Bioaccumulation Models: State of the Application at Large Superfund Sites

by Karl Gustavson, Trina von Stackelberg, Igor Linkov, and Todd Bridges

BACKGROUND: Sediment remediation for persistent organic contaminants such as polychlorinated biphenyls is typically conducted on the basis of contamination in fish and risks to those consuming the fish (including humans and wildlife). These contaminated sediment sites, often managed under the U.S. Environmental Protection Agency Superfund program, can be very large, complex, and expensive to remediate. Food web bioaccumulation models are quite important in determining remedial actions at the sites – they are often used to establish sediment cleanup levels and to compare the effect of various remedial scenarios on fish tissue concentrations. There are no prescribed methods for selecting and applying these methods at contaminated sites; as a result, their application can differ markedly at various sites. This technical note reviews the application of the models at four large contaminated sediment Superfund sites to document the state of the practice and to draw conclusions and recommendations from that combined experience.

INTRODUCTION: The purpose of the Superfund program is to protect human health and the environment from releases of hazardous substances. At contaminated sediment sites, the primary human exposure pathway to contaminants (particularly those sites with persistent hydrophobic contaminants such as PCBs) is through consumption of fish that have accumulated contaminants from the sediment. Sediment remediation is used to achieve a desired risk level associated with the ingestion of contaminated fish tissue; i.e., sediment contaminant concentrations are reduced to reduce fish tissue contaminant concentrations. However, the spatial extent of sediment remediation cannot be established by monitoring fish at a site, so sediment contaminant concentrations are used to delineate areas for remediation. As a result, understanding the relationship between sediment and fish tissue contaminant concentrations is essential to accurately define acceptable levels of sediment contaminant concentrations and to predict the impact remedial actions will have on desired risk levels.

Food web bioaccumulation models are used to describe the relationship between contaminant concentrations in sediment, water, and fish. In practice, they are frequently used to estimate fish contaminant concentrations resulting from exposure to specified sediment and water contaminant concentrations. The models are also used to back-calculate the sediment contaminant concentrations associated with acceptable levels of fish tissue contaminant concentrations.

There are several bioaccumulation models for these purposes (Imhoff et al. 2004; Weisbrod et al. 2007). Since the design and complexity of models vary greatly, as do modeling needs at sites and the availability of site-specific data, recent guidance from the U.S. Environmental Protection

Agency (EPA) on remediation of contaminated sediment (USEPA 2005) provides little guidance except:

> *The development of the sediment RGs [remedial goals] may involve a variety of different approaches that range from the simple application of a bioaccumulation factor from sediment to fish or more sophisticated food chain modeling. The method used and the level of complexity in the back calculation from fish to sediment should be consistent with the approaches used in the human health and ecological risk assessments.*

Arnot and Gobas (2004) describe the evolution of bioaccumulation models. Initially, they were simple models based on equilibrium partitioning from water until they became more advanced foodweb models that include dietary uptake from various food web components. Mass-balance bioaccumulation models are typically used for modeling food web transfer of persistent organic contaminants at sediment Superfund sites. The models estimate either the steady-state or time-varying concentration of fish based on the uptake of contaminants from water, diet and elimination through respiration, egestion, growth dilution, and metabolism (though for compounds such as PCBs, metabolism is assumed to be zero). The Thomann et al. (1992) and Gobas (1993) models and variations on those have gained the widest use and acceptance (Adams et al. 2005).

The models rely on a combination of site-specific data (e.g., contaminant concentrations in water and sediment), parameters that are literature-derived (e.g., chemical uptake or elimination rate constants), and other parameters that can be both (e.g., feeding preferences informed by site-specific information).

There are no specific protocols for the use and development of foodweb bioaccumulation models at Superfund sites, although there is general guidance on the use of environmental models at Superfund sediment sites (USEPA 2005). This guidance states that "where numerical models are used, verification, calibration, and validation typically should be performed to yield a scientifically defensible modeling study." In this context, verification refers to establishing that the model code does what it purports and that it is consistent with the theory behind the model. Calibration is the process of using site-specific information over some time period to adjust model parameters and obtain optimal agreement between measured and modeled data. Validation refers to running the calibrated model on an independent data set to establish that the calibrated model is predictive of independent conditions. Importantly, the guidance also specifies that models should be validated post-remedial action to provide a basis for their enhancement and to improve future model performance.

Food web models have been applied at many sites to understand the relationship between contaminant concentrations in sediment and fish tissue. They are also used to estimate sediment concentrations that pose a health risk to humans who consume exposed fish. It is not surprising that model application has varied, considering the differences between site conditions, modeling needs, practitioners, and a number of models from which to choose. The intent of this paper is to survey the application of these models at some of the largest Superfund sites, to document the state of the practice, and to draw conclusions and recommendations from that combined experience.

REVIEW OF THE APPLICATION OF FOOD WEB BIOACCUMULATION MODELS: The selection and application of food web models were reviewed at four large Superfund sites, the Housatonic River, MA; Fox River, WI; Duwamish River, WA; and the Hudson River, NY. These sites were selected because they are among the largest Superfund sediment sites, fish tissue contamination with PCBs is a major driver of risk, and food chain models play a major role in decision making. The food web models used at the sites are listed in Table 1. Total PCBs were modeled at all these sites.[1] Efforts to use simpler approaches to predict fish tissue PCB concentrations on the basis of sediment PCB concentrations (such as biota-sediment accumulation factors (BSAFs)) have often been rejected at large Superfund sites. Typically, this is because the BSAFs did not adequately represent the relationship between sediment and tissue concentrations (e.g., on the Fox [Exponent, Inc. 1999][2], Housatonic [Weston 2004a][3], and Passaic [Iannuzzi et al. 2011] Rivers). In addition, models based on empirical relationships have little predictive power since management alternatives are generally intended to result in concentrations below those that have been observed, and there is evidence that the ratio of tissue concentration to sediment concentration is concentration-dependent (e.g., accumulation factors are not constant across sediment concentrations) (Morrison et al. 1996, Cretney and Yunker 2000). This results in an application of the model outside the range of observed data. Finally, there is an assumption of equilibrium implicit in any bioaccumulation factor approach – both equilibrium between the organism and sediment or water, and between sediment and the overlying water column. Particularly in dynamic systems, these equilibrium assumptions are readily violated.

Table 1. Food web models selected for use at four Superfund Sites		
Site	**Model**	**Model Ref**
Fox River	FRFOOD (Thermo RETEC 2001)	Gobas (1993)
Housatonic River	Food Chain Model (FCM), adapted from QEAFDCHN 1.0[1]	QEA (2001a, b)[2]; Thomann (1992)
Duwamish River	Food Web Model (FWM) (Windward Environmental 2007)	Arnot and Gobas (2004)
Hudson River	FISHRAND (TAMS Consultants et al. 2000a, Books 3 & 4)	Gobas (1993)
[1] "FCM differs from QEA (1999), and several other published applications of QEAFDCHN, in that the benthic invertebrate concentrations are modeled mechanistically rather than through the application of empirically derived bioaccumulation factors (BAFs). The rationale behind this approach is described in detail in Section C.1.1 of the Model Calibration Report (Weston 2004b, p. C.1-4)." [2] The Housatonic modeling documentation does not provide a stand-alone reference for the model; rather, it says it was used in the Hudson and Fox and gives those references. However, the cited references are good descriptors of the model.		

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[1] The Housatonic River also modeled nine individual congeners (PCB-77, PCB-101, PCB-118, PCB-123, PCB-126, PCB-138, PCB-156, PCB-177, and PCB-183, and the Hudson River modeled five individual congeners (BZ#4, BZ#28, BZ#52, BZ#[90+101] and BZ#138). Total PCBs at the Hudson River are defined as the sum of the trichlorinated and higher congeners to correspond with the Aroclor-based data collected in earlier years.

[2] "Evaluations of pre-1998 and recent data show that total PCB concentrations in sediment and fish in the Fox River are not directly related to each other by any simple empirical function. Thus, tissue PCB concentrations cannot be accurately predicted from sediment PCB concentrations alone." (Exponent, Inc. 1999, p. 21).

[3] "Although appealing for their simplicity and empirical basis, [Bioconcentration factors (BCFs) and biota-sediment accumulation factors (BSAFs)] cannot adequately represent the complexity of PCB bioaccumulation in the aquatic food web in the Housatonic River." (Weston 2004a, p. 5-21).

Generally, the four models applied at these sites used either the Gobas model construct (Gobas et al. 1993) (Fox, Duwamish, and Hudson) or the Thomann model construct (Housatonic) (Thomann 1989; Thomann et al. 1992). The models have many similarities and model fish tissue concentration resulting from various uptake processes minus excretion processes (Burkhard 1998). The model used on the Housatonic River is described as a "dietary exchange model" while the Gobas models are based on thermodynamic-based exchange (Barber 2008). Details in model design, theory, and performance have been explored in depth by other authors (Barber 2003, 2008; Burkhard 1998, Burkhard et al 2004, Mackay and Fraser 2000) and will not be addressed in this technical note. Housatonic was the only one of the four sites that didn't use the Gobas model. The rationale was "Because the Gobas models are based on chemical fugacity principles rather than the conservation of mass, these models were not selected for the mass-balance-based Housatonic River modeling framework." (Weston 2004, p. 5-38).

All the models can be applied assuming steady state or dynamically (Burkhard et al. 2004). Only the food web model applied at the Duwamish site used a strictly steady state approach that assumed that environmental contaminant concentrations would not change over time (e.g., seasonal variations, inter-annual variations, or short-term disturbances) (Windward Environmental 2007). Other model applications were linked to a sediment and contaminant fate and transport model for estimating non-steady state (dynamic) accumulation of contaminants in organisms. The Duwamish application also included a probabilistic component to consider the uncertainty in estimated parameter values (see below for further discussion). The Hudson River's time-varying model incorporated a two-dimensional probabilistic approach to address both variability (e.g., distributions of concentrations across species-specific fish populations) and uncertainty (e.g., the uncertainty bounds around the population distribution).

Stated Purposes of Modeling. The objective of food web bioaccumulation modeling at Superfund sites is typically to 1) predict and compare the results of remedial actions on fish tissue concentrations, or 2) develop a risk-based sediment cleanup concentration on the basis of the relationship between contaminant concentrations in fish and sediment. The stated purposes of the foodweb modeling at the four sites are described below.

