Lower Duwamish Waterway Group

Port of Seattle / City of Seattle / King County / The Boeing Company

Lower Duwamish Waterway Remedial Investigation

FOOD WEB MODEL MEMORANDUM 1: OBJECTIVES, CONCEPTUAL MODEL, AND SELECTION OF FOOD WEB MODEL DRAFT

Prepared for

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Bellevue, WA

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Prepared by: Windward environmental LLC

200 West Mercer Street, Suite 401 • Seattle, Washington • 98119

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Acronyms

Acronym	Definition
BSAF	biota-sediment accumulation factor
dw	dry weight
EPA	US Environmental Protection Agency
ERA	ecological risk assessment
FS	Feasibility Study
FWM	food web model
HHRA	human health risk assessment
LDW	Lower Duwamish Waterway
LDWG	Lower Duwamish Waterway Group
OC	organic carbon
PCBs	polychlorinated biphenyls
QEA	Quantitative Environmental Analysis, LLC
ROC	receptor of concern
RBG	risk-based goal
RI	Remedial Investigation
RI/FS	Remedial Investigation/Feasibility Study
SQT	sediment quality threshold
TMDL	total maximum daily load
ww	wet weight

1.0 Introduction

A comprehensive dataset of chemical concentrations in sediment and tissue has been collected in the Lower Duwamish Waterway (LDW) to define the nature and extent of contamination and to conduct baseline risk assessments in the Phase 2 Remedial Investigation (RI). These data will also be used to support a food web model (FWM) for the LDW. The FWM is needed for two applications. As part of the RI, risk-based goals (RBGs) for fish and crab tissue will be established based on the results of the ecological and human health risk assessments (ERA and HHRA), and those tissue RBGs will be translated into sediment quality thresholds (SQTs)[1] using the FWM. In the Feasibility Study (FS), the FWM will also be used as one tool to evaluate residual risks associated with various sediment cleanup scenarios.

Three memoranda will be submitted describing the FWM, including a rationale for the selection of a model, the modeling approach, and the results of preliminary modeling runs. This memorandum is the first of these three FWM deliverables. Section 2 of this memorandum describes the uses and objectives of the FWM. Section 3 describes the conceptual approach to food web modeling, including the conceptual bioaccumulation model for the LDW, the species to be modeled, and the assumed pathways of chemical uptake. Section 4 provides justification for the selection of a FWM, and discusses how the selected model meets the necessary specifications and objectives for the project. Section 5 lists model parameters. Section 6 contains references cited. A series of conceptual bioaccumulation model figures is presented at the end of the document.

2.0 Uses and Objectives of the FWM

The FWM will be used in two different applications in the Phase 2 RI/FS:

- To estimate SQTs associated with RBGs in fish and crab tissue
- To estimate concentrations in fish and crab tissue resulting from various sediment cleanup scenarios in the FS

Figure 2-1 illustrates how the FWM will be used in the RI/FS process.

[1] SQTs are chemical concentrations in sediment associated with specific acceptable risk estimates. SQTs may be derived for multiple exposure scenarios

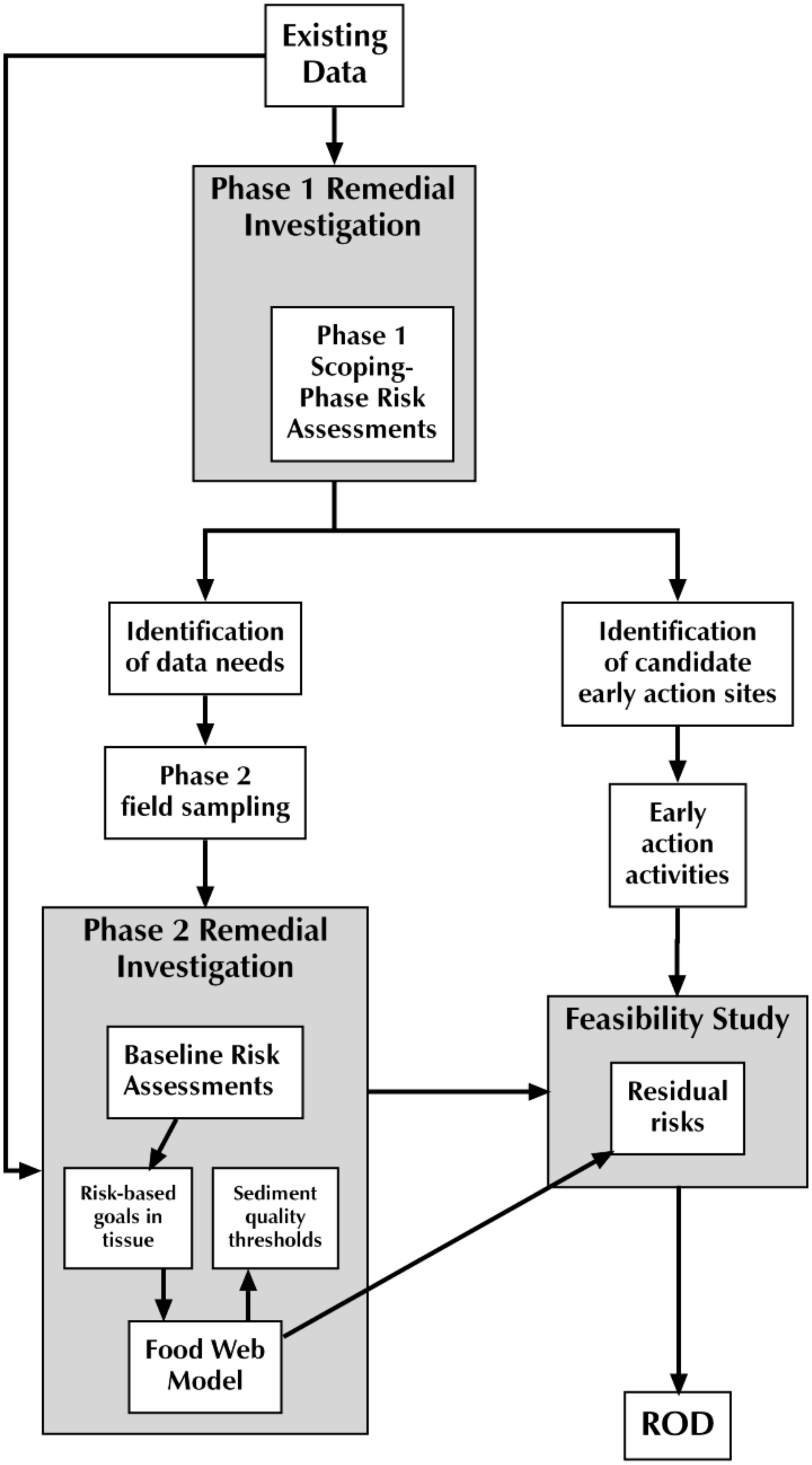

Figure 2-1. FWM relationship to RI/FS process

For estimation of SQTs from tissue-based RBGs, the FWM will be used to answer the following question:

- What chemical concentration(s) in sediment are predicted to result in fish and crab tissue concentrations equal to risk thresholds for ecological and human receptors under a range of exposure scenarios

The FS will include an analysis of alternative remedial designs. To evaluate these designs, the FWM will be used in the FS to answer the following question:

- What chemical concentrations are predicted in fish and crab tissues over a range of anticipated sediment concentrations associated with various sediment cleanup scenarios?

Based on these intended applications of the FWM, the objective for the FWM is as follows:

- To investigate the relationship between concentrations of chemicals in sediment and fish and crab tissue at different spatial and temporal scales in the LDW

3.0 Conceptual Approach

The purpose of an FWM is to predict the transfer of chemicals through an ecosystem. Simplifying assumptions must be made when using a FWM because ecosystems are complex and dynamic environments that cannot be fully characterized in a quantitative manner without a high level of uncertainty. Simpler models focus on parameters and processes that contribute to the most significant movement of a given chemical among different media in an ecosystem (water, sediment, and tissue). Because numerous assumptions and estimates are required in modeling, the modeling process is necessarily iterative. For the model to be used as an effective tool, these assumptions and estimates must be clearly articulated to and accepted by stakeholders. This section describes the conceptual bioaccumulation model for the LDW, and provides an introduction to the simplifying assumptions required to model chemical concentrations in key species to meet the needs of the Phase 2 RI/FS, as discussed above.

