Lower Duwamish Waterway Group

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

# *Lower Duwamish Waterway Remedial Investigation*

## FOOD WEB MODEL MEMORANDUM 2: MODELING APPROACH

Prepared for

**The U.S. Environmental Protection Agency**
**Region 10**
Seattle, WA

**The Washington State Department of Ecology**
**Northwest Regional Office**
Bellevue, WA

**November 10, 2005**

**Prepared by:** Windward environmental LLC

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

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## Acronyms

| Acronym | Definition |
|---|---|
| **BPTC** | base predicted tissue concentration |
| **COC** | chemical of concern |
| **cPAH** | carcinogenic polycyclic aromatic hydrocarbon |
| **DOC** | dissolved organic carbon |
| **Ecology** | Washington State Department of Ecology |
| **EFDC** | Environmental Fluid Dynamics Computer Code |
| **EPA** | US Environmental Protection Agency |
| **ERA** | ecological risk assessment |
| **FS** | feasibility study |
| **FWM** | food web model |
| **HHRA** | human health risk assessment |
| **HQ** | hazard quotient |
| **$K_{ow}$** | octanol-water partition coefficient |
| **LDW** | Lower Duwamish Waterway |
| **MPAF** | model predictive accuracy factor |
| **NLOC** | non-lipid organic carbon |
| **NLOM** | non-lipid organic matter |
| **NPTC** | new predicted tissue concentration |
| **PAH** | polycyclic aromatic hydrocarbon |
| **PCB** | polychlorinated biphenyl |
| **POC** | particulate organic carbon |
| **QAPP** | quality assurance project plan |
| **RBG** | risk-based goal |
| **RI** | remedial investigation |
| **RI/FS** | remedial investigation/feasibility study |
| **RM** | river mile |
| **SPAF** | species predictive accuracy factor |
| **SPD** | species percent difference |
| **SQT** | sediment quality threshold |

| Acronym | Definition |
|---|---|
| **SWAC** | spatially weighted average concentration |
| **TBT** | tributyltin |
| **TEF** | toxic equivalency factor |
| **TEQ** | toxic equivalent |
| **TOC** | total organic carbon |

## Glossary

| | |
|---|---|
| **Base parameterization** | Parameterization resulting from the first calibration of the initial parameterization for the LDW-wide spatial scale (LDW initial parameterization). This parameterization will be used in the sensitivity and uncertainty analyses. |
| **LDW Initial parameterization** | Parameterization resulting from initial best approximate value for each input parameter at the LDW-wide spatial scale. |
| **Model performance criterion** | A criterion used for model performance evaluation after initial calibration. The criterion is predicted tissue concentrations for all species within a factor of 5 of empirical data. |
| **Model performance evaluation metrics** | Metrics developed to quantify model performance |
| **Model performance goal** | A goal set as a target for continued model calibration. The goal is predicted tissue concentrations for all species within a factor of 3 of empirical data. |
| **Parameterization** | 1) Set of input values entered for the model parameters<br>2) Process of selecting input values for model parameters |
| **Subsection of the LDW** | Area smaller than the LDW-wide area to be modeled for certain species (e.g., tissue sampling area 2 or tissue sampling subarea 3 of tissue sampling area 3) |

## 1.0 Introduction

A comprehensive dataset of chemical concentrations in sediment and tissue samples 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 based on the model of Arnot and Gobas (Arnot and Gobas 2004). The FWM is needed for two applications. As part of the RI, risk-based goals (RBGs) for fish and crab tissue[1] 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)[2] 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 alternatives.

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 second of these three FWM deliverables, and focuses on key approaches required for model development and evaluation. Section 2.0 of this memorandum summarizes the chemicals that will be modeled using the selected FWM, and Section 3.0 describes specifically how polychlorinated biphenyls (PCBs) will be modeled. Section 4.0 presents the areas of the LDW to be modeled. Section 5.0 presents the modeling approach for the LDW-wide spatial scale, and the modeling approach for subsections of the LDW. Section 5.0 also describes calibration and associated analysis tools that will be used to refine the FWM prior to its final uses in the Phase 2 remedial investigation/feasibility study (RI/FS). Section 6.0 contains quality assurance and quality control measures, and Section 7.0 contains references cited.

## 2.0 Chemicals to Be Modeled

The baseline ERA and HHRA will be conducted using Phase 1 and Phase 2 data to estimate risks assuming no remedial actions occur, as discussed in Section 3.3 of the Phase 2 work plan (Windward 2004c). The results of these baseline risk assessments will be used to identify chemicals that could trigger remedial action (i.e., risk drivers), and will thus aid in defining the list of chemicals to be modeled.

[1] Clam RBGs will be developed in the HHRA. The clam RBGs will then be translated into SQTs using biota-sediment accumulation factors.

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

In the Phase 2 RI, RBGs in tissue will be estimated for risk-driving chemicals from dietary exposure pathways. RBGs are acceptable[3] chemical concentrations in biota (i.e., fish, crabs, clams, or benthic invertebrates). RBGs will then be translated into SQTs using either the FWM or other tools.

Baseline risk estimates have not been completed; however, the Phase 1 risk estimates provide preliminary results (Windward 2003a, b). Based on the exposure scenarios evaluated in the Phase 1 HHRA, the following chemicals were identified as chemicals of concern (COCs)[4] (i.e., having a cancer risk estimate greater than 1 in 1,000,000 or a hazard quotient [HQ] greater than 1 for non-carcinogenic health effects) for a dietary exposure pathway: polychlorinated biphenyls (PCBs), arsenic, carcinogenic PAHs (cPAHs), tributyltin (TBT), and mercury. The Phase 1 ERA identified PCBs, arsenic, and copper as warranting additional analysis in the baseline ERA because tissue concentrations exceeded established dietary effects levels for survival, growth, or reproduction in at least one fish or wildlife species.[5]

The final list of chemicals to be modeled as risk drivers for the Phase 2 RI/FS will be determined following completion of the baseline risk assessments, and will be based on risk results, consideration of background information, and the spatial distributions of risk-driving chemicals. It is clear that modeling of PCBs will be required. The Arnot and Gobas (2004) FWM is well suited for modeling PCBs.

The physical and chemical properties of any other chemicals for which RBGs are derived will define the approach to the development of sediment SQTs. The FWM to be used for the Phase 2 RI/FS was designed for hydrophobic organic compounds that are not readily metabolized. Therefore, if RBGs are calculated for other chemicals that are either metabolized (e.g., polycyclic aromatic hydrocarbons [PAHs]) or otherwise regulated by organisms (e.g., certain metals in fish), an approach for evaluating the linkage between concentrations of these chemicals in sediment and tissue other than the FWM would need to be determined in coordination with the US Environmental Protection Agency (EPA) and the Washington Department of Ecology (Ecology).

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[3] Health-protective if equaled or not exceeded; for wildlife and human health, this concentration is calculated using the dietary exposure model.

[4] A larger number of chemicals were identified as COCs for human health based on direct sediment contact scenarios. Food web modeling is not required for these scenarios because no dietary pathway is involved.

[5] A larger number of chemicals were identified as COCs for benthic invertebrates. Risks to benthic invertebrates will be evaluated in the ERA based on direct exposure to sediment; food web modeling is not required.