Housatonic River (Weston 2006):
- Predict average PCB concentrations in aquatic biota and assess relative performance among various remedies for reducing contaminant concentrations in biota.
- Quantify the historical and current relative contribution of various PCB source media (e.g., water, sediment) to bioaccumulation in target species.
- Estimate the time required for PCB concentrations in fish tissue and other biological compartments to be reduced to levels established during the risk assessment process, based on various response and restoration scenarios.

Fox River (ThermoRetec Consulting Corporation 2001a):
- Estimate concentrations of PCBs in multiple trophic levels in the aquatic food web (i.e., benthic insects, phytoplankton, zooplankton, and fish).
- Estimate risk-based sediment quality thresholds (SQTs) by running the model in "reverse" to calculate sediment concentrations that correspond to fish tissue concentrations.

- Estimate long-term human health and ecological risk reduction from selected remedial action levels in the RI/FS.

Duwamish River (Windward Environmental 2007):
- Estimate the relationship between total PCB concentrations in tissue and sediment.
- Estimate sediment PCB concentrations that correspond with risk to human health from eating fish tissue contaminated with PCBs. Risks from PCBs resulting from various cleanup alternatives were also estimated with the model.

Hudson River (TAMS Consultants, Inc. et al. 2000a):
- Determine when PCB levels in the fish population will recover to levels meeting human health and ecological risk criteria under continued no action.
- Determine whether remedies other than no action can significantly shorten the time required to achieve acceptable risk levels.
- Determine if there are contaminated sediments now buried and effectively sequestered from the food chain that are likely to become "reactivated" following a major flood, resulting in an increase in contamination of the fish population.

Trophic Level, Species, and Age Class of Modeled Organisms. A range of species and trophic levels are generally required to appropriately represent bioaccumulation through the food web. Selection of organisms was dependent on the model used, important species at the site, and whether tissue monitoring data were available for comparison to model predictions. An emphasis is placed on including necessary components while avoiding unnecessary complexity (Weston 2006). Table 2 summarizes the species and rationales used at the four sites.

Spatial Domain and Consideration of Fish Migration. Models predict fish tissue concentrations over a specified area. These areas are typically designated because they represent areas of contiguous hydrology or habitat types (for example, water areas between dams). Particularly important is matching the spatial scale of a modeling unit to the scale of an organism's exposure. The reviewed sites show wide variation in the size and segmentation of modeled areas (Table 3).

Migration among exposure areas or into uncontaminated areas is important in the modeling of contaminant uptake in fish. Clearly, whether or not a fish is actually exposed to predicted water and sediment contaminant concentrations will markedly affect whether a model application can accurately predict tissue contaminant concentrations. At the sites reviewed, a few modifications were made to account for the migration of fish, but mostly it was assumed that modeled fish remained in the exposure unit.

At the Housatonic River, Weston (2006) concludes "the exact nature of fish movements is difficult to predict. However, for the purposes of bioaccumulation modeling, it is reasonable to assume that PCB exposure to largemouth bass (and other fish) has occurred mainly in the reach from which fish were collected." A species-specific review of the life history was conducted that concluded that largemouth bass, sunfish, bullheads, and minnow exposures would occur within the designated subreaches; white sucker and yellow perch were expected to be more wide-ranging, but movement between areas was not simulated within the food chain model for two reaches (5 and 6). For the other two reaches (7 and 8), yellow perch (used only in an interspecies

extrapolation analysis) and white sucker use of areas was assumed to be proportional to habitat quality and was estimated using "weighted averages based on habitat quality factors" (Weston 2006, p. 2.4-10).

Table 2. Trophic levels and species included in foodweb models at sites.		
Site	**Trophic Level, Species, and Age**	**Comments**
Housatonic River	Invertebrates: water column organisms, epibenthic organisms, and benthic infaunal organisms. Fish: three trophic levels, five species: Predators (largemouth bass, 0-9+ years); foragers (minnows and sunfish, 0-5+ years); bottom feeders (bullheads and white sucker, 0-5+ years).	Fish species were chosen on the basis of their contribution to fish biomass, availability of tissue PCB data, representation of ecological niches, and importance in the risk assessments (Weston 2006, p. 2.4-4). For invertebrates, finer divisions were not made because site-specific PCB data indicated that there were no differences between feeding classes (Weston 2006, p. 2.4-1).
Fox River	Phytoplankton, zooplankton, benthic invertebrates (oligocheates and chironmomids), and fish (shiner, gizzard shad, carp, perch, walleye, rainbow smelt, and alewife)[1]; young-of-year and adults were considered for carp, alewife, perch and walleye.	Based on a review of the scientific literature and knowledge of regional fisheries biologists (ThermoRetec Consulting Corporation 2001a, p. 3-1).
Hudson River	Phytoplankton, zooplankton, benthic invertebrates, and fish. The food web included two forage fish (pumpkinseed, spottail shiner), white perch (semi-anadramous, semi-piscivorous), yellow perch, brown bullhead (demersal), largemouth bass (piscivorous), and striped bass (piscivorous, migratory). Forage fish represent predominantly yearling fish and piscivorous fish represent fish greater than 10 cm in length. The model predicts population distributions rather than specific age classes.	Selection of fish species for modeling body burdens was based on: 1) importance for fishing, 2) abundance, 3) importance in diet of other fish, 4) whether the selected species is representative of particular habitats or trophic levels, and 5) whether the selected species is representative of other fish species. Selected species were agreed upon in conjunction with NYSDEC, USEPA, and NOAA (TAMS Consultants, Inc. et al. 2000a, p. 9 of Bks3&4).
Duwamish River	Phytoplankton/algae, zooplankton, filter-feeding benthic invertebrates, scavenger / predator / detritivore benthic invertebrates, and fish. Three species of adult fish (English sole, Pacific staghorn sculpin, and shiner surfperch), two species of adult crabs (dungeness and slender crabs) and soft-shell clams (considered a filter-feeding benthic invertebrate) were selected. Juvenile fish, but not from any particular species, were modeled.[2]	Species were receptors of concern in the ecological risk assessment or served as key prey species for other receptors in the ERA or in the human health risk assessment (Windward Environmental 2007, p. 12).
[1] Rainbow smelt and alewife were only for the lower river reach and Lake Michigan (Green Bay zones 1 and 2). [2] "Juvenile fish in the FWM [food web model] represent small fish that would serve as prey for fish and crab species, such as Pacific staghorn sculpin and crabs" (Windward Environmental 2007, p. 40).		

Table 3. Size of areas encompassed by food web model predictions.	
Location	River Miles
Housatonic River (Weston 2006)	
Reach 5a	4.9 (40 acres)
Reach 5b	2.1 (26 acres)
Reach 5c	3.1 (43 acres)
Reach 5d	44 acres
Reach 6	0.6 (68 acres)
Reach 7a	1.5
Reach 7b	0.8
Reach 7c	0.8
Reach 7d	5.1
Reach 7e	0.7
Reach 7f	5.9
Reach 7g	0.6
Reach 7h	2.7
Reach 8	1.1
Fox River (RETEC Group, Inc., and Natural Resources Technology, Inc. 2002)	
Little Lake Butte des Morts Reach	6
Appleton to Little Rapids Reach	20
Little Rapids to De Pere Reach	6
De Pere to Green Bay Reach (Green Bay Zone 1)	7
Green Bay Zone 2	7.6 miles from the Fox River mouth into Green Bay
Hudson River (TAMS Consultants, Inc., et al. 2000a)	
Thompson Island Pool	5 (RM 188-193)
Stillwater	8 (RM 168-176)
Waterford	2 (RM 155-157)
Duwamish River (Windward Environmental 2007)	
Duwamish River	5.25
NA = Not applicable; these are broad and shallow backwater areas above area 6; river miles are not appropriate. RM = River mile. Sources: Housatonic River: Weston et al. 2006, Table 1-1; Weston, Inc. 2004a, Tables 2-2, 2-3; Fox River: RETEC Group, Inc. and Natural Resources Technology 2002, pp 1-6 to 1-7; Duwamish River: Windward Environmental 2007, p. 13; Hudson River: TAMS Consultants, Inc. et al. 2000a, p. 51, Books 3 and 4.	

In the Duwamish River, there was only one modeling area over the 5.25-mile study area. It was assumed that fish and crab species used all areas equally and a surface-weighted average concentration (SWAC) was used to represent PCB sediment concentrations. No adjustments were made for species that may move out of the site for part of the year. However, it was recognized

that there was uncertainty in that decision. The summary report (Windward Environmental 2007) indicates that "fish and crab species may preferentially use some areas of the LDW (Lower Duwamish Waterway) with more suitable habitat (e.g., better food sources or refuge from predators) more than other areas" and that "some species may leave the LDW for part of the year." A separate analysis[1] was conducted to evaluate whether smaller exposure areas would be appropriate for the modeled species. Results indicated that smaller exposure areas could be appropriate for shiner surfperch and staghorn sculpin. The analysis also indicated that smaller areas were not appropriate for English sole and the crab species because they were wide-ranging relative to the smaller areas. Ultimately, the lower 5.25 miles of the river was used for all species.

In the Fox River, the top three reaches of the system are separated from one another by dams, so migration between the reaches is not an issue. These reaches are long – one reach is 20 miles long; possible variable exposure within the reaches is not considered. Fish within the lower two units (the 6 miles above the mouth of Green Bay to 7.6 miles into Green Bay) were assumed to receive 100 percent of their PCB exposure within the combined area.

The upper Hudson River is separated by a series of locks and dams, which generally impede significant migration across pools. However, the model did evaluate the white perch (a semi-anadramous species) in the upper river as well as striped bass in the lower river (a highly anadramous species), both of which experience exposures over larger geographical areas.

Model Inputs. As described above, foodweb model inputs are from a range of sources. Model inputs of chemical concentrations in environmental compartments are almost always site-specific (though they will include estimates based on partitioning or from fate and transport models), while the organism contaminant uptake and elimination rates are generally specified in the model. Other components such as species feeding preferences can be a mixture of both. Because the models used at the sites were different (or were different iterations of the same model construct), there is little consistency in parameters among the applications reviewed here; therefore there is not a one-to-one comparison of input parameters across sites. A comprehensive review of individual model inputs and their function is beyond the scope of this paper. This section summarizes the descriptions provided in the model documentation.[2]

Contaminant data. Environmental contaminant concentrations form the basis of every foodweb model. The derivation of the concentrations used as input to the models varies. Sediment and water concentrations can be estimated from a linked sediment and contaminant fate and transport model or from point estimates of environmental concentrations (e.g., area/time average contaminant concentrations).[3] At the reviewed sites, PCB exposure concentrations in water and

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[1] Woodward Environmental 2007, p. 13: "Statistical analyses were conducted at the tissue sampling areas scale (ANOVAs) to explore absolute differences in total PCB concentrations in tissue among areas and at the tissue sampling subareas scale (regressions) in order to explore relationships between total PCB concentrations in tissue vs. sediment. This information was used to draw conclusions about how well the FWM is expected to perform at the scale of the modeling areas."