3.1 Conceptual Bioaccumulation Model

The generalized conceptual bioaccumulation model for the LDW is presented in Figure 3-1 (located at the end of this document). Figure 3-1, although relatively complex, represents a simplification of the estuarine ecosystem within the LDW. Various boxes or "compartments" are included in the conceptual bioaccumulation model, each representing a group of species or abiotic media that may influence chemical transfer and bioaccumulation. Figure 3-1 also shows pathways for chemical uptake through dietary and water routes as well as pathways for chemical transfer between various abiotic media. Table 3-1 presents the compartments depicted in the generalized conceptual model (Figure 3-1) and the organisms and media assumed to be represented by that compartment.

Table 3-1. Compartments in the generalized conceptual bioaccumulation model

"Compartment" in Conceptual Bioaccumulation Model	Biota or Environmental Media Represented by Each Compartment
Phytoplankton	plants and algae in the water column
Water column detritus	non-living organic matter in the water column and associated bacteria and fungi (e.g., feces, small pieces of dead plants and animals)
Zooplankton	planktonic animals and animals living on pilings or rocks above sediment surface
Benthic algae	benthic algae and vascular plants (e.g., macroalgae, periphyton, benthic diatoms)
Sediment	suspended sediment (clay, silt, and sand) in bottom water
	bed sediment (clay, silt, sand, and gravel)
Sediment-associated detritus	detritus in bottom water and porewater (e.g., feces and small pieces of dead plants and animals)
Sediment-associated bacteria and fungi	bacteria and fungi living on sediment-associated detritus
Epibenthic invertebrates	invertebrates living on the sediment, including crabs, amphipods, echinoderms, gastropods, polychaetes oligochaetes, etc.
Infaunal invertebrates	invertebrates living in the surface sediment and exposed to porewater, including oligochaetes, polychaetes, amphipods, bivalves, echinoderms, etc.
Demersal fish	fish living on or near the sediment associated with bottom waters and sediment, including English sole, sand sole, starry flounder, and Pacific staghorn sculpin
Benthopelagic fish	fish that move between the bottom water and the water column, including shiner surfperch, pile perch
Pelagic fish	fish living and feeding in the water column (e.g., eulachon)
Small fish as prey	juvenile benthopelagic, demersal, and pelagic fish
Water column water	water above the sediment surface that is less influenced by fluxes from sediment resuspension than bottom water
Porewater	water between bedded sediment particles that is assumed to be in equilibrium with sediment-bound chemicals
Bottom water	water at or near the sediment surface that experiences fluxes of chemicals from re-suspension of sediments and is the layer closest to porewater to receive chemicals via diffusion

3.2 Species to be Modeled

The target species to be modeled in the FWM are either receptors of concern (ROCs) in the ERA or serve as key prey species for other receptors in the ERA or HHRA. Target species that will be modeled using the FWM include:

- English sole as a representative of demersal fish that consume primarily invertebrates; English sole are an ROC in the ERA, serve as prey for wildlife ROCs, and are consumed by humans

- Pacific staghorn sculpin as a representative of demersal fish that consume both invertebrates and small fish; Pacific staghorn sculpin are an ROC in the ERA and serve as prey for wildlife ROCs
- Shiner surfperch as a representative of benthopelagic fish; shiner surfperch serve as prey for wildlife ROCs and are consumed by humans
- Dungeness and slender crabs as representatives of epibenthic invertebrates; crabs are an ROC in the ERA, serve as prey for wildlife ROCs, and are consumed by humans

For each target species, Phase 1 and/or Phase 2 tissue chemistry data exist that can be used to calibrate the FWM.

Other biotic compartments to be modeled in the FWM are phytoplankton, zooplankton, benthic invertebrates, and small prey fish. These biotic compartments are being modeled to complete the trophic transfer of chemicals from abiotic media to the target fish and crab species presented above. Phytoplankton and zooplankton will serve as prey for benthic invertebrates and small prey fish; benthic invertebrates and small prey fish will serve as prey for the target fish and crab species. While Phase 2 benthic invertebrate tissue chemistry data are available for calibration of the benthic invertebrate compartment, no empirical tissue chemistry data exist for phytoplankton, zooplankton, or small prey fish for model calibration. Calibration of the FWM will be discussed further in FWM Deliverable 2.

As determined from historical fish surveys as well as recent trawling, beach seining, and limited gill netting in the LDW, no resident, higher-trophic-level, pelagic fish inhabit the LDW. Based on this information and past consultations with fish experts, no resident pelagic fish have been identified as an ecological receptor of concern or as a component of seafood consumed by people fishing in the LDW. Therefore, pelagic fish will not be included in the FWM for the LDW.

Clams are also part of the HHRA seafood exposure assessment as shellfish and part of the ERA as wildlife prey. Clam tissue concentrations will be modeled using a biota-sediment accumulation factor (BSAF) rather than the FWM. Benthic invertebrates are also part of the ERA as fish and wildlife prey. As stated above, these species will be modeled in the FWM as prey for fish and crab species. However, for the calculation of ecological risks to birds and mammals, a BSAF will be used to estimate benthic invertebrate chemical concentrations included in exposure estimates.

3.3 SIMPLIFIED CONCEPTUAL BIOACCUMULATION MODEL

As stated above, ecosystems are complex and dynamic environments that are difficult to model. For this reason, simplified food web models were developed for the three fish species and two crab species identified in Section 3.2. These simplified models were developed to illustrate the assumed major routes of chemical uptake for these fish and crab species. For hydrophobic organic chemicals, dietary uptake is generally assumed to be the primary pathway of uptake for higher-trophic-level species (Gobas et al. 1999). Chemical partitioning through aqueous pathways can also be important, particularly for lower trophic level species and for chemicals that are less hydrophobic (Russell et al. 1999). Figures 3-2 through 3-6 (located at the end of the document) provide a simplified graphical representation of the assumed pathways for chemicals in the food web for the LDW as a whole (Figure 3-2), and for Dungeness crab and slender crab (Figure 3-3), English sole (Figure 3-4), Pacific staghorn sculpin (Figure 3-5), and shiner surfperch (Figure 3-6).

Assumptions relating the generalized conceptual bioaccumulation model to the simplified conceptual bioaccumulation models are listed in Table 3-2. These assumptions were made based on the nature and types of empirical data, as well as the relative importance of each compartment to chemical transfer through the food web.

Table 3-2. Assumptions relating the simplified conceptual bioaccumulation model to the generalized conceptual bioaccumulation model

Compartment in Simplified Conceptual Bioaccumulation Model	Generalized Conceptual Bioaccumulation Model Compartment(s) Represented	Reason / Comments
Phytoplankton	Phytoplankton and suspended detritus (with associated bacteria and fungi)	Literature values for phytoplankton generally include all particles in water column < 236 µm (Mackintosh et al. 2004)
Benthic invertebrates	Infaunal and epibenthic invertebrates (except crabs which are epibenthic invertebrates and have their own compartment)	Empirical data for LDW benthic invertebrates includes both infaunal and epibenthic invertebrates. LDW fish are assumed to consume both equally.
Sediment	sediment, detritus, bacteria, and fungi (all from the bottom water/sediment interface)	LDW sediment samples include all detritus and organisms living in the sediment
Water-column water and porewater	Bottom water	No LDW-specific data are available for bottom water or porewater for bioaccumulative chemicals. Gobas and QEA models use "porewater" and water column water (either empirical or calculated from sediment) to represent bottom water. Bottom water in the model will be represented by exposure to specified fractions of water column water and porewater.

