



Missouri University of Science and Technology  
Scholars' Mine

---

Civil, Architectural and Environmental  
Engineering Faculty Research & Creative Works

Civil, Architectural and Environmental  
Engineering

---

01 Jan 2005

## Spatial Bioaccumulation Modeling in a Network of Bayous

Ronaldo Luna

Missouri University of Science and Technology, [rluna@mst.edu](mailto:rluna@mst.edu)

Karen H. Watanabe

Andrew J. Wilding

Follow this and additional works at: [https://scholarsmine.mst.edu/civarc\\_enveng\\_facwork](https://scholarsmine.mst.edu/civarc_enveng_facwork)

 Part of the [Civil Engineering Commons](#)

---

### Recommended Citation

R. Luna et al., "Spatial Bioaccumulation Modeling in a Network of Bayous," *Environmental Modeling and Software*, Elsevier Ltd., Jan 2005.

The definitive version is available at <https://doi.org/10.1016/j.envsoft.2005.08.003>

This Article - Journal is brought to you for free and open access by Scholars' Mine. It has been accepted for inclusion in Civil, Architectural and Environmental Engineering Faculty Research & Creative Works by an authorized administrator of Scholars' Mine. This work is protected by U. S. Copyright Law. Unauthorized use including reproduction for redistribution requires the permission of the copyright holder. For more information, please contact [scholarsmine@mst.edu](mailto:scholarsmine@mst.edu).

# Spatial Bioaccumulation Modeling in a Network of Bayous

Ronaldo Luna<sup>a\*</sup>, Karen H. Watanabe<sup>b</sup>, and Andrew J. Wilding<sup>a</sup>

<sup>a</sup> *Department of Civil, Architectural and Environmental Engineering, University of Missouri-Rolla, Rolla, MO 65409, USA*

<sup>b</sup> *Department of Environmental and Biomolecular Systems, Oregon Health & Science University, Beaverton, OR 97006, USA*

## Abstract

A software system, Spatial Network Bioaccumulation Model (SNBM), was developed to model the bioaccumulation of polycyclic aromatic hydrocarbons (PAHs) in aquatic food webs. The SNBM uses a geographic information system as an engine to (i) store the spatial representation of input parameters (the data related to the ecosystem), (ii) to transfer input and output data to and from the food-web bioaccumulation model, and (iii) display the predicted food-web organism concentrations over a base map of the field site. The bioaccumulation model is a time-dependent, set of first-order ordinary differential equations that are solved numerically. Many sampling locations can be analyzed using the SNBM in one individual run. We demonstrate the system for a steady-state simulation of three PAHs, naphthalene, phenanthrene and benzanthracene in a food-web for spotted gar (*Lepisosteus oculatus*) from the LaBranche Wetlands, Louisiana, USA. The predicted food-web organism concentrations are plotted at their respective sampling location.

---

\* Corresponding author: Department of Civil, Architectural and Environmental Engineering, University of Missouri-Rolla, Rolla, MO 65409. Phone: 1.573.341.4484; Fax: 1.573.341.4729; Email: [rluna@umr.edu](mailto:rluna@umr.edu).

## **Software availability**

Name of Software: Spatial Network Bioaccumulation Model

Developers: Ronaldo Luna, Ph.D., P.E. and Karen Watanabe, Ph.D.

Contact Address: R. Luna, Department of Civil, Architectural and Environmental  
Engineering, University of Missouri-Rolla, Rolla, MO 65409, USA.

K. Watanabe, Department of Environmental and Biomolecular Systems, Oregon Health  
& Science University, Beaverton, OR 97006, USA

Telephone: (573) 341-4484

Fax: (573) 341-4729

Email: [rluna@umr.edu](mailto:rluna@umr.edu) or [watanabe@ebs.ogi.edu](mailto:watanabe@ebs.ogi.edu)

Availability: free download: [http://www.tulane.edu/~bio\\_fate](http://www.tulane.edu/~bio_fate) (version 2.13 and 3.0)

## **1. Introduction**

The biological fate of aquatic chemical contaminants is dependent upon a number of environmental conditions (e.g., nutrients, population, species, etc.) present in the aquatic or riverine system. The environmental conditions can be represented as a two-dimensional spatial feature, a collection of interconnected lines (riverine system) integrated with a biological food web. Benthic invertebrates that reside in contaminated sediments are in an intermediate trophic level in the food chain and their small home range provides a different exposure relative to the predators (e.g., fish) that feed on them. This known heterogeneity could lead to inaccurate predictions of contaminant bioaccumulation in the food chain and its estimated impact upon an ecosystem and human health. For organic compounds with high octanol-water partition coefficients ( $\log K_{ow} > 5.0$ ), biomagnification through the food chain

has greater significance in bioaccumulation and spatial representation of a food web model would provide a more realistic representation of the biological fate of contaminants.

Existing bioaccumulation modeling methodologies (Connolly and Tonelli, 1985; Thomann, 1989; Barber et al., 1991; Gobas, 1993; Madenjian and Carpenter, 1993; Endicott and Cook, 1994; Morrison et al., 1996; Morrison et al., 1997) do not explicitly account for spatial variability in the contaminated environment and its impact on bioaccumulation (Stewart and Loar, 1993). Spatial and temporal averages of environmental parameters are used as inputs into these models to yield steady-state predictions of contaminant concentration in the food web animals. Thomann et al. (1991) integrated bioaccumulation modeling with a spatial fate and transport model of PCBs in the Hudson River estuary by utilizing averaged water concentration predictions from their fate and transport model as inputs for the bioaccumulation model. However, predictions from a deterministic fate and transport model cannot account for known “hot spots” of contamination and as such could not predict the effect of “hot spots” on bioaccumulation. More recently, Linkov, et al. (2002) described a method of incorporating spatial and temporal characteristics in determining human health risks from the consumption of PCB contaminated winter flounder in the coastal waters of New York and New Jersey. Using 1m x 1m grid cells to represent the area of interest, a spatial sub-model (Schell and Linkov, 1999) was used to simulate a random-walk of fish foraging to produce a monthly time series of exposure point concentrations (i.e., sediment and water concentrations). They state, “The exposure point concentrations for each time step is the average concentration across the cells that a fish encounters within its foraging area for a specified time period.” In this paper, we describe a computational software system that facilitates the use of individual sampling site data to account for known

variability in the environment when predicting chemical concentrations in the organisms of an aquatic food web.

Costanza and Maxwell (1991) developed a Spatial Modeling Package integrating a raster-based GIS with dynamic modeling software, STELLA that attempts to represent a large areal extent and requires parallel processing due to its computational intensity. Our objective is to use a much simpler, vector-based spatial representation such as routes and events within a network representing an aquatic system. The benefit of this approach is its computational efficiency and reduced spatial redundancy and memory. It focuses on the interconnected waterways of interest and their spatial representation as a network of interconnected linear features. Once a spatial representation is complete, an interface between the GIS and a bioaccumulation model provides seamless model operation.

