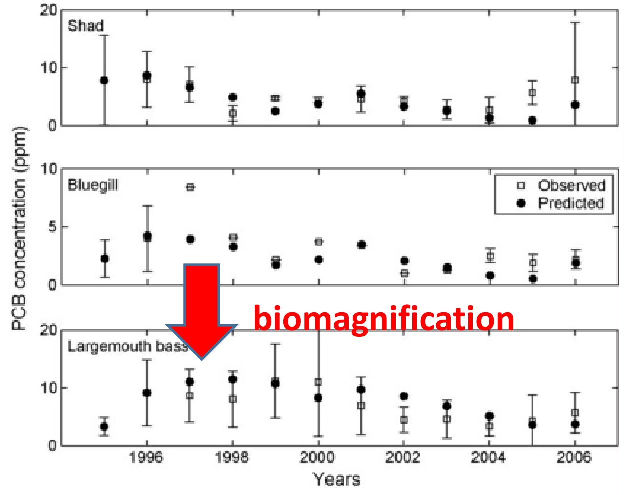
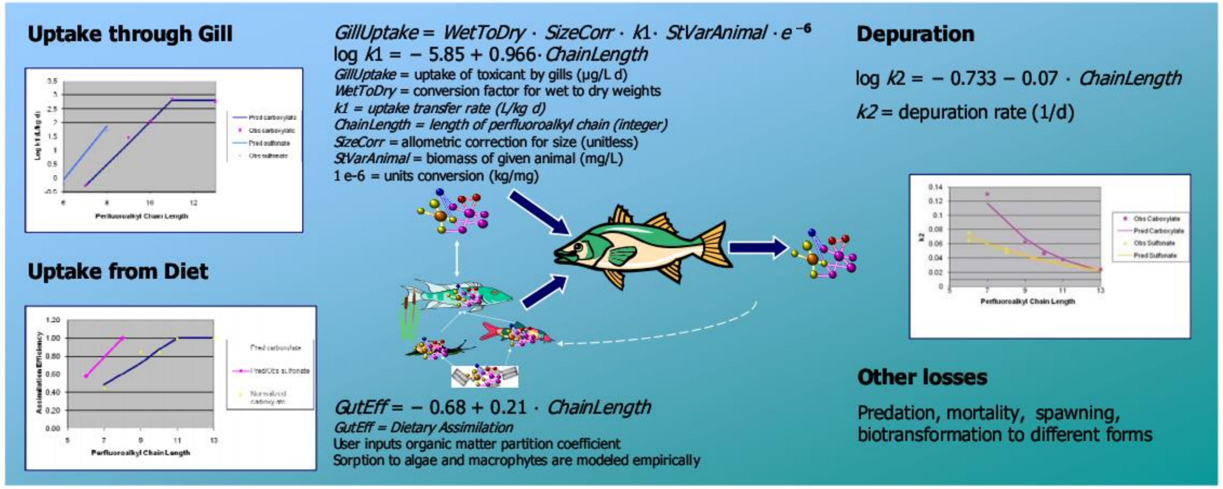


Fig. 3 – Predicted and observed total PCB fillet concentrations (wet-weight) over twelve years in three fish species for Lake Hartwell TCA. Observed values are concentrations averaged by fish species measured at a central sample site in TCA (SV-107) in April of each year.

Predicted PCB in fish is similar to observed

PFOS PROCESSES IN AQUATOX



$GillUptake = WetToDry \cdot SizeCorr \cdot k1 \cdot StVarAnimal \cdot e^{-6}$

$\log k1 = -5.85 + 0.966 \cdot ChainLength$

GillUptake = uptake of toxicant by gills (µg/L d)
WetToDry = conversion factor for wet to dry weights
k1 = uptake transfer rate (L/kg d)
ChainLength = length of perfluoroalkyl chain (integer)
SizeCorr = allometric correction for size (unitless)
StVarAnimal = biomass of given animal (mg/L)
1 e-6 = units conversion (kg/mg)

$\log k2 = -0.733 - 0.07 \cdot ChainLength$

k2 = depuration rate (1/d)

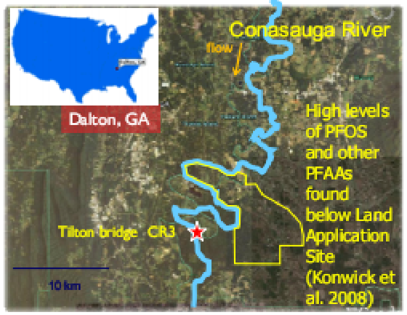
$GutEff = -0.68 + 0.21 \cdot ChainLength$