## 3.0 PCB Modeling Approach

As discussed in Section 2.0, PCBs are a known risk driver for the LDW based on the results of the Phase 1 risk assessments (Windward 2003a, b). PCBs will be modeled for this project to generate SQTs and to estimate fish and crab concentrations so that residual risks associated with various remedial alternatives can be calculated. The form of PCBs to be modeled (total PCBs [sum of Aroclors] vs. individual PCB congeners vs. toxic equivalents [TEQs]) is discussed below.

PCBs have been analyzed in sediment and tissue samples from the LDW as Aroclors, as individual PCB congeners, or both, depending on the sampling location. Risk estimates for the Phase 2 RI will be made using both total PCBs (as Aroclors) and PCB congener data (Windward 2004c). Because the FWM will attempt to establish the linkage between tissue RBGs, which are based on risk assessment results, and SQTs, understanding the manner in which PCB risks will be estimated in the Phase 2 HHRA and ERA is important in order to understand the PCB modeling approach. A technical memorandum currently being prepared summarizes the risk estimation methods that may be used in the Phase 2 HHRA and ERA, and provides rough risk estimates for PCBs. This memorandum will be submitted to EPA and Ecology in December 2005.

Because both total PCBs (as Aroclors) and dioxin-like PCB congener data will be used in the baseline risk assessments, the relationship between total PCBs (as Aroclors) and PCB-TEQ was evaluated. The two data sets are highly correlated, therefore, if predictions of PCB-TEQs in tissue are needed for the residual risk assessment, the relationship between total PCBs and PCB-TEQ could be used to predict PCB-TEQs. The evaluation of these two data types is presented below.

The Phase 2 tissue sampling conducted in 2004 included the analysis of 108 fish and crab samples, 14 clam samples, and 20 benthic invertebrate composite samples for total PCBs (as Aroclors). As specified in the quality assurance project plans (QAPPs) for these events (Windward 2004a, b), a minimum of one-third of the samples of each tissue type analyzed for total PCBs were also analyzed for all 209 individual PCB congeners. The samples targeted for PCB congener analyses were selected to cover the range of total PCBs and to provide spatial coverage (Windward 2005a, b). A total of 62 composite tissue samples, including a subset of each tissue type, were analyzed for PCB congeners (Table 3-1) to provide the data necessary to estimate the risks from dioxin-like PCB congeners. The average total PCB concentration and TEQ[6] for each species/tissue type ranged over approximately a factor of 25; the minimum and maximum concentrations ranged more widely (Figure 3-1). Total PCBs (as Aroclors) and TEQ were highly correlated in tissue with an $R^2$ value across all

[6] Based on mammalian toxic equivalency factors (TEFs) from Van den Berg et al. (1998)

sample types of 0.95 (Figure 3-1). The raw PCB congener data are presented in Windward (2005c).

**Table 3-1. Summary of total PCB (as Aroclors) concentrations and TEQ data for LDW benthic invertebrate, clam, fish, and crab samples**

| Sample Type | Number of Samples | Average Total PCB (as Aroclor sum) (µg/kg ww) | Average TEQ from PCB Congeners (ng/kg ww) |
|---|---|---|---|
| Benthic invertebrate composite | 8 | 394 | 5.51 |
| Clam | 8 | 222 | 2.45 |
| Dungeness crab-edible meat | 3 | 136 | 2.68 |
| Dungeness crab-hepatopancreas | 2 | 3,620 | 61.5 |
| English sole-fillet | 7 | 955 | 17.1 |
| English sole-whole body | 7 | 2,020 | 33.4 |
| Pile perch-fillet | 1 | 192 | 4.83 |
| Shiner surfperch-whole body | 9 | 3,190 | 49.7 |
| Slender crab-edible meat | 4 | 155 | 3.98 |
| Slender crab-hepatopancreas | 2 | 918 | 25.0 |
| Staghorn sculpin-whole body | 8 | 749 | 13.1 |
| Starry flounder-fillet | 1 | 300 | 5.40 |
| Starry flounder-whole body | 1 | 458 | 7.94 |
| Striped perch-fillet | 1 | 442 | 11.3 |

A similar correlation of PCBs as the sum of Aroclors and as TEQs was also found for surface sediment. Demonstration of this relationship is important because sediment is a key input parameter to the FWM. Thirty-three sediment samples collected as part of the Round 1 and 2 sediment sampling events in early 2005 were analyzed for both PCB Aroclors and a subset of individual PCB congeners (including the dioxin-like PCB congeners to calculate a TEQ). Concentrations of PCBs in sediment expressed as a sum of Aroclors and as TEQ were also highly correlated (Figure 3-2; $R^2 = 0.96$).