Within a GIS, the most relevant type of network analysis is the prediction of network loading such as the transport of water and sediment in a river system, where correctly predicting the flow, magnitudes and location of floods due to storms provides a means for advanced emergency service planning. Network analysis software applications are available commercially in some GIS software packages, and their popularity has become more prevalent with desktop systems. What is not very common is the use of the spatial data model (e.g., a network model) to represent information along the linear feature and the integration of the spatial model with a computational model (e.g., the food-web bioaccumulation model). A network that spatially references the bioaccumulation model utilizes dynamic segmentation, and the definition of routes, and events that are built upon the geographically referenced arcs and nodes. Other investigators have exploited the use of river networks to model the chemical fate, transport and bioaccumulation in river basins taking advantage of the EPA's BASINS system. This ambitious system, called GISTOX

(Hellweger, et al. 2001), used the generalized information in the reaches of a river for steady-state transport in one dimension and a pre-set food web. Hellweger et al. described the functionality of this system, however the methods and results were not presented in enough detail to assess its attributes relative to the SNBM. Software applications within a GIS framework are becoming common in environmental modeling, such as watershed modeling, water management and ecological impact, pesticide non-point source input (Shen, et al. 2005, Schluter, et al. 2005, and Ropke, et al. 2004, respectively). More specifically, work to integrate water quality modeling within a GIS are Hartnett and Nash (2004); Halls (2003) and Bhuyan, et al. (2003), but few address bioaccumulation as mentioned above.

Our study focuses on Bayou Trepagnier in the LaBranche Wetlands, Louisiana, USA to assess the bioaccumulation of past industrial wastewater discharges into a network of bayous. The LaBranche wetlands are located in St. Charles Parish bordering the southwest shores of Lake Pontchartrain about 20 miles west of New Orleans, Louisiana, USA (Figure 1). These wetlands have been historically affected by the industrial waste and land development in St. Charles Parish. A low salinity lagoon to the north, Lake Pontchartrain, provides most of the flow to the system of bayous via tidal fluctuations and wind effects. Bayou Trepagnier is located within the LaBranche wetlands and is the subject site for this paper.

Bayou Trepagnier is a low-gradient tidal stream that flows approximately 3 miles through wetlands from the rear fence of a major refinery. This bayou joins Bayou LaBranche, which flows into Lake Pontchartrain. Bayou Trepagnier was the wastewater receiving stream for about 80 years ending in 1995, resulting in contaminated sediments with high levels of heavy metals and organic compounds (Flowers et al., 1998). In February of 1995, the Louisiana Department of Wildlife and Fisheries authorized diverting the effluent from the bayou to the

Mississippi River. Of particular interest were the polycyclic aromatic hydrocarbons (PAHs) that were measured at high levels even several years after the point source loading of effluent was diverted. Wetland streams have not been adequately studied prior to the 1970s and the value of wetlands and the consequences of wetland drainage and destruction were not appreciated (Mitsch and Gosselink, 1986). However, it is well recognized that tidal wetlands provide important habitat for wildlife and support commercial fisheries by providing an important coupling for movement of organisms and nutrients between wetlands and estuaries (Flowers et al., 1998).

This paper describes the development of the Spatial Network Bioaccumulation Model (SNBM), a GIS-based system that couples geographic representation with a food-web bioaccumulation model. As an example, we present a detailed case study for the bioaccumulation of naphthalene with simulation results also reported for phenanthrene, and benzanthracene in the spotted gar (*Lepisosteus oculatus*) food web. Results for steady-state conditions are displayed at several locations along the network of bayous.

## **2. Software System**

The goal of the system described herein is to spatially track measured concentrations of contaminants and compute aquatic biota chemical concentrations to facilitate the evaluation of contaminant effects in the ecosystem. Both steady-state and transient bioaccumulation models are available in the system, however, only the steady-state version is demonstrated here. The system requires a set of electronic vector or raster-based maps for the research study site to locate the analysis geographically. Each sampling site is identified by the user and then model input data are gathered through the graphical user interface (GUI). These data include: environmental parameters for the water column and the sediments; the concentration of each chemical of interest (Table 1); and the conceptual food web, input in

matrix form (Table 2). With these input parameters, concentrations for each species in the food web are computed by solving the system of equations in the bioaccumulation model. For the time-dependent model, this is a coupled set of first order ordinary differential equations, and at steady-state, the set reduces to algebraic equations. Every station or segment along the bayou can be dynamically computed for each simulation and the results can be displayed interactively.

Arcview<sup>®</sup> 3.2 and ArcGIS Arcview<sup>®</sup> 8.3 by ESRI<sup>®</sup>, were used to develop two different versions of the SNBM: one using the Avenue programming language (version 2.13) and the other using Visual Basic (version 3.0). A GUI was developed to run within Arcview<sup>®</sup> to prompt users for input data, calculate the output results, and display output to a map. While this program's interface is user-friendly, it is a tool designed for researchers. Input of information is simple, as described in Table 1, but knowledge about the input is required to understand the output results.

## **2.1. Spatial Data**

Electronic maps are widely available from multiple sources, however large scale maps at 1:24,000 scale (USGS 7.5' quads) are not completely available. Typically the areas close to populated areas or sites of interest are available electronically. For Bayou Trepagnier several thematic layers were readily available and imported into the GIS (Figure 1). The thematic layers available were: hydrography, highways, utilities, man-made structures and others. These vector based thematic layers are in the form of "shape files" in the ESRI GIS software and are often available from the USGS. Additionally, field data collected via Global Positioning System (GPS) were converted into electronic maps for import into the GIS and used in combination with the other thematic layers. Figure 2 shows Bayou Trepagnier



highlighted within the system of bayous. This process could be done for any research site in question.

## **2.2. GIS Customized Development**

Customization in Arcview<sup>®</sup> is done through its included upper level object-oriented programming language, Avenue or Visual Basic. The GUI is created by writing scripts to produce message and dialog boxes. The message boxes and user-dialogs are used extensively, since the program maintains constant interaction with the user to collect data and control operation. This GUI can be divided into three main categories: Preprocessing, Bioaccumulation numerical modeling routines, and Post-Processing. The numerical modeling routines pass user-entered input data to an external program developed in C. This C-code is the computational engine for the food-web bioaccumulation model and computes chemical concentrations for several organisms in the food web at different spatial locations. The post-processing portion takes the predicted chemical concentrations and plots them on a map using symbols to show relative concentrations. A more detailed description of these procedures is presented in the following sections and shown in flowchart form (Figure 3).