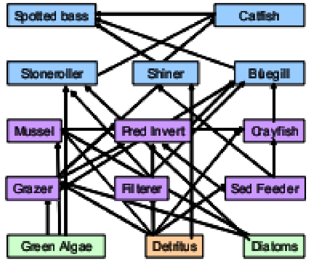
GutEff = *Dietary Assimilation*
User inputs organic matter partition coefficient
Sorption to algae and macrophytes are modeled empirically

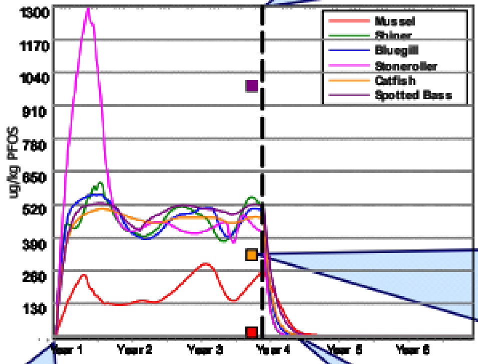
Predation, mortality, spawning, biotransformation to different forms

PFOS IN RIVERS

PFOS input set to zero to examine recovery







AQUATOX predicts PFOS in biota within the range of measured data (squares) but does not reproduce observed differences among species

Species initialized with zero PFOS; assumed constant loading of PFOS in water at concentration equal to mean measured value at site

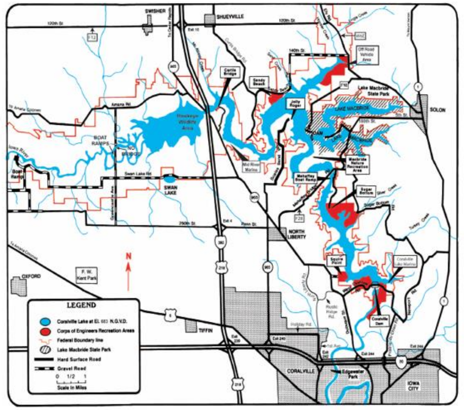
Simulated recovery occurs quickly in the absence of PFOS loading to the system

Predicted and observed PCB tissue conc. (Rashleigh et al. 2008), PFOS dynamics (Rashleigh et al. 2012)

AQUATOX was developed originally for use in Ecological Risk Analysis and can be readily applied in Economic Benefit Analysis

Coralville Reservoir Iowa
long-term contamination with dieldrin

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



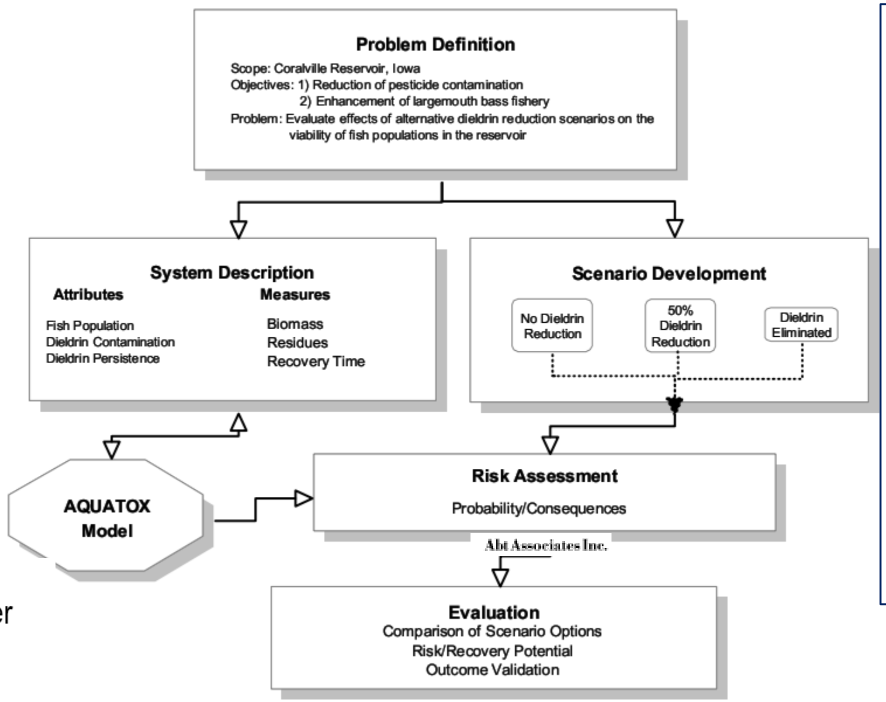
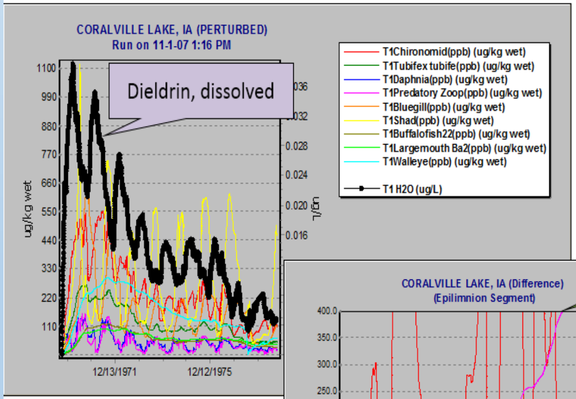


