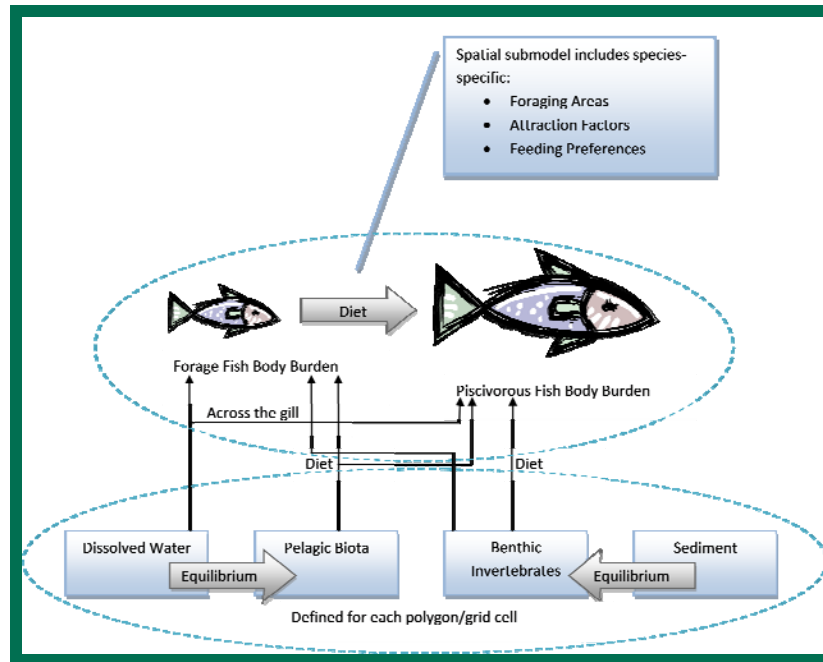# ESTCP
# Cost and Performance Report

## (ER-200917)



## Improvement, Verification, and Refinement of Spatially Explicit Exposure Models in Risk Assessment - FishRand

**August 2015**

# REPORT DOCUMENTATION PAGE

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# ACRONYMS AND ABBREVIATIONS

| | |
|---|---|
| AFB | Air Force Base |
| | |
| CERCLA | Comprehensive Environmental Response, Compensation, and Liability Act |
| CERCLIS | Comprehensive Environmental Response, Compensation, and Liability Information System |
| | |
| DDD | dichlorodiphenyldichloroethane |
| DDE | dichlorodiphenyldichloroethylene |
| DDT | dichlorodiphenyltrichloroethane |
| DoD | Department of Defense |
| | |
| ERM | Effect Range-Medium |
| ERL | Effect Range-Low |
| ESTCP | Environmental Security Technology Certification Program |
| | |
| FR | FishRand |
| | |
| GIS | geographical information system |
| | |
| ICF | Inner City Fund International |
| | |
| mg/kg | milligrams per kilogram |
| | |
| NCP | National Oil and Hazardous Substance Pollution Contingency Plan |
| NPL | National Priorities List |
| NSSC | U.S. Army Natick Soldiers Systems Center |
| | |
| PCB | polychlorinated biphenyls |
| | |
| RCRA | Resource Compensation and Recovery Act |
| RI/FS | Remedial Investigation/Feasibility Study |
| RPD | relative percent difference |
| | |
| SERDP | Strategic Environmental Research and Development Program |
| SWAC | surface-area weighted average concentrations |
| | |
| TSERAWG | Tri-Service Environmental Risk Assessment Work Group |
| | |
| USACE | U.S. Army Corps of Engineers |
| USEPA | U.S. Environmental Protection Agency |
| | |
| ww | wet weight |

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# ACKNOWLEDGEMENTS

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# EXECUTIVE SUMMARY

Regulatory decision-making at contaminated sediment sites are typically informed by the results of human health and ecological risk assessments. Bioaccumulation of sediment-associated contaminants through aquatic food webs often represents the predominant pathway of concern in these risk assessments. Site data provides an indication of current conditions. However, predictive models are required to evaluate the impact of potential management alternatives.

Bioaccumulation models predict fish tissue concentrations under one or more future scenarios. Although the mechanistic process of bioaccumulation is well-understood, particularly for heavy organic compounds such as polychlorinated biphenyls (PCB), dioxins, and many pesticides (e.g., dichlorodiphenyltrichloroethane [DDT]), none of the models in current use account for the influence of spatial heterogeneity in contaminant distribution in combination with fish foraging behaviors and strategies. Similarly, temporal changes in contaminant concentrations are infrequently evaluated.

The project team demonstrated the application of a probabilistic, spatially-explicit, and dynamic bioaccumulation model, referred to as FishRand at two Army sites. Those results are compared to the currently accepted practice of a deterministic application and a probabilistic, but not spatially-explicit application. In all cases, the mathematical framework of the bioaccumulation model is based on the well-recognized "Gobas Model," which has been used at many sites.

The data requirements for FishRand are similar to those required for any bioaccumulation model, although more information is required on fish foraging areas and strategies than would otherwise be developed. Exposure concentrations in surface sediments rely on the commonly used geographical information system (GIS)-based characterizations of site data. All modeling and results presented in this report are based on the original version of the FishRand model, which did not provide a direct, quantitative linkage to GIS files (e.g., .SHP files), as will be discussed. However, since this effort was completed, the model has been updated to provide a direct linkage to GIS files. The latest version of the model is available from http://el.erdc.usace.army.mil/trophictrace/.

The project team developed the application for total PCBs, two individual PCB congeners, and three homologue groups at one site; and DDT, dichlorodiphenyldichloroethylene (DDE), and dichlorodiphenyldichloroethane (DDD) at the other site. The spatially-explicit model consistently predicts tissue concentrations that closely match both the average and the variability of observed data across contaminants and environments. The probabilistic framework allows direct linkages to ecological assessments of impacts to fish populations. Because the model explicitly distinguishes between "uncertainty" (e.g., lack of knowledge) and "variability" (e.g., population heterogeneity), different output statistics are generated depending on whether the results are used to support risk assessments for fish consumers (either human or ecological) or direct risks to fish.

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# 1.0    INTRODUCTION

The Department of Defense (DoD) faces legacy contamination at approximately 6,000 nationwide sites (Government Accountability Office Report, 2005), many of which contain sediment-associated organic contaminants likely to bioaccumulate in aquatic food webs leading to the potential for human health and ecological impacts through fish consumption. Bioaccumulation models quantifying the relationship between sediment exposures and resulting tissue concentrations have been in use for many years to support remedial decision-making. However, the predictive power of these models remains a concern. Participants at a recent combined Strategic Environmental Research and Development Program (SERDP)/Environmental Security Technology Certification Program (ESTCP) workshop identified the "evaluation of food web models in setting remedial goals and long-term monitoring requirements" as a critical research area. This was particularly evident when using these models as the basis for evaluating potential risk reductions associated with site-specific management actions (Thompson et al., 2012). It is recognized that bioaccumulation represents the exposure pathway of primary concern for many sediment-originating contaminants. Predicted aquatic-organism concentrations provide exposure estimates for human health and ecological risk assessments, which provide risk-based frameworks for back-calculating remedial levels in sediments. Because bioaccumulation models quantify the relationship between sediment-exposure concentrations and resulting tissue levels in aquatic organisms, these models strengthen the available tools used in the decision-making process at sediment sites.

Bioaccumulation modeling approaches range from deriving empirical trophic relationships based on site-specific data, to dynamic, mechanistic models. Of the available bioaccumulation models, the FishRand (FR) model presented here is the only one that simulates fish foraging behavior over GIS-defined spatially-variable sediment and water exposure concentrations using a dynamic (time-varying) mathematical framework. The project team presented the results of applying the FR model under several different exposure scenarios at two separate DoD sites to demonstrate its strengths and potential limitations.

## 1.1    BACKGROUND

Bioaccumulation models rely on sediment and water exposure concentrations to drive exposure and uptake in aquatic food webs incorporating site-specific data on trophic levels, species foraging strategies, and feeding preferences. Frequently, the bioaccumulation models are highly detailed and increasingly complex in their representation of the food web (Arnot and Gobas, 2004; Windward Environmental, 2010; Lopes et al., 2012; Gobas and Arnot, 2010) and yet in almost all cases rely on simple averaging techniques such as surface-area weighted average concentrations (SWAC) to describe potential exposures (Gustavson et al., 2011). These averaging techniques poorly capture the spatial and temporal variability of the majority of contaminated-sediment sites.

Because bioaccumulation models quantify the relationship between sediment-exposure concentrations and subsequent tissue levels in aquatic organisms, these models represent a key link in the suite of tools used to support decision-making at sediment sites. Results of bioaccumulation modeling are used as inputs to human health and ecological risk assessments. They are also used to evaluate how temporal changes in the contaminant concentrations of aquatic organisms change over time following remedial actions or other management alternatives at

sediment sites. The focus of this effort was to explore improvements in predictive capacity associated with use of a spatially-explicit bioaccumulation model.

## 1.2    OBJECTIVE OF THE DEMONSTRATION

To demonstrate the application of a spatially-explicit bioaccumulation model run under three scenarios:

1.  Deterministic Case: Deterministic sediment and water exposure concentrations defined as arithmetic averages, or SWACs, consistent with typical exposure characterization.