3.3.1 Dietary uptake

The diets of the fish and crab species to be modeled are likely to be variable because these species are known to be relatively opportunistic feeders (Fresh et al. 1979; Miller et al. 1977; Stevens et al. 1982; Wingert et al. 1979). Thus, their diets are likely to vary with prey availability both seasonally and spatially throughout the LDW. Although dietary information for these species is not available from the LDW, several dietary studies have been conducted for these species in Puget Sound or in some cases on the Pacific coast (Table 3-3). The results of these studies are assumed to reasonably represent the diets of these fish and crabs within the LDW, and have formed the basis for the simplified food webs shown in Figures 3-2 through 3-6. In the simplified food webs (Figures 3-2 through 3-6), all invertebrates consumed by fish will be represented by LDW benthic invertebrate samples. Benthic invertebrate samples provide average lipid content information for model input, and tissue chemical concentrations for calibration. On a biomass basis, benthic invertebrate sample were dominated by oligochaetes, polychaetes, amphipods, and small clams. Diets of the modeled species will be discussed in more detail in FWM deliverable 3, where the assumed relative percentages of dietary prey items will be presented.

Table 3-3. Dietary data used to construct the LDW food web

SPECIES	LOCATION OF STUDIES	SOURCE OF DIETARY DATA
Dungeness crab	Grays Harbor, WA	Stevens et al. (1982)
Slender crab	not available; continue to research	To be determined (assumed to be similar to Dungeness crab with fewer fish in diet)
English sole	Nisqually Estuary, West Point, Alki Point, Point Pully	Fresh et al. (1979) Wingert et al. (1979)
Pacific staghorn sculpin	Nisqually Estuary, West Point, Alki Point, Point Pully, Northern Puget Sound	Miller et al. (1977) Fresh et al. (1979) Wingert et al. (1979)
Shiner surfperch	Nisqually Estuary, West Point, Alki Point, Point Pully, Northern Puget Sound	Miller et al. (1977) Fresh et al. (1979) Wingert et al. (1979)
Small fish (prey for Dungeness crab and Pacific staghorn sculpin)	Northern Puget Sound (juvenile English sole), Pacific coast (juvenile shiner surfperch)	Gordon (1965) Bane and Robinson (1970) Boothe (1967) Miller et al. (1977)

Diets of organisms also include living or non-living matter (e.g., carcasses, detritus, incidental sediment). For the FWM, all detritus consumed by benthic filter feeders, detritivores, scavengers, or bottom feeders will be represented by sediment. Detritus consumed by water column organisms will be represented by phytoplankton. For each of the compartments that represent detritus, the total organic carbon content will account for detrital material.

3.3.2 Aqueous uptake pathways

Aqueous partitioning is generally described using a three-phase model including particulate organic carbon, dissolved organic carbon, and the truly dissolved phase in water (Arnot and Gobas 2004). The truly dissolved portion is the fraction assumed to be most bioavailable for aqueous uptake (McCarthy 1983; McCarthy and Jimenez 1985).

The generalized conceptual bioaccumulation model includes three types of water: the water column, bottom water, and porewater (Figure 3-1). Organisms are exposed to different concentrations of chemicals in different water types. The organisms residing in each water layer are summarized in Table 3-1. Organisms living solely in the water column are phytoplankton, zooplankton, and suspended bacteria and fungi associated with detritus. Benthopelagic and demersal fish and some epibenthic invertebrates (e.g., shrimp) spend part of their time in the water column and part of their time in bottom water. Infaunal invertebrates and demersal fish are in contact with bottom water, sediments, and the associated porewater. Organisms that live solely in bottom water or on the sediments are epibenthic invertebrates, benthic algae, and some bacteria and fungi. Some infaunal organisms and bacteria and fungi spend all their time in the sediment (porewater). Other infaunal invertebrate species, specifically filter feeders, ventilate 100% bottom water. Assumptions regarding the percentage of each type of water exposure will be detailed in FWM deliverable 3.

For the simplified food web models (Figures 3-2 through 3-6), bottom water is not included as a compartment and is instead represented by a combination of exposure to water-column water and porewater. There are no empirical chemical concentration data for bioaccumulative chemicals in bottom water or porewater in the LDW. Food web models often use porewater concentrations (either empirical or calculated from sediment) to account for aqueous uptake of chemicals from bottom water and porewater. Empirical relationships have been established between organic carbon-normalized chemical concentrations in the sediment, organic carbon-water partitioning coefficient (K_{OC}), octanol-water partitioning coefficient (K_{OW}), and concentrations of particulate organic carbon and dissolved organic carbon (McCarthy 1983; McCarthy and Jimenez 1985). Although these relationships are uncertain, they may be less uncertain than calculating the chemical concentrations in bottom-water, which is dependent on many factors, including flow rates and both physical and biological disturbances. Therefore, specified fractions of water column water and porewater will be used to represent bottom-water in the FWM.

4.0 Food Web Model Selection

This section presents model-specific specifications, models that were considered, the model selected for the LDW, and the rationale for its selection.

4.1 Model-Specific Specifications

The following model-specific specifications (or selection criteria) were developed to assess the suitability of available FWMs to meet the stated objective in Section 2, and thereby meet the specific needs for the Phase 2 RI/FS.

- Model can be used to predict sediment chemical concentrations in the LDW from specified chemical concentrations in tissue and water
- Model can be used to predict chemical concentrations in fish and crab tissue in the LDW from specified chemical concentrations in sediment and water based on empirical chemical concentrations

- Model can be used to predict chemical concentrations in fish and crab tissue in the LDW from specified chemical concentrations in sediment and water based on anticipated sediment chemical concentrations associated with various sediment cleanup scenarios
- Model can represent a reasonable simplification of what is known about the LDW food web and the likely pathways of chemical transfers among trophic levels
- Model is fully documented, including all equations, code, and assumptions for input parameters
- Model can be applied to different areas of the LDW given sufficient location-specific data
- Parameter uncertainty can be systematically quantified
- Model can be used to predict chemical concentrations in tissue or sediment with the degree of accuracy necessary to make RI/FS decisions
- Model has been used and accepted at other Superfund sites

4.2 General Evaluation of Food Web Models

Several models were considered for application in the LDW to meet the objective presented in Section 2 and the specifications presented above. Two general types of models were considered:

- An empirical statistical model derived solely from site-specific data
- Mechanistic models based on theoretical relationships describing chemical bioaccumulation through the food chain; the mechanistic models evaluated are Gobas-type equilibrium models and Quantitative Environmental Analysis, LLC's (QEA) bioaccumulation model

Each of the specific models considered is described and evaluated for use in the LDW RI/FS in the following sections.

4.2.1 Empirical statistical model

4.2.1.1 Empirical model description

A statistical model based on empirical relationships between measured chemical concentrations in sediment and biota was considered because it would be based entirely on site-specific data. To assess the potential application of this type of model in the LDW, regression relationships between concentrations of total polychlorinated biphenyls (PCBs) in sediment and tissues were evaluated. Tissue chemistry data from 2004 were regressed against spatially weighted average total PCB concentrations in sediment over the subarea or area from which tissue samples were collected. Specifically, shiner surfperch and Pacific staghorn sculpin tissue data were regressed separately against subarea-scale concentrations in sediment calculated using inverse-distance weighted interpolations. Each of the following regression models was considered for each species:

- PCBs in tissue (ww) vs. PCBs in sediment (dw)
- PCBs in tissue (ww) vs. organic carbon (OC)-normalized PCBs in sediment
- Lipid-normalized PCBs in tissue vs. PCBs in sediment (dw)
- Lipid-normalized PCBs in tissue vs. OC-normalized PCBs in sediment

The best model for each species and tissue type was determined based on the smallest 95% confidence interval at a tissue concentration arbitrarily set at 1,000 µg/kg ww (Table 4-1).