One of the criteria in the design of this GIS application was to make the application as portable as possible for use at other study sites. Thus, the software should be flexible for use by other researchers with interest in modeling bioaccumulation of contaminants in other ecosystems and foodwebs. To do this, users need to supply site-specific spatial data, environmental conditions, input parameters and concentrations, and properties and definition of the foodweb (in the form of feeding preferences and metabolic rate constants). The site specific data is described as user input in the next section, specifically Tables 1 and 2 provide an example of the type of data required for the model, listing the appropriate references.

### 2.3. Pre-Processing – User Input

Initialization of the Spatial Network Bioaccumulation Model prepares the program to carry out the rest of the tasks needed for completion, such as opening files and setting default variables. As the user proceeds, a choice between the steady-state or transient (time dependent) model is provided. As mentioned before, only the transient model is not being discussed in this paper. Following the steady-state selection, the program allows the user to create a new input file or locate a pre-existing file. To create a new file the program displays a dialog, which prompts the user to enter a number of locations along the bayou where the bioaccumulation model will compute food web organism concentrations. Each location requires fourteen parameters that will be passed to the external C-code (Figure 4 and 5). Default data is initially displayed in the input areas, allowing the user to either accept these or enter site-specific values. Also, checks are performed on all user-entered data to assure that it is in the correct format.

### 2.4. Bioaccumulation Numerical Modeling Routines

Once the input file is initialized, it is converted into the proper format for use by the bioaccumulation model. The input file is passed to an external process (out of Arcview<sup>®</sup>), to compute chemical concentration values in the food web organisms. Gobas (1993) describes the model equations in detail and we summarize them here for each type of organism.

In plankton and aquatic insects, the whole body concentration,  $C_i$ , is represented by

$$\frac{dC_i}{dt} = k_{ui} C_{wD} - k_{ei} C_i, \quad (1)$$

where  $i$  is an indicator for plankton or aquatic insects,  $k_{ui}$  is the uptake rate constant and  $k_{ei}$  is the elimination rate constant assuming a single compartment model of the organism. At

steady-state, following Gobas' assumption that  $k_{ui}/k_{ei} = L_i K_{ow}$  this equation reduces to  $C_i = L_i K_{ow} C_{WD}$ , where  $L_i$  is the lipid fraction of the organism.

The whole body concentration (Landrum et al., 1992),  $C_j$ , in crayfish or shrimp is represented by.

$$\frac{dC_j}{dt} = k_{sj} C_s - k_{ej} C_j, \quad (2)$$

where,  $j$  is an indicator for crayfish or shrimp,  $C_s$  is the sediment concentration,  $k_{sj}$  is the uptake rate constant from the sediment and  $k_{ej}$  is the elimination rate constant from the organism. At steady-state, following the assumption of Gobas that

$$k_{sj}/k_{ej} = (L_j d_{oc}) / (OC_s d_l), \text{ equation (2) reduces to } C_j = C_s d_{oc} L_j / OC_s d_l,$$

where  $d_{oc}$  is the density of organic carbon,  $L_j$  is the lipid fraction,  $OC_s$  is the organic carbon fraction of the sediment and  $d_l$  is the density of lipids.

The toxicant concentration in fish,  $C_f$ , is described by

$$\frac{dC_f}{dt} = k_{uf} C_{WD} + k_{Df} C_{Df} - (k_{elimf} + k_{egestf} + k_{metf} + k_{growthf}) C_f, \quad (3)$$

which, at steady-state, reduces to

$$C_f = \frac{k_{uf} C_{WD} + k_{Df} C_{Df}}{k_{elimf} + k_{egestf} + k_{metf} + k_{growthf}}. \quad (4)$$

In equation (3),  $C_{Df}$  is the concentration of toxicant in the food,  $k_{uf}$  is the rate constant for uptake through the gills,  $k_{Df}$  is the dietary uptake rate constant,  $k_{elimf}$  is the elimination rate constant through the gills,  $k_{egestf}$  is the fecal egestion rate constant,  $k_{metf}$  is the metabolic rate constant, and  $k_{growthf}$  is the growth rate constant. Each rate constant is calculated as a function of the following input parameters: water temperature, octanol water partition coefficient, fish lipid fraction, and fish weight. See Gobas (1993) for the relationships between the rate constants and the input parameters.

The differential equations are solved using a 4<sup>th</sup> order Runge-Kutta algorithm (Press et al., 1992) programmed in ANSI-C and runs as a separate program, called from within the Avenue or Visual Basic script, and runs on the Component Object Model (COM) level. The C-code saves the output values as a text file, which is retrieved by the GIS and can be saved to the user's local directory as a database file (DBF). Finally, this DBF is displayed as an editable table. The advantages of using DBFs over text files include ease of: (i) querying; (ii) value retrieval; and (iii) modification. Also, the GIS program recognizes the DBF as an attribute storage file for use in a thematic display, which increases the ease of adding data to the map (ESRI, 1996). After all calculations have been made, the Spatial Network Bioaccumulation Model proceeds to spatial representation of the output values on the site map.

## **2.5. Spatial Post-Processing**

After selecting a food web organism and chemical of interest, symbols are displayed onto the site map showing the chemical concentration range predicted for that organism. First, the program displays dialogs to gather user input on which organism and chemical (toxicant) to plot (Figure 5). Then, a new theme is created (from saved data) with a group of sampling points, one for each of the geographic locations being analyzed. The program then locates the DBF file for this theme as well as the output DBF file from the bioaccumulation routine. For this, a database query was written to retrieve the quantitative results by selecting all records for the chemical of interest. Then, the record for the first point is chosen and the value of contamination for the chosen organism is retrieved from the table. These two steps are repeated for the subsequent points. Then, these queried values are added to the recorded DBF file for the theme. By adding these values to the DBF file, not only can the results be plotted, but the actual contamination concentration value will show up in the attributes of the

point when clicked. Finally, the previously plotted dots are changed into graduated symbols and the color of the symbols is changed to be uniform.

Throughout the execution, intermediate information is saved in a virtual table (Vtab) to provide a view of multiple tabular data sources (ESRI, 1998; Razavi, 1999). Vtabs are stored solely in RAM (random access memory) so, disk access time is not an issue. Since storing data in a Vtab is not permanent, commands to write the data to disk are given numerous times throughout the program to ensure that the calculated data are not lost.

After the Spatial Network Bioaccumulation Model has been executed, the user has the opportunity to re-plot data to the map. The same output file is used as in the original plot, but different chemicals and organisms may be chosen. This allows the user to examine the body burdens of several chemicals in an organism, or body burden of one chemical in several organisms without additional runs. Re-plotting may be done by clicking a customized button on the toolbar and then going through the dialog and choosing an organism and chemical as before. This merely reruns the plotting portion of the previous script, allowing different choices for the toxicant and organism. However, if the input parameters need to be changed the entire routine should be run again as another case to model and study.