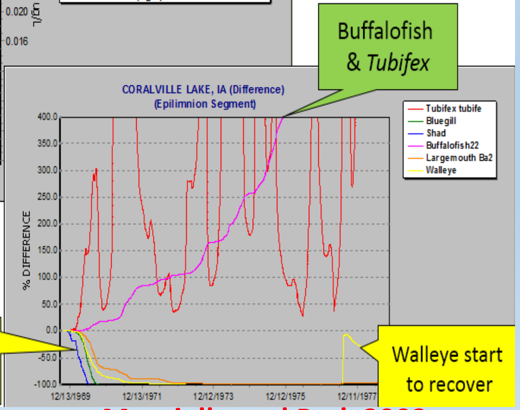
Table 5-13: Total Social Benefits of Fish Population Recovery at Coralville Reservoir (undiscounted, 2003$)

Year	Recreational Benefits	Commercial Benefits		Non-use Benefits[a]		Total Benefits[a]	
		Low	High	Low	High	Low	High
1969	$0	$0	$0	$0	$0	$0	$0
1970	$0	$0	$0	$0	$0	$0	$0
1971	$0	$0	$0	$0	$0	$0	$0
1972	$0	$0	$0	$0	$0	$0	$0
1973	$0	$0	$0	$0	$0	$0	$0
1974	$0	$0	$0	$0	$0	$0	$0
1975	$0	$0	$0	$0	$0	$0	$0
1976	$0	$0	$0	$0	$0	$0	$0
1977	$0	$0	$0	$0	$0	$0	$0
1978	$758	$0	$0	$0	$0	$758	$758
1979	$1,667	$0	$0	$0	$0	$1,667	$1,667
1980	$5,317	$28,912	$65,052	$0	$0	$34,229	$70,369
1981	$28,965	$24,123	$54,276	$720,183	$1,537,796	$773,271	$1,621,037
1982	$157,362	$20,425	$45,957	$720,183	$1,537,796	$897,970	$1,741,115
1983	$540,723	$15,883	$35,736	$720,183	$1,537,796	$1,276,789	$2,114,255
1984	$627,895	$11,178	$25,152	$720,183	$1,537,796	$1,359,257	$2,190,843
1985	$427,714	$8,729	$19,639	$720,183	$1,537,796	$1,156,625	$1,985,149
1986	$326,687	$7,220	$16,245	$720,183	$1,537,796	$1,054,090	$1,880,728
Total, undiscounted	$2,117,087	$116,470	$262,057	$4,321,098	$9,226,775	$6,554,656	$11,605,920

Abt Associates Inc. 2005

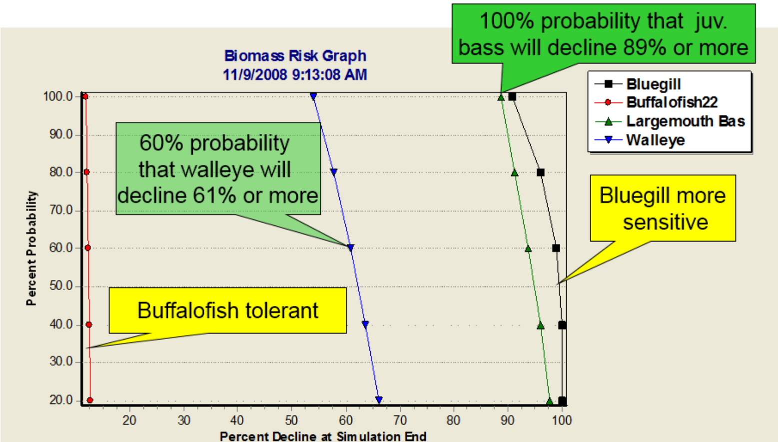
Dieldrin bioaccumulates & declines over 20 years
with fish mortality, but tolerant buffalofish, *Tubifex* prosper