Table 4-1 Comparison of regression equations and sediment concentration confidence intervals at a fish tissue total PCBs concentration of 1,000 µg/kg-ww

Y-Variable[a]	X-Variable[a]	Predicted Sediment Conc. (µg/kg dw) for Tissue Conc. of 1,000 µg/kg ww	95% Lower Bound (µg/kg dw)	95% Upper Bound (µg/kg dw)	Width of CI (µg/kg dw)
Shiner surfperch					
log[tissue]	log[sediment]	88.4	4.19	1,864	1,860
log[lipid-normalized tissue]	log[sediment]	74.6	2.54	2,194	2,191
log[tissue]	log[OC-norm sediment]	102[b]	8.16[b]	1,270[b]	1,261[b]
Log[lipid-normalized tissue]	**log[OC-norm sediment]**	**92.1[b]**	**6.73[b]**	**1,260[b]**	**1,253[b]**
Sculpin					
log[tissue]	sediment	792	-534	2,118	2,652
log[lipid-normalized tissue]	sediment	722	-451	1,895	2,346
log[tissue]	OC-norm sediment	710[b]	-128[b]	1,548[b]	1,676[b]
sqrt[lipid-normalized tissue]	**OC-norm sediment**	**559[b]**	**-84.4[b]**	**1,202[b]**	**1,286[b]**

[a] Variables were log- or square root-transformed if data were non-normal or the shape of the regression curve was not linear

[b] Rescaled to non-normalized sediment concentration

Rows in **bold** correspond to the best regression model for each species

Log – $\log_{10}$ transformed data

Sqrt – square-root transformed data

OC norm – organic carbon-normalized sediment concentration

CI – confidence interval

As shown in Table 4-1, the confidence intervals at 1,000 µg/kg total PCBs in tissue ranged over two to nearly three orders of magnitude for all models considered. Because of the uncertainty in these relationships, an empirical statistical model based on these data would have a high degree of uncertainty at tissue and sediment concentrations of interest. Additionally, it was determined that because no empirical LDW tissue data are available for these two fish species at concentrations less than 108 to 1,320 µg/kg ww, depending on the species, a statistical model would be required to extrapolate outside the range of available data, where the model cannot be confirmed to apply.

4.2.1.2 Empirical model evaluation

Benefits for use as LDW FWM

- Based solely on site-specific data
- Because of its simplicity, the model could be readily communicated to stakeholders
- Because of its simplicity, uncertainty can be readily quantified
- Simple and cost effective

Limitations to use as LDW FWM

- Because the confidence interval for prediction of sediment concentrations is more than two orders of magnitude, such a model would be highly uncertain
- Because no LDW data are available at very low tissue concentrations, the model would likely be required to extrapolate beyond the available data
- Model assumes sediment chemical concentrations explain chemical concentrations in fish tissue; therefore, it ignores the water pathway and dietary influences

4.2.2 Gobas model with updates

The original Gobas (1993) model is a four-compartment, steady-state, mass-balance bioaccumulation model. The Gobas model was originally developed to describe bioaccumulation of PCBs in the Great Lakes food web. Several iterations of the model have subsequently been developed, including both refinements and simplifications. The iterations of the Gobas model discussed below were considered for application in the LDW.

4.2.2.1 Gobas (1993)

The four biotic compartments of the original Gobas (1993) model are phytoplankton/macrophytes, zooplankton, benthic invertebrates, and fish. Chemical concentrations for phytoplankton/macrophytes, zooplankton, and benthic invertebrates are derived using equilibrium partitioning equations, while chemical concentrations for fish are calculated using kinetic equations for uptake and loss. Uptake mechanisms for fish include uptake from water via the gills and uptake from the diet. Loss mechanisms for fish include metabolism, growth dilution, loss to water via gills, and fecal egestion. This model forms the basis for many subsequent updates and iterations of Gobas-type models.

4.2.2.2 TrophicTrace

TrophicTrace was developed for the U.S. Army Corps of Engineers for management of dredged materials (von Stackelberg and Burmistrova 2003). Among other models (i.e., human health and ecological risk models, and a bioaccumulation model for metals), TrophicTrace includes a mechanistic bioaccumulation model for hydrophobic organic chemicals, based on the model of Gobas (1993). This model differs from the Gobas (1993) model, however, because it relies on user-supplied BSAFs rather than equilibrium partitioning equations to predict chemical concentrations in benthic invertebrate tissue.

4.2.2.3 Morrison (1996)

In 1996, the Gobas model was updated to account for the high degree of variability observed in bioaccumulation of organic chemicals by benthic invertebrates and thus improve benthic invertebrate model predictions for the Lake Erie food web. Separate mechanistic steady-state model equations were developed for benthic filter feeders and benthic scavengers based on sediment, water, and invertebrate data from Lake Erie (Morrison et al. 1996).

4.2.2.5 Arnot and Gobas (2004)

Based on recent advances in understanding of bioaccumulation processes from field and laboratory studies (Gobas and MacLean 2003; Gobas et al. 1999; Nichols et al. 2001; Roditi and Fisher 1999),) and from improvements in data availability for model parameterization (SETAC Supplemental Archives S1 and S2), the Gobas model has recently been further refined (Arnot and Gobas 2004). New elements added to the model include: 1) a new model for partitioning chemicals into organisms; 2) kinetic models for predicting chemical concentrations in algae, phytoplankton, and zooplankton; 3) new allometric relationships for predicting gill ventilation rates in a wide range of aquatic species; and 4) the inclusion of a mechanistic model for predicting gastrointestinal magnification[2] of organic chemicals in a range of species.

Chemical concentrations in phytoplankton are calculated assuming aqueous uptake and loss via the respiratory surface, and loss via growth dilution. Chemical concentrations in zooplankton, invertebrates, and fish are calculated assuming uptake from water via the respiratory surface and uptake from the diet. Losses include metabolism, growth dilution, loss to water via the respiratory surface, and fecal egestion. Chemical concentrations in filter-feeding invertebrates are calculated assuming uptake via ingestion of plankton and suspended solids, and uptake from

[2] Gastrointestinal magnification is the process by which a chemical's concentration in the ingested tissue fraction increases as it passes through the gut as a result of digestion and absorption relative to the slow uptake of the chemical. This process results in a greater concentration gradient between the organism and its food, and can partially explain the mechanism of biomagnification up the food chain.

water via the respiratory surface. Filter-feeders are linked to sediments via ingestion of suspended sediments.

4.2.2.6 Gobas-type models evaluation

Benefits for Use as LDW FWM

- Gobas-type models are well established and have gained widespread acceptance. The US Environmental Protection Agency (EPA) has made extensive use of a Gobas-type model to derive bioaccumulation factors, bioconcentration factors, and food-chain multipliers in the baseline HHRA and ERA development of the Great Lakes Water Quality Initiative criteria (EPA 1993, 1994).
- Gobas-type models have been used at numerous Superfund sites for various purposes. For example, Gobas-type models have been used for calculating SQTs in the 1996 RI/FS for the Fox River (GAS and SAIC 1996) and the Sheboygan River ERA (EVS and NOAA 1998), and for predicting chemical concentrations in biota in the Hudson River (TAMS 2000). In each of these Superfund site applications, model-predicted tissue concentrations were found to be accurate to within a factor of 5 of empirical tissue concentrations.
- The models can be fully parameterized using LDW and literature data
- The models can be run in Excel, making them cost-effective to run
- The models can be readily modified to accommodate additional complexity in the LDW foodweb, if necessary

Limitations to Use as LDW FWM

- Model includes many variables, resulting in inherent uncertainty
- Parameterization of the model can be controversial

4.2.3 QEA model

The QEA model (QEA 2001a, b) is similar to the Gobas-type models in terms of pathways and processes modeled (respiration rates, growth rates, assimilation efficiencies). The main differences are that: 1) the QEA model simulates energy (kJ/g C) transfer while the Gobas-type models use chemical concentration (µg/kg ww), and 2) the QEA model is a steady-state model that can be tied to a fate and transport model and run in successive time steps (assuming steady-state at each time step).