### **3. Simulation of naphthalene in Bayou Trepagnier, LA, USA**

A case study is presented here to demonstrate the capabilities of the SNBM. The input parameters were derived from field-measured data (e.g., sediment and water concentration, water temperature, and feeding preferences based on gut contents analysis), and data reported in the literature (e.g., octanol-water partition coefficient, densities, lipid fractions, and metabolic rate constant). The field data were collected in March of 1997 from Bayou Trepagnier in the LaBranche Wetlands, Louisiana, and the analytical methods used to measure sediment, water and gar tissue concentrations of naphthalene, phenanthrene, and

benzanthracene were described in Watanabe et al. (2005). Sediment and water concentration measurements were made at three sites along the Bayou. Tables 1 and 2 describe the input conditions used to simulate the whole-body organism concentration in the different species of the spotted gar food web.

The SNBM was used to make predictions of naphthalene, phenanthrene, and benzanthracene concentrations in the spotted gar and its prey (Table 3). Using the spatial post-processing feature of the SNBM, results are overlaid on the site map for naphthalene concentrations in plankton, crayfish, mixed small fish (e.g., *Cyprinodon variegatus*, *Gambusia affinis*, and *Poecilia latipinna*), and spotted gar (Figure 6). Spatial dependence in the predicted naphthalene concentrations is apparent in Figure 6 for crayfish and gar. The crayfish and grass shrimp were modeled as being in equilibrium with the sediments, thus their predicted concentrations reflect sediment naphthalene concentrations, which was highest at BTP071 followed by BTP060 and BTP105. In addition, predicted crayfish and grass shrimp body burdens are the highest in the food web because of their exposure to the sediments and the relatively higher concentration of PAHs in the sediments compared to water. Our unpublished data measuring the sediment, water, and tissue concentrations of different PAHs from samples collected in the LaBranche wetlands in 2002, show that some crayfish and grass shrimp have higher concentrations (typically of phenanthrene) than the small fish, but no comparison was made to measured gar tissue concentration.

Predicted gar naphthalene concentrations are highest at BTP071 (6.3  $\mu\text{g}/\text{kg}$ ) followed by BTP060 (5.7  $\mu\text{g}/\text{kg}$ ) and BTP105 (3.7  $\mu\text{g}/\text{kg}$ ). They are within the range of concentrations (3 to 12  $\mu\text{g}/\text{kg}$ ) measured in gar captured between September 1996 and March 1997 (Watanabe et al., 2005). Gar naphthalene concentrations measured in single fish captured in March 1997 at BTP071, BTP060, and BTP105 were 12, 6.2, and 7.9, respectively. The measured

values are higher than the predicted concentrations in general, and could be due to model input parameter uncertainty (e.g., too high metabolic rate constant, or the incomplete definition of the small fish feeding) or measurement uncertainty. Since the only data available are from one fish captured per sampling site, it is difficult ascertain whether this is a model structure issue.

#### **4. CONCLUSIONS**

The SNBM integrates Gobas' aquatic food-web model with a GIS engine. It utilizes site-specific input parameters rather site-wide averages in order to allow the user to address spatial variability the food-web bioaccumulation model predictions. This demonstration of the SNBM uses the steady-state food web bioaccumulation model. The model predicts organism concentrations based on data from the heterogeneous aquatic environment, but in reality we know that the gar traverse a much larger area than, say, the crayfish or grass shrimp. The framework of this system, specifically the geographic information system, is amenable to incorporating information on organism home ranges which will allow us to more realistically predict food-web organism concentrations. The intent of the Spatial Network Bioaccumulation Model is that the GIS application and code is portable to other users that have a different site and foodweb to be studied. If a scientist is interested in studying bioaccumulation in a different ecosystem and food-web, they will need: (i) a baseline map of the aquatic system and input parameters; (ii) the spatially referenced sampling locations; (iii) the foodweb and species parameters as outlined in Tables 1, 2, and 3. Often, feeding preferences are not known for a particular species, and one must use the best available data first from the site, and then from the literature for determining the feeding preferences. Metabolic rate constants may also be unknown in which case methods such as interspecies extrapolation could be used to determine the appropriate rate constant.

The SNBM is intended to facilitate the analysis of the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs. Through user-friendly dialog boxes it provides prompts for input data, or the model can be run from input text files. A possible outcome of using the SNBM is to stimulate insight into spatial relationships between organism bioaccumulation and the environment.

### **Acknowledgments**

The authors would like to thank the Center for Bioenvironmental Research at Tulane and Xavier Universities and its staff in the Field Core, Analytical Core and the Data Management Core for their contributions to making this investigation possible. We would also like to acknowledge Drs. T. Bianchi, and G. Flowers who provided us with data used in the model. This material is based upon work supported by the National Science Foundation under Grant No. 9808363, and the US Department of Energy under Grant No. DE-FG21-93EW-53023.



## References

- Barber, M.C., Suárez, L.A. and Lassiter, R.R., 1991. Modelling bioaccumulation of organic pollutants in fish with an application to PCBs in Lake Ontario salmonids. *Can. J. Fish. Aquat. Sci.*, 48: 318-337.
- Bhuyan, S.J., Koelliker, J.K., Marzen, L.J. and Harrington, J.A., 2003. An integrated approach of water quality assessment of a Kansas watershed. *Environmental Modelling & Software*, 18(5) 473-484.
- Chapman, R.F., 1982. *The Insects: Structure and Function*. Harvard University Press, pp. 934.
- Connolly, J.P. and Tonelli, R., 1985. Modelling kepone in the striped bass food chain of the James River Estuary. *Estuarine, Coastal and Shelf Science*, 20: 349-366.
- Costanza, R. and Maxwell, T., 1991. Spatial ecosystem modelling using parallel processors. *Ecol. Model.*, 58: 159-183.
- Endicott, D.D. and Cook, P.M., 1994. Modeling the partitioning and bioaccumulation of TCDD and other hydrophobic organic chemicals in Lake Ontario. *Chemosphere*, 28: 75-87.
- ESRI, 1996. In: Avenue™ Customization and Application Development for ArcView®, Environmental Systems Research Institute, Inc., pp. 189-197.
- ESRI, 1998. ArcView® Help Files.
- Flowers, G.C., Suhayda, J.N., Clymire, J.W., McPherson, G.L., Koplitz, L.V. and Poirrier, M.A., 1998. Impact of industrial effluent diversion on Bayou Trepagnier, Louisiana. *Environmental and Engineering Geoscience*, IV: 77-91.
- Geyer, H.J., Scheunert, I., Bruggemann, R., Matthies, M., Steinberg, C.E., Zitko, V., Kettrup, A. and Garrison, W., 1994. The relevance of aquatic organisms' lipid content to the