2.  Probabilistic Case: Non-spatially explicit but probabilistic sediment and water exposure concentrations (e.g., exposure concentrations were defined by distributions rather than point estimates, and not by a deterministic SWAC).

3.  Spatially-Explicit Case: Sediment (and water, if appropriate) exposure concentrations were spatially defined, and aquatic organism foraging activities were simulated over GIS-based representations of exposure.

The results of a set of runs were compared to each other and to site-specific data and goodness-of-fit statistics were developed to evaluate potential improvements in prediction accuracy attributable to the way in which exposures were captured when holding all other cross-scenario inputs consistent. Bioaccumulation modeling results were used as inputs to risk assessments (see Regulatory Drivers, Section 1.3), and were used to predict changes in tissue concentrations associated with implementation of remedial or management alternatives. Although predicted tissue concentrations serve as inputs to human health and ecological risk assessments, we noted that predicted risk was linear with respect to fish tissue concentrations. The key metric to evaluate model performance was thus predicted versus observed fish tissue levels.

## 1.3    REGULATORY DRIVERS

During the mid-1980s, risk assessment emerged as the primary tool that supported decision-making for potential remediation at hazardous waste sites under programs such as the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) (commonly referred to as Superfund), and the Resource Compensation and Recovery Act (RCRA) (U.S. Environmental Protection Agency [USEPA], 1989; 1992a; 1992b; 1998). The U.S. Army is also responsible for environmental management of its properties, including remedial studies of contaminated sites. To such an extent that bioaccumulation represents the key pathway of concern for sediments contaminated with heavy organics, modeling tools and approaches that efficiently predict contaminant exposures in fish tissues, and appropriate inputs to human health and ecological risk assessments are both needed. Federal guidance recognizes assessment to populations of species, of habitats, and the heterogeneity of contamination (USEPA, 1992a; 1992b; 1998). An understanding of contaminant fate in the environment is essential in the required predictive ecological risk assessment that is specific to published guidance (USEPA, 1998). This is consistent with DoD Technical Guidance (Tri-Service Environmental Risk Assessment Work Group [TSERAWG], 2000; 2002). For sediment-contaminated sites, tiered approaches that start with simple comparisons between sediment concentrations and sediment-based benchmarks are used. For example, use of Effects Range-Medium (ERM), and Effects Range-Low (ERL) (Long

and Morgan, 1990; O'Connor, 2004). However, ERMs and ERLs do not address potential impacts associated with bioaccumulation of contaminants through the food web to aquatic organisms that are subsequently consumed by human and ecological receptors. Thus, bioaccumulation models are required to predict expected contaminant concentrations in aquatic organisms.

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## 2.0    TECHNOLOGY

This section provides a brief overview of the spatially-explicit approach of FR, including a brief description of the mathematical framework and underlying conceptual assumptions. A full description of the technology can be found in the accompanying Final Report. (Johnson, 2014)

### 2.1    TECHNOLOGY DESCRIPTION

In areas of localized contamination, exposure of aquatic organisms to varying concentrations of sediment and water contaminants, are a function of spatial factors and species biology, including foraging strategies, feeding preferences, and habitats. Due to local variability in species behavior and contaminant distributions, species with overlapping foraging areas from the same site may experience significantly different contaminant exposures as they overlap with preferred foraging and migratory areas. Predicted exposure estimates and subsequent human health and ecological risk projections typically assume static exposures of receptors to contaminant concentrations that are characterized by a descriptive statistic (e.g., a mean or maximum). The level of health protection is unknown, and in a dynamic system, results may not represent actual exposures of aquatic organisms. Further, uncertainty and variability in underlying input parameters are not accounted for in these static exposures.

The FR calculates seasonal, chemical, and species-specific body burdens based on time- and spatially-varying sediment and water exposure concentrations. These data are used to calculate deterministic toxicity quotients or in refined ecological risk assessment models are used to estimate population-level risks for fish, or as inputs to ecological and human health risk assessment models for higher-order fish-consuming receptors. Figure 1 depicts a conceptual schematic of the relationship across compartments in the FR model.
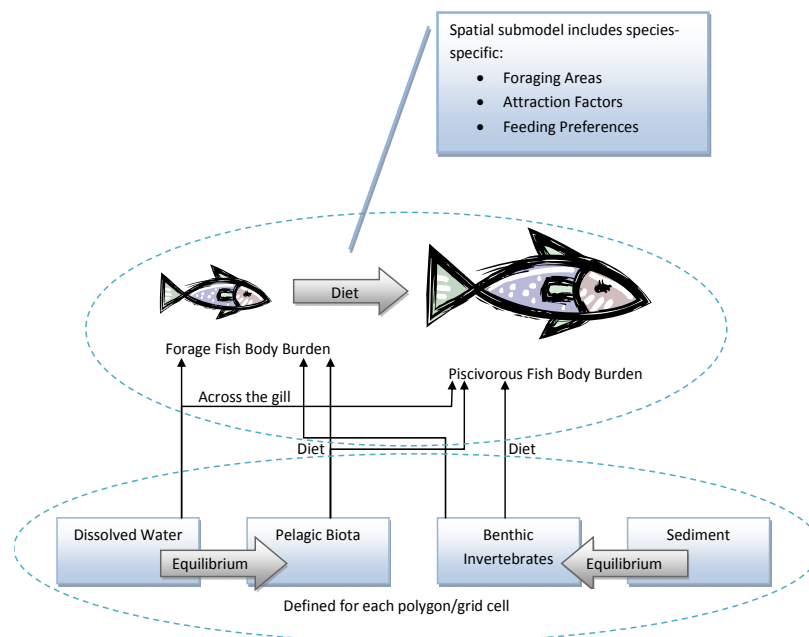


**Figure 1. Schematic of compartments in the FR model.**

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The FR model assumes that anglers or ecological receptors are sampling (catching) fish from a population, and every individually-caught fish is obtained from a larger distributed population. In addition to population variability, uncertainty in the distribution of the true population exists. This is attributable to uncertainty in the input parameters, which are included in the FR approach. In some cases, the literature indicates that specific parameters may contribute to uncertainty or variability in the output distribution (von Stackelberg et al., 2002a; Kelly et al., 2007). Hence, the FR model separates "uncertain" from "variable" inputs as opposed to explicitly modeling the uncertainty in a variable input. For a full description of how these assumptions lead to the computed nested Monte-Carlo subroutines, please refer to the Final Report.

FR predicts fish body burdens in aquatic food webs given site-specific exposure conditions. One key aspect to this is a complete understanding of the relationship between sediment and water concentrations (i.e., to understand how sediment interacts with water and how concentrations in either media change over time as a result of this interaction). Although fish are primarily exposed to bioaccumulative contaminants through sediment sources, significant dynamics might exist that allow sediments to release contaminants. For example, through various flux mechanisms that might result from disequilibrium between sediment and water—an important consideration to capture with respect to exposure. FR is not a sediment fate and transport model—these issues need to be addressed outside the realm of the bioaccumulation model. It is likely that deficiencies attributed to the bioaccumulation model actually result from an imperfect understanding of the sediment-water interaction and dynamics.

FR allows users to specify probability distributions for model inputs, and users can specify whether a parameter contributes predominantly to "uncertainty" or population "variability." Uncertainty and variability should be viewed separately in risk assessment because they have different implications to regulators and decision makers (Thompson and Graham, 1996). For example, there is "true" uncertainty (e.g., lack of knowledge) in the estimated concentrations of sediment and water to which aquatic organisms are exposed. Concurrently, parameters contributing to contaminant bioaccumulation display variability. Variability is a population measure, and provides a context for a deterministic point estimate (e.g., average or reasonable maximum exposure). Variability typically cannot be reduced, only better characterized and understood. In contrast, uncertainty represents unknown but often measurable quantities. Often times, uncertainty is reduced by obtaining additional measurements of the uncertain quantity. Quantitatively separating uncertainty and variability allows an analyst to determine the fractile of the population, for which a specified risk occurs, and the uncertainty bounds or confidence interval around that predicted risk (von Stackelberg et al., 2002a).

If uncertainty is large relative to variability (i.e., it is the primary contributor to the range of risk estimates), and if the differences in cost among management alternatives are high, additional collection and evaluation of information is recommended before making management decisions for contaminated sediments. Alternatively, including variability in risk estimates allows decision makers to quantitatively evaluate the likelihood of risks above and below selected reference values or conditions (e.g., average risks as compared to 95th percentile risks).

**2.2     TECHNOLOGY DEVELOPMENT**

The FR model is a spatially-explicit aquatic bioaccumulation model that was originally developed to support decision-making at the Hudson River Superfund Site (assuming single, non-spatially explicit reach-wide exposure concentrations in sediment and water). It was used to compare remedial alternatives (and no action) on the basis of predicted fish tissue concentrations. The mathematical engine of the model is based on the work of Dr. Frank Gobas (Gobas, 1993), which is run in dynamic time-varying mode and augmented to allow all inputs to be defined by distributions or ranges and not by point estimates, including the spatially-explicit foraging module to better characterize exposures for migratory and wide-ranging fish species.