4.2.3.1 QEA model evaluation

Benefits for Use as LDW FWM

- Model is well established and has been applied in a variety of environments (including Housatonic River Superfund projects), with predicted tissue concentrations accurate within a factor of 5 of empirical concentrations
- The model can be parameterized using LDW and literature data

- Model can be made incrementally more sophisticated without further programming (i.e., model can incorporate organism movement between subsections of the LDW and a time series of predictions, although these increased levels of sophistication would require extensive additional data for parameterization)

Limitations to Use as LDW FWM

- Model includes many variables, resulting in inherent uncertainty
- Parameterization of the model can be controversial
- Some model elements may be more complex than justified by project needs (e.g., data on movement of modeled species among subsections of the LDW, incorporation of age-related changes in environmental conditions or biological responses)

4.3 SELECTED FOOD WEB MODEL

Based on the evaluation of the FWMs discussed in Section 4.2, the Arnot and Gobas (2004) model was selected for use in the LDW RI/FS. Primary reasons for selection of this model are:

- Gobas-type models have been applied in various other systems including Superfund sites, and have been well accepted by EPA and stakeholders
- The Arnot and Gobas (2004) model represents the latest refinements of the Gobas model and these refinements make the model both more realistic and potentially more accurate
- The Arnot and Gobas (2004) model framework is easier to run and make adjustments to (Excel spreadsheet with all code accessible)

The ability of the Arnot and Gobas (2004) model to meet the objectives and specifications presented in Section 4.1 is discussed in Section 4.3.1. Section 4.3.2 discusses the performance of Gobas-type models in other systems.

4.3.1 Ability to meet objectives and specifications

To satisfy the needs of the LDW RI/FS and answer the questions stated in Section 2.0 for each application of the FWM, the Arnot and Gobas (2004) model must meet each of the model-specific specifications presented in Section 4.1. The ability of the model to meet each specification is presented below.

Model can be used to predict sediment chemical concentrations in the LDW from specified chemical concentrations in tissue and water

Gobas-type models have been used to calculate sediment concentrations associated with tissue thresholds in other systems. A Gobas-type model was used to calculate SQTs in the 1996 RI/FS for the upper Fox River (GAS and SAIC 1996) and for the Sheboygan River ERA (EVS and NOAA 1998).

Model can be used to predict chemical concentrations in fish and crab tissue in the LDW from specified chemical concentrations in sediment and water based on empirical chemical concentrations

The Arnot and Gobas (2004) model, and models similar to it, have demonstrated an ability to predict fish tissue concentrations from sediment and water concentrations in both riverine and estuarine environments. Model performance in other systems is described in Section 4.3.2.

Model can be used to predict chemical concentrations in fish and crab tissue in the LDW from specified chemical concentrations in sediment and water based on anticipated sediment chemical concentrations associated with various sediment cleanup scenarios

The Arnot and Gobas (2004) model can be used in conjunction with estimates of future chemical concentrations in sediment to predict future chemical concentrations in tissue.

Model can represent a reasonable simplification of what is known about the LDW food web and the likely primary pathways of chemical transfer among trophic levels

The structure of the Arnot and Gobas (2004) model is compatible with the simplified LDW conceptual bioaccumulation model (see Section 3.0).

Model is fully documented, including all equations, code, and assumptions for input parameters

Arnot and Gobas (2004) discuss all equations and parameters in the model. Model component tables for application of this model to the LDW are being prepared that list equations and parameters with associated symbols, units, assumptions, uncertainties, sources, and proposed future actions. These tables will be submitted with FWM deliverable 3.

Model can be applied to different areas of the LDW given sufficient location-specific data

The Arnot and Gobas (2004) model can theoretically be applied at any environmental scale assumed to relate to the "exposure area" for that organism. Exposure areas for each target species will be presented in FWM deliverable 2.

Parameter uncertainty can be systematically quantified

Uncertainty analyses can be conducted through iterative parameter entry or use of probability distributions. Parameter uncertainty for the application of the Arnot and Gobas (2004) model in the San Francisco Bay project was evaluated using Monte Carlo analysis. A systematic approach for assessment of model sensitivity and parameter uncertainty will be described in FWM deliverable 2.

Model can be used to predict chemical concentrations in tissue or sediment with the degree of accuracy necessary to make RI/FS decisions

Preliminary human health risk calculations made using the 2004 fish and crab chemistry data show that chemical concentrations in seafood will need to be substantially reduced to reach any risk-based goal based on tribal seafood consumption rates. Consequently, the model performance must be adequate at chemical concentrations lower than those that currently exist in the system. The underlying equations and assumptions of the Arnot and Gobas (2004) model are expected to provide a reasonable estimate across the range of chemical concentrations associated with tissue RGBs and sediment concentrations likely to be discussed in the FS, therefore this model should be a useful tool in providing information for RI/FS decision making. Model accuracy in other systems is described in Section 4.3.2.

Model has been used and accepted at other Superfund sites

Gobas-type models have been used at numerous Superfund sites. For example, a Gobas-type model was used to calculate SQTs in the 1996 RI/FS for the upper Fox River (GAS and SAIC 1996) and in the Sheboygan River ERA (EVS and NOAA 1998), and to predict concentrations in biota in the Hudson River (TAMS 2000). Application of Gobas-type models to these sites is discussed further in the following section (Section 4.3.2).

4.3.2 Application and performance of Gobas models

Models based on the original Gobas (1993) approach have been used in a broad range of environments (i.e., lakes, rivers, and estuaries) (Gobas 1993; Gobas and Wilcockson 2003b; Gobas et al. 1998). The original Gobas model, when applied to Lake Ontario, predicted average fish tissue concentrations within a factor of 1.8 (Gobas 1993). Burkhard (1998) reviewed the capabilities of the Gobas (1993) model and the Thomann et al. (1992) model (a predecessor to the QEA model), to predict chemical concentrations in fish tissue from Lake Ontario, and concluded that the Gobas model provided slightly more accurate predictions of chemical concentrations in fish tissue. Morrison et al. (1997) applied an updated version of the Gobas model to PCBs in Lake Erie. Ninety-five percent of empirical PCB concentrations in invertebrates and fish were within a factor of 2 of the predicted concentrations (Morrison et al. 1997). Gobas et al. (1998) developed a time-dependent, multimedia, mass-balance simulation model of the environmental distribution and food-chain accumulation of organic contaminants in aquatic ecosystems (ECOFATE), and applied it to the Fraser River in British Columbia. The model was parameterized for dioxins and furans. Predicted chemical concentrations for mountain white fish and rainbow trout tissue were within a factor of 1.1 to 1.3 of empirical concentrations, with the model slightly overpredicting concentrations. In 2002, a modified version[3] of the Gobas (1993) model was used to model the bioaccumulation dynamics of hydrophobic organic contaminants in the Anacostia River (Foster et al. 2002). In 2003, an updated version of the Gobas model was applied to PCBs in San Francisco Bay (Gobas and Wilcockson 2003b). This FWM used the same uptake and loss equations as the Arnot and Gobas (2004) version except that it also predicts PCB concentrations in birds, bird eggs, and marine mammals.[4] The San Francisco Bay Regional Water Quality Control Board applied the model to establish a total maximum daily load (TMDL) and implementation plan for PCBs in San Francisco Bay. Empirical PCB concentrations in two polychaete species and two fish species were within factors of 1.6 and 1.1, respectively, of predicted concentrations. A technical report from an early phase of its implementation is available online (Gobas and Wilcockson 2003a). The final report is in draft form and is not currently available to the public.

A good fit between predicted and empirical fish tissue PCBs concentrations has also been reported for Superfund site applications. When the model was applied to the Hudson River (TAMS 2000), annual predicted concentrations in four fish species at three locations for up to 16 years of data (depending on species and location) were generally within the 95% confidence interval of annual median concentrations. Predicted tissue PCB concentrations were mostly within a factor of 2 and were all within a factor of 3 of empirical concentrations (relative percent difference ranged from <1% difference to 188% difference) (TAMS 2000). When the model was applied to the Fox River (GAS and SAIC 1996), estimated fish tissue PCB concentrations were generally within the range of empirical values. Forage fish (alewife, shiners, shad, and smelt) were somewhat underpredicted (0.3 to 1.2 times empirical). PCB concentrations in yellow perch model predictions were 1.6 to 4 times empirical concentrations (based on limited data). Predicted PCB concentrations in walleye, perch, and carp were 0.6 to 2.2 times empirical values. When the model was applied to the Sheboygan River (EVS and NOAA 1998), predicted tissue PCB concentrations were generally within a factor of 5 of empirical concentrations in smallmouth bass.