- toxicity of lipophilic chemicals: toxicity of lindane to different fish species. *Ecotoxicol Environ Saf*, 28: 53-70.
- Gobas, F.A.P.C., 1993. A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario. *Ecol. Model.*, 69: 1-17.
- Halls, J.N., 2003. River run: an interactive GIS and dynamic graphing website for decision support and exploratory data analysis of water quality parameters of the lower Cape Fear river. *Environmental Modelling & Software*, 18(6), 513-520.
- Hartnett, M. and Nash, S., 2004. Modelling nutrient and chlorophyll<sub>a</sub> dynamics in an Irish brackish waterbody. *Environmental Modelling & Software*, 19(1), 47-56.
- Landrum, P.F., Lee, H., II. and Lydy, M.J., 1992. Toxicokinetics in aquatic systems. Model comparisons and use in hazard assessment. *Environ. Toxicol. Chem.*, 11: 1709-1725.
- Linkov, I., Burmistrov, D., Cura, J. and Bridges, T.S., 2002. Risk-based management of contaminated sediments: consideration of spatial and temporal patterns in exposure modeling. *Environ Sci Technol*, 36: 238-246.
- Madenjian, C.P. and Carpenter, S.R., 1993. Accumulation of PCBs by Lake Trout (*Salvelinus namaycush*): an individual-based model approach. *Can. J. Fish. Aquat. Sci.*, 50: 97-109.
- Mitsch, W.J. and Gosselink, J.G., 1986. *Wetlands*. Van Nostrand Reinhold Co., New York, pp. 5392.
- Morrison, H.A., Gobas, F.A.P.C., Lazar, R. and Haffner, G.D., 1996. Development and verification of a bioaccumulation model for organic contaminants in benthic invertebrates. *Environ. Sci. Technol.*, 30: 3377-3384.

- Morrison, H.A., Gobas, F.A.P.C., Lazar, R., Whittle, D.M. and Haffner, G.D., 1997. Development and verification of a benthic/pelagic food web bioaccumulation model for PCB congeners in western Lake Erie. *Environ Sci Technol*, 31: 3267-3273.
- Press, W.H., Teukolsky, S.A., Vetterling, W.T. and Flannery, B.P., 1992. *Numerical Recipes in C*. Cambridge University Press, New York, pp. 994.
- Razavi, A.H., 1999. ArcView<sup>®</sup> GIS/Avenue<sup>™</sup> Developer's Guide. In: ArcView<sup>®</sup> GIS/Avenue<sup>™</sup> Developer's Guide, pp. 177-184.
- Röpke, B., Bach, M. and Frede, H-G., 2004. DRIPSa DSS for estimating the input quantity of pesticides for German river basins. *Environmental Modelling & Software*, 19: 1021-1028.
- Schell, W.R. and Linkov, I., 1999. Priorities in forest radioecology: Model development for integrated assessment of toxic element transport. In: I. Linkov and W.R. Schell (Editors), *Contaminated Forests: Recent Developments in Risk Identification and Future Perspectives*, Kluwer, Amsterdam, pp. 1-14.
- Schlüter, M., Savitsky, A.G., McKinney, D.C. and Lieth, H., 2005. Optimizing long-term water allocation in the Amudarya River delta: a water management model for ecological impact assessment. *Environmental Modelling & Software*, 20: 529-545.
- Shen, J., Parker, A. and Riverson, J., 2005. A new approach for a Windows-based watershed modeling system based on a database-supporting architecture. *Environmental Modelling & Software*, 20 (9): 1127-1138.
- Stewart, A.J. and Loar, J.M., 1993. Spatial and temporal variation in biomonitoring data. In: *Biological monitoring of aquatic systems*, Lewis Publishers, Boca Raton, FL, pp. 381.
- Thomann, R.V., 1989. Bioaccumulation model of organic chemical distribution in aquatic food chains. *Environ Sci Technol*, 23: 699-707.

Thomann, R.V., Mueller, J.A., Winfield, R.P. and Huang, C., 1991. Model of fate and accumulation of PCB homologues in Hudson Estuary. *Journal of Environmental Engineering*, 117: 161-178.

van der Linde, A., Hendricks, A.J. and Sijm, D.T.H.M., 2001. Estimating biotransformation rate constants of organic chemicals from modeled and measured elimination rates. *Chemosphere*, 44: 423-435.

Watanabe, K.H., Lin, H., Bart Jr., H.L., Martinat, P., Means, J.C., Kunas, M.L. and Grimm, D.A., 2005. Bayesian estimation of kinetic rate constants in a food web model of polycyclic aromatic hydrocarbon bioaccumulation. *Ecol. Model.*, 181: 229-246.

## Figure Captions

Fig. 1. Project site vicinity maps.

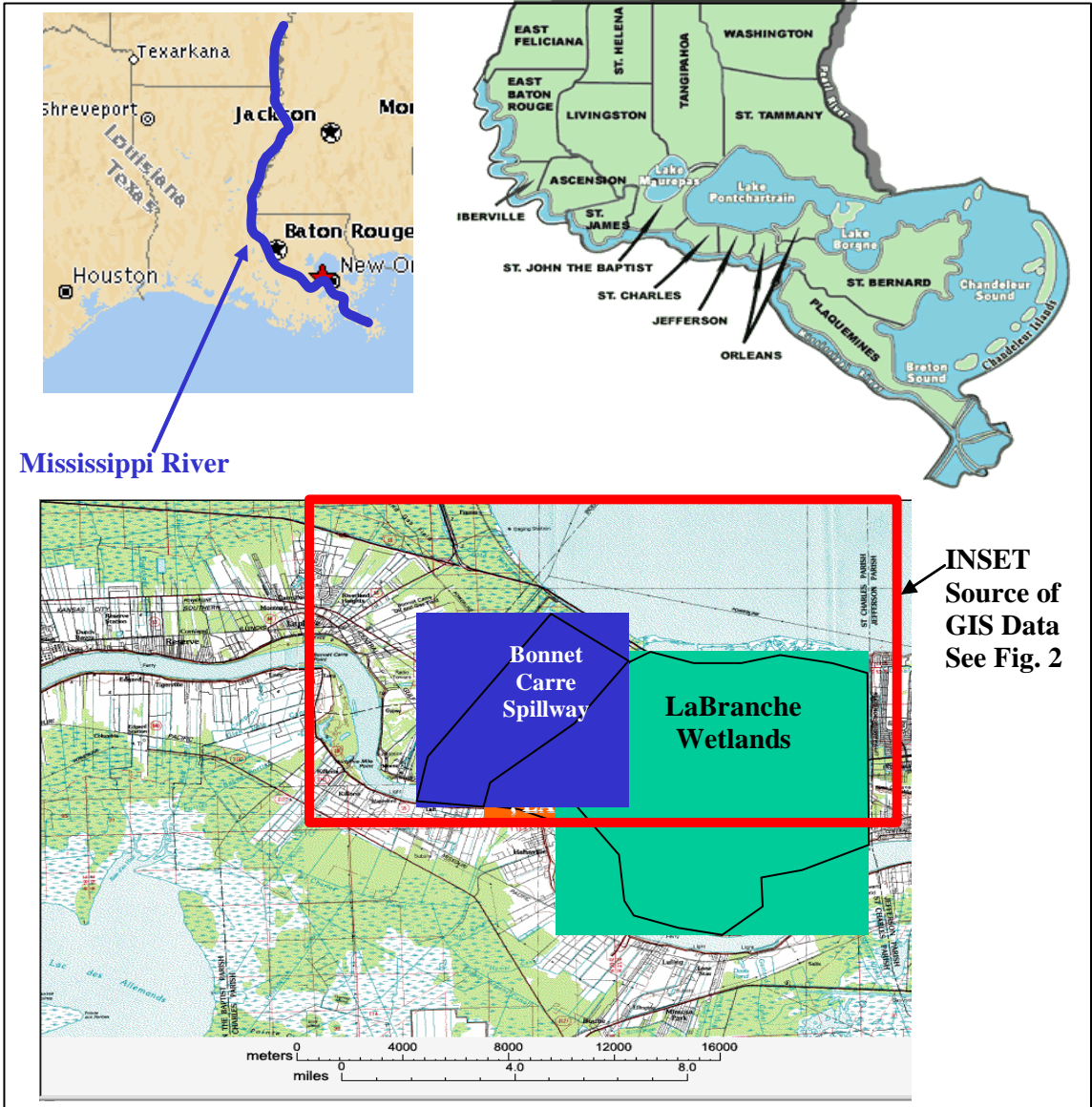
Fig. 2. GIS base maps available for the subject site.