This section describes the development of the FR Spatially-Explicit Model. Many original publications and presentations provide details of the development and application of this model. For example:

- von Stackelberg, K., 2013. Platform presentation on spatially-explicit bioaccumulation modeling at the SedNet conference in Lisbon, Portugal. http://www.sednet.org/2013-presentations.htm.

- von Stackelberg, K., 2013. Decision analytic strategies for integrating ecosystem services and risk assessment. *Integrated Environmental Assessment and Management* 9(2):260-268.

- von Stackelberg, K., 2012. The FishRand spatially-explicit bioaccumulation model. Platform presentation at the North America SETAC Annual Meeting, November 2012, Long Beach, CA.

- von Stackelberg, K., 2012. Incorporating fish behavior in bioaccumulation modeling. Invited platform presentation at the North America SETAC Annual Meeting, November 2012, Long Beach, CA.

- von Stackelberg, K., 2012. Bioaccumulation and Potential Risk from Sediment-Associated Contaminants in Dredged Materials. Platform presentation at Dredging 2012, Dredging in the 21st Century, San Diego, CA.

- von Stackelberg, K., M. Johnson, and W.T. Wickwire, 2012. Spatially-Explicit Exposure and Ecological Risk Modeling Tools: SEEM and FISHRAND. Platform Presentation at the SETAC Europe Annual Meeting, May 2012, Berlin, Germany.

- von Stackelberg, K., 2010. Spatially-Explicit Bioaccumulation Modeling. Presented at the Society for Environmental Toxicology and Chemistry Annual Meeting, November 2010, Portland, OR.

- Sunderland, E.S., C.D. Knightes, K. von Stackelberg, and N.A. Stiber, 2010. Environmental fate and bioaccumulation modeling at the U.S. Environmental Protection Agency: Applications to inform decision making. In Modelling of Pollutants in Complex Environmental Systems Volume II. United Kingdom: ILM Publications.

- Johnson, M.S., M. Korcz, K. von Stackelberg, and B. Hope, 2009. Spatial analytical techniques for risk based decision support systems. In Decision Support Systems for Risk

Based Management of Contaminated Sites. Marcomini, A., Suter, G.W. and A. Critto, Eds. Springer-Verlag.

- von Stackelberg, K.,W.T. Wickwire, and D. Burmistrov, 2005. Spatially-explicit exposure modeling tools for use in human health and ecological risk assessment: SEEM and FISHRAND-Migration. pp. 279–288. In: Environmental Exposure and Health, 2005. Aral MM, Brebbia CA, Maslia ML and Sinks T (eds.), United Kingdom: WIT Press.

- von Stackelberg, K., D. Burmistrov, I. Linkov, J. Cura, and T.S. Bridges, 2002. The use of spatial modeling in an aquatic food web to estimate exposure and risk. *Sci Total Environ* 288(1-2):97-110.

- Linkov, I., D. Burmistrov, J. Cura, and T.S. Bridges, 2002. Risk-based management of contaminated sediments: consideration of spatial and temporal patterns in exposure modeling. *Environ Sci Technol* 36(2):238-246.

- von Stackelberg, K., D. Vorhees, I. Linkov, D. Burmistrov, and T. Bridges, 2002. Importance of uncertainty and variability to predicted risks from trophic transfer of contaminants in dredged sediments. *Risk Analysis* 22(3):499-512.

- USEPA, 2000. Phase 2 Revised Baseline Modeling Report for the Hudson River Remedial Investigation/Feasibility Study. Prepared by Limno-Tech, Inc., Menzie-Cura and Associates, Inc., and TAMS Consultants, Inc. for USEPA. December, 2000. www.epa.gov/hudson.

The model has been applied in both the non- and spatially-explicit modes for several different sites on behalf of the U.S. Army Corps of Engineers (USACE). It has also been applied under a Small Business Innovation Research Grant as part of a larger decision analytic framework (von Stackelberg, 2013). Technology development for the FR model has focused on improving how exposure is defined, both in terms of spatially-explicit exposure concentrations and simulating fish foraging behavior relative to those spatially-defined exposures. Decision-makers cannot control the ways in which fish behavior and physiology interact with exposure concentrations. However, decision-makers can control spatial patterns of contaminant concentrations. The basic uptake equations are kept as conservative as possible, while adding greater realism to the ways in which exposure influences predicted uptake.

## 2.3   ADVANTAGES AND LIMITATIONS OF THE TECHNOLOGY

This technology provides a number of analytical advantages. While limitations exist, appreciation and comprehension of these limitations within the context of each user's specific modeling goals should permit uncomplicated management of the technology.

The advantages of this technology include:

- Avoidance from selecting the site or contamination area as the only spatial context;

- Direct simulation of fish foraging strategies over GIS-defined, spatially-explicit sediment and water exposure fields;

- Easier description and translation of model mechanics to stakeholders;

- Better analysis of population risk;

- Accessible design and user-determined complexity encourages use of technology;

- Provision of relative indicators of sensitivity, and assistance in the understanding of factors that contribute most to exposure, and hence risk;

- Provision of quantitative estimates bounding uncertainty and variability in exposure/risk estimates; and

- Provision of more usefully formatted fish body burden estimates (probability distributions) that link to other analyses (e.g., risk assessments, economic forecasts, injury determinations, etc.).

The limitations of this technology include:

- Simplified bioaccumulation options/assumptions (true of any bioaccumulation model);
- Subjectivity of habitat suitability as defined by attraction factors;
- Lack of direct link to GIS output (e.g., .SHP files) since users much manually draw the exposure fields;
- Unaccounted dynamic habitats and resultant changes in wildlife usage;
- Simplified foraging strategies (lacking important considerations such as competition for limited resources, bioenergetics, and fluctuating food availability);
- Lack of quantifiable uncertainty in the variability, e.g., a second-order probabilistic analysis in which a variability distribution (mean and standard deviation) are also specified as distributions. For example, a distribution for lipid content specified by a mean and standard deviation, each themselves consisting of means and standard deviations; and
- Increased model complexity linked to increasing calibration challenges.

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## 3.0 PERFORMANCE OBJECTIVES

The objectives for this project are provided in Table 1 below.

**Table 1. Performance objectives.**

| Performance Objective | Data Requirements | Success Criteria | Results |
|---|---|---|---|
| **Quantitative Performance Objectives** | | | |
| Verify FR results for a number of fish species across two sites and two different contaminants | See Table 2-1 in Final Report | Comparison of FR predicted fish body burdens with analytical results from site; an improvement relative to non-spatially explicit results and lowest RPD | RPDs for spatially-explicit case consistently improved over deterministic or probabilistic |
| Improve and refine FR | Feedback from peer reviewers and workshop panelists | Favorable feedback regarding refinements | The only direct recommendation for FR was to consider inclusion of a direct linkage to GIS |
| **Qualitative Performance Objectives** | | | |
| Ease of use | Feedback on usability of the model and time required | Risk assessors and non-risk assessors will be able to learn to apply FR, practical examples of use | Held a hands-on workshop with all users successfully using the model with their own datasets |
| Develop a publication from the workshop highlighting current thinking on spatial models in risk assessment – applications, benefits versus risks of using, improvements | Preparation of the final publication using notes/feedback from workshop participants | Acceptance for publication in a peer reviewed journal | A publication is currently in preparation |
| Development of a user guide | Information on how to use and set up models to include relative comparisons of options | Feedback from users at training sessions | Held a hands-on workshop with all users successfully using the model with their own datasets |
| Final Technical Reports | Results of field validation | If performance criteria are met | Completed |
| | Results and final conclusions/ recommendations | | |

## 3.1 VERIFY FISHRAND RESULTS

This objective involves comparing model predictions to observed data to evaluate whether there is an improvement in prediction accuracy when exposures are better characterized. As described previously, the approach was to apply the bioaccumulation model under three scenarios with the way in which exposure was characterized as the only difference in assumptions across scenarios.

Background information for each of the sites is provided in Section 4.0, model inputs in Section 5.0, and detailed performance results in Section 6.0.

## 3.2    IMPROVE AND REFINE FISHRAND

Workshops were conducted to explore broader value of spatial models, and application of the models by the scientific community and regulators. Model improvements were discussed, and addressed four key questions:

1. What are spatially-explicit exposure models and why are they valuable?
2. How have the models been applied?
3. Are there regulatory impediments to their use?
4. Are there limitations to the models and can they be improved?

Workshop participants were asked to develop a list of considerations for model improvement and functionality. The only recommendation specific to FR was to provide a direct link to GIS output files (e.g., ".shp" files) rather than requiring users to redraw exposure concentrations. As the model was developed when GIS use was less common and expensive for routine use, the direct link was not initially included. Resource constraints combined with the software development platform of the original FR model precluded adding in the direct linkage to GIS output at the time these analyses were developed. However, the version of the model publicly available through USACE does include the direct GIS linkage as FR has now been reprogrammed in a Java-based programming environment.

Workshop participants focused their recommendations on how to increase use of spatially-explicit models to support regulatory decision-making rather than on technical aspects of the model itself. These recommendations included identifying factors impeding regular use of spatially-explicit models generally, such as few precedents for their use, misguided perceptions as to their purpose, traditional regulatory practices, when such models are considered during the site assessment process, and specific technical concerns, including the quality of input data.