5.0 Food Web Model Parameters

For its application to the LDW, the Arnot and Gobas model currently has 12 site-specific input parameters (Table 5-1) and 28 literature-based parameters (Table 5-2). FWM deliverable 3 will describe model parameterization in more detail, discussing site-specific data, literature sources, uncertainty, and assumptions made for each parameter. The results presented in deliverable 3 will be assessed, in consultation

[3] Uptake by invertebrates was calculated using empirically derived bioaccumulation factors rather than equilibrium partitioning equations, and fish growth rates and feeding rates were calculated using site-specific or species-specific data rather than empirically derived equations

[4] Chemical concentrations in marine mammals, birds, or bird eggs will not be modeled in the Phase 2 ERA for the LDW

with the EPA and the Washington State Department of Ecology, to determine whether additional data would improve model accuracy.

Table 5-1. Site-specific parameters for the Arnot and Gobas (2004) model

MODEL COMPONENT
Biological
Weight of the organism (species-specific)
Lipid fraction of the organism (species-specific)
Non-lipid organic matter fraction of the organism (species-specific)
Water fraction of the organism (species-specific)
Environmental / Sediment
Chemical concentration in sediment
Sediment organic carbon content
Environmental / Water
Total chemical concentration in the water column[a]
Concentration of dissolved organic carbon in the water column
Concentration of particulate organic carbon in the water column (approximated as the difference between TOC and DOC)
Mean water column temperature
Dissolved oxygen concentration in the water column
Concentration of suspended solids in the water column

[a] Will be based on empirical data or output from King County hydrodynamic model

Table 5-2. Literature-based parameters for the Arnot and Gobas model

MODEL COMPONENT
Biological
Fraction of the diet consisting of each prey item (species-specific)
Fraction of overlying water ventilated (species-specific)
Fraction of porewater ventilated (species-specific)
Lipid fraction of the organism (phytoplankton & zooplankton)
Non-lipid organic carbon fraction of the phytoplankton
Non-lipid organic matter fraction of the organism (zooplankton)
Water fraction of the organism (phytoplankton & zooplankton)
Rate constant for metabolic transformation of the chemical
Scavenging efficiency of particles absorbed from the water
Resistance to chemical uptake through aqueous phase for algae, phytoplankton, and aquatic macrophytes
Resistance to chemical uptake through organic phase for algae, phytoplankton, and aquatic macrophytes
Proportionality constant expressing the sorption capacity of non-lipid organic matter to that of octanol
Dietary absorption efficiencies of lipid in fish, crabs, invertebrates, zooplankton
Dietary absorption efficiencies of non-lipid organic matter in fish, crabs, invertebrates, zooplankton
Dietary absorption efficiencies of water for fish, crabs, invertebrates, zooplankton

Model Component
Environmental / Porewater
Density of the organic carbon in sediment
Environmental / Water
Disequilibrium factor for dissolved organic carbon partitioning
Disequilibrium factor for particulate organic carbon partitioning
Proportionality constant describing similarity in phase partitioning of dissolved organic carbon in relation to that of octanol
Proportionality constant describing similarity in phase partitioning of particulate organic carbon in relation to that of octanol
Chemical Properties
Octanol-water partition coefficient
Henry's Law constant

6.0 References

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Conceptual Bioaccumulation Model Figures