Fig. 3. System Overview Flowchart

Fig. 4. Example Input Parameters. Dialog boxes shown from version 2.13 for the input parameters and the help file describing the input parameter units.

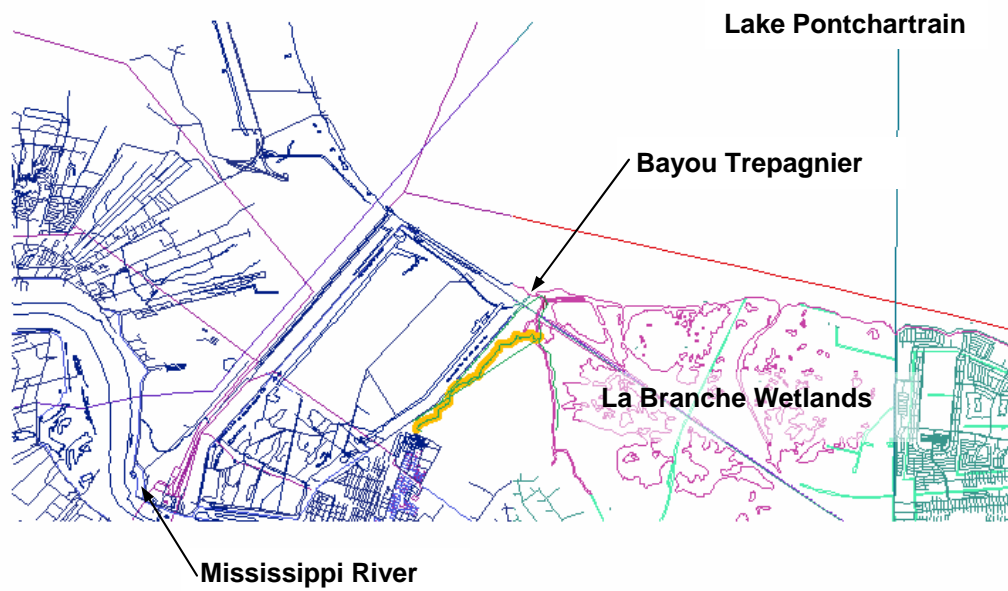
Fig. 5. Plotting Interface Dialogs for Post-Processing

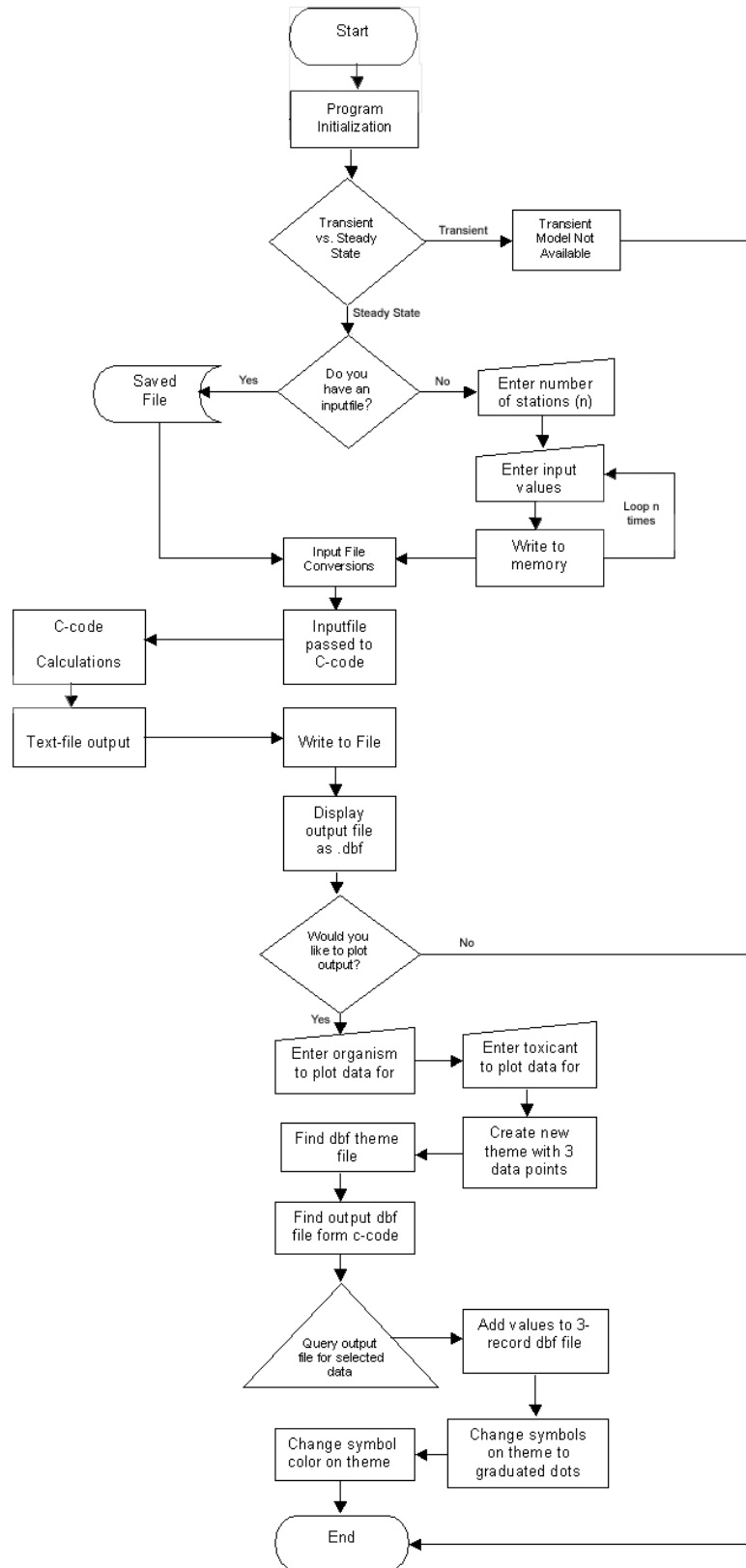
Fig. 6. Predicted naphthalene concentration ( $\mu\text{g}/\text{kg}$ ) for food web organisms at different locations.