## 3.3    EASE OF USE

A 2-day workshop held in April 2010 with attendees from DoD, industry, and government allowed participants to use the model based on both the demonstration datasets contained within the model and their own data. Participants were invited to provide comments, which focused on strategies for increasing general use of spatially-explicit models (Wickwire et al., 2011).

## 3.4    PUBLICATION DEVELOPMENT

A publication for submission to the peer-reviewed literature is in preparation.

# 4.0  DESCRIPTION OF THE MODELING SITES

## 4.1  U.S. ARMY NATICK SOLDIERS SYSTEMS CENTER (NSSC) SITE DESCRIPTION

The U.S. Army Natick Soldiers Systems Center (NSSC) site is located approximately 17 miles west-southwest of Boston in the town of Natick, Middlesex County, Massachusetts. The facility occupies a small peninsula extending from the eastern shoreline of the South Pond of Lake Cochituate and encompasses approximately 74 acres. NSSC has been a permanent U.S. Army installation since October 1954. The installation's mission includes research and development activities in food engineering, food science, clothing, equipment, materials engineering, and aeronautical engineering.

NSSC was listed as a Superfund site based on contamination in groundwater and was added to the USEPA National Priorities List (NPL) in May 1994. The groundwater is undergoing treatment and removal, and other on-site investigations are ongoing, pursuant to CERCLA and the National Oil and Hazardous Substances Pollution Contingency Plan (NCP). The Comprehensive Environmental Response, Compensation, and Liability Information System (CERCLIS) identification number for the Site is MA1210020631. The U.S. Department of the Army is the lead agency responsible for environmental cleanup at this site. Primary documents that provide information for this site include Inner City Fund (ICF) International (2008 and 2009). Data were not provided electronically and were extracted from hard copy files. All the original data as presented in source documents for both NSCC and Tyndall Air Force Base (AFB) are provided in the "Final Report."

In addition, full details on site location and history, site geology and hydrogeology, and contaminant distribution are described in the "Final Report."

## 4.2  TYNDALL AFB

The primary document providing the information for modeling is the Draft Feasibility Study (Weston Solutions, Inc., 2009). Sediment and fish data, as well as model inputs and outputs from the FR model are provided in the Final Report.

In addition, full details on site location and history, site geology and hydrogeology, and contaminant distribution are described in the "Final Report."

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# 5.0  TEST DESIGN: MODEL APPLICATION

Parameterization of the FR model evaluation relied exclusively on existing data, typical of what would be provided during a Remedial Investigation/Feasibility Study (RI/FS) conducted at Superfund sites or other types of site characterization. Both demonstration sites had FSs available as referenced below, and these provided the spatially-explicit sediment and water exposure concentrations, as well as the fish concentrations used for comparing predicted model outputs. In addition, fish lipid content and total organic carbon were based on site-specific data. Benthic and pelagic invertebrate lipid content and Log $K_{ow}$ were obtained from the literature as neither of these sites conducted invertebrate sampling programs.

The modeling application presented here relied on publicly available data from the RI/FS process, and as such, there were existing conceptual models of the aquatic food web. This is a necessary step that is not unique to an application of the FR model and would be required irrespective of the chosen modeling approach. The conceptual model identifies the linkages across components in the food web in a general sense, e.g., the specific fish species and their foraging preferences expressed as compartments across trophic levels. In general, the food web should capture all relevant exposure pathways, but not be so detailed as to be redundant. For example, it is generally not necessary to identify individual benthic invertebrate species unless there are clear differences in parameters that would influence exposure (e.g., lipid content) in the context of fish feeding preferences. An oligochaete would differ from a clam, but would not differ from other soft-bodied, burrowing organisms.

The conceptual model of bioaccumulation in the aquatic food web must link to the larger conceptual model of site exposures and interactions, and these are developed together with the risk assessors and other analysts working at the site. The application of the bioaccumulation model relies on data obtained from the sampling program and the approach must be tailored to identify the species relevant to decision-making at the site (e.g., fish consumption pathway). Typical contaminated sediment sites rely on a suite of models and analyses to support decision making. USEPA (2009) provides a primer for those not experienced in the development and use of models at sediment sites. It explains the objectives of modeling; how models are developed and applied; how they are used to predict the effectiveness of management alternatives; and, finally, an approach for addressing uncertainties in model predictions.

## 5.1  MODEL INPUTS

### 5.1.1  NSSC SITE MODEL INPUTS

All model inputs were identical across the three scenarios except for the way in which sediment exposure concentrations were defined. Please refer to the Final Report (Johnson, 2014) for details.

### 5.1.2  TYNDALL AFB MODEL INPUTS

Please refer to the Final Report (Johnson, 2014) in which a summary of the input data in common to all scenarios and locations, except for feeding preferences, is provided.

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# 6.0    PERFORMANCE ASSESSMENT

This section provides a summary of the performance assessment for both sites. Because a number of the performance objectives relate equally to both sites (e.g., are fundamental to the FR model), these are not separately described for each model application, but are combined. Model performance at each of the sites is described separately.

## 6.1    NSSC SITE PERFORMANCE ASSESSMENT

The key performance criterion is predicted model results versus observed tissue concentrations under each of the three scenarios.

### 6.1.1    Predicted Versus Observed Model Results

Table 2 provides a summary of predicted model outputs under the three scenarios as compared to fish data for the NSSC site. Figure 2 provides these same data graphically.

**Table 2. Results of predicted versus observed and RPD across scenarios for the NSSC site.**

| Species | Observed Mean (mg/kg ww) | Deterministic Case (mg/kg ww) | Probabilistic (No Spatial) (mg/kg ww) | Spatially-Explicit Model Results (mg/kg ww) | RPD Deterministic | RPD Probabilistic | RPD Spatially-Explicit |
|---|---|---|---|---|---|---|---|
| **Yellow Perch** | | | | | | | |
| PCB-052 | 0.016 | 0.037 | 0.155 | 0.015 | 78% | 162% | -7% |
| PCB-153 | 0.289 | 0.156 | 0.191 | 0.281 | -60% | -41% | -3% |
| Cl-4 Tetrachlorobiphenyls | 0.124 | 0.122 | 0.351 | 0.122 | -1% | 96% | -1% |
| Cl-5 Pentachlorobiphenyls | 0.247 | 0.328 | 0.53 | 0.323 | 28% | 73% | 27% |
| Cl-6 Hexachlorobiphenyls | 0.938 | 0.745 | 0.903 | 1.130 | -23% | -4% | 19% |
| Total PCBs | 2.266 | 1.56 | 2.12 | 2.260 | -37% | -7% | 0% |
| **Bluegill** | | | | | | | |
| PCB-052 | 0.008 | 0.016 | 0.079 | 0.006 | 69% | 164% | -21% |
| PCB-153 | 0.072 | 0.049 | 0.043 | 0.086 | -39% | -51% | 17% |
| Cl-4 Tetrachlorobiphenyls | 0.045 | 0.05 | 0.171 | 0.049 | 10% | 116% | 8% |
| Cl-5 Pentachlorobiphenyls | 0.087 | 0.111 | 0.192 | 0.108 | 24% | 75% | 22% |
| Cl-6 Hexachlorobiphenyls | 0.240 | 0.239 | 0.283 | 0.362 | 0% | 16% | 41% |
| Total PCBs | 0.582 | 0.623 | 0.79 | 0.848 | 7% | 30% | 37% |
| **Largemouth Bass** | | | | | | | |
| PCB-052 | 0.023 | 0.054 | 0.231 | 0.021 | 81% | 164% | -8% |
| PCB-153 | 0.348 | 0.161 | 0.198 | 0.276 | -74% | -55% | -23% |
| Cl-4 Tetrachlorobiphenyls | 0.149 | 0.175 | 0.502 | 0.146 | 16% | 109% | -2% |
| Cl-5 Pentachlorobiphenyls | 0.321 | 0.379 | 0.622 | 0.331 | 16% | 64% | 3% |
| Cl-6 Hexachlorobiphenyls | 1.154 | 0.81 | 1.000 | 1.160 | -35% | -14% | 1% |
| Total PCBs | 2.767 | 1.76 | 2.420 | 2.410 | -44% | -13% | -14% |