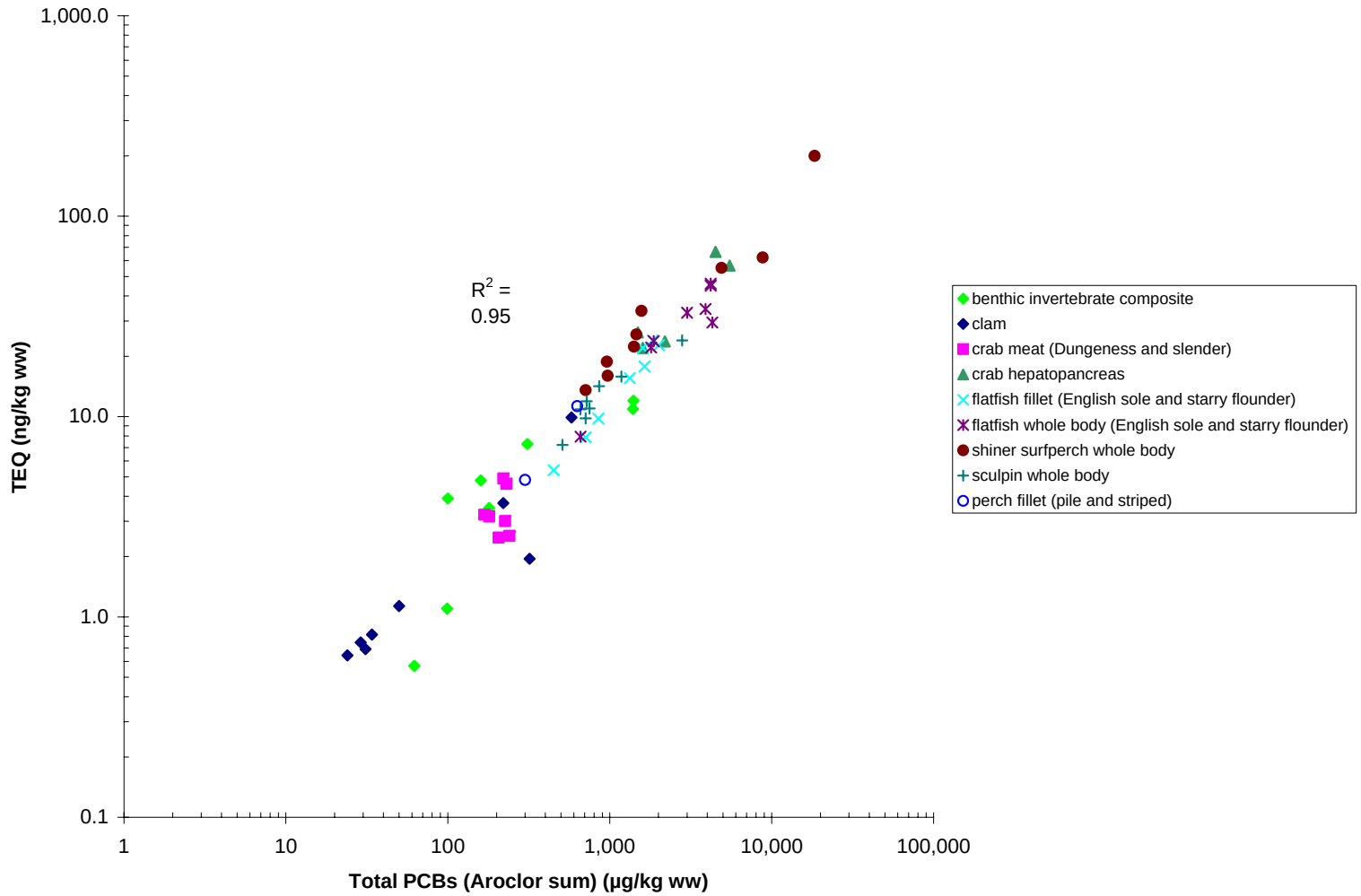


**Figure 3-1. Total PCB concentration (Aroclor sum) vs TEQs for LDW benthic invertebrate, fish, crab, and clam tissue samples collected in Phase 2**

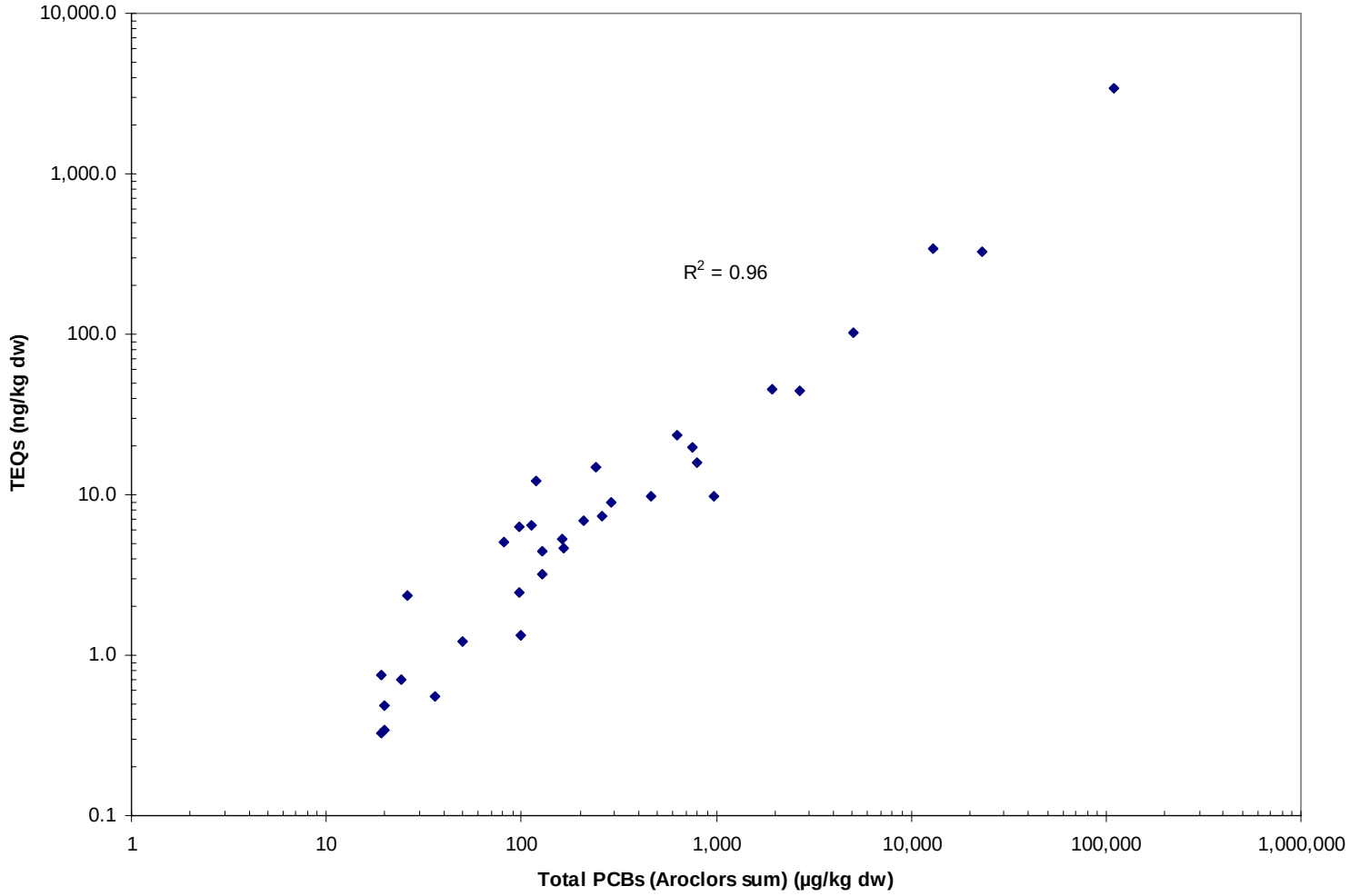


**Figure 3-2. Total PCB concentrations (Aroclor sum) vs TEQs for LDW surface sediments collected in Phase 2**

The consistency of these correlations indicates that modeling total PCBs (as Aroclors) should allow SQTs, RBGs, and residual risk estimates to be made that are health-protective of the overall risk attributable to PCBs. This relationship, and its relevance to remedial decision making, will be further explored with EPA and Ecology following their review of the preliminary PCB calculations memorandum as well as a review of approaches used at other Superfund sites.

## 4.0 Spatial Areas to Be Modeled

The spatial areas of the LDW to be modeled are based on both the scales over which risks will be estimated as well as the potential exposure areas (home ranges) of the fish and crab species being modeled (i.e., English sole, Dungeness and slender crabs, shiner surfperch, and Pacific staghorn sculpin).

As described in the Phase 2 Work Plan, human health risks based on seafood consumption and most ecological risks will be calculated for site-wide exposure. The resulting RBGs will be derived from site-wide considerations. As a result, SQTs will generally be calculated on a site-wide basis. Therefore, the FWM will initially be calibrated on an site-wide basis. Section 5.0 describes the calibration approach.

In the uncertainty analysis for the HHRA and ERA, risk predictions for particular human populations or ecological receptors may also be of interest at spatial scales smaller than the entire LDW. Modeling subsections of the LDW (see Section 5.7) may be relevant for species with home ranges smaller than the LDW, and may contribute to an understanding of uncertainty in the baseline[7] and residual risk assessments. Moreover, use of the FWM to evaluate residual risk after remedial actions or recovery times could involve applications of the model to spatial scales smaller than the entire LDW. Therefore, following initial calibration, the ability of the FWM to predict empirical tissue data for LDW subsections will also be evaluated. Calibration of the FWM for these LDW subsections is described in Section 5.6.