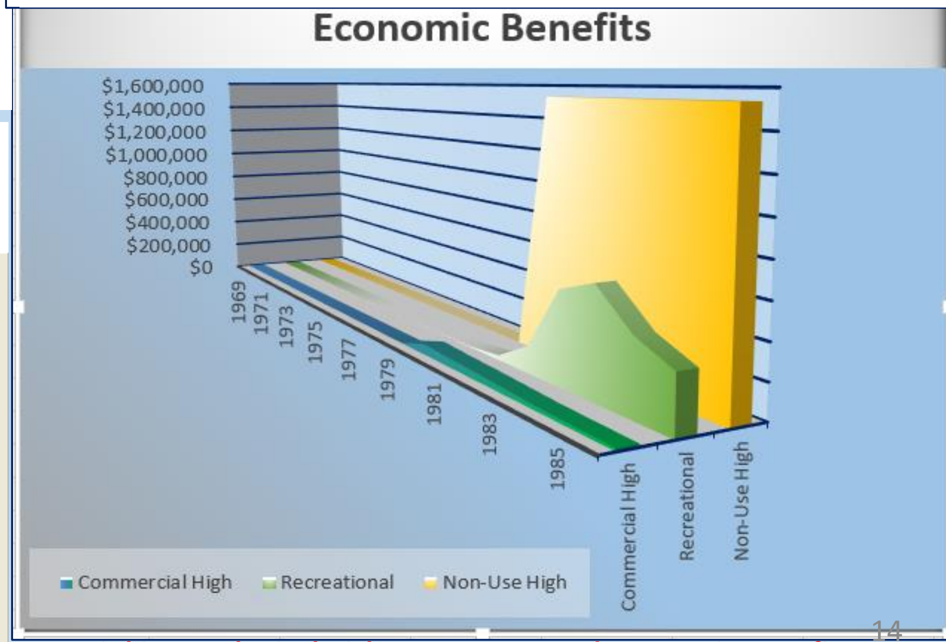




Mauriello and Park 2002

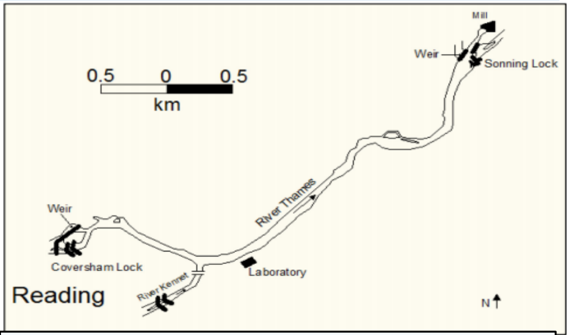
Probability of decline in biomass (end of 1st year) can be estimated based on uncertainty





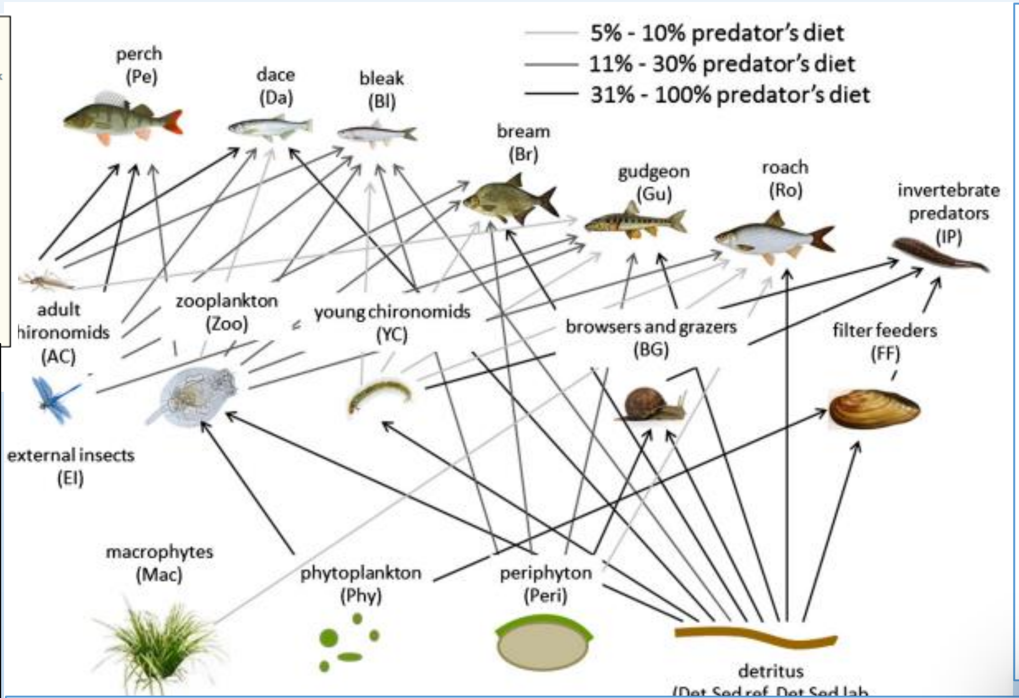
Linking Ecological Risk Assessment and Economic Benefits