RPD = relative percent difference calculated as (predicted-observed)/average (predicted-observed)
green values indicate lowest RPD; blue values indicate within 50% of observed
PCB = polychlorinated biphenyls        mg/kg = milligrams per kilogram        ww = wet weight
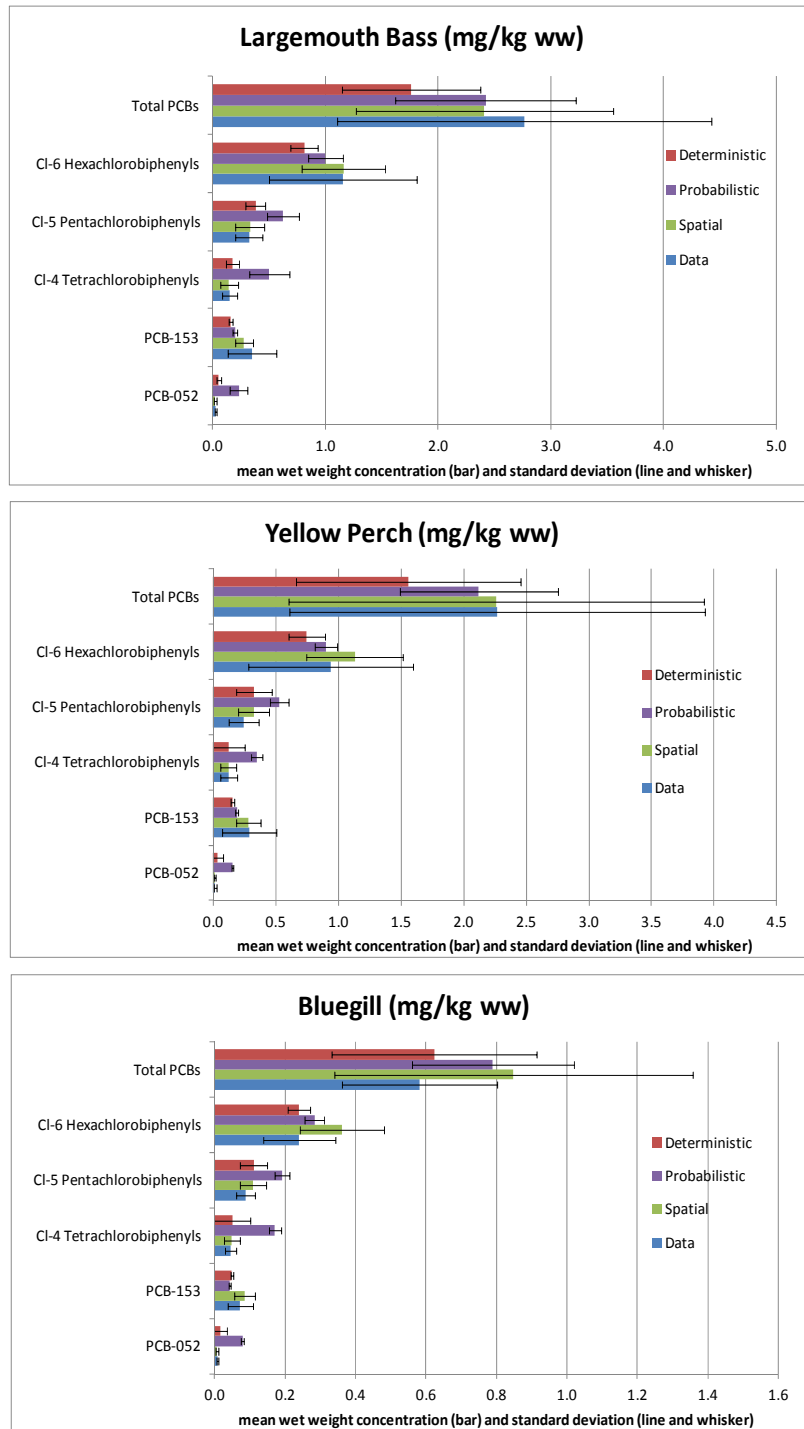
**Figure 2. Results of predicted versus observed across scenarios for the NSSC site.**

Figure 2 and Table 2 provide the results of the model to data comparison for three of the four modeled species (no data were available for pumpkinseed), including largemouth bass, the predator species of most interest from a human health perspective: yellow perch and bluegill. The lowest RPDs across scenarios are highlighted in green (Table 2), and comparisons within 50%, which indicate highly satisfactory model performance are shown in blue.

Taken together, Table 2 and Figure 2 show that across species and individual contaminant types, the spatially-explicit model shows the most consistent and lowest RPDs across individual congeners, homolog groups, and total PCBs. However, the absolute difference across scenarios and contaminants is insignificant, save for the Deterministic Case, which consistently shows the worst performance relative to either the Probabilistic or Spatially-Explicit Cases. Nonetheless, the spatially-explicit model shows either blue or green RPDs across all contaminants and species, in contrast to either of the other approaches, suggesting the spatially-explicit exposure characterization better captures the relationship between sediment and water exposures, fish foraging strategies, and PCB uptake. Figure 2 additionally shows the comparison of standard deviations across the scenarios, and again, the spatially-explicit case performs better with respect to capturing the variance in the data in addition to capturing the central tendency. This can be important for subsequent ecological risk calculations that may require exposure distributions across the population rather than deterministic estimates of tissue concentrations, for example, using joint probability curves or other probabilistic risk methods.

## 6.2    TYNDALL AFB PERFORMANCE ASSESSMENT

The key performance criterion is predicted model results versus observed tissue concentrations under each of the three scenarios.

### 6.2.1   Predicted Versus Observed Model Results

Table 3 summarizes the predicted model output under the three scenarios as compared to fish data for the Tyndall Site. The red values in the table represent the lowest RPD across scenarios. RPDs between 0% and 50% demonstrate excellent model performance and are highlighted in blue in Table 3.

**Table 3. Results of predicted versus observed and RPD across scenarios for the Tyndall AFB site.**

| Species and Area | Observed Mean (mg/kg ww) | Deterministic Case (mg/kg ww) | Probabilistic (No Spatial) (mg/kg ww) | Spatially-Explicit Model Results (mg/kg ww) | RPD Deterministic | RPD Probabilistic | RPD Spatially-Explicit |
|---|---|---|---|---|---|---|---|
| **Pinfish Area 1** | | | | | | | |
| DDD | 0.058 | 0.040 | 0.098 | 0.059 | -37% | 51% | 1% |
| DDE | 0.040 | 0.018 | 0.049 | 0.040 | -77% | 19% | -1% |
| DDT | 0.017 | 0.023 | 0.042 | 0.050 | 27% | 83% | 96% |
| DDx | 0.116 | 0.054 | 0.107 | 0.142 | -73% | -8% | 20% |
| **Killifish Area 1** | | | | | | | |
| DDD | 0.149 | 0.105 | 0.258 | 0.147 | -35% | 53% | -2% |
| DDE | 0.190 | 0.032 | 0.088 | 0.065 | -142% | -73% | -98% |
| DDT | 0.014 | 0.064 | 0.116 | 0.132 | 127% | 156% | 161% |
| DDx | 0.353 | 0.138 | 0.275 | 0.301 | -88% | -25% | -16% |

**Table 3. Results of predicted versus observed and relative percent difference across scenarios for the Tyndall AFB site (continued).**

| Species and Area | Observed Mean (mg/kg ww) | Deterministic Case (mg/kg ww) | Probabilistic (No Spatial) (mg/kg ww) | Spatially-Explicit Model Results (mg/kg ww) | RPD Deterministic | RPD Probabilistic | RPD Spatially-Explicit |
|---|---|---|---|---|---|---|---|
| **Killifish Area 2** | | | | | | | |
| DDD | 0.304 | 0.752 | 1.890 | 0.474 | 85% | 145% | 44% |
| DDE | 0.253 | 0.338 | 0.751 | 0.222 | 29% | 99% | -13% |
| DDT | 0.175 | 3.250 | 10.500 | 0.138 | 180% | 193% | -23% |
| DDx | 0.731 | 3.640 | 9.390 | 0.570 | 133% | 171% | -25% |
| **Killifish Areas 1 and 2** | | | | | | | |
| DDD | 0.248 | 0.752 | 1.890 | 0.474 | 101% | 154% | 63% |
| DDE | 0.304 | 0.338 | 0.751 | 0.222 | 11% | 85% | -31% |
| DDT | 0.053 | 3.250 | 10.500 | 0.138 | 194% | 198% | 89% |
| DDx | 0.605 | 3.640 | 9.390 | 0.570 | 143% | 176% | -6% |
| **Pinfish Area 5** | | | | | | | |
| DDD | 0.013 | 0.007 | 0.016 | 0.007 | -59% | 21% | -59% |
| DDE | 0.014 | 0.018 | 0.031 | 0.173 | 27% | 78% | 171% |
| DDT | 0.004 | 0.023 | 0.100 | 0.023 | 140% | 184% | 140% |
| DDx | 0.031 | 0.033 | 0.155 | 0.034 | 8% | 134% | 10% |
| **Killifish Area 5** | | | | | | | |
| DDD | 0.028 | 0.020 | 0.050 | 0.027 | -33% | 57% | -3% |
| DDE | 0.053 | 0.032 | 0.055 | 0.226 | -50% | 3% | 124% |
| DDT | 0.007 | 0.071 | 0.323 | 0.069 | 163% | 191% | 162% |
| DDx | 0.088 | 0.105 | 0.031 | 0.088 | 17% | -96% | 0% |

RPD = relative percent difference calculated as (predicted-observed)/average (predicted-observed)
green values indicate lowest RPD; blue values indicate within 50% of observed
DDD = dichlorodiphenyldichloroethane          DDE = dichlorodiphenyldichloroethylene          DDT = dichlorodiphenyltrichloroethane

In general, Table 3 shows that the majority of the blue and green comparisons are for the Spatially-Explicit Case, which indicates the most consistent predictions relative to observed data. For risk assessment purposes, particularly human health risks, results for DDD/DDE/DDT are typically combined and quantified as total DDx. In this context, the Spatially-Explicit Case performs optimally, within 20% across all sites and species, and represents excellent performance.