English sole appear to be found less often in low salinity conditions (Toole et al. 1987). Therefore, in addition to LDW-wide modeling, English sole may also be modeled in two subsections of the LDW (a northern and a southern subsection) based on the location of the salt wedge and salinity information (Table 4-1).

Pacific staghorn sculpin and shiner surfperch will be modeled at an LDW-wide scale, and also at the spatial scales of the four individual fish and crab tissue sampling areas and a subset of the fish and crab tissue sampling subareas (Table 4-1; Figure 4-1). These scales were selected because local experts expressed opinions at a March 31, 2004, meeting that the foraging movements of these species may be as large as the

[7] The baseline risk assessments will be based on empirical data. However, insights gained through modeling may be helpful in reducing exposure uncertainties.

LDW but could also be as small as a tissue sampling subarea (approximately 0.26 mi).

**Table 4-1. Areas to be modeled for each species**

| Species | LDW-wide | 2 Subsections of LDW Based on Salinity Information | Tissue Sampling Areas | Tissue Sampling Subareas[a] |
|---|---|---|---|---|
| English sole | X | X | | |
| Shiner surfperch | X | | X | X |
| Pacific staghorn sculpin | X | | X | X |
| Crabs | X | | | |

[a] The model will be run for a subset of the tissue sampling subareas. Subareas will be selected to cover a range of total PCB concentrations in sediment and tissue.

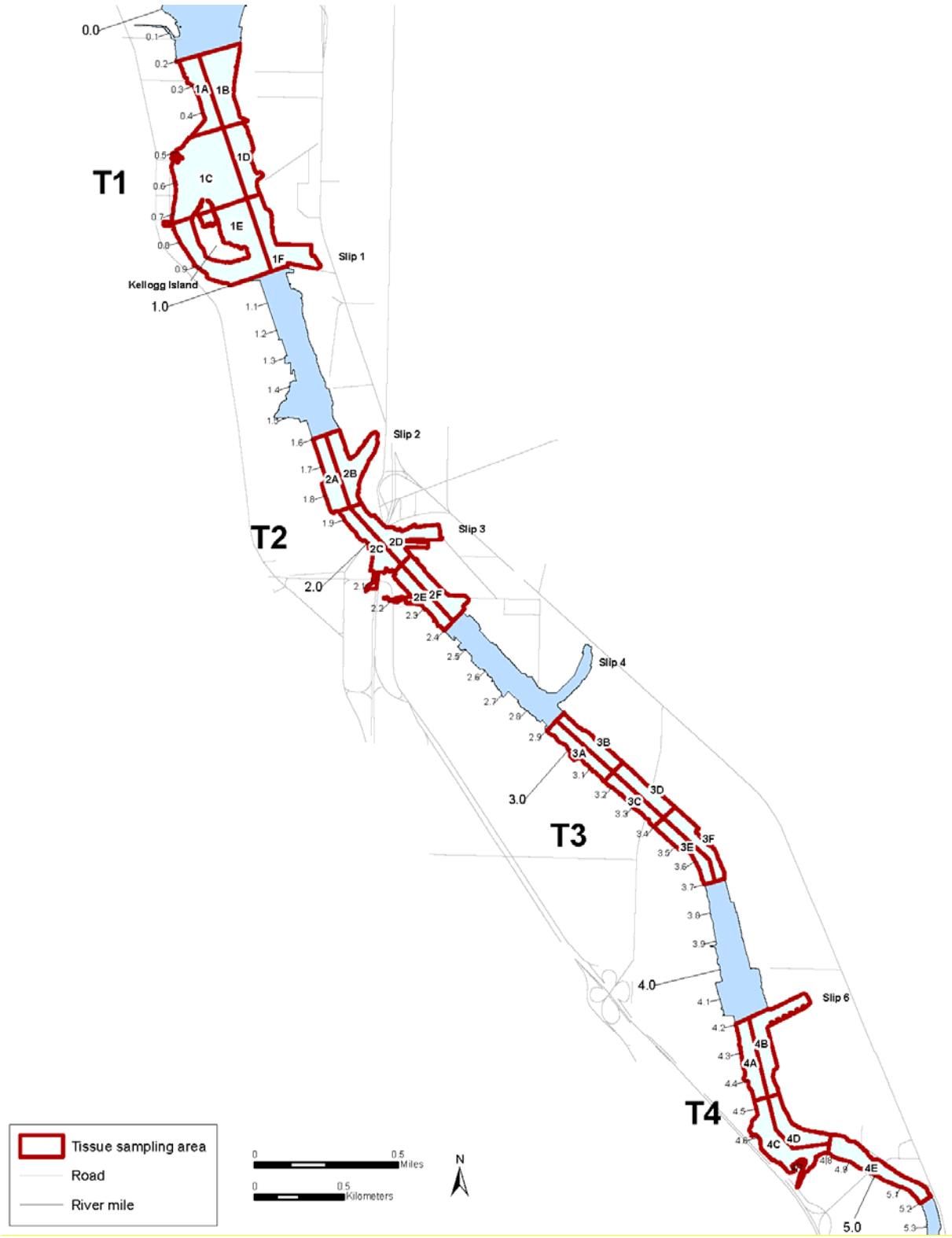


**Figure 4-1. Fish and crab tissue sampling areas**

## 5.0 Modeling Approach

No model can be verified to be an exact representation of the system being modeled because all natural systems are open systems subject to randomness and uncertainty (Oreskes et al. 1994). Model structures are only approximate representations of true ecosystem structures and relationships, and models require input parameters that are incompletely known. In addition, measurements of population and ecosystem parameters are approximations because no study can capture all variations of all parameters affecting bioaccumulation.

Model validation is defined as the process of ensuring that the model is reasonably parameterized for the designated purpose. To fully validate a model, model output would be compared to a dataset not used in calibration (Banks and Carson 1984; Oreskes et al. 1994). In this sense, the LDW FWM will not be "validated" (i.e., an independent dataset will not be used to validate the FWM). However, through careful parameterization, initial calibration, sensitivity analyses, uncertainty analyses, and further calibration, the FWM can be optimized to the extent necessary to meet project needs.

This section describes the process that will be followed to parameterize, calibrate, and evaluate the performance of the LDW FWM. This process is presented schematically in Figure 5-1. For the LDW-wide spatial scale, the FWM will first be parameterized with initial best estimates of parameter values (LDW initial parameterization; see Section 5.1). If the FWM with the initial parameterization does not meet the model performance criterion, then the FWM will be calibrated (Section 5.3). If initial calibration activities can meet the model performance criterion of predicted tissue concentrations for all species within a factor of 5 of empirical data (Section 5.2), then sensitivity and uncertainty analyses (Sections 5.4 and 5.5) will proceed. If the FWM cannot be calibrated to meet the model performance criterion, further actions will be determined in consultation with EPA and Ecology.

After sensitivity and uncertainty analyses are completed for the site-wide scale, the FWM will be applied to several subsections of the LDW (Sections 4.0 and 5.6). If the base parameterization with location-specific parameter values for each subsection does not immediately meet the model performance criterion, then the FWM will be calibrated for each subsection of the LDW, focusing on parameters with location-specific data. Subsection models that meet the model performance criterion will be selected for further calibration activities. Once the LDW-wide spatial scale and all subsections have been initially calibrated and subsections of the LDW have been selected for further calibration, further calibration activities will begin for all selected spatial scales and locations. Those parameterizations that meet the model performance criterion or goal (Section 5.2) will be selected and subjected to final uncertainty analyses. Final calibration and uncertainty analyses will be presented in the Phase 2 RI.