[2] The amount of information provided in the model documentation reports varied across sites; the Housatonic River (Weston 2006) and Hudson River (TAMS Consultant, Inc. et al. 2000a) reports provided more information than others.

[3] In this context, point estimates refer to an environmental concentration over a specified area at a point in time, rather than, for example, the contaminant concentration in a specific sediment sample.

sediment were based on a combination of monitoring results and fate and transport modeling. Sediment concentrations were typically described as organic carbon normalized (mg PCBs/kg organic carbon (OC)) to better address bioavailability and variability. A description of the available data for each site follows.

Housatonic: Model simulations required sediment PCB concentrations (mg/kg OC); PCB concentration of particulate organic matter in the water column (mg/kg OC); dissolved PCB concentrations in water (μg/L), and dissolved PCB concentration in sediment pore water (μg/L) – pore water and particulate organic matter PCB concentrations were determined by modeling partitioning processes supported by site-specific studies. Sediment contaminant concentrations were specified for the biologically active zone (the depth of sediments to which organisms are exposed), the depth of which varied depending on whether EFDC, a combined hydrodynamic, sediment transport, and contaminant fate and transport model, was used to predict PCB concentrations or whether empirical (measured) data were being used. When contaminant data were estimated using the EFDC model, the thickness of the biologically active zone varied on a "reach-species" basis between 4 cm and 7 cm. When the estimates were based on empirical data (which they were during one component of the calibration [see below]), OC-normalized PCB concentrations in the active layer of sediment (6 in./15 cm) were used (Weston 2006, p. 2.4-36). Data were extracted from the site's database and the arithmetic mean of each reach/time period was used (Weston 2004b, attachment C.14). The PCB exposure concentrations were aggregated for each reach (e.g. 6,7,8); subreach averages were not derived (e.g., 7a,7b, 7c, etc.) (Weston 2006, p. 2.4- 36).

Fox: The food web model on the Fox River required input of sediment and water PCB concentrations. The calibration of the food web model (described below) used either empirical "point estimates" of contaminant concentrations or concentrations generated by the linked contaminant transport models (Whole Lower Fox River Model and the Enhanced Green Bay Toxics Model). Empirical point estimates of total PCB concentrations in the top 10 cm of sediments in each river reach were a SWAC interpolated from surface sediment bed maps populated by the site's database. PCB concentrations in water were the soluble fraction (filtered water; the reach-wide mean or upper confidence limit of the mean (UCL), also derived from the site database) (ThermoRetec Consulting Corporation 2001a, p. 3-3). The linked contaminant transport models provided sediment PCB concentrations for the upper 10 cm and PCB concentrations in whole (unfiltered) water samples.[1]

Duwamish: PCB concentrations in the water column, porewater, and sediment were included in the site's food web model. Water column PCB concentrations were derived from site data via the EFDC hydrodynamic and contaminant fate modeling; the dissolved fraction was estimated by modeling three-way PCB partitioning between particulate organic carbon, dissolved organic car-

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[1] The rationale for using dissolved PCB concentrations in the point calibrations (not total PCBs as provided by the linked contaminant transport models) was: "Filtered water total PCB concentrations were used rather than estimated water total PCB concentrations, because when filtered and estimated total water concentrations of total PCBs were compared, it was found that water concentrations of total PCBs varied seasonally over time. Filtered water total PCB concentrations varied less than estimated total water concentrations. The variation was observed to be dependent on the degree of phytoplankton production. In order to not have PCB concentrations in phytoplankton counted twice, filtered water concentrations rather than total water concentrations were used as inputs in the calibration for the FRFood Model (ThermoRetec Consulting Corporation 2001a, p. 3-4)."

bon, and the freely dissolved phase. Porewater PCB concentrations were estimated assuming equilibrium partitioning with the sediment (Windward Environmental 2007, p. 7). The average sediment PCB concentration at the site was a SWAC developed from sediment concentrations within the site's database.[1] The sampling depth(s) for designating surface sediment PCB concentrations was not provided in the Duwamish foodweb modeling report.

Hudson: The FISHRAND model requires freely dissolved water and sediment concentrations as inputs. For the Hudson River application, the model used monthly dissolved water and annual sediment concentrations generated by the HUDTOX fate and transport model (TAMS Consultants, Inc. et al. 2000a, pp. 27 and 74 of Books 3 and 4) expressed as distributions representing uncertainty around a mean estimate (lognormal specified by a mean and standard deviation). The input distributions for sediment were estimated based on the assumption that aquatic organisms are exposed to a sediment mixture consisting of 75% cohesive (fine-grained) sediments and 25% non-cohesive sediments. The model assumed a biologically active zone (bioturbation or mixing depth) of 10 cm.

Other Model Parameters:

Housatonic: Weston (2006) summarizes the parameters in the food web model and their basis (see Table 2.5-3, Weston 2006). Of the 30 parameters described, approximately one third are site-specific or have site-specific components. For example, invertebrate lipid contents were literature-derived; fish lipid concentrations were derived from site-specific data. Protein concentrations were literature-derived. The energy density of sediments as a food source was also literature-derived. Growth rates for fish were estimated from site-specific data (except that the age of minnows, sunfish, and bullheads, which was used in growth rate estimation, was estimated on the basis of literature data)[2]; for invertebrates, growth rates were literature-derived. Respiration rates were literature-derived. K_{ow} values, used as model inputs and to derive other partitioning parameters, had literature-derived and site-specific components. Contaminant/food assimilation efficiency ratios (which varied with the K_{ow} of compound) for water column fish, bottom-feeding fish, and invertebrates, were literature-derived. Contaminant elimination via respiratory exchange and fecal elimination were combined and simulated as a "lumped" process: literature values and previous applications of the bioaccumulation model were used to select the gill elimination constant and associated resistance factor. A literature-derived PCB uptake efficiency of one was used for fish and invertebrates.

Diet composition for species was established on the basis of literature reviews and site-specific knowledge. Evaluations of stomach contents were not available to provide site-specific information on fish diet composition (Weston 2006, 2.4-15). Feeding preferences varied by age class of fish and by reach (for minnows and largemouth bass only). For largemouth bass, the age class of fish prey was also designated for different age class fish.[3] For bullhead and white suckers, it was

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[1] Windward Environmental 2007 (p. 24): "SWAC calculated using IDW [inverse distance weighting] on October 20, 2006, based on 1,264 samples [collected since 1990] from the LDW baseline surface sediment database."

[2] Growth rates were estimated on the age-weight relationships from sampled fish (including from other water bodies within the watershed). The relationship was modified to adjust for growth only during the growing season.

[3] While crayfish make up a substantial portion of adult largemouth bass diet (17-31 percent) and bullhead (as much as 50 percent), they are not included in the diet composition, however, they are assumed to be similar in PCB concentration to fish and benthic invertebrates (Weston 2004b, p.24).

assumed that 20 percent of diet was sediment/detritus. In downstream reaches (7 and 8), feeding preferences from upstream reaches (5 or 6) that had the most similar habitat were used (Weston 2004b, p. 24). A sample table showing food preferences is provided below (Table 4). It was assumed that benthic infauna feed 100 percent from the sediment bed and water column invertebrates 100 percent from suspended particulate matter. Sediment-derived energy sources were assumed to range from a minimum of 35 percent to a maximum of 75 percent for all reaches.

Table 4. Sample feeding matrix for white suckers on the Housatonic River.						
Prey	Age Class 0+	Age Class 1+	Age Class 2+	Age Class 3+	Age Class 4+	Age Class 5+
Sediment detritus	0	20	20	20	20	20
Infauna invertebrates	0	0	0	0	0	0
Water column invertebrates	20	0	0	0	0	0
Epifauna invertebrates	80	80	80	80	80	80
Fish	0	0	0	0	0	0
Source: Weston 2004b, Table 21.						

Fox: The Fox River model documentation (ThermoRetec Consulting Corporation 2001a) provides little information on model components or the source of their values. The report discusses diet composition, lipid contents, and organism weights. It is expected that model input values other than environmental variables (contaminant concentrations, organic carbon content, etc.) were literature-derived or model default parameters.

Values for diet composition of fish (species and percent prey based on weight or volume of prey) were determined from a literature search. For walleye, site-specific evaluations of fish stomach contents were used. Diet composition was used as a calibration variable so values could vary between river reaches. No information is provided for organisms other than fish.

Duwamish: Windward Environmental (2007, p. 8, 22) provides a description of model inputs and their sources. They document that the food web model required the selection of values for 114 input parameters.[1] Information on these values was derived from site-specific data and the literature (including default values used in previous applications of the food web model). Probability distributions were developed for 95 parameters, and point estimates were used to characterize 19 parameters. Site-specific data were used to derive values for eight environmental parameters: sediment PCB concentrations, sediment total organic carbon, PCB concentrations in water, and five water quality parameters (total suspended solids, dissolved oxygen, dissolved organic carbon, particulate organic carbon, and temperature). For those values with sufficient information to develop probability distributions, statistics (mean, mode, and standard deviation) were generated and either a normal or triangular distribution was assumed to represent the uncertainty around the mean estimate.

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[1] Many parameters, e.g., weight, lipid content, and dietary fractions, are duplicated for each of the different organisms in the food web; i.e., there are not 114 parameters for each organism.

Dietary scenarios were established for all species except phytoplankton and zooplankton by considering "ecology, behavior, feeding observation studies, and stomach content analyses" (Windward Environmental 2007, p. 45). Stomach content analyses (apparently from Puget Sound and the region, but none was site-specific) were the dominant sources except for clams, which were based on "literature and best professional judgment." Different dietary scenarios were created to represent the variability and uncertainty in the diets and to support the probabilistic approach used in the modeling; triangular distributions were assumed for each dietary item.