AQUATOX was successfully applied in risk assessment of two common house-hold products in the large and complex ecosystem of the River Thames, UK (Lombardo et al. 2015). Currently it is being used as the framework for an integrated environmental risk assessment of the Yangtze River (Scholz-Starke et al.2013)



AQUATOX facilitates examination of complex aquatic foodwebs, such as in the River Thames, and the responses to ecotoxicological processes leading to the direct and indirect effects of chemicals. For example, in this risk assessment of LAS, a toxic polar surfactant, and TCS, which inhibits photosynthesis, AQUATOX was used to assess"bottom-up" and "top down" joint responses in defensible, realistic simulations.

In an even more ambitious project, AQUATOX is being used in a joint German-Chinese integrated risk assessment of the Yangtze River, including the Three Rivers Gorge, one of the largest reservoirs in the world with a drainage basin occupied by 400 million people with urban and industrial wastes, and pesticides from extensive and heavily cultivated fields.



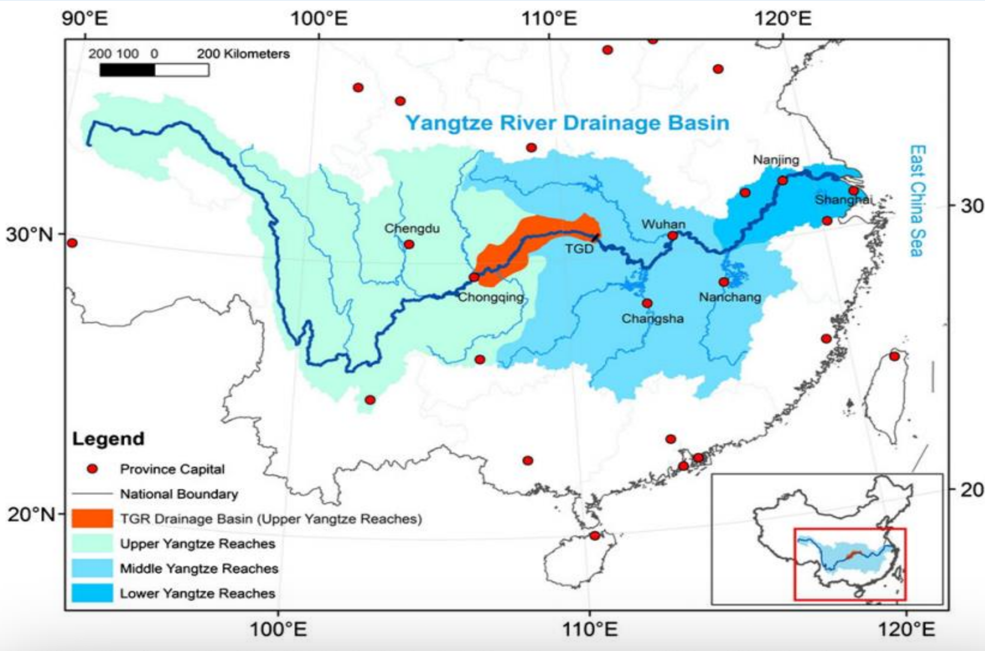


Fig. 1 Map of the Yangtze River Basin (*light to dark blue*) and the Three Gorges Reservoir (*TGR*; *red*). TGD *Three Gorges Dam*