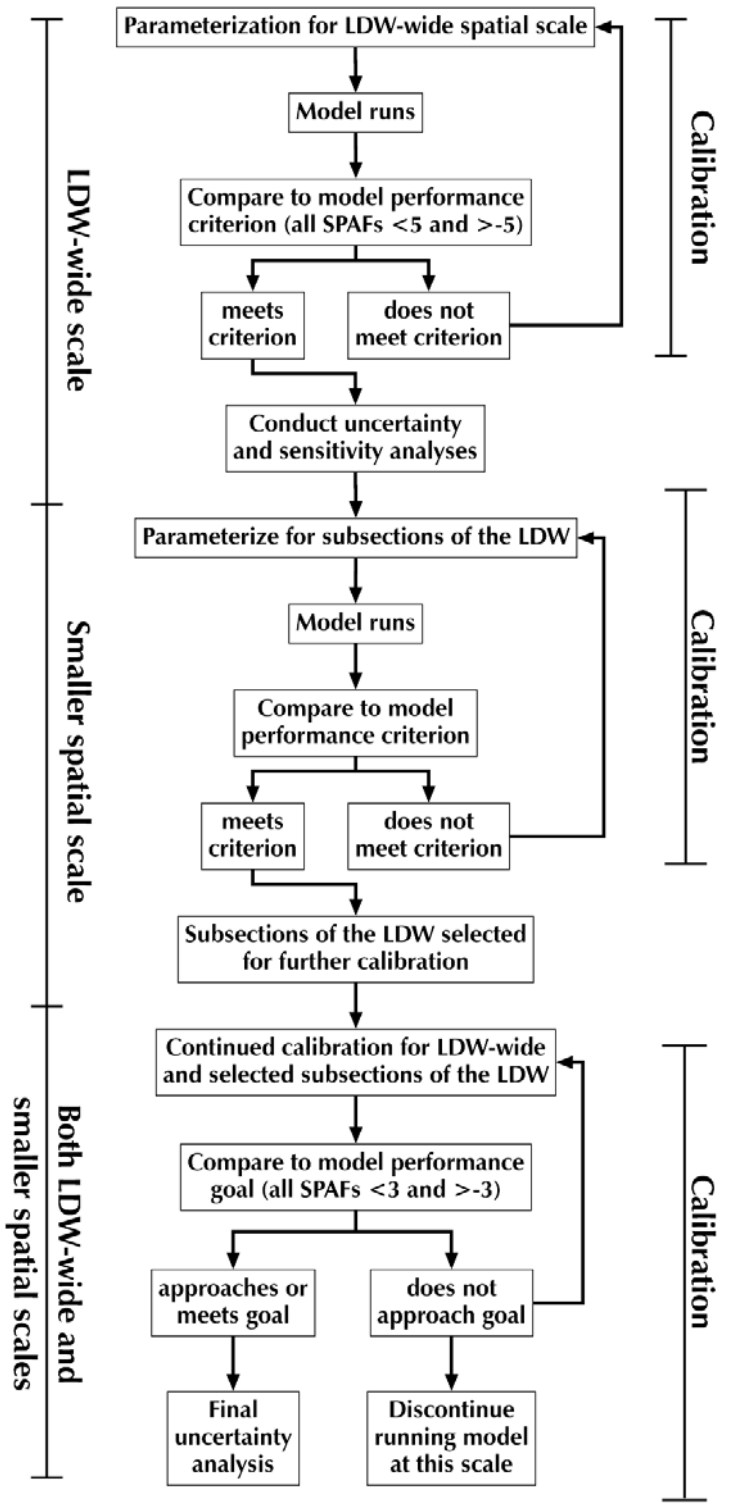


**Figure 5-1. Parameterization and calibration cycle**

## 5.1 MODEL PARAMETERIZATION APPROACH

Before any model runs can be conducted, the FWM must be fully parameterized (i.e., specific values must be provided for each model input parameter). Parameterization is an iterative process. Multiple lines of evidence will be explored to select the initial best approximation and the reasonable upper and lower bound estimates for each input parameter value. Sources of information for model parameterization will include site-specific data from Phase 1 and Phase 2 investigations, and either site-specific or other information available from the grey literature, agency reports, and peer-reviewed literature. The FWM will initially be parameterized with the best approximate average value for the LDW-wide exposure area. This parameterization will be called the initial parameterization. Examples of the types of data currently available for parameterization of the FWM and methods for selecting and deriving parameter values are given below.

**Site-specific empirical data –** Site-specific data are available for numerous input parameters to the FWM (e.g., organism weights and lipid fractions, water quality parameters, chemical concentrations in sediment, organic carbon content of sediment). Statistical distributions of these site-specific data are generally available on an LDW-wide spatial scale. Available summary statistics for these types of parameters include the mean, geometric mean, maximum, and minimum.

A large site-specific dataset is available for sediment parameters, but the sample locations do not equally represent the LDW spatially. Therefore, spatially weighted average concentrations (SWACs) will be used for these parameters. The method used to calculate the SWACs will be determined in consultation with EPA and Ecology.

**Modeled data –** Total PCB concentrations in the water column will be determined based on the output of a hydrodynamic model calibrated with various LDW site data (e.g., current velocities, salinity, total suspected solids [TSS], metals, and PCBs). This model, the Environmental Fluid Dynamics Computer Code (EFDC), was calibrated by King County to LDW and Elliott Bay site conditions as part of the Water Quality Assessment for the Duwamish River and Elliott Bay (King County 1999). The EFDC model is being re-calibrated for PCBs with new water data collected in 2005 (King County 2005); the recalibration is expected to be completed in March/April 2006. The EFDC model will be used to provide PCB water concentrations on a LDW-wide basis as well as on subsections of the LDW. The PCB water concentrations assumed for the initial parameterization will be based on the model output associated with the King County Water Quality Assessment (King County 1999); when recalibration of the EFDC model is complete based on the 2005 water data being collected by King County, updated PCB water concentrations will be used.

**Literature values –** Site-specific data are not available for all input parameters (e.g., dietary absorption efficiencies of non-lipid organic matter [NLOM] by invertebrates). Literature-based values will be used for these parameters. Many of the literature values to be used have been used for previous applications of the Arnot and Gobas

model (Arnot and Gobas 2004; Gobas and Wilcockson 2003). For organism diets, different scenarios will be developed to reflect the variability and uncertainty of dietary fractions. This information and the specific methods used to determine each parameter's range of values will be presented in FWM Deliverable 3.

## 5.2 MODEL PERFORMANCE EVALUATION METRICS

Two model performance evaluation metrics will be used to evaluate the results of a given model run relative to empirical data. These metrics are:

- the species predictive accuracy factor (SPAF)
- the model predictive accuracy factor (MPAF)

The metrics are indications of a "factor difference" between predicted and empirical values, a common measure of model performance (Gobas 1993; Morrison et al. 1997; ThermoRetec 2001). These metrics complement one another in evaluating model performance. Both metrics will be generated for each model run.