Hudson: The FISHRAND model used for the Hudson River requires probability distributions for user-defined inputs. In addition, the Gobas model rate constants can be specified by distributions as well. Tables 6-1, 6-2, and 6-3 of Books 3 and 4 (TAMS Consultants, Inc. et al. 2000a) summarize the input distributions used for the modeling. The approach was to minimize the number of inputs and rely primarily on site-specific data for key parameters. Site-specific inputs included: lipid content of fish, dietary preferences of modeled species (based largely on site-specific stomach analyses augmented by the literature), fish weight, total organic carbon, and temperature. Literature-derived values were used for growth rate and Log K_{ow}, although these two inputs were used as calibration parameters.

Model Calibration and Validation. Following initial model setup, food web models are calibrated by adjusting the "calibration parameters" to provide optimal fit to collected fish tissue data. There are no pre-defined calibration variables; these are chosen by model developers and will vary across sites. Once a model is considered calibrated, it is validated by comparing model output from the calibrated model to a new set of empirical data. Again, there are no specified procedures or performance criteria for model validation. The approaches used for calibration and validation at the studied sites are described in this section.

Calibration Procedures:

Housatonic River: Food chain model output (PCB tissue concentrations for a given species/reach/age) was calibrated during two phases on the basis of its ability to predict measured fish tissue concentrations. The Phase 1 Calibration period, from 1995 through 2000, used both empirical contaminant exposure data (data gathered during the calibration period) and output from EFDC, which modeled water and sediment concentrations. The objective of Phase 1 "was to ensure that, without requiring substantial manipulation of the model code, and using best initial estimates of model parameters, model performance was acceptable across a range of reaches, organism types, and PCB congeners" (Weston 2006, p. 3.3-8). The Phase 2 Calibration period used only EFDC exposure inputs from January 1, 1990 through June 30, 2000. Field-collected tissue PCB data (collected between 1998 and 2000) were compared to model output from October 1, 1998 – the timepoint closest to the majority of the EPA tissue collections in Reaches 5 and 6. Results from the phase 2 calibration are considered the final calibration results for food chain model (Weston 2006, p. 3.6-1).

Fox River: The model's ability to predict fish tissue contaminant concentrations was calibrated in two stages. First, the model was calibrated using empirical data (reach-wide sediment and water average contaminant concentrations) to derive fish tissue concentrations. Here, the sediment PCB concentrations were SWACs derived from bed sediment maps based on data collected from 1989 through 1998 (ThermoRetec Consulting Corporation 2001b). The model's average

fish tissue PCB concentration was compared to the average PCB concentration in fish (by reach and species) collected between 1989 and 1998. In the second stage, output from the site's contaminant transport model was used to provide sediment and water concentrations (presumably the average PCB concentrations) from 1989 to 1995 for input to the food chain model. Predicted fish tissue concentrations were then generated using the food chain model. Linear extrapolation of the food chain model results was used to estimate fish tissue concentrations out to 1998.[1] Model output was then compared to fish concentrations over the 1989–1998 time period. There were only sufficient fish data at four of the five reaches to compare to model output. Model results for invertebrates were not calibrated.

Duwamish: Calibration of the Duwamish food web model was probabilistic. Parameter values were randomly selected from their probability distributions (resulting in a parameter set) and the model run to yield an estimate of PCB concentrations in tissues of the modeled species. PCB concentrations in water were represented as a distribution, while PCB sediment concentrations were a point estimate (a single SWAC was used). Predicted PCB concentrations in tissues were then compared with the mean tissue PCB concentration measured in each modeled species. The parameter sets that had a difference greater than a factor of 2 (ratio of estimated to empirical total PCB concentrations in tissue [or its inverse] for a given species) were rejected. A best-fit parameter set – the set that produced estimates most similar to the empirical data (lowest mean ratio across all species with empirical data) was then identified. Benthic invertebrates (clams) were not included in the calibration of the foodweb model. No empirical data existed for phytoplankton, zooplankton, or juvenile fish, so the model was not calibrated for those species.

Hudson: The FISHRAND calibration approach relied on statistical methods applicable to non-linear models. A sensitivity analysis based on elasticities (the effect of a percentage change in an input on the dependent variable) was used to select several of the most important parameters for calibration. Likelihood profiles, a Bayesian calibration method, were used to select ranges of variation and to assign corrected prior distributions for these parameters. Finally, parameter distributions were updated using Bayesian Monte Carlo techniques to incorporate the full range of experimental data to derive posterior distributions for the model parameters within the range of observed data. (That is, a distribution could not incorporate values that had not been observed). This process is known as Bayesian Updating. The approach optimizes the agreement between predicted and empirical fish concentration distributions by adjusting the input distributions identified as most sensitive through the likelihood profiling. The model was calibrated for two river reaches and the calibrated model applied to the third river reach.

Tissue Data Used in the Calibration:

Housatonic: Between 1998 and 2000, samples of 11 species of fish were collected and analyzed. These data were used for the final calibration of the model (phase 2 calibration). Additional fish tissue PCB data (from 1980 through 2004) were available from Reaches 5 and 6; these data sets were used only for model validation. The Housatonic River was the only application that calibrated model output to invertebrate contaminant concentrations. Weston (2004b, p. 6.3-14) describes four primary sources of calibration data for invertebrate tissue PCB concentrations: invertebrate D-net samples, oligochaete bioaccumulation data, crayfish tissue data, and tree

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[1] It is not stated why the contaminant transport model only predicted surface and water concentrations to 1995.

swallow stomach contents. However, the D-net samples (mean PCB concentrations measured in the D-net invertebrate samples) [1] were focused on in the calibration; it was only indicated whether the other invertebrate data sources corroborated results from the D-Net samples.

Fox River: Fish tissue contaminant concentration data were available from several sampling efforts between 1989 and 1998. The amount of data varies by reach, species, and year (Thermo-Retec Consulting Corporation 2001a, Table 3-6).

Duwamish: Tissue PCB concentration data used to compare to model output and calibrate the model were from sampling efforts in 1997, 2004, and 2005. The 1997 effort had samples only from Dungeness crabs (two meat samples and one hepatopancreas sample) and shiner surfperch (three composites of 10 fish per composite). The 2004 data set was the most extensive; however, a large dredging event took place that year and fish tissue concentrations were significantly higher than they were before or after (Windward Environmental 2007, p. 52). As a result, two data sets were used in the calibration: "calibration 1" included 2004 fish data and "calibration 2" excluded it. Empirical PCB concentration data were not available for phytoplankton, zooplankton, and juvenile fish tissues.

Hudson: NYSDEC has been collecting fish tissue data on an Aroclor basis since 1977 for various species at different locations (described in Table 4-5 in TAMS Consultants, Inc. et al. 2000a). In addition, EPA collected fish and analyzed them on a congener basis during 1993. The EPA sampling program also collected invertebrates (the only year for which invertebrates were collected).

Performance Criteria: In all the modeling applications, the models' ability to predict empirical fish tissue concentrations was quantitatively evaluated. The criteria for acceptance of model performance are listed in Table 5. Weston (2006) emphasized that the criteria were not absolute criteria for model acceptance or rejection, but one of a number of measures to judge the utility of the model.

Calibration parameters: Typically in model calibration, a number of model parameters are varied to minimize the difference between predicted and observed tissue contaminant concentrations. In most cases, the most sensitive parameters are used as those provide the greatest adjustments in terms of predictions. The modeling reports typically emphasized that the values of the calibration variables needed to be plausible and reflect knowledge of the site. For the Fox, Housatonic, and Hudson Rivers, specific variables were chosen for calibration; in the Duwamish, a probabilistic approach was taken that encompassed most variables in the model.

Housatonic: The "vast majority" of calibration adjustments were made during phase 1 calibration (see above) where parameters were adjusted within the ranges of plausible values that were identified prior to the analysis. Model parameterization remained "essentially unchanged" during the phase 2 calibration. The report emphasizes that there was a strong preference to retain the "best estimate" values identified prior to calibration. The following parameters are identified as having "small-scale refinements" during the calibration process: feeding preferences matrices

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[1] Composite samples of predators and shredders collected in 1999; samples were predominantly epifauna with a small amount of infauna (e.g., oligochaetes) (Weston 2004b).

(invertebrates and fish); chemical uptake assimilation efficiencies; cyprinid respiration rates; energy density of POM (Weston 2004b, p. C.3-10).

Table 5. Performance criteria for food web models selected at 4 Superfund Sites.		
Site	Calibration	Validation
Fox River	Agreement of plus or minus one-half order of magnitude between the predicted and measured mean and 95th upper confidence limit of the fish tissue concentrations.	No separate validation, so no validation performance metric.
Housatonic River	Fish and invertebrates: ratio of total PCBs (central tendency, wet weight and lipid normalized) should be within a factor of 2.	Fish: ratio of total PCBs (central tendency, wet weight and lipid normalized) should be within a factor of 2.5; invertebrates should be within a factor of 3.
Duwamish River	Calibration was conducted within the model's probabilistic framework. The parameter sets that resulted in estimated concentrations with a difference greater than a factor of 2 (comparing model predictions to measured means) were rejected.	No separate validation, so no validation performance metric.
Hudson River	The calibration was done using Bayesian updating. Although no formal performance criteria are identified in the report, it was determined that, overall, the FISHRAND model predicts mean wet weight Tri+ PCB fish body burdens to within a factor of two, and typically significantly less than that.	Several approaches were used to validate the FISHRAND model. One method was to calibrate FISHRAND for one river segment, and then to run the model for a different river segment. Satisfactory agreement for both river miles implied model validity across locations in the Hudson River. In addition, a calibration was conducted using only part of the available dataset, and then the model results were compared with the remaining portion of the dataset. The posterior distributions obtained using only the partial dataset were compared to the posterior distributions obtained using the full dataset. Finally, the partial-data calibrated model was run for the forecast period and these results were compared to the full-data calibrated model results. Good agreement across all three metrics implied confidence in the performance of the model. No specific validation metrics were defined.

Fox River: The report (ThermoRetec Consulting Corporation 2001a, p. 3-3) indicates that dietary inputs for the food web species were generally based on average consumption, but modified as necessary for calibration purposes. Lipid concentrations for fish were also treated as a calibration variable.[1] The model was parameterized for each reach and its specific food web (Wisconsin Department of Natural Resources (WDNR) and USEPA 2002, p. 6-21). These parameters were varied "within the published range of values" until PCB concentrations in the modeled fish matched measured values as closely as possible. Little additional information is provided regarding the model's input variables and the source of model input. It is expected that other input values were literature-derived or model default parameters.