Unfortunately, the data available for this site are single samples of composite fish, precluding a comparison of variance between predicted and observed. However, graphical comparisons of predicted versus observed are provided in Figure 3.
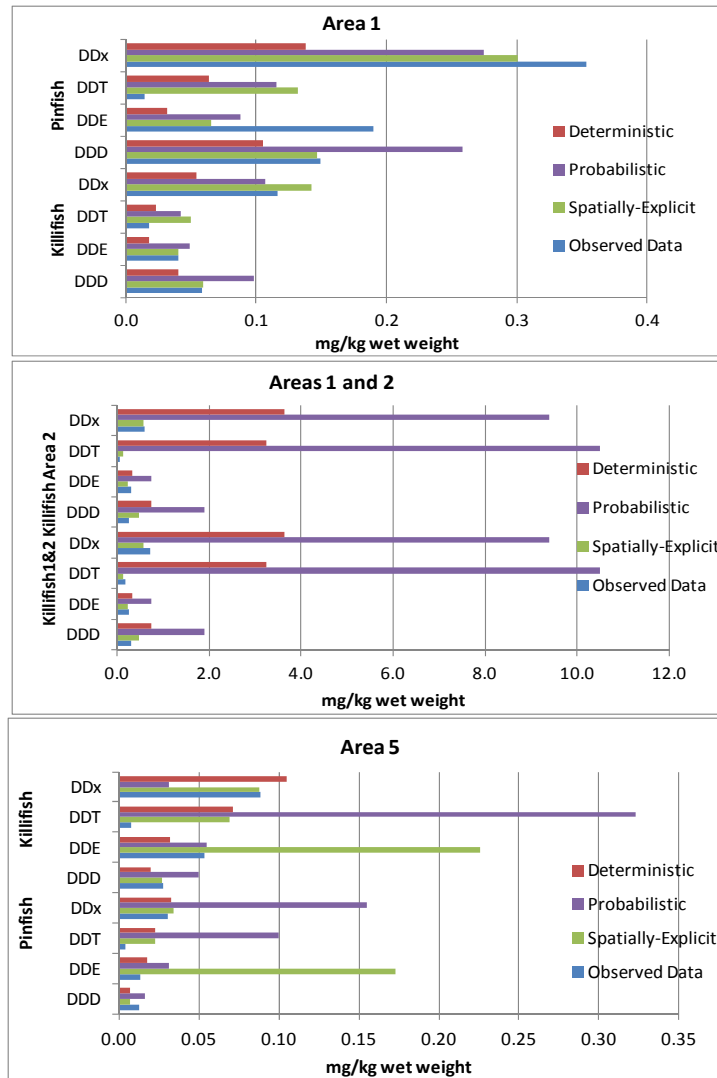
**Figure 3. Results of predicted versus observed across scenarios for the Tyndall AFB site.**

As shown in Table 3 and Figure 3, the probabilistic model performs particularly poorly for Areas 1 and 2 combined, largely a function of the high standard deviation in sediment concentrations attributable to the significant heterogeneity in concentrations across both areas. The spatially-explicit model tends to perform best, particularly in areas of spatial heterogeneity such as Area 1 and Areas 1 and 2 combined. By contrast, in Area 5, the advantages of the spatially-explicit approach are less evident. At sites with less spatial heterogeneity, (e.g., Area 5), a deterministic approach functions nearly as well.

Another observation from Table 3 and Figure 3 is that results for DDE are often under-predicted while results for DDT are over-predicted. One explanation for this is that DDE is a known metabolite of DDT in both fish and mammals. While the model allows for a metabolic term, data are insufficient to specify this term. Although it is possible to use the metabolic rate constant (currently set to zero, e.g., no metabolism) as a calibration parameter, this was not done for the current application. Further evidence for DDT metabolism is demonstrated by comparing the

proportion of each isomer to total DDx across sediment and fish (Figure 4). The Y-axis shows the proportion of DDD, DDE and DDT in total DDx for fish and sediment across Areas. The red bar denotes the percentage of total DDx represented by DDD, green is DDE and blue is DDT. The bars are mean percentages, with error bars described as one standard error from the mean.
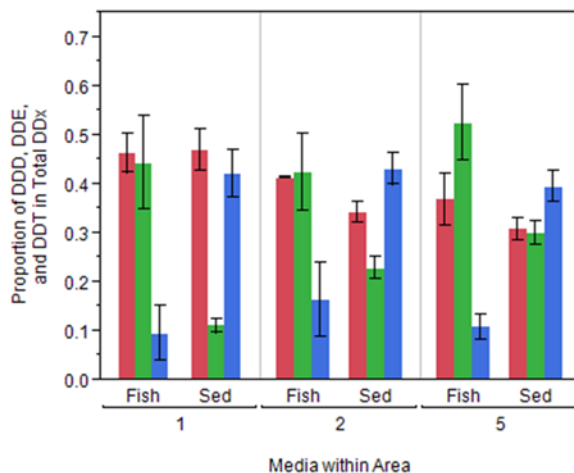


**Figure 4. Data-based proportion of DDD, DDE and DDT in total DDx in fish and sediment by area (1, 2, and 5) at the Tyndall AFB site.**

This figure shows that while the proportion of DDD (red bars) is similar across fish and sediment samples within an Area, the proportions of DDE (green bars) and DDT (blue bars) across fish and sediment samples are essentially reversed. For example, the proportion of DDE in total DDx in fish from Area 1 is approximately 0.45 (DDE comprises 45% of total DDx), while it is closer to 0.1 (DDE comprises only 10% of total DDx) for sediment, suggesting either enrichment relative to sediment or metabolism of DDT to DDE within fish. Similarly, the blue bars, which represent the proportion of DDT in total DDx, differ significantly between fish and sediment within an Area. This figure also highlights differences across Areas at the Tyndall Site, particularly for sediment. Areas 1 and 2 show very similar patterns, while Area 5 is very different. Proportions for fish are more similar, but do show some differences, particularly in enrichment of DDE in Area 5 (greater than 50%) relative to Areas 1 and 2 (approximately 45%). These differences have implications for the modeling, since the same Log $K_{ow}$ is used for a contaminant across areas (e.g., DDE has the same Log $K_{ow}$ regardless of area).

In its simplest terms, Log $K_{ow}$ represents the relationship between sediment organic carbon and lipid in organisms, so that if the proportion of DDE changes across areas, the model has no way to capture that apparent difference in the relationship, given that feeding preferences, metabolic rates, etc., are also the same across areas.

## 6.3    DISCUSSION OF RESULTS

The procedure to develop these two site-specific applications involved using data typically available from an RI/FS or similar process. The approach was to parameterize the site-specific food webs using existing data augmented with information from the literature. Once these inputs were determined, they were consistently applied across scenarios, which differed only in their characterization of exposure concentrations. This included a Deterministic Case (deterministic

SWAC, in both cases characterized by an arithmetic average); a Probabilistic Case (probabilistic sediment exposure concentrations but not spatially-explicit); and, a Spatially-Explicit Case. Both sites differed in their physical characteristics (NSSC is a freshwater lake while Tyndall AFB is an estuarine and brackish coastal system), and in the contaminants considered (PCBs and individual PCB congeners at the NSSC site; DDD/DDE/DDT at Tyndall AFB). Additionally, the spatial characteristics of exposure varied across scenarios, particularly at the Tyndall site. Area 5 is a relatively homogeneous area, with lower sediment concentrations, and essentially one single hot spot (SED175). Area 1 and Areas 1 and 2 together are highly heterogeneous, with sediment concentrations ranging from non-detectable to 100s of parts per million. The utility of the FR model in cases of heterogeneous contamination is evident in the results, which demonstrate the least value-added for Area 5 relative to other areas of the Tyndall Site and as compared to the NSSC Site. However, another factor to consider in the assessment for the Tyndall Site is that pinfish are largely (90%) tied to water rather than to sediment. Water concentrations were specified as point estimates across all scenarios (nominally set at approximately the detection level or less).