Mississippi River

INSET  
Source of  
GIS Data  
See Fig. 2







Input for Steadystate		Help	
Enter the data below and press OK:		<p>Location ID is the identification number of the specific test site.            Location ID should have a maximum of six characters.            Date should be entered in the following format : mm/dd/yy            Water Temperature should have units of degrees Celcius.            Water Organic Matter Concentration should have units of Kilograms per Liter.            Sediment Organic Carbon Fraction should have no units.            Lipid Density should have units of Kilograms per Liter.            Sediment Organic Carbon Density should have units of Kilograms per Liter.            Water Organic Matter Density should have units of Kilograms per Liter.            Toxicant is the contaminant present in the water.            Log Octanol Water Partition Coefficient has no units.            Total Water Concentration of Toxicant should have units of micrograms per Liter.            Sediment Concentration should have units of micrograms per Kilograms, dry weight.</p>	
Location ID	btp060	OK	
Date	1/29/97	Cancel	
Water Temperature	9.48	Help	
Water Organic Matter Concentration	0.0000103		
Sediment Organic Carbon Fraction	0.090		
Lipid Density	.9		
Sediment Organic Carbon Density	.9		
Water Organic Matter Density	1		
Toxicant	Napthalene		
Log Octanol Water Partition Coefficient	3.3		
Total Water Concentration of Toxicant	0.0400		
Sediment Concentration	95.36		
			OK

**Organism**

Please select the organism for which you would like to plot data.

- Plankton
- Aquatic insects
- Terrestrial Arthropods
- Crawfish
- Grass Shrimp
- Small Fish
- Spotted Gar

OK Cancel

**Toxicant**

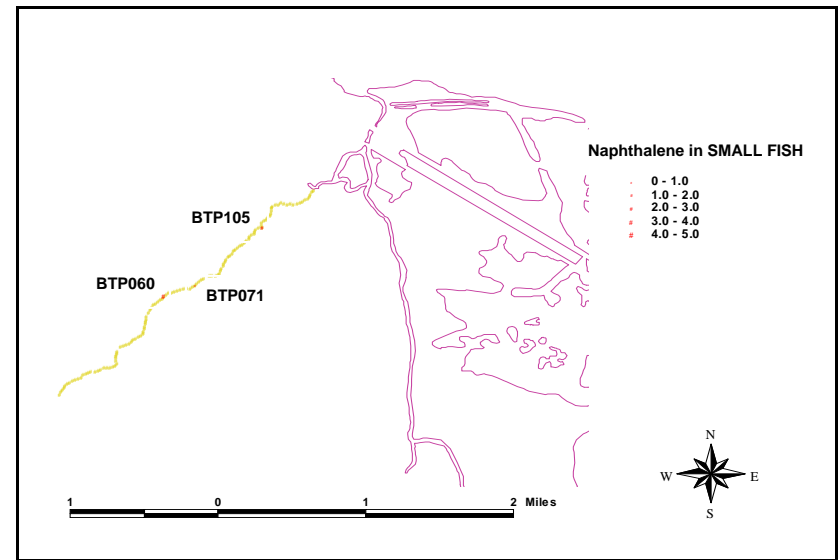
Please select the toxicant for which you would like to plot data.

- Naphthalene
- Phenanthrene
- Anthracene
- Chrysene
- Benz(a)anthracene
- Benzo(a)pyrene
- Dibenzo(a,h)anthracene

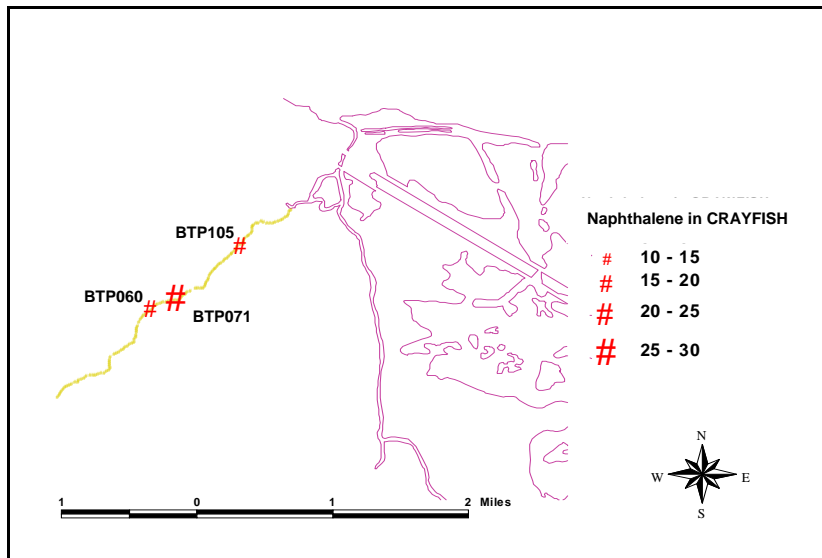
OK Cancel



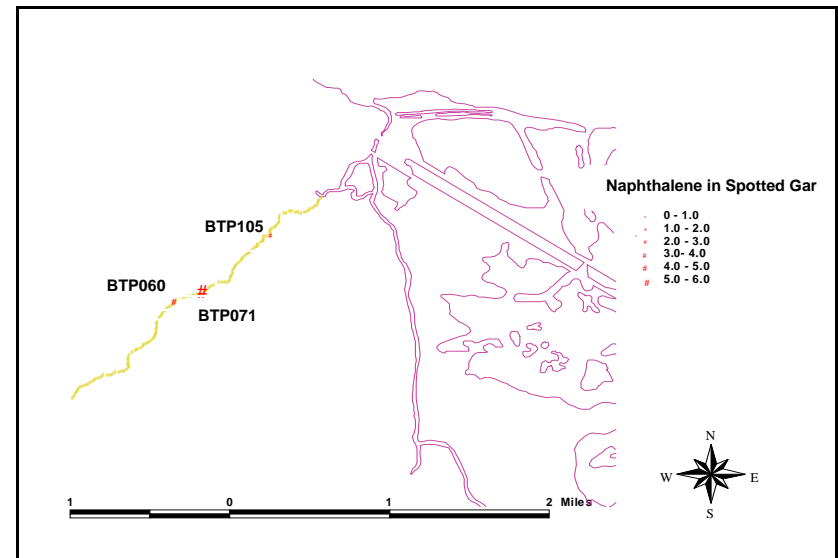
(a) PLANKTON



(b) SMALL FISH



(c) CRAYFISH



(d) SPOTTEDGAR

Table 1: Model input parameter values for simulation of naphthalene, phenanthrene, and benzantracene in the spotted gar food web.