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[1] It appears that the lipid concentrations used in the model were always the mean lipid concentration for that reach (ThermoRetec Consulting Corporation 2001a, p. 3-4).

Duwamish: Windward Environmental (2007) indicates that probability distributions were developed for 95 parameters. All of these could be considered calibration variables. This includes environmental data such as PCB concentrations in water, total suspended solids, sediment organic carbon, and temperature.

Hudson: To determine the best parameters for calibration, a sensitivity analysis was conducted using an analytical solution to the Gobas model. The sensitivity analysis focuses on the relationship between predicted fish body burden and the rate constants as well as user-defined parameters. The elasticity of each parameter is estimated by obtaining the partial derivative of each parameter with respect to predicted tissue concentration. Elasticities are used to interpret the effect of a percentage change in the independent variable on the dependent variable. This is known as likelihood profiling. The final parameters selected for calibration include: total organic carbon, Log K_{ow}, growth rate coefficient (for largemouth bass), and percent lipid in fish.

Calibration Results: The general conclusions of the calibration are presented here. Greater specificity regarding the output of the models for selected fish is provided below under, "Review of Example Model Output and Performance."

Housatonic: Weston (2004b) outlined food chain model calibration results based on input from empirical data and from EFDC. For invertebrates, using the food chain model fed by empirical data, the conclusion was that the results were in strong agreement (see Figure 1)[1] and simulations of PCBs in epifauna were "well within the factor of 2 performance measure" (Weston 2006, p. 3.6-8). A similar conclusion was reached for the EFDC-linked model calibration (phase 2). Invertebrate sampling was not conducted in reaches other than 5 and 6. For fish, using empirical data, the report indicates that overall the model-simulated fish tissue concentrations were within the calibration targets (Weston 2006, p. 3.6-10). The linked model produced simulated PCB tissue concentrations that were within a factor of two of the mean for measured PCB concentrations for all fish/reach combinations except minnows in the downstream portion of Reaches 5 and 6 (Weston 2006, p. 3.6-8).

Overall, Weston (2006) concludes that the phase 2 calibration produced simulated PCB concentrations that were within the model performance measures and that it produced a bioaccumulation model that is "relatively unbiased overall."

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[1] Results for epifauna are described while those for infauna and zooplankton are not. Weston (2006, p. 3.6-2) states "The field data include all three invertebrate types, but are dominated in numbers and biomass by epifauna (particularly chironomids and bivalves); therefore, the epifauna invertebrate category is the most relevant for comparison to field data."
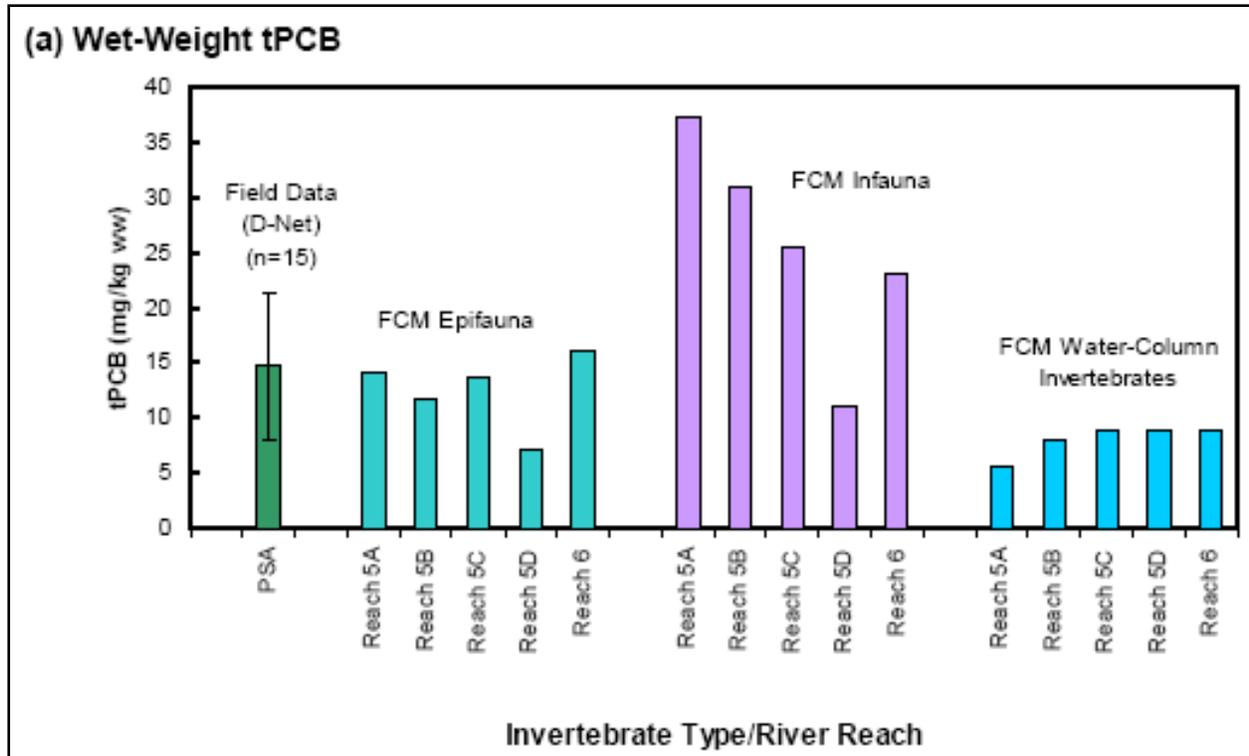
Figure 1.   Mean total PCB concentrations measured in the D-net invertebrate samples compared to the invertebrate concentrations simulated by FCM for each invertebrate type and river reach. Source: Figure 6.3-9, Weston 2004b.

Fox River: Model output was compared to the mean and 95 percent UCL whole fish tissue concentrations (e.g., Table 6 provides empirical data and model predictions from the Little Lake Butte des Morts reach). The model documentation report (ThermoRetec Consulting Corporation 2001a, pp 3-4) indicated that for all reaches and zones, output from the calibrated model was "well within one-half order of magnitude of observed concentrations of total PCBs for the mean and 95% UCL." Within the upper reaches, the point calibrations were within observed values, generally between 0.6 to 1.5 times the mean. For the lower reaches (Green Bay zones 1 and 2), predicted tissue concentrations for walleye, perch, and carp were 0.6 to 2.2 times observed values. Alewife, shiners, shad, and smelt were generally under-predicted; they were between 0.3 and 1.2 times the observed values (ThermoRetec Consulting Corporation 2001a, p. 3-4). The report concluded "Based upon both the point calibrations and the calibrations using the output from the hydrodynamic model, the FRFood Model was deemed suitable for projections within the Lower Fox River."

Duwamish: The calibration process identified parameter sets that estimated total PCB concentrations for all species within a factor of 2 of empirical data. Of the parameter sets that met the performance criteria, the mean factor difference was 1.4 and 1.5 for the two calibrations (against the data that included and excluded the 2004 samples). The best-fit parameter sets for both calibrations had a 1.2-fold mean difference. Modeling using the best-fit parameter sets for both calibrations produced mean concentrations that were similar to empirical data for each species; however, the model results were generally higher. The parameter set that was selected for the calibration excluded the 2004 fish tissue data sediment "Because tissue data from 2004 may have

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been influenced by the large dredging events that took place months before tissue samples were collected." (Windward Environmental 2007, p. 64).

Table 6. Results of the Lower Fox River Model Calibration.								
				Observed Total PCB		Predicted Total PCB		
Species	Number of Samples	Number of Detects	Detection Frequency	Mean	95% UCL	Mean	95% UCL	Units
Location: Little Lake Butte des Morts								
Water (filtered)	46	40	87	0.011	0.015			µg/L
Surface Sediments (I_d)	51,261	51,261	100	3,699	3,749			µg/kg
Gizzard Shad	4	4	100	296	530	263	358	µg/kg
Golden Shiner	2	2	100	993	1,140	723	868	µg/kg
Yellow Perch	1	1	100	363	363	1,266	1,443	µg/kg
Carp	30	30	100	1,992	2,957	2,374	2,639	µg/kg
Walleye	13	11	85	1,159	3,800	1,756	2,109	µg/kg
Source: ThermoRetec Consulting Corporation 2001a.								

Hudson: Table 6-4 of TAMS Consultants, Inc. et al. (2000a) and Figures 6-6 through 6-9 in the same document provide the comparison of predicted means to observed data across species and river reaches. Figure 6-10 provides quantile-quantile plots (e.g., comparison across the entire predicted distribution). In general, most predicted body burdens were within 50 percent of observed on a mean basis.

Validation Results: As described earlier, validation refers to running the calibrated model on an independent data set to establish that the calibrated model is predictive of independent conditions (USEPA 2005). Weston (2006) describes that "although there are several approaches to model calibration and validation, perhaps the most common procedure is to use only a subset of the data record for calibration. Once final parameter values are determined, model performance is evaluated by the goodness-of-fit between measured and simulated values using the remaining data."

Housatonic: The major component of the validation process was "temporal" validation which occurred over a longer time and used data independent of the calibration period. The food chain model was run using EFDC exposure inputs from January 1, 1979 through December 31, 2004. The EFDC model provided data on the PCB concentration in sediment and particulate organic matter. Fish tissue data were compared to model results from the date of collection for each fish tissue sample.

Model performance over the validation period was assessed by comparing predicted to measured PCB concentrations for the modeled species. Weston 2006 (p. 3.6-31) concludes "Overall, model simulations of central tendencies were within a factor of 2.5 of the data for all modeled species

and all reaches." However, the report also describes that "two measures of central tendency with large sample sizes (n > 6) fall outside the factor of 2.5 validation performance measure" and that "measured tPCB concentrations for smaller sample sizes are more variable, but were always within a factor of 5 of the simulated concentrations, and usually within a factor of 2." (Weston 2006, 3.6-22). The report further concluded that "the high variability and low sample sizes for most species/age/reach combinations limit the temporal analysis; however, both model results and data suggest that any changes in mean tissue tPCB concentrations over the validation period were small, if any" (Weston 2006, p. 3.6-28). No invertebrate tissue PCB data were available that were independent of the calibration data set, so model-data validation comparisons were not made.