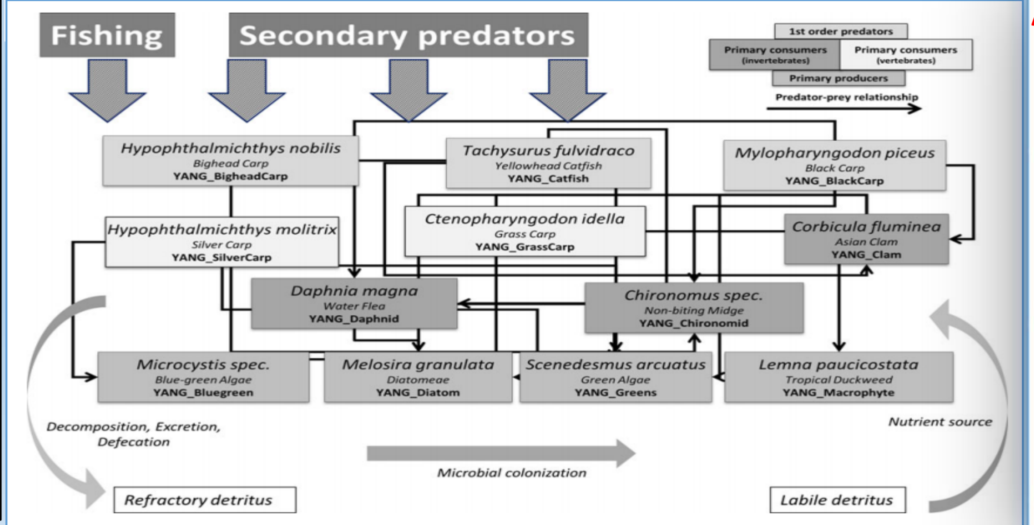
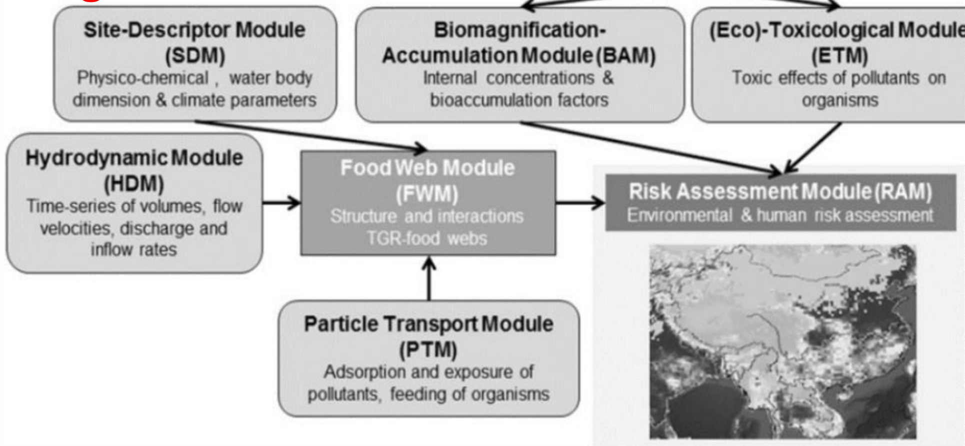


Fig. 8 The simplified "connectedness" food web of the river simulation as implemented in the AQUATOX model. *Arrows* point from predators to prey

AQUATOX is framework for integrated risk assessment



Numerous endpoints facilitate analyses and document conclusions; transparent model output meets regulatory and litigation requirements

Interpretation facilitated by qualitative and quantitative endpoints (concentration, process rates, limitations to photosynthesis)

Wide variety of stressors can be simulated together or separately

Designed to *isolate stressor effects*

- **Perturbed** simulation *with* stressor
- **Baseline** simulation *without* stressor

paired simulations

- **Joint plots** of baseline and perturbed results (for example, biomass, chlorophyll *a*, DO, Secchi depth)
  - Difference graphs – subtract perturbed results from baseline
  - Steinhaus plots – quantitative differences: dissimilarity indices
  - Biomass maximum, minimum, mean, mode, variance, std dev. for given or repeating period
  - Trophic state indices – especially algal concentrations
  - Summary output
    - Biomass of commercial spp. (oysters, shrimp. Redfish, etc.)
    - Gross primary production
    - Net primary production
    - Annual secondary production
    - Communiuty respiration
    - Turnover
    - Production/Respiration
    - Time to recovery for persistent & biomagnified contaminants
    - Percent exceedance and duration graphs (example: *"Phyto. Chlorophyll (ug/L) is exceeded 12.1% of the time."*)