Input Description	Variable	Value			Source <sup>a</sup>
		BTP060	BTP071	BTP105	
Water temperature	T <sub>w</sub> (°C)	19.8	19.2	19.2	CBR Field Core
Total water concentration	C <sub>WT</sub> (ug/L)				
naphthalene		0.053	0.058	0.035	CBR Analytical Core
phenanthrene		0.0067	0.01	0.005	CBR Analytical Core
benzantracene		0.0	0.0	0.0	CBR Analytical Core
Water suspended organic matter	OM <sub>w</sub> (kg/L)	1.03x10 <sup>-5</sup>	1.03x10 <sup>-5</sup>	2.55x10 <sup>-5</sup>	T. Bianchi, personal communication <sup>b</sup>
Sediment concentration	C <sub>s</sub> (ug/kg)				
naphthalene		84.9	119.3	53.8	CBR Analytical Core
phenanthrene		80.4	114.9	57.8	CBR Analytical Core
benzantracene		142.8	173.8	103.5	CBR Analytical Core
Sediment organic carbon fraction	OC <sub>s</sub>	0.09	0.09	0.073	G. Flowers, personal communication <sup>c</sup>
Lipid density	d <sub>L</sub> (kg/L)	0.9	0.9	0.9	Gobas (1993)
Organic carbon density	d <sub>OC</sub> (kg/L)	0.9	0.9	0.9	Gobas (1993)
Organic matter density	d <sub>OM</sub> (kg/L)	1.0	1.0	1.0	Gobas (1993)
Metabolic rate constant	K <sub>metf</sub> (1/day)	0.1	0.1	0.1	van der Linde (2001) <sup>d</sup>
Octanol-water partition coeff.	K <sub>OW</sub>				
naphthalene		2.0 x 10 <sup>3</sup>	2.0 x 10 <sup>3</sup>	2.0 x 10 <sup>3</sup>	Hazardous Substances Data Bank
phenanthrene		3.7 x 10 <sup>4</sup>	3.7 x 10 <sup>4</sup>	3.7 x 10 <sup>4</sup>	Hazardous Substances Data Bank
benzantracene		4.1 x 10 <sup>5</sup>	4.1 x 10 <sup>5</sup>	4.1 x 10 <sup>5</sup>	Hazardous Substances Data Bank
Lipid fractions:					
Plankton	L <sub>p</sub>	0.05	0.05	0.05	For zooplankton (Gobas, 1993)
Aquatic insect	L <sub>ai</sub>	0.05	0.05	0.05	Mosquito (Chapman, 1982)
Small crayfish	L <sub>cr</sub>	0.021	0.021	0.021	measured
Grass shrimp	L <sub>sh</sub>	0.022	0.022	0.022	measured
Small fish	L <sub>sf</sub>	0.032	0.032	0.032	Mosquitofish (Geyer et al., 1994)
Spotted Gar	L <sub>gar</sub>	0.06	0.06	0.06	Mean lipid fraction (Geyer et al., 1994)
Weights (kg):					
Small fish	V <sub>sf</sub>	0.0002	0.0002	0.0002	Mosquitofish (Geyer et al., 1994)
Gar	V <sub>gar</sub>	0.64	0.64	0.64	CBR Field Core
Feeding preferences	P <sub>feed</sub>	see Tbl. 2			P. Martinat, personal communication

<sup>a</sup> CBR stands for the Tulane/Xavier Center for Bioenvironmental Research

<sup>b</sup> Total suspended particulate as upper bound for concentration of suspended organic matter. Value for BTP071 set at measured value at BTP060.

<sup>c</sup> Sediment total carbon fraction used as an upper bound for the sediment organic carbon fraction. Values for BTP060 and BTP071 from measured value at BTP082 and BTP 105 set a measured value for BTP104 in September, 1995.

<sup>d</sup> Reported range for metabolic rate constant of PAHs is 0.1-1.0 day<sup>-1</sup>.

Table 2: Feeding preferences used in the model simulations.

	<i>Prey</i>						
<i>Predator</i>	plankton	aquatic insect	terrestrial arthropod	crayfish	grass shrimp	small fish	spotted gar
plankton	0	0	0	0	0	0	0
aquatic insect	0	0	0	0	0	0	0
terrestrial arthropod	0	0	0	0	0	0	0
crayfish	0	0	0	0	0	0	0
grass shrimp	0	0	0	0	0	0	0
small fish	0.5	0.5	0	0	0	0	0
spotted gar	0	0.03	0.33	0.03	0.16	0.45	0

Table 3: Output table of chemical concentrations ( $\mu\text{g}/\text{kg}$ ) in all foodweb organisms.

(several stations and chemical chemicals shown).

<b>Station Location</b>	<b>Date</b>	<b>Chemical</b>	<b>Plankton</b>	<b>Aquatic Insect</b>	<b>Crayfish</b>	<b>Grass Shrimp</b>	<b>Small Fish</b>	<b>Spotted Gar</b>
BTP105	3/20/97	Naphthalene	3.322	3.322	15.477	16.214	2.129	3.696
BTP060	3/20/97	Naphthalene	5.180	5.181	19.810	20.753	3.320	5.740
BTP071	3/20/97	Naphthalene	5.669	5.669	27.837	29.162	3.632	6.316
BTP105	3/20/97	Phenanthrene	4.769	4.769	16.627	17.419	3.104	2.852
BTP060	3/20/97	Phenanthrene	9.001	9.002	18.760	19.653	5.870	4.894
BTP071	3/20/97	Phenanthrene	13.435	13.435	26.810	28.087	8.743	7.177
BTP105	3/20/97	Benz(a)anthracene	0.000	0.000	29.783	31.201	0.000	1.771
BTP060	3/20/97	Benz(a)anthracene	0.000	0.000	33.325	34.912	0.000	2.053
BTP071	3/20/97	Benz(a)anthracene	0.000	0.000	40.542	42.472	0.000	2.410