Fox River: Performance of the calibrated food chain model was not validated on an independent data set. This is not explicitly mentioned in the model documentation report (ThermoRetec Consulting Corporation 2001a), but all available fish data were used in the calibration exercise (ThermoRetec Consulting Corporation 2001a, Table 3-6).[1]

Duwamish: There were no independent data sets to evaluate the selection of the best-fit parameter set selected during the calibration. No formal validation was conducted.

Hudson: Several approaches were used to validate the FISHRAND model. One method was to calibrate FISHRAND for one river mile, and then to run the model for a different river mile. Satisfactory agreement for both river miles implied model validity across locations in the Hudson River. In addition, a calibration was conducted using only part of the available dataset, and then the model results were compared with the remaining portion of the dataset. The posterior distributions obtained using only the partial dataset were compared to the posterior distributions obtained using the full dataset. Finally, the partial-data calibrated model was run for the forecast period and these results compared to the full-data calibrated model results. Good agreement across all three metrics implied confidence in the performance of the model. Finally, model results were compared to 1998 and 1999 data (which had not been used in the calibration).

Review of Example Model Output and Performance. At the reviewed sites, model runs encompassed several fish species, sometimes in different age classes, over many different areas (e.g. river reaches), resulting in a large amount of output from each species/reach/age class combination. Appendix A focuses on large adult (typically predator) fish in the modeled systems to evaluate the input to and output from the bioaccumulation modeling process. These fish are important because they are frequently targeted by fish consumers and they are the apex of the modeled food chains. If multiple areas are being modeled at a site, a representative area was chosen to illustrate techniques used and results generated at the site. Appendix A compares model output to individual fish tissue samples for the studied sites. These plots clearly indicate the high variability in fish tissue concentrations, even for fish lumped together as cohorts; model output is

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[1] The central question is whether 1998 fish data were independent of the calibration data set. The answer is not apparent from the model's documentation report or supporting material (Thermo RETEC Consulting Corporation 2001a; Wisconsin Department of Natural Resources (WDNR) and the RETEC Group, Inc. 2002). However, Table 3-6 in ThermoRetec Consulting Corporation (2001a) (Table 6 here) indicates that 11 walleye samples were included in the calibration (no years are given). In Figure 3-3, which shows the available empirical fish data (Figure A1 here), 11 walleye samples are also depicted; 6 of these are from 1998 sampling. This strongly suggests that there was not an independent validation data set.

shown as a single data point. These are important plots as they represent the end result of modeling process.

Sensitivity Analyses

Housatonic: A quantitative sensitivity analysis ("local sensitivity analysis"[1]) was conducted on the Housatonic's food web model. The purpose was to identify model parameters that exert the greatest effect on the model output. Input parameters were increased and decreased by 10 percent and then 33 percent to examine the effect on modeled tissue concentrations. The site's documentation report indicates that parameters with the greatest sensitivity are those for which more accurate values are needed, and they are most important for understanding the behavior of the modeled system. The most sensitive parameter values were related to organism bioenergetics (growth, respiration), toxicokinetics (particularly contaminant assimilation efficiency), and feeding preferences.

Fox River: No formal sensitivity analysis was undertaken for this model.

Duwamish: A sensitivity analysis of the model's individual input parameters was performed. A correlation analysis identified the 20 parameters that correlated most strongly with tissue concentration estimates (i.e., had the highest average absolute r-values).[2] A "nominal range sensitivity analysis" was then conducted on the 20 variables. This analysis varied the input values one at a time from minimum to maximum values,[3] while maintaining all other parameters at their best-fit values. The magnitude of the effect that this variation had on resulting fish tissue PCB concentrations was then documented.

The results of the correlation coefficient analysis and the sensitivity analysis were different. The correlation analysis indicated the parameters that most strongly correlated with tissue results were PCBs in the water column (for phytoplankton and zooplankton), dietary adsorption efficiencies (for crabs) and lipid content (for various species), dietary preferences (for shiner surfperch, juvenile fish, Pacific staghorn sculpin) and porewater ventilation by benthic invertebrates (for English sole) (Windward Environmental 2007, p. 69). The sensitivity analysis indicated that parameters that most influenced modeled fish tissue PCB concentrations were water column total PCBs, log KOW, and density of lipids; benthic invertebrate parameters had an effect on fish and crabs (Windward Environmental 2007, p. 71).

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[1] Weston 2006: "The local sensitivity analysis method evaluates the effect on model outputs resulting from varying only one of the model inputs, while holding all other inputs at their nominal or base-case values. The difference in the model output due to the change in the input variable is called the sensitivity, and is represented as a percentage change relative to the nominal solution."

[2] The following description is provided: "Pearson product-moment correlation coefficients (r-values) were calculated to characterize the strength of correlations between each FWM parameter and estimated total PCB concentrations in tissues. For each parameter, the absolute values of the correlation coefficients were averaged across all species in the FWM to get a general sense of the degree of covariance between a given parameter and predicted total PCB concentrations in tissues of all species combined."

[3] The minimum to maximum values of a parameter were those that still achieved +/- 2-fold the average empirical fish tissue PCB concentrations.

Hudson: The probabilistic framework used for this site started with the afore-mentioned sensitivity analysis (e.g., likelihood profiling to identify best parameters for calibration). In addition, correlation analyses were developed for the final, calibrated model. For each iteration in the Monte Carlo framework, an individual input is paired with the predicted tissue concentrations to develop correlations between inputs and outputs.

Uncertainty Analysis.

Housatonic: An uncertainty analysis was conducted on the food chain model output (tissue PCB concentrations) and input parameters (PCB exposure outputs from EFDC and FCM bioaccumulation variables). Monte Carlo analyses included a mix of point estimates and probability distributions for the input parameters to the model. The main result summarized by Weston 2006 (p. 3.8-11) is that the uncertainty of the final results of the simulations (modeled PCB concentrations in fish) is greater than the variability in the sampling data.

Fox River: No formal uncertainty analysis.

Duwamish: The sensitivity analysis was also considered an uncertainty analysis. The documentation report (Windward Environmental 2007) states "Nominal range sensitivity analysis can also be referred to as an uncertainty analysis because it provides information about how uncertainties in model parameters affect the reliability of the model's output" and that the sensitivity analysis provides "a measure of the relative influence that parameter has on the uncertainty of FWM tissue estimates."

Hudson: The probabilistic framework allowed for model input parameters to be specified by distributions identified as either "variable" (contributing more to differences in uptake across the population) versus "uncertain" (contributing more to uncertainty in any given population percentile). The result was predictions of population distributions of PCBs in fish tissue with associated uncertainty. Correlation analyses were also run for the final, calibrated model (Tables 8-1 through 8-4 in TAMS Consultants, Inc. et al. 2000a).

CONCLUSIONS: At the sites reviewed, different food web bioaccumulation models were used and their application (static or dynamic) varied. There was, however, consistency in the purpose of modeling. The models were routinely applied to predict and compare the results of remedial actions on fish tissue concentrations or to develop a risk-based sediment cleanup concentrations on the basis of the relationship between contaminant concentrations in fish and sediment. The importance of these analyses to site decision-making reflects the importance of the modeling. Remedial decisions will often be made or justified on the basis of model results.

The reviewed areas were waterways located across the United States and they varied greatly in size and hydrology, so it is not surprising they showed wide diversity in the modeled species and size of the areas (0.7 to 20 river miles) encompassed by predictions (Tables 2 and 3). The large size of the exposure areas reflects a primary uncertainty in food web contaminant modeling. The working assumption is commonly that fish are exposed equally across the exposure area; while it's known this assumption is generally incorrect, information to refine the fish-exposed areas is typically not available. During calibration and validation of the model, fish are assumed to have accumulated contaminants throughout the modeled area. The veracity of this assumption would

depend on fish movement, size of the area, and presence of natural barriers to migration; still, the movement and exposure history of individual fish in a calibration or validation data set is unknown.

There was wide variation both within and among sites in the amount of fish tissue data used to calibrate or verify model predictions. In this regard, there are no established best practices for the number of samples and time points that should support model application. However, USEPA (2000, 2008) has developed technical guidance for using fish tissue data to monitor remedy effectiveness, including advice on appropriate sample sizes of fish based on a review of population variability. These types of evaluations are appropriate for planning the number of fish and sampling dates to support bioaccumulation modeling.

The bioaccumulation models consist of numerous parameters, and the development of the models for a particular site is relatively complex. (For example, the Duwamish River food web model required 114 user-defined inputs, and yet was run in the simplest, steady-state mode.) Many parameters are literature-derived. In general, the only site-specific data used in the reviewed model applications relate to contaminant and organic carbon concentrations in environmental media, organism mass and lipid measurements, water temperature, and potentially dietary preferences. That the multitude of literature-derived parameters are applied identically between sites with such disparate geography, hydrology, and biologic assemblages seems to indicate that either processes driving contaminant uptake are well understood and highly uniform across sites or perhaps that individual parameter values are less important when combined and adjusted through calibration.

Calibration and validation procedures also varied across sites. All sites used empirical fish tissue concentrations to calibrate the model, however, in several cases there were no data available to independently verify or validate the calibrated model's performance. The selection of calibration parameters was not consistent across the four sites evaluated, although total organic carbon and percent lipid in fish were used in more than one model application. Calibration is often complicated by the fact that there is not a unique solution set for the given parameters. Further, calibrating a model to less data is actually easier than calibrating to multiple years of highly variable conditions. For example, all things being equal, it will be significantly easier to calibrate a model for a site with only a few samples collected annually for one or two years versus a site with samples from multiple locations over several years or within a year. When calibrating to a longer-term dataset, or to a dataset with greater spatial resolution, a single model parameterization (e.g., same uptake rates, same lipid, etc.) is required to predict observations, which is far more challenging than calibrating to a single location or collection effort. This represents a significant complication in comparing bioaccumulation model performance between sites, as it is generally not explicitly accounted for in any comparison.

Foodweb bioaccumulation models typically predict the mean of the modeled fish tissue concentrations, which is relevant to human or predator consumption of those fish species. However, the large variation in empirical fish tissue concentrations is not reflected by the apparent precision of modeling estimates. A cursory review of the fish tissue concentration data presented in Appendix A shows that data from the same species and age class (when available) that were

collected in the same area at the same time[1], can vary by an order of magnitude or more. This variability could result from fish tissue collection efforts and the need to focus more on collecting as similar of individual fish (both physiologically and in terms of temporal and spatial exposure) as possible. Or, it could just be the variability in contaminant concentrations that should be expected from similar fish in the modeled environments. If model outputs do not accurately portray that variability, they establish false expectations of accuracy. When the models are used to compare and differentiate trends in fish tissue concentrations under various remedial scenarios (as they commonly are in Superfund Feasibility Studies), that false sense of accuracy can be carried forward.