The SPAF will be the main metric used during calibration because it is a species-specific indication of FWM performance. The SPAF is calculated in one of two ways (Equation 5-1 or 5-2), depending on the relative magnitude of predicted and empirical tissue chemical concentrations for a given species.

The SPAF is calculated as follows if predicted tissue chemical concentrations are higher than empirical tissue chemical concentrations:

$$\text{SPAF} = \frac{\text{predicted tissue chemical concentration}}{\text{empirical tissue chemical concentration}} \qquad \textbf{Equation 5-1}$$

The SPAF is calculated as follows if predicted tissue chemical concentrations are lower than empirical tissue chemical concentrations:

$$\text{SPAF} = \frac{\text{empirical tissue chemical concentration}}{\text{predicted tissue chemical concentration}} \times -1 \qquad \textbf{Equation 5-2}$$

For Equation 5-2, a negative sign is automatically assigned to the SPAF to indicate an underprediction. Although it is conventional to have the predicted value always divided by the empirical value, Equation 5-2 ensures that factor differences will always be greater than 1 (not a fraction).

The SPAF enables a comparison of model results for each species relative to empirical data for that species. Because a negative sign is assigned to the SPAF for each species where the FWM underpredicts the empirical data, the SPAF indicates both the magnitude of difference from empirical data and whether the prediction was above or below empirical data.

The statistic used to represent the "empirical data" for the SPAF will be the arithmetic mean[8] of chemical concentrations for all composite samples of a given species at a given scale. Data from different datasets (Phase 1, 2004, and 2005) may be combined or evaluated separately, in consultation with EPA and Ecology.

The MPAF is the average of the absolute value of SPAFs for all species. Thus, MPAF provides a true average factor difference for the FWM without providing information regarding over- or underprediction. This metric provides a quick analysis of how the model is doing for all species combined.

For each iterative step of the calibration process (see Section 5.3), a set of calibration parameters will be tested and model performance will be measured by SPAFs and MPAFs. For the initial calibration, a performance criterion threshold of predictions within a factor of 5 of empirical data (< 5 and > -5 for all SPAFs) will be used. A model performance standard of "within a factor of 5" for all species was set for Gobas models on the Fox River (ThermoRetec 2001) and Hudson River (TAMS 2000). The goal for the final calibration phase is to be "within a factor of three" of empirical tissue data. A model parameterization that meets the model performance standard will be used in the RI/FS. If the model cannot be calibrated to meet this standard, LDWG will discuss various options with EPA and Ecology.

In addition to the SPAF and MPAF, absolute difference metrics such as predicted concentration minus empirical concentration or observed concentration minus predicted concentration divided by observed concentration may be calculated for each species. These metrics could be assessed for each individual species across model runs and/or across all species within one model run to determine whether variations represent uncertainty or bias in the model output. These metrics may be useful for further statistical evaluations of model performance.

## 5.3 INITIAL CALIBRATION APPROACH

Calibration is the iterative process of comparing model results to empirical data, and using the discrepancies between the two to guide the selection of alternative parameter values to improve the model's performance. Calibration consists of establishing values for each model parameter that maximize the fit between the model output (predicted chemical concentrations in tissue) and empirical data (measured chemical concentrations in tissue), while remaining within plausible ranges for each parameter within the LDW or a similar ecosystem. This process is repeated until the pre-established model performance criterion or goal is achieved, or, if not met, until model failure is declared (Banks and Carson 1984).

[8] A mean will only be calculated if more than one composite sample is available for the species at that scale.

For the initial calibration of the LDW-wide spatial scale, those parameters that the model has been proven highly or moderately sensitive to in the past (Arnot 2005) and those with high variability or uncertainty will have their values adjusted. The Arnot and Gobas (2004) model has been automated so that various parameterizations can be rapidly run and results from each model run efficiently compared. All modifications to the base parameterization will be documented.

In addition to altering single parameters sequentially for calibration, dietary fraction estimates will be tested by running several dietary scenarios created during the parameterization phase. Dietary scenarios will be evaluated on a species-specific basis, and will be presented in FWM Deliverable 3

The resulting parameterization from the initial calibration of the LDW-wide scale will be called the base parameterization. This parameterization and the results of the initial calibration will be presented in FWM Deliverable 3. If the model performance criterion (all SPAFs < 5 and > -5) is achieved, sensitivity and uncertainty analyses will be completed on the base parameterization (Sections 5.4 and 5.5), and presented in FWM Deliverable 3. After these analyses are completed, subsections of the LDW will be evaluated (Section 5.5). If the FWM cannot be calibrated to within a factor of 5 at any spatial scale, further actions will be determined in consultation with EPA and Ecology.

## 5.4 SENSITIVITY ANALYSIS APPROACH

Sensitivity analysis involves the investigation of how changes in input parameters affect model output. The sensitivity analysis identifies parameters that most influence model predictions. These analyses provide the basis for determining calibration parameters, and also for selecting parameters to be evaluated in the uncertainty analysis. Particularly sensitive parameters merit relatively closer scrutiny.

Two types of sensitivity analyses will be conducted. One method will decrease each parameter value by 10% to assess the relative influence of each parameter on model output. The second method will alter each selected parameter value by a larger amount representing a range of the most probable values (e.g., one standard deviation). Varying parameters by 10% will identify which parameters the model is most sensitive to as a result of the mathematical formulation of the model. Varying parameters by a fraction of their known (or estimated) range of variability will identify which parameters the model is most sensitive to as a result of inherent variability or uncertainty in the parameters themselves.

### 5.4.1 Sensitivity Analysis with 10% Change

The sensitivity of the model to each input parameter will be assessed by independently decreasing each input parameter value by 10% to determine the change in model output. Output will be most influenced by those parameters to

which the model is more sensitive and less influenced by those parameters to which the model is less sensitive. To assess the influence of these parameter changes on model predictions, resulting estimates of tissue concentrations will be compared to predictions from the base parameterization rather than empirical tissue concentration data. Comparison to empirical data occurs as part of the calibration process (Section 5.3).

Unless otherwise indicated in Table 5-1, each parameter listed will be tested independently by decreasing its value by 10%. Species-specific parameters that have different values for each species (e.g., lipid fraction, weight, water fraction) will be adjusted simultaneously for all species. The simultaneous adjustment is done to simplify the sensitivity analysis task, with the goal of identifying parameters for additional assessment as part of the uncertainty analysis and calibration activities. Table 5-1 presents parameter-specific considerations for the sensitivity analysis.

Most parameters calculated by equations are not included in the sensitivity analysis because previous sensitivity analyses have found that the model is not sensitive to them (Arnot 2005), or because re-parameterizing them would be a great endeavor beyond the scope of this modeling effort.