Figures 5 and 6 provide another graphical view of the comparison between model predictions and site data for the Tyndall Site and NSSC Site, respectively. Note that Figure 5 is on a log scale for ease of comparison since several of the model predictions were so much higher (e.g., for the Deterministic and Probabilistic scenarios) than observed data. The values shown in Figure 6 are as follows: all data points in the dataset are presented. For model output across scenarios, the mean, 5th percentile and 95th percentiles are presented. This figure shows that typically, the predicted 5th to 95th percentile ranges from the Spatially-Explicit scenario largely capture the range of observed data, and in all cases, compare most favorably relative to either the Deterministic or Probabilistic scenarios.
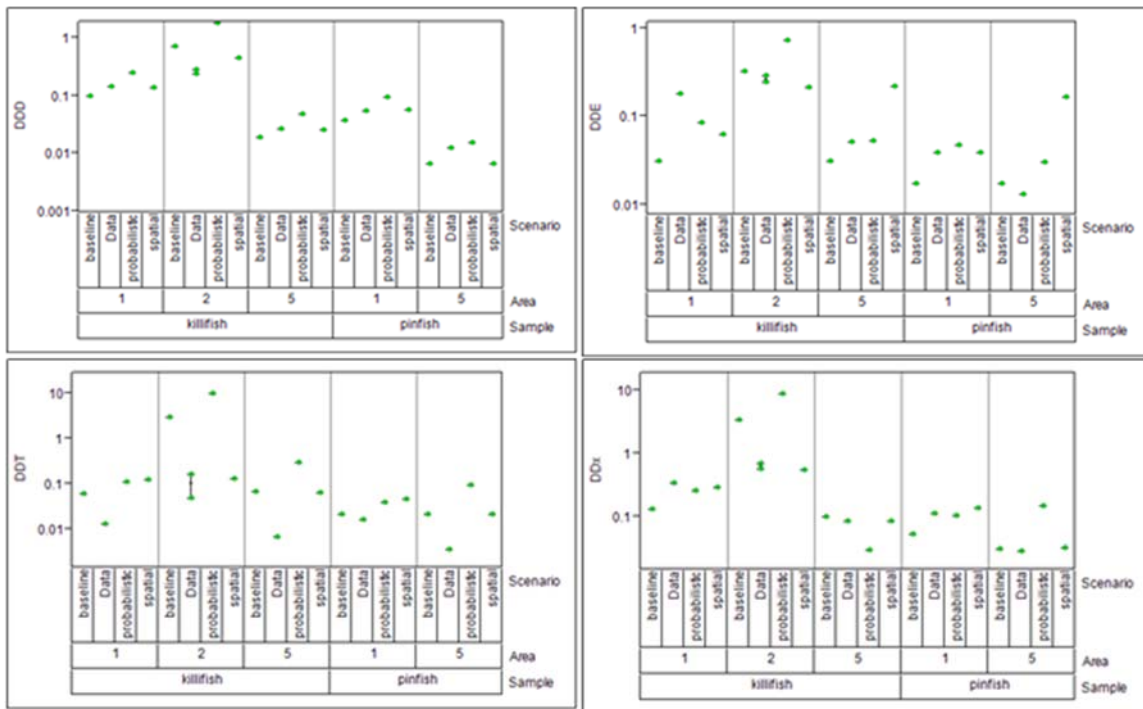


**Figure 5. Comparison of model predictions to site data for the Tyndall AFB site.**
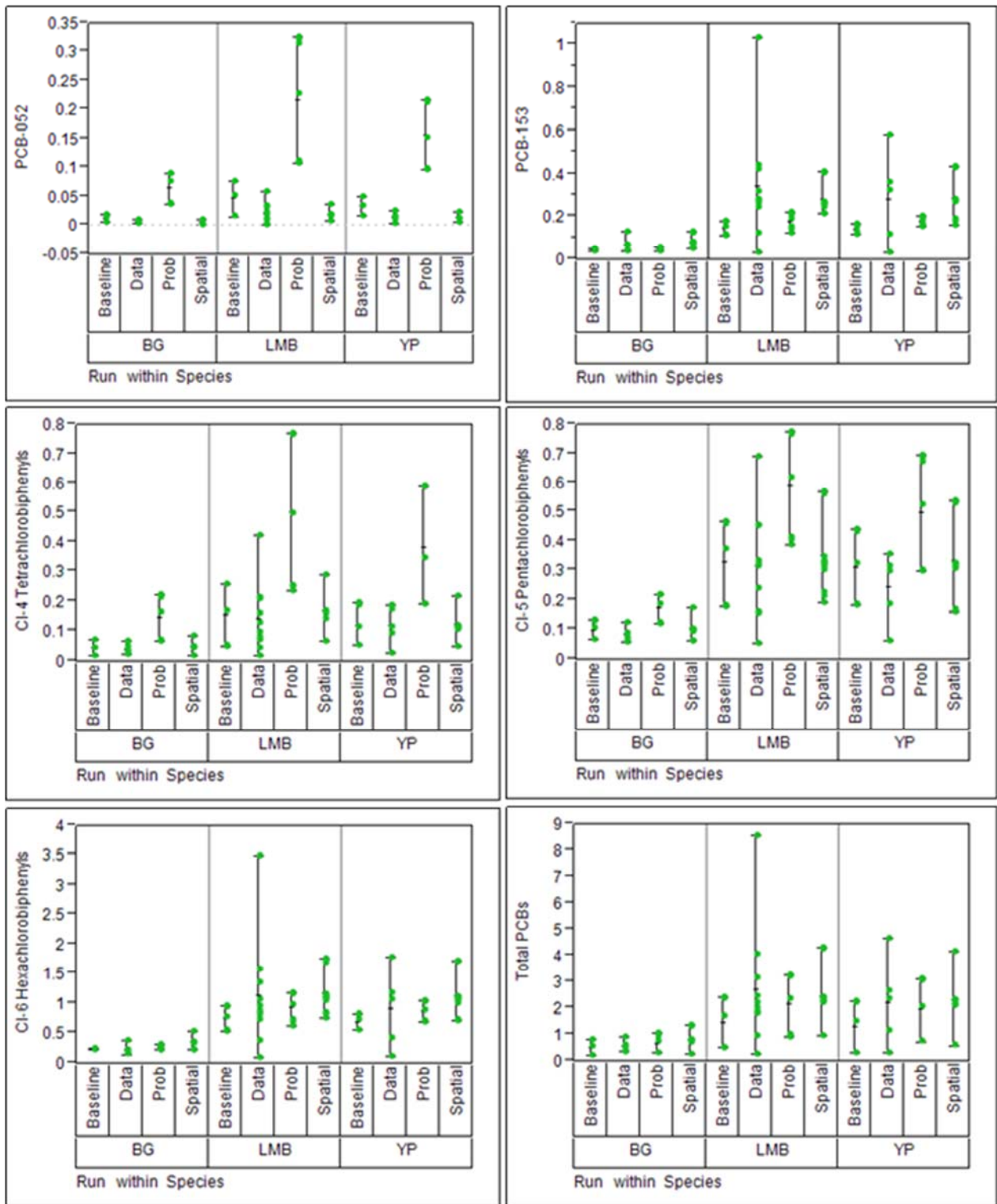(Note the log scale for ease of comparison)

**Figure 6. Comparison of model predictions to site data for the NSSC site.**

### 6.3.1 Model Calibration and Verification

In general, site-specific application of a model requires calibration and verification (USEPA, 2005; 2009). Models are based on a combination of data combined with a scientific understanding of physical and chemical processes. Most of the equations in a model include numerical coefficients. To the extent that site data are available, some of the coefficients are based on the fit of the equations to data, and others are taken to be universal constants based on laboratory studies (e.g., growth rate in fish). Where site-specific data are limited, coefficients may be values from scientific literature. For example, the modeling framework presented here is based on the well-established mathematical framework developed by Gobas (1993) and further refined by Arnot and Gobas (2004). Calibration of a model is the process of adjusting its coefficients to attain optimal agreement between predicted values and actual site data. Most commonly, model calibration consists of fine-tuning the model to provide the best fit to site data. The model is then verified by running the calibrated model without adjusting any inputs or adjusted coefficients to an independent data set, either using data from a different time period or geographic location (within the same site), or by excluding a portion of the data set to be used to compare with the results. Calculated and actual values are compared, and if an acceptable level of agreement is achieved, the model is considered verified. If not, then further analysis of the model is performed, leading to refinements that should improve the accuracy of the model.

For both sites presented here, the initial model parameterization led to an acceptable comparison between predicted and observed tissue concentrations without a formal calibration. However, this does not necessarily represent a typical application; particularly for larger, more complex sediment sites for which calibration is usually required (Gustavson et al., 2011). Oftentimes, this is attributable to the availability of larger datasets, particularly those representing more than one point in time. In both the applications presented here, data were only available for one sampling time, thus, it is not possible to evaluate model performance over time, which would be an important criterion at sites where greater temporal resolution in data are available, and for potential model deficiencies where calibration could be more evident. Site-specific model calibration focuses on adjustments to inputs that are potentially uncertain and for which the bounds on the data are generally wide.

An exhaustive discussion on model calibration and verification is beyond the scope of this document. However, much is known about sensitivity in modeling parameters for bioaccumulation models. For example, see von Stackelberg et al., 2002a; Gustavson et al., 2011; Barber, 2008; Burkhard, 1998; Ianuzzi et al., 1996; Imhoff et al., 2004), and site-specific model applications (most sites make their modeling documents publicly available, e.g., Hudson River, Duwamish, Portland Harbor, etc.). In general, bioaccumulation models are particularly sensitive to changes in Log $K_{ow}$, lipid content, total organic carbon, assimilation efficiency, growth rate, and feeding preferences, although the exact order of sensitivity will vary according to site-specific characteristics and data. Specific guidance on model calibration is given in USEPA (2005) and associated references.

### 6.3.2 Implications for Risk Management

Both of these sites are not particularly highly contaminated, which to some extent limits the utility of a more complex spatially-explicit model. By and large, for both sites, the deterministic model

performs reasonably well enough to support simplistic predictions of average fish tissue concentrations. However, the site-wide average total PCB sediment concentration at NSSC (1.4 mg/kg) is well within cleanup levels and remedial objectives derived at other sites (see for example, a compilation of remedial objectives assembled by the Interstate Technology Regulatory Council at http://www.itrcweb.org/contseds_remedy-selection/Default.htm#AppendixA/1AppendixACaseStudies.htm%3FTocPath%3DAppendix%2520A.%2520Case%2520Studies%7C_____0. Also, the Sediment Management Workgroup hosts a Major Contaminated Sediment Sites Database at http://www.smwg.org/MCSS_Database/MCSS_Database_Docs.html); similarly, no cleanup has been proposed at the Tyndall Site on the basis of contaminants in fish or fish consumption. This presents a challenge with respect to demonstrating the clear benefits of a spatially-explicit approach, in that both of these sites will not require remedial activities based on fish consumption as an exposure pathway.