In the reviewed applications, uncertainty analyses were conducted by assigning a distribution of values to individual model parameters and evaluating the effect of that distribution on modeled fish tissue concentrations (i.e., parameter uncertainty was evaluated).[2] When the uncertainty distributions of input parameters are combined in model runs, the range of model results can easily exceed the variability actually seen in the modeled systems (e.g., Weston 2006). These uncertainty analyses do not address model structure uncertainty, i.e., equations and values are assigned to simulate a biologic function, but it is unknown whether that representation accurately portrays the modeled biologic function. Additionally, the uncertainty analyses do not represent the model's accuracy for predicting actual fish tissue contaminant concentrations (termed model error (Arnot and Gobas 2004)). The commonly-applied uncertainty analyses represent the variation in the model's output when parameters are varied. Ultimately, the model's accuracy in predicting future fish tissue contaminant concentrations is unknown.

Any assessment of bioaccumulation model performance and parameterization is complicated by the fact that rarely, if ever, is the bioaccumulation model operating in isolation. At a minimum, all bioaccumulation models require sediment and water exposure concentrations, total organic carbon, and water temperature. These vary spatially and temporally, and are described by empirical data or other models, and represent a source of uncertainty in bioaccumulation model predictions. In some cases, bioaccumulation models represent one module of a complex, integrated modeling system and the bioaccumulation module "picks up" very distinctly where the fate and transport and hydrodynamic models leave off. Any uncertainties in the underlying exposure concentrations will ultimately be reflected, perhaps unjustly, in the performance of the bioaccumulation model.

The bioaccumulation of organic contaminants through sediment-based food webs is relatively well-understood. However, there is substantial uncertainty associated with predicting future conditions, particularly when these predictions incorporate the impact of remedial technologies on contaminant exposures. There is a tension between model complexity and data availability. More complex models require greater effort to parameterize, and introduce more uncertainty. At the same time, simple models may not appropriately represent complex systems. Given the high variability in observed environmental conditions and the high level of uncertainty associated with predicting future conditions, increased model complexity may not be warranted.

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[1] At least the year of collection; specific collection dates are sometimes not provided.
[2] It's important to note that parameter distributions are also uncertain and, in many cases, the distributions were estimated based on very little site specific data or simply the range of literature values.

POINTS OF CONTACT: For additional information, contact Karl Gustavson (703-603-8753, *Karl.E.Gustavson@usace.army.mil*) or the Program Manager of the Dredging Operations and Environmental Research Program, Dr. Todd S. Bridges (601-634-3626, *Todd.S.Bridges@usace. army.mil*). This technical note should be cited as follows:

> Gustavson, K., T. von Stackelberg, I. Linkov, and T. Bridges. 2011. *Bioaccumulation models: State of the application at large Superfund sites*. DOER Technical Notes Collection. ERDC TN-DOER-R17. Vicksburg, MS: U.S. Army Engineer Research and Development Center.

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Appendix A: Examples of Model Input and Output from Examined Sites

Fox River, Little Lake Butte Des Morts Segment: Table A1 summarizes the fish data that were used in the calibration and validation procedure in the Little Lake Butte des Morts segment of the Fox River, WI. Figure A1 (from ThermoRetec Consulting Corporation 2001a) shows the calibration data (empirical data) and the modeled concentrations of PCBs in adult carp and walleye in the Little Lake Butte des Morts reach of the Fox River. The modeled fish tissue concentrations stem from the fate and transport model output from 1989-1995; the trend of this output (linear extrapolation) is then given to 1998. As described above, the calibration data represent all of the empirical fish data used in the modeling.

Table A1. Summary of the calibration and validation input and analysis for carp and walleye on Little Lake Butte des Morts.[1]						
Calibration			**Validation**			
Period	**Data sets**	**# Fish**	**Period**	**Data sets**	**# Fish**	**Model report conclusion**
1989 to 1998	1989, 1992, 1996, 1998	30 carp and 11 walleye[2] from the reach	No independent validation data set			Predicted walleye and carp were well within the observed range of data.
[1] Period refers to the time span over which data are considered; data sets are the years from which data from the corresponding period have been taken; # fish represents the number and species (if applicable) used in the procedure; the conclusion summarizes the analysis from the site report.						
[2] Two walleye samples were ND (ThermoRetec Consulting Corporation 2001, Table 3-6)						
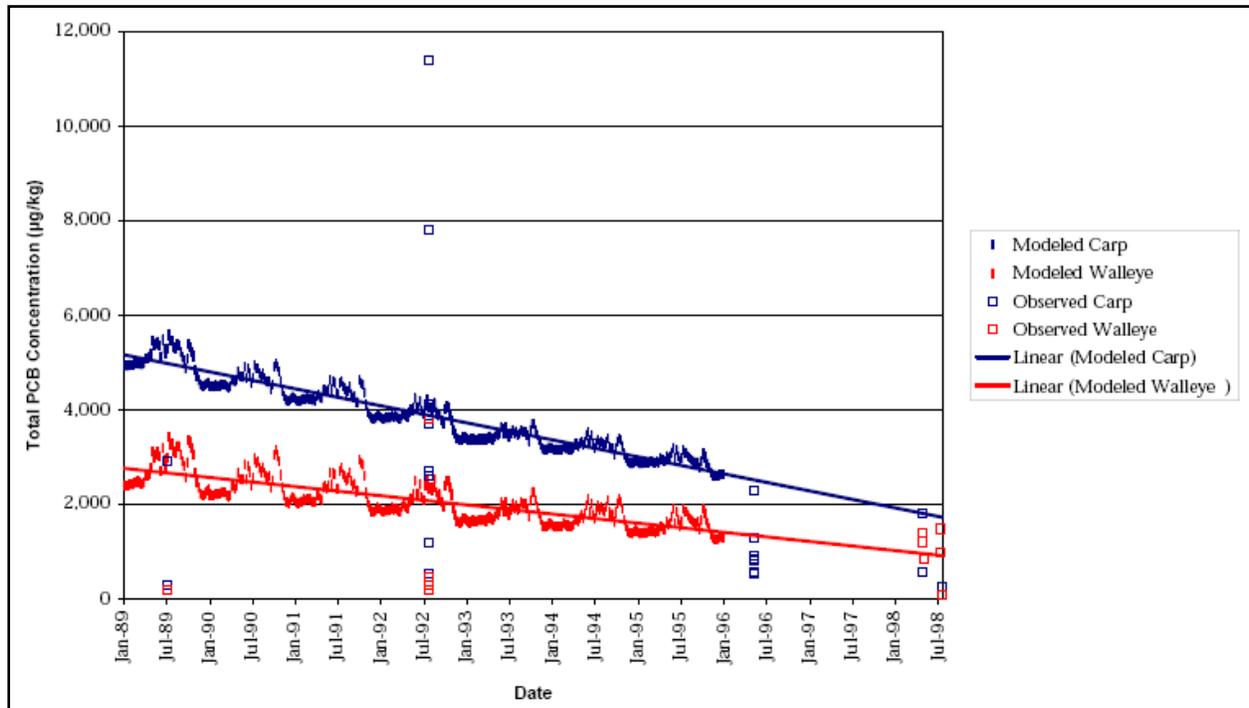
Figure A1. Output from FRFood Calibration in Little Lake Butte des Morts of the Fox River, WI. Total PCB concentrations of modeled fish tissue compared to measured fish tissue concentrations. Source: ThermoRetec Consulting Corporation 2001a.

Housatonic River, Reaches 5 and 6: Table A2 summarizes the fish data that were used in the calibration and validation procedure for adult largemouth bass in reaches 5 and 6 of the Housatonic River. Figure A2 (from Weston 2006) shows the calibration data and the model output for mature largemouth bass. The simulated data result from feeding the output of the EFDC model into the food web model. Note that the data in this figure are the independent validation data - the calibration data are not presented.

Table A2. Summary of the calibration and validation input and analysis for largemouth bass in Reaches 5 and 6 of the Housatonic River.						
Calibration			**Validation**			
Period	**Data sets**	**# fish**	**Period**	**Data sets**	**# Fish**	**Model Report Conclusion**
1998 to 1999	1998, 1999	38 fish captured from areas 5a, 5b, 5c, and 6	1979-2004	1990, 1994, 2002	33 fish captured from areas 5b and 6	Measured concentrations were variable – modeled performance was good
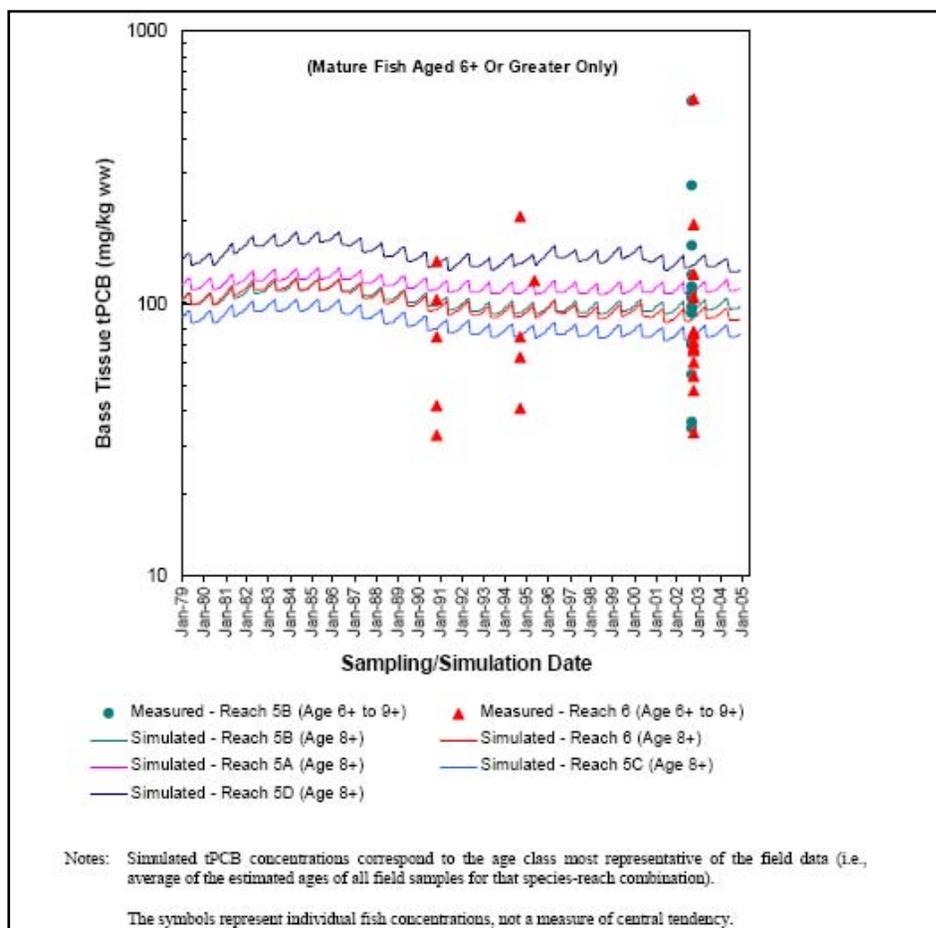
Figure A2. Simulated and measured PCB concentrations in mature largemouth bass over time in the Housatonic River reaches 5 and 6. The PCB concentrations (depicted by symbols) represent individual fish tissue samples used in the model validation. Model simulations, solid lines, indicate model results for age classes that represent each reach.