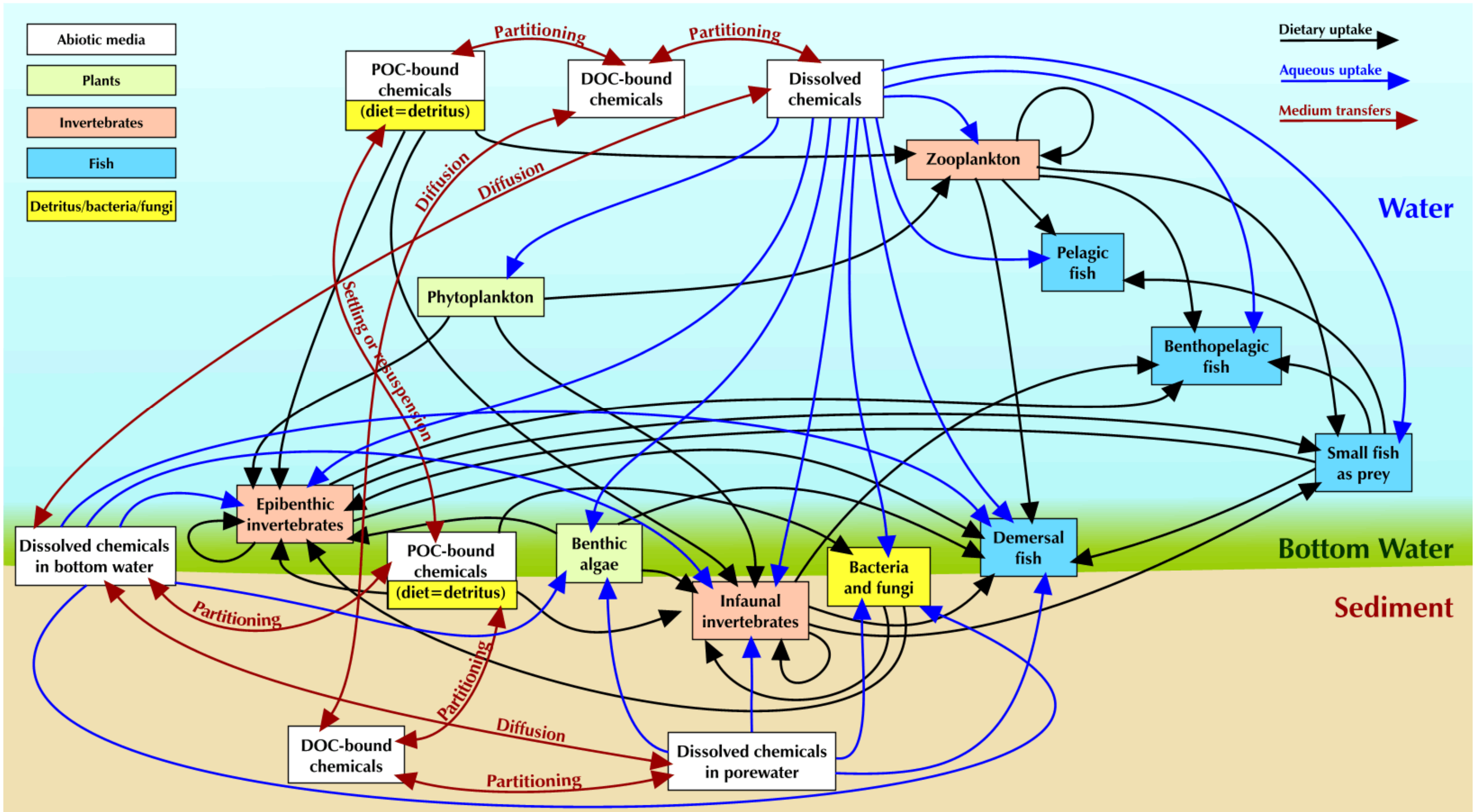

Figure 3-1. Generalized LDW food web model

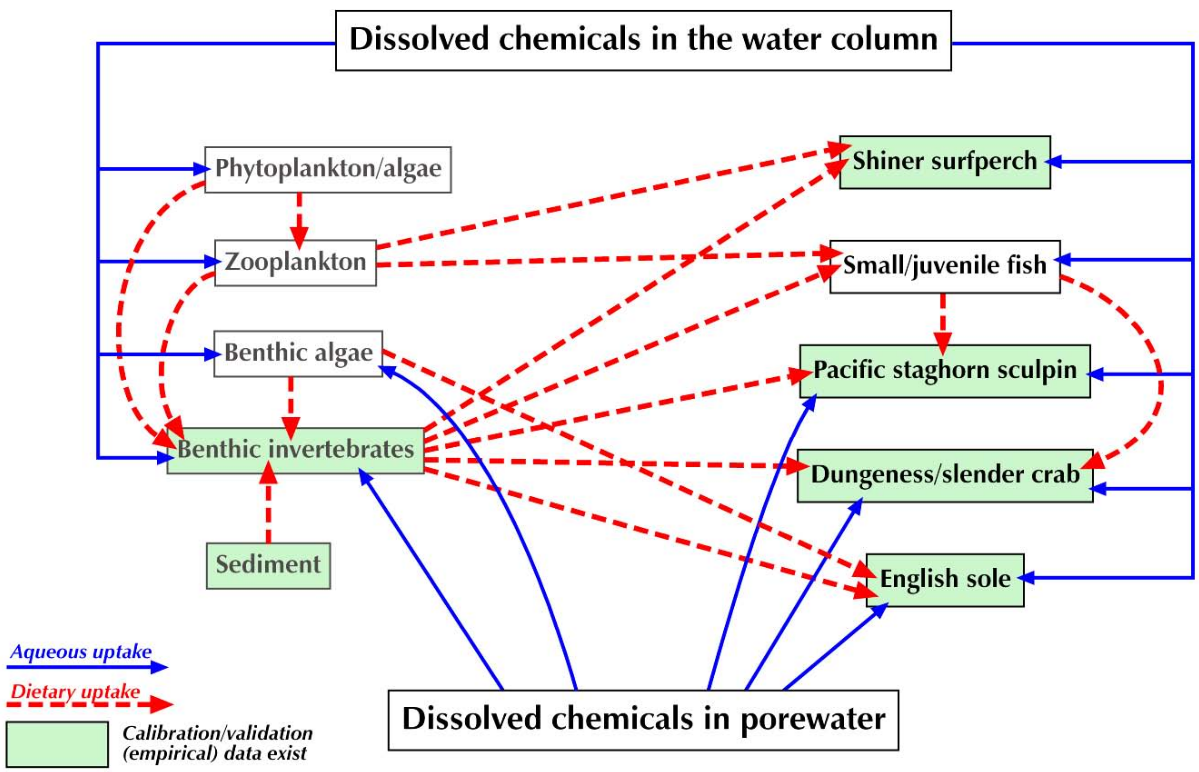

Figure 3-2. Simplified dietary and aqueous uptake routes for LDW biota

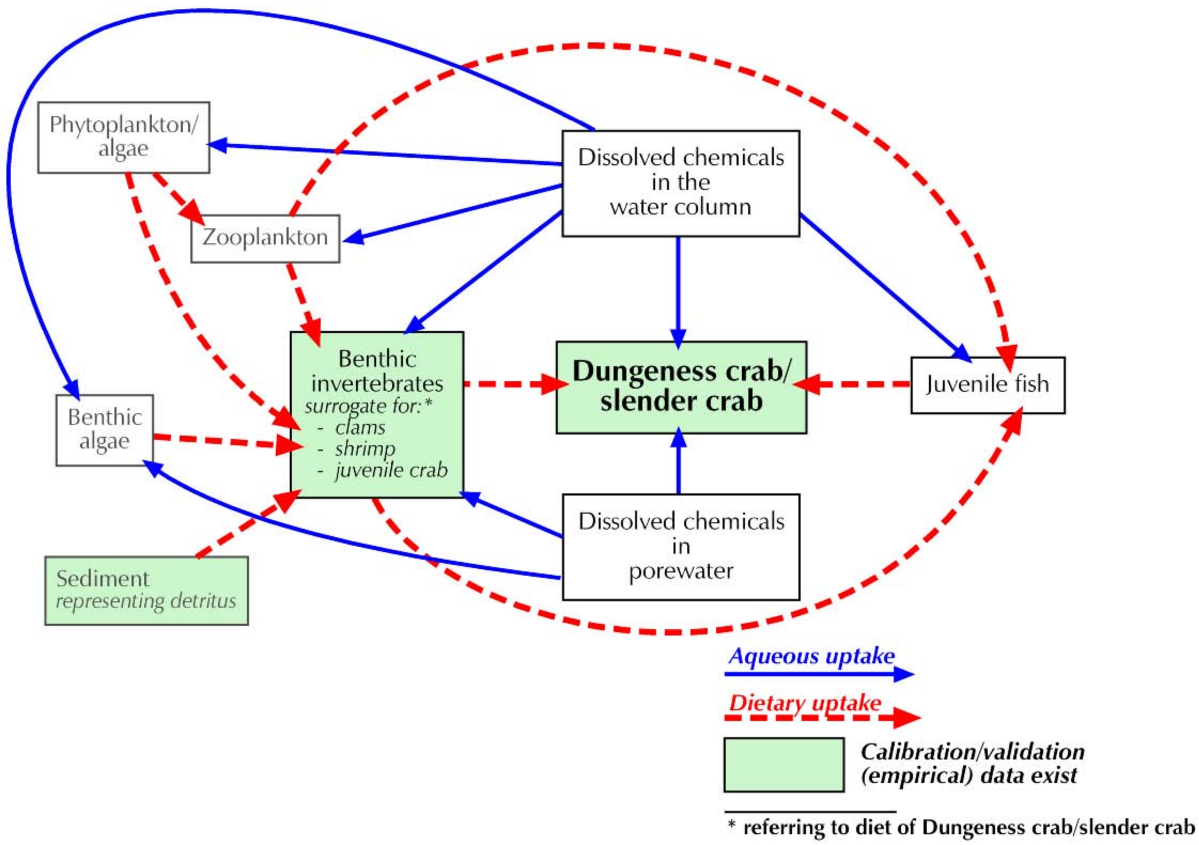

Figure 3-3. Simplified dietary and aqueous uptake routes for Dungeness crab and slender crab