**Table 5-1. Parameter-specific considerations for sensitivity analysis**

| MODEL COMPONENT | SENSITIVITY ANALYSIS CONSIDERATIONS |
|---|---|
| **Variables parameterized with site-specific data** | |
| **Biological** | |
| Weight of the organism (species-specific) | All species will be adjusted simultaneously |
| Lipid fraction of the organism (species-specific) | All species will be adjusted simultaneously |
| NLOM fraction of the organism (species-specific) | This parameter will be tested during the model run for water fraction of the organism, because NLOM is related to water fraction as follows:<br>NLOM = 1 - water fraction - lipid fraction |
| Water fraction of the organism (species-specific) | All species will be adjusted simultaneously |
| **Environmental/Sediment** | |
| Chemical concentration in sediment | SWAC (spatially weighted average concentration) estimates will be influenced by the scale being modeled |
| Sediment total organic carbon (TOC) content | SWAC estimates will be influenced by the scale being modeled |
| **Environmental/Water** | |
| Total concentration of a chemical in the water column | Investigates the effect of variability and uncertainty of water concentration estimates |
| Concentration of dissolved organic carbon (DOC) in the water column | Investigates the effect of variability and uncertainty of DOC concentrations |
| Concentration of particulate organic carbon (POC) in the water column (approximated as the difference between TOC and DOC) | Will be adjusted independently of DOC during a separate model run |
| Mean water column temperature | Higher temperatures lead to lower dissolved oxygen |

| MODEL COMPONENT | SENSITIVITY ANALYSIS CONSIDERATIONS |
|---|---|
| Concentration of suspended solids in the water column | Affects the feeding rate of filter feeders |
| **Variables parameterized with literature-based data** | |
| **Biological** | |
| Fraction of the diet consisting of each prey item (species-specific) | Dietary fractions will be evaluated during calibration by testing different dietary scenarios |
| Relative fraction of porewater and overlying water ventilated (species-specific) | fraction porewater + fraction overlying water = 1<br>All species will be adjusted simultaneously |
| Lipid fraction of the organism (phytoplankton and zooplankton) | Included with lipid fraction of the organism model runs, as indicated above |
| Non-lipid organic carbon (NLOC) fraction of the phytoplankton | This parameter will be tested during the model run for water fraction of the organism, because NLOC is related to water fraction as follows:<br>NLOC = 1 - water fraction - lipid fraction |
| NLOM fraction of the organism (zooplankton) | Adjusted relative to % moisture and % lipids (NLOM = 1 - % moisture - % lipids). The model runs for % moisture and water fraction of organism will characterize the model sensitivity to NLOM. |
| Water fraction of the organism (phytoplankton and zooplankton) | Included with water fraction of the organism model runs, as indicated above |
| Rate constant for metabolic transformation of the chemical | For poorly metabolized chemicals, such as PCBs, the value is assumed to be zero. To assess model sensitivity, the model will be run at 0.001 (Arnot 2005) and 10% lower. |
| Scavenging efficiency of particles absorbed from the water | Directly affects feeding rate of filter feeders only |
| Resistance to chemical uptake through aqueous phase for phytoplankton | Directly affects rate constant for aqueous uptake ($k_1$) of phytoplankton only |
| Resistance to chemical uptake through organic phase for phytoplankton | Directly affects rate constant for aqueous uptake ($k_1$) of phytoplankton only |
| Proportionality constant expressing the sorption capacity of NLOM to that of octanol | Affects biomagnification (used to calculate the gastrointestinal tract-to-organism partition coefficient) |
| Dietary absorption efficiencies of lipid in fish, crabs, invertebrates, zooplankton | All species adjusted simultaneously |
| Dietary absorption efficiencies of NLOM in fish, crabs, invertebrates, zooplankton | All species adjusted simultaneously |
| Dietary absorption efficiencies of water for fish, crabs, invertebrates, zooplankton | All species adjusted simultaneously |
| **Environmental/Porewater** | |
| Density of the organic carbon in sediment | Positively correlated with freely dissolved chemical concentration in the porewater |
| **Environmental/Water** | |
| Disequilibrium factor for DOC partitioning | Directly affects the freely dissolved water concentration |
| Disequilibrium factor for POC partitioning | Directly affects the freely dissolved water concentration |
| Proportionality constant describing similarity in phase partitioning of DOC in relation to that of octanol | Directly affects the freely dissolved water concentration |

| MODEL COMPONENT | SENSITIVITY ANALYSIS CONSIDERATIONS |
|---|---|
| Proportionality constant describing similarity in phase partitioning of POC in relation to that of octanol | Directly affects the freely dissolved water concentration |
| **Chemical Properties** | |
| Octanol-water partition coefficient (log $K_{OW}$) | 10% decrease and increase based on antilog of log $K_{OW}$ |
| **Variables Calculated by Model Equations** | |
| **Biological** | |
| Rate constant for growth of aquatic organisms ($k_G$) | This parameter is calculated in the model relative to organism mass. The value generated by the model equation will be decreased 10%. Will be adjusted simultaneously for all organisms. |
| Feeding rate ($G_D$) | Will be adjusted simultaneously for all organisms |
| **Environmental** | |
| Freely dissolved chemical concentration in the porewater ($C_{WD,P}$) | Tests effects of potential inaccuracies of empirical equation used to calculate this parameter. |
| Dissolved oxygen concentration in the water column ($C_{OX}$) | Co-dependent with water temperature, higher temperatures lead to lower dissolved oxygen. Effects gill ventilation rate of invertebrates and fish. |

All parameter adjustments will be calculated automatically from the base parameterization. The sensitivity analysis will be processed in batches and the results from all parameterizations will be output to a single table. The results will be evaluated using a species percent difference (SPD) metric (Equation 5-3) that will be automatically reported for each model run for each species.

$$SPD = \frac{NPTC - BPTC}{BPTC} \times 100 \qquad \textbf{Equation 5-3}$$

Where:

SPD = species percent difference
NPTC = new predicted tissue concentration
BPTC = base predicted tissue concentration

Changes that increase the predicted tissue concentration will be positive and those that decrease the predicted tissue concentration will be negative. Parameters will be ranked by maximum SPDs for any species. The results will be evaluated to determine which parameters to focus on during calibration and uncertainty analyses.

### 5.4.2 Sensitivity Analysis with Upper and Lower Bound Estimates

Parameter sensitivity will also be assessed by altering each parameter value according to its plausible range (e.g., one standard deviation) or upper and lower bound estimates. This analysis will involve two model runs for each parameter, one for the upper bound estimate and another for the lower bound estimate. All parameters from Table 5-1 for which a range of values can be established will be included in this sensitivity analysis. The plausible range of values will be determined in consultation with EPA and Ecology, and will be presented in FMW Deliverable 3.

The SPD metric (Equation 5-3) will also be used to assess the results of the upper and lower bound estimate sensitivity analysis. Parameters will be ranked by maximum SPDs. Results will be evaluated together with results from the 10% sensitivity analysis approach to determine which parameters to focus on during calibration and uncertainty analyses.

## 5.5 UNCERTAINTY ANALYSIS APPROACH

Uncertainty analyses evaluate the effect of uncertainty in input parameters on model output. The purpose of an uncertainty analysis is to characterize quantitatively the combined effect of each parameter's uncertainty on model output (i.e., predicted concentrations of chemicals in tissue). This information is useful not only for refining the model calibration, but also for interpreting final model output.

Monte Carlo simulations will be used to investigate the effects of parameter variability and uncertainty on model predictions. Distributions, rather than point estimates, will be assigned to input parameters, as appropriate (i.e., if data are available and the FWM is sensitive to a given parameter). In a Monte Carlo simulation, the FWM is run hundreds to thousands of times. For each FWM iteration, distributions are generated for input parameters and used in the FWM to generate a distribution of predicted tissue concentrations. The result is a range of model predictions reflecting different combinations of input parameter values. Taken together, the model output values represent the cumulative probability of different outputs based on the user specifications for variable input parameters. Specifications include user-defined probability and range limits.