Duwamish River: The foodweb model at the Duwamish River was not run in a dynamic application; it estimated fish tissue concentrations assuming that environmental contaminant concentrations do not change over time. The sediment SWAC was 380 ug/kg dw; water concentrations were considered probabilistically – the best-fit parameter was 1.22 or 1.11 µg/L (Calibration 1 and 2, respectively).

Table A3. Calibration and validation input and analysis for fish and crab in the Duwamish River.						
Calibration			**Validation**			
Period	**Data sets**	**# Composite Samples[1]**	**Period**	**Data sets**	**# Fish**	**Model Report Conclusion**
1990-2006[2]	1997, 2004, 2005	Slender crab: 13/1 Dungeness Crab: 12/5 Sculpin: 28/4 Surfperch: 49/25 Sole: 42/21	No independent validation data set			Estimated PCB concentrations in fish and crab tissues were generally similar to mean empirical data
[1] Data provided for Calibration 1/Calibration 2. Calibration 1 included the fish and crab data from 2004, Calibration 2 excluded it (see text for explanation). [2] Period over which the sediment concentrations were averaged.						

Figures were not available in the model documentation report (Windward Environmental 2007) that displayed the individual empirical data points for the fish and crab tissue in the Duwamish (nor were tables of the individual data). Figure A3 shows the range of empirical data included in calibration 2 (that excluded the 2004 data set). The modeled (predicted) total PCB concentrations in fish and crab tissues were those associated with the best-fit parameter sets for calibration 2. The estimates associated with the best-fit parameter sets were generally higher than the mean empirical data, with the exception of shiner surfperch.

Hudson River: Results of the calibration and validation are shown in Figure A4. TAMS Consultants, Inc. et al. (2000a) also provides tables of relative percent difference on an annual basis between predicted and observed concentrations. TAMS Consultants, Inc. et al. (2000b) (responses to the peer review comments) provides additional validation results for 1998 and 1999 (the calibration utilized data from 1977 to 1997). "Updating" refers to the Bayesian Updating used to calibrate the model. Numbers in the figure title (e.g., "189") refer to river miles.
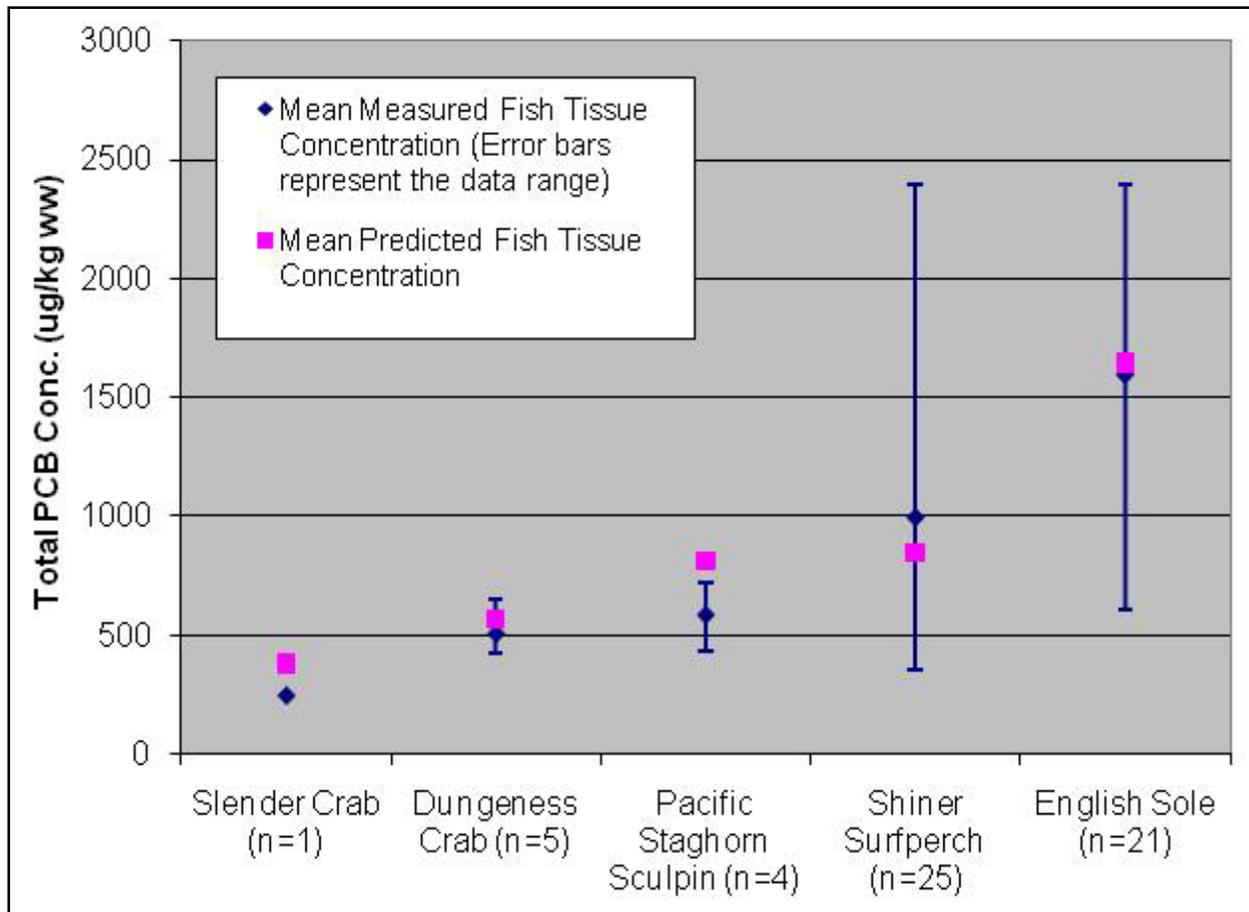
Figure A3. Measured and predicted total PCB concentrations in fish and crab from the Duwamish River. Bars represent the range of measured data. The number of composite samples (n) is in parentheses. Data source: measured fish tissue mean and range, Windward Environmental 2007, Table D.5-2; mean predicted fish tissue concentration Windward Environmental 2007, Table D.6-4 (for a SWAC of 380 ug/kg).
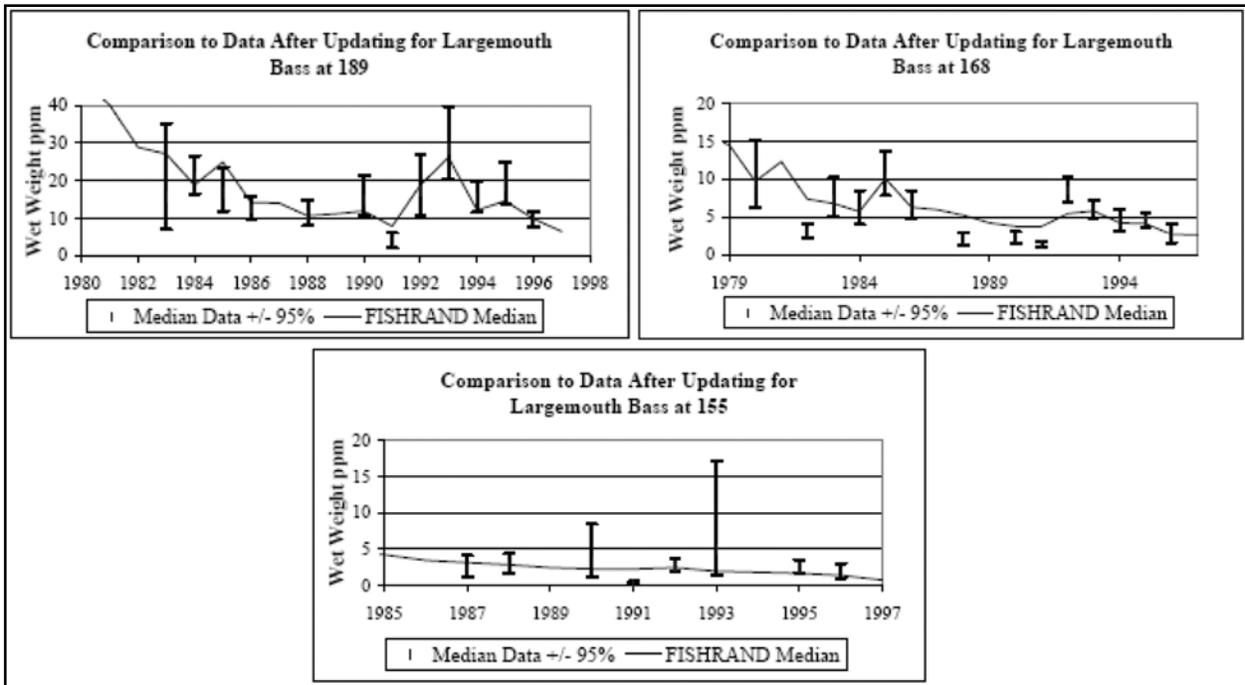
Figure A4. Comparison of median predicted fish concentrations on a wet-weight basis. Results for River Mile 155 are based on running the final calibrated model (validation). Source: Figures 6-6 through 6-11 of TAMS Consultants, Inc. et al. (2000a).