Nonetheless, irrespective of absolute concentrations, it is straightforward to demonstrate that an evaluation of remedial alternatives is facilitated through use of the spatially-explicit approach. In the deterministic case, implementation of a remedial alternative will require deriving a new site-wide average concentration, while in the spatially-explicit case, it is possible to more realistically simulate the impact of specific actions, such as removing hot spot areas or all areas above a certain threshold. But in order to use the model in this way, it is necessary to first demonstrate confidence in the predictions. At the NSSC site, the FR model consistently predicted tissue concentrations within 50% across all PCB congeners, homologs, and total PCBs for largemouth bass, a top-level predator fish that would be the focus of decision making. The deterministic model was less consistent and did not perform as well on an individual congener basis, raising concerns about how well the model is really capturing exposures.

By definition, developing and evaluating remedial alternatives is a spatially-explicit process. Certain areas may be targeted for removal actions, or other management options such as capping. All of this spatial information will be lost when using deterministic approaches that rely on single, site-wide estimates of exposures.

# 7.0    COST ASSESSMENT

This section describes the costs associated with parameterizing and running the FR model. The cost assessment does not include costs associated with collecting the data, as these are assumed to occur regardless of whether the FR model is applied or not. In addition, the costs associated with developing GIS-based graphics of site concentrations are not included, as these would likely be generated whether or not a bioaccumulation model was being run. Therefore, only the costs associated with parameterizing and running the model are presented.

## 7.1    COST MODEL

The key costs associated with application of the model include creating the FR input files. This involves obtaining the input data through a combination of site-specific data already available along with literature reviews. Table 4 provides a summary of these costs described in greater detail in the following subsections.

**Table 4. Cost Model for an application of the FR spatially-explicit model.**

| Cost Element | Data Tracked During the Demonstration | Costs | |
|---|---|---|---|
| **Baseline site characterization – use of existing GIS data** | • Personnel required and associated labor <br> • Assumes GIS-based site characterization already exists <br> • Requires modeler to set up FR spatial files <br> • Complexity of spatial characterization will increase costs | Modeler will typically spend 2 weeks organizing the spatially-explicit inputs, and total organic carbon, temperature etc. Assumes 80 hours @ $80/hour. A deterministic model, all things equal, would require at least 60 hours. | $6,400 |
| **Food web parameterization** | Unit: $ per species <br> • Labor per species in the food web; assumes literature review combined with site-specific data | Modeler or junior analyst will typically spend 1 week per species. Generally a minimum of three fish species. This effort would be required for a deterministic model. | $10, 000 |
| **Computer run-time** | • Time required per run | • Not a direct cost | 15 min – 1 hour |
| **Calibration and verification** | • Personnel time | • Most difficult to predict and variable cost | $1,500 - $8,000 |
| **Post-processing** | Unit: $ per workbook <br> • Macros can be written to facilitate Excel-based workbook linkages | Modeler or analyst will typically spend 1 day per run (assumes five chemicals, one site, five species) | $640 |

## 7.2    COST DRIVERS

Costs for developing input files for use of FR depend on the complexity of the application (e.g., complexity of the food web being modeled), and data availability (e.g., site-specific versus literature-based). The cost evaluation assumes that a conceptual model of aquatic food web

exposures already exists as was the case for the two demonstration sites here. Cost estimates assume that the bioaccumulation model is being developed in conjunction with a suite of other site assessment tools and that appropriate data are already being collected as part of a larger site characterization process, such as an RI/FS or similar framework.

The least predictable and potentially most significant cost driver in any modeling application is the calibration and verification process. Different aquatic food webs might exist at complex sediment sites with different linked habitat areas (e.g., freshwater, estuarine, and marine). In addition, differences in population characteristics across locations might exist (e.g., specific species, feeding preferences, growth rates, etc.). Although no explicit calibration was required for the two demonstration sites presented herein, it may not represent a typical application. For example, development of the bioaccumulation model for the Hudson River Superfund Site (www.epa.gov/hudson) required extensive calibration, and that process resulted in some 40% of overall costs associated with bioaccumulation model development. This is an example of a site with over 20 years' worth of fish tissue data, and measured sediment and water exposure concentrations for only a few of those years.

## 7.3    COST ANALYSIS

Bioaccumulation modeling applications include simple, steady-state, deterministic applications to probabilistic, and time-varying applications. The cost differential between parameterizing the FR model versus another model is greatest for the simplest approach as compared to a full FR application. As mentioned previously, the cost estimates developed here assume that the bioaccumulation model is only one part of a larger site evaluation process, and that bioaccumulation model development leverages ongoing data collection activities and does not require an independent dataset or separate sampling program.

The level of effort required to acquire the data necessary to parameterize the food web (e.g., feeding preferences, habitat use or attraction factors, and lipid and weight of the organisms) will depend on the overall complexity of the site, and should be proportional to the resources expended for other site characterization activities. There is no prescriptive proportion, but estimates based on professional experience suggest that something on the order of 20% of overall site characterization costs would be attributable to the bioaccumulation modeling.

Depending on the site complexity, there are options available for model parameterization that can be more expensive and correspondingly provide more information for decision-making. For example, two key inputs, feeding preferences and habitat use (or foraging area) can either be based on literature values or professional judgment all the way to detailed, site-specific studies. Feeding preferences, whether site-specific or from the literature, are based on gut content analyses. Expending resources to evaluate gut contents from fish collected on site may not be warranted for small sites. Similarly, different kinds of tag-recapture studies provide data on site fidelity and use for specific species. Depending on the type of sensor used, and whether the data are temporally collated or simply obtained from two points in time, very detailed information can be gathered on where fish are spending their time, which can be directly incorporated to a spatially-explicit and probabilistic model like FR. Again, for large, complex sediment sites, the additional effort to develop site-specific information to support model development may be warranted given the potential expected costs of remediation or implementation of other management alternatives.

# 8.0    IMPLEMENTATION ISSUES

Implementing the FR model is uncomplicated given appropriate data inputs. However, the quality and quantity of data available from the site characterization process is a key consideration in the successful implementation of the model. In practice, data availability is a limiting factor with respect to model implementation. At many sites, data are not necessarily representative in time or space. Often, there is only one sampling event for sediment or fish or both, and the bioaccumulation model must capture the relationship between sediment exposures and resulting tissue concentrations based on this one sampling event. Similarly, often the bioaccumulation model is held accountable for potential limitations in understanding the relationship between sediment and water. For many, if not all, bioaccumulative contaminants, the assumption is that a bulk sediment concentration represents the relevant exposure metric with an incomplete understanding of: 1) how sediment concentrations may be changing over time (e.g., net deposition, net erosion, and so on); 2) the relationship between sediment and water (e.g., low flow and highly dissolved concentrations at certain times of the year, or resuspension events that carry contaminants to other areas in either the dissolved or particulate phases); and 3) potential sources and flux mechanisms (e.g., groundwater recharge, bioturbation, and mechanisms for releasing "buried" sediments). These kinds of interactions would typically require hydrodynamic and fate and transport modeling. However, occasionally, the bioaccumulation model is expected to capture exposures that may not be truly understood from a fate and transport perspective.

A challenge in bioaccumulation modeling has been in understanding what is meant by true exposures. The FR model tries to overcome this limitation, and does so by: 1) providing a mechanism for characterizing spatial heterogeneity in sediment (and water) exposure concentrations; and 2) simulating fish movement probabilistically rather than by using static approaches, including site averages, site-use factors, and similar deterministic adjustments. However, both foraging strategies of individual fish (e.g., spatial and temporal, in addition to appreciating what those prey items are, and whether they are primarily associated with sediment or water sources) combined with spatial heterogeneity in contamination contribute to population exposures. An understanding of species-specific fish biology is always desirable from a modeling perspective. Therefore, an implementation issue with respect to the model is how much site-specific data is available regarding fish biology. Tag-recapture studies and gut content analyses both provide important information relevant to the modeling. Oftentimes, these data are not obtained easily given limited resources (see above under costs). However, knowledge gaps in these areas might represent a significant source of uncertainty when parameterizing the model.
In general, a site-specific application of any model involves model calibration and verification.

Calibration is the process of making adjustments to a small number of input parameters to achieve the best fit between predicted model output and monitoring data. Verification (referred to as validation by USEPA, 2009) is the process of running a calibrated model and comparing the results to an independent data set not used in model calibration. In practice, it is difficult to have enough data to accomplish both calibration and verification using independent data sets. Therefore, many bioaccumulation models combine calibration with verification in one step. Also, if sufficient data are available, another approach is to divide the data in half, and use one half for calibration and the other half for verification. Sometimes it is possible to apply the model in one location (e.g., river reach) for calibration, and use data from another reach or operable unit for model verification.

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# APPENDIX A

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