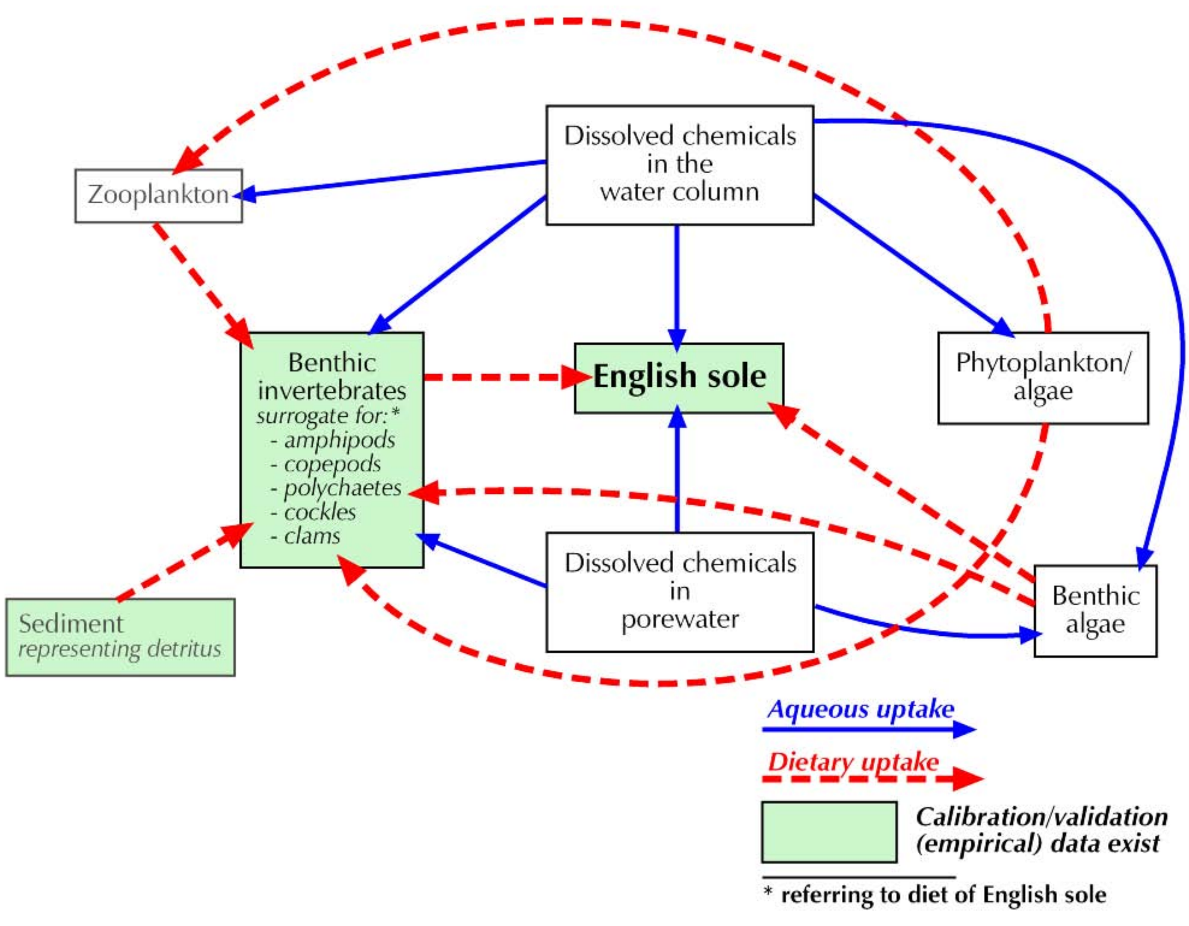

Figure 3-4. Simplified dietary and aqueous uptake routes for English sole

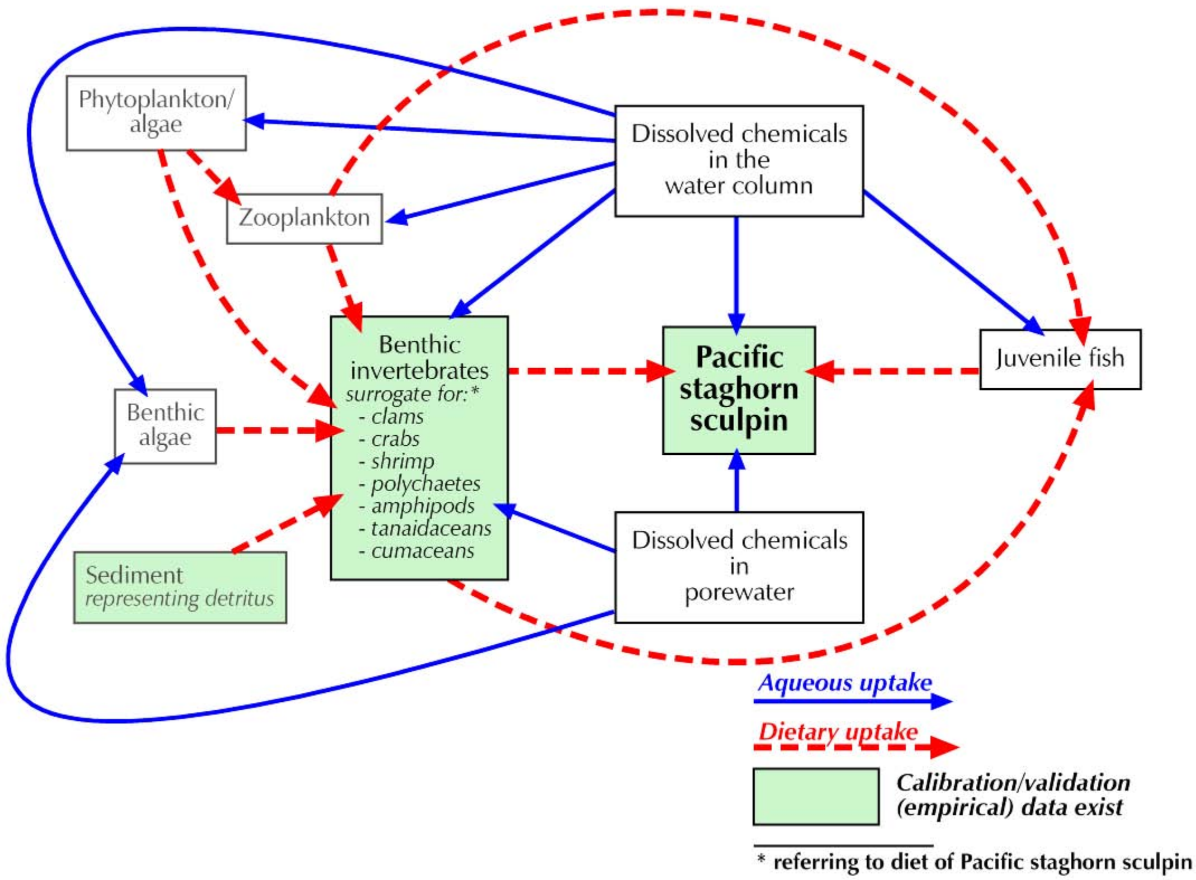

Figure 3-5. Simplified dietary and aqueous uptake routes for Pacific staghorn sculpin

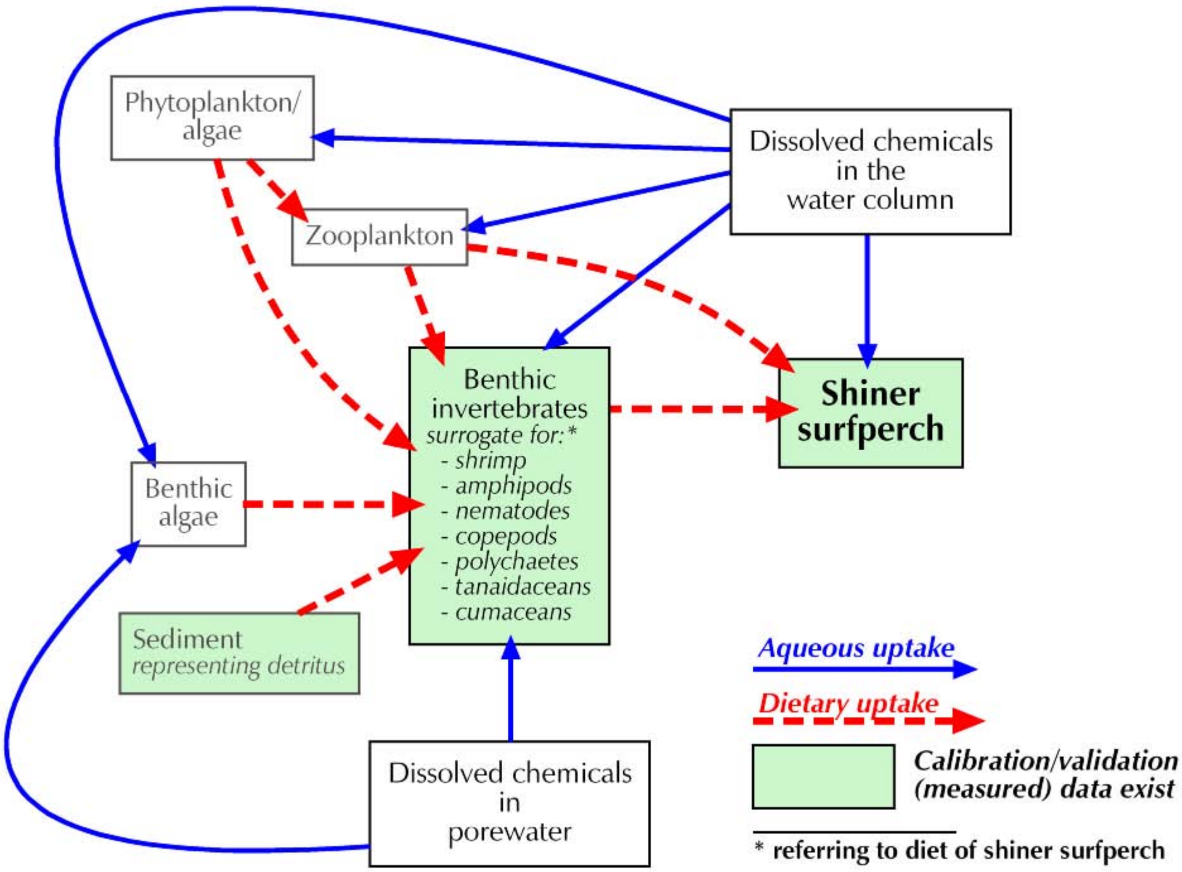

Figure 3-6. Simplified dietary and aqueous uptake routes for shiner surfperch