There are several advantages to Monte Carlo modeling over the use of point estimates. A point estimate approach may be used to bound model predictions by using upper bound estimates for all input parameters, but this approach, unlike Monte Carlo, provides no information on the expected likelihood of such an outcome. Providing model predictions as a distribution quantifies the impacts of model input variability and uncertainty on model predictions as well as the expected probability of different predictions.

Before conducting a Monte Carlo simulation, the distributions to be used for those parameters must be established. All parameters for which an empirical distribution exists will have a distribution generated that matches the data as closely as possible. For other parameters with limited data, the type of the distribution (e.g., flat, triangular) to be used to represent the parameter will be determined based on the nature of the studies the data were derived from (e.g., does the data represent a full range of values or just several point estimates). Some parameters with low sensitivity, based on the sensitivity analysis, will be included only as point estimates in the Monte Carlo simulations. All distribution assumptions will be documented in FWM Deliverable 3 and discussed with EPA and Ecology.

An initial uncertainty analysis will be conducted on the base parameterization for the LDW-wide spatial scale. The results from this analysis will guide further calibration of the LDW-wide spatial scale and guide initial calibration of the subsections of the LDW.

Final uncertainty analyses will be conducted for the LDW-wide scale and/or subsections of the LDW, depending on which are selected for application in the Phase 2 RI/FS based on their performance and spatial needs of RI/FS analyses.

## 5.6 Approach to Evaluate Model Performance for Subsections of the LDW

As discussed in Section 4.0, in addition to the LDW-wide spatial scale, the FWM will be parameterized and calibrated for each species for each LDW subsection presented in Table 4-1.

For each LDW subsection to be modeled, changes will be made to the LDW base parameterization to reflect location-specific data. Examples of parameters that may change among subsections of the LDW are:

- chemical concentration in sediment
- sediment TOC
- tissue parameters such as lipid content, weight, and percent moisture
- water parameters may also be varied, depending on the variability of the data

Because most parameter values are not specific to the different LDW subsections to be evaluated, those few parameters that are location specific and which the FWM is sensitive, as determined in the sensitivity analyses, will be the focus of LDW subsection model calibration. After an initial calibration, LDW subsection model performance will be compared with empirical data specific to that subsection. LDW subsections that result in predicted concentrations within a factor of 5 of empirical data for each species may be considered for future use in the RI/FS. If the FWM is not predictive for LDW subsections at the scale of interest, plausible reasons for the difference in the predictive ability of the FWM between LDW subsections will be contemplated to assess whether modeling results at the smaller scale are useful.

## 5.7 Continued Calibration of the Model for LDW-wide and Selected Subsections of the LDW

Insights gained through the model calibration process, including results of the sensitivity and uncertainty analyses, LDW subsection results, and additional data exploration, will be used to guide further calibration of the FWM for LDW-wide and selected subsections of the LDW. The precise order of adjustments to the model parameterization will depend on the results of the sensitivity and uncertainty analyses, considering both parameter sensitivity and uncertainty ranking as well as the nature and degree of characterization of the uncertainty.

Continued calibration of the LDW-wide and subsections of the LDW (see Figure 5-1) will occur simultaneously. Any changes made at the LDW-wide spatial scale to non-location specific data, such as organism diets or porewater ventilation, will be incorporated into the LDW subsection parameterizations, and the effect on model performance will be evaluated. If alterations in parameterization from the continued calibration at the LDW-wide scale result in poor model performance for many LDW subsections and the loss in model performance cannot be regained from calibration of those LDW subsections, then the calibration at the LDW scale may be reconsidered. If model performance is worsened only at a small percentage of the LDW subsections, then the LDW-wide calibration will be accepted.

Initial calibration at the LDW-wide spatial scale will determine whether the FWM is capable of predicting tissue chemical concentrations within a reasonable range (within a factor of 5) of empirical tissue concentrations for each species. If certain species are not meeting the performance criterion threshold in the initial calibration (SPAFs > 5 or < -5), those species will be targeted for additional calibration, such as changes to dietary composition. Continued calibration will determine whether the FWM's performance can be further enhanced (moving towards a goal of SPAFs < 3 and > -3) through additional calibration or modeling at a different spatial scale, while staying within plausible ranges for parameter values. If the calibration process does not approach the model performance goal (Section 5.2), then other options, including the potential modeling of a subset of individual PCB congeners, will be discussed with EPA and Ecology.

Changes to the base parameterization at the LDW-wide scale and subsections of the LDW will be reported in FWM Deliverable 3. These parameterizations will be further tested after King County PCB water data (King County 2005) and recalibrated EFDC model predictions for PCBs in water become available in the spring of 2006.

Thus, complete evaluation and selection of LDW spatial scales and locations will not occur until after FWM Deliverable 3. After these spatial scales and locations have been evaluated and selected, a Monte Carlo uncertainty analysis (as described in Section 5.5) will be performed for parameterizations selected for use in the RI/FS, and presented in the Phase 2 RI. Final calibration of the FWM at the LDW-wide scale and for subsections of the LDW will also be presented in the Phase 2 RI, and all assumptions will be fully documented.

For each application of the FWM (e.g., to estimate concentrations in fish and crab tissue resulting from various sediment remediation alternatives in the FS), the parameterization that best matches the scale of interest will be used to address a given FWM application if the parameterization for that location (LDW-wide or a subsection) meets the model performance criterion or model performance goal. Specifically, if for a given species a given LDW subsection parameterization results in a SPAF < 5 and > -5, then it may be used to address FWM applications for that species specific to that location. If for a given species, the LDW subsection

parameterizations result in substantially lower (i.e., more predictive) SPAFs for subsections of the LDW relative to the LDW wide parameterization SPAF, the subsection predictions will be evaluated together to address LDW-wide applications of the FWM for that species. For example, if the LDW-wide parameterization results in a SPAF > 5 or < -5 for shiner surfperch, but all four tissue sampling area parameterizations result in SPAFs < 3 and > -3, all four tissue sampling area predictions would be evaluated together to address LDW-wide applications of the FWM for shiner surfperch. If only some subsections of the LDW result in substantially lower SPAFs than the LDW-wide parameterization, plausible reasons for the difference in the predictive ability of the FWM between subsections will be contemplated to assess which scale is most useful. If only the LDW-wide parameterization results in SPAF < 5 or > -5, then it will be used to predict LDW-wide residual risks or SQTs associated with average exposure over the LDW.

## 6.0 Quality Assurance and Quality Control

To ensure confidence in the quality of model runs, various quality assurance/quality control measures will be implemented. The following steps will be taken:

- A box model showing the mathematical relationships in the FWM will be included in FWM Deliverable 3 to illustrate model mechanics.
- Model runs will be automated to the extent possible to minimize data input errors.
- All model equations and their interdependencies in the computer program will be independently reviewed by Jon Arnot and Windward personnel prior to initial model runs to ensure that the FWM is running correctly.
- All input parameters will be reviewed by a Windward staff person, independent from the modeler, prior to each model run.

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