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Puget Sound Regional Toxics Model: Enhancements, Data Integration, and Reduction Target Evaluation

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July 2012

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EAP: Environmental Assessment Program.
W2R: Waste 2 Resources Program.
WQP: Water Quality Program.

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Abstract

The Puget Sound Regional Toxics Model (PSRTM) is a model of contaminant fate and transport and bioaccumulation that was developed during Phase 2 of the Puget Sound Toxics Loading Analysis (PSTLA). During initial model simulations of polychlorinated biphenyls (PCBs) in Puget Sound, several critical data gaps were identified. These gaps limited the usability of the model for evaluating source control strategies. New regional loading and biota data for a variety of toxic contaminants were collected in Phase 3 of the PSTLA to fill the identified gaps and reduce uncertainty in the model inputs.

This project will incorporate the newly collected monitoring data into the model and update the previous PCB model. Additionally, the capability to simulate polybrominated diphenyl ethers (PBDEs), selected polycyclic aromatic hydrocarbons (PAHs), copper, lead, and zinc will be developed. The model will be calibrated for each of the modeled contaminants, and sensitivity and uncertainty analyses will be conducted.

Model scenarios will be run to estimate contaminant loading reductions and time requirements to meet various environmental quality targets (e.g., Ecosystem Recovery Targets defined by the Puget Sound Partnership). These scenarios will inform the development of an overall source reduction strategy to protect the Puget Sound ecosystem, and will demonstrate the utility of the model as a tool for exploring management options.

Background and Project Overview

Toxic Contamination Concerns in Puget Sound

Human activities introduce a wide range of contaminants into the Puget Sound ecosystem, many of which are harmful to humans and aquatic life. While not necessarily released at dangerous levels, toxic contaminants that enter the inland marine and estuarine waters of the Sound can remain for long periods of time due to the system's bathymetry (i.e., deep and narrow interconnected basins separated by shallow sills) and the persistence of many contaminants. As a result, toxics may circulate and accumulate in some inlets and embayments of Puget Sound, increasing their exposure to aquatic organisms.

Contaminants in the water column and sediments of Puget Sound can exert significant adverse biological effects on the organisms that come into contact with them (PSP, 2006). The toxic effects of these contaminants on aquatic organisms can be acute and/or chronic, including neurological problems, reproductive and developmental abnormalities, immune-response suppression, cancer, endocrine disruption, and death. Some toxics concentrate in animal tissues and magnify as they move up through the Puget Sound food web, accumulating in forage fish (e.g., herring) and bottom fish species and ultimately affecting salmon, seals, and orcas. These contaminants are also a significant concern for human health, especially for individuals who frequently consume fish and other aquatic organisms with high contaminant levels.

Toxic contaminants have long been recognized as a serious concern in Puget Sound (e.g., Dexter et al., 1981; Romberg et al., 1984; PTI, 1991; PSAT, 2003; Redman et al., 2006). Despite cleanup efforts and targeted actions to reduce point sources, many sites in Puget Sound contain persistent toxic substances that were banned decades ago, such as polychlorinated biphenyls (PCBs) and some polybrominated diphenyl ethers (PBDEs). These and other toxics that have not been banned, such as polycyclic aromatic hydrocarbons (PAHs) and heavy metals (e.g., copper, lead, and zinc), continue to enter the Sound via surface runoff (including stormwater), groundwater discharges, municipal and industrial wastewater outfall pipes, and atmospheric deposition. Addressing the problem of toxic contaminants in the Puget Sound ecosystem remains an ongoing challenge and a priority for environmental managers and the general public (PSP, 2008: Action Agenda Priority C.1.1).

Numerical Modeling of Toxic Contaminants in Puget Sound

From 2006 to 2011, the Washington State Department of Ecology (Ecology) worked in collaboration with the Puget Sound Partnership (PSP) and other state and federal agencies to conduct a multi-phase Puget Sound Toxics Loading Analysis (PSTLA[1]). The overall goal of the PSTLA was to provide scientific information to guide decisions about how best to direct resources and prioritize strategies for controlling toxic contaminants in the Puget Sound basin. PSTLA studies provided improved understanding of the timing, quantities, sources, and delivery

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[1] Ecology's website for the PSTLA, from which all project publications can be accessed, is at www.ecy.wa.gov/programs/wq/pstoxics/index.html.

pathways of contaminant loading to Puget Sound, as well as their transport and fate in the aquatic ecosystem.

Phase 2 of the PSTLA included development of numerical models of toxic constituents in Puget Sound. Ecology developed the Puget Sound Regional Toxics Model (PSRTM; previously called the "Puget Sound Toxics Box Model" or "Ecology box model") to simulate the movement of toxic contaminants within and between Puget Sound waters, sediments, and the wide variety of aquatic organisms in the ecosystem. Such models are an important tool for the evaluation of management alternatives, allowing comparison of the ecosystem response under various source control scenarios.

For the PSRTM, Pelletier and Mohamedali (2009) integrated three previously published model applications:

- Box model of water circulation and transport (Babson et al., 2006).
- Mass balance model of contaminant fate and transport (Davis, 2004).
- Food web bioaccumulation model (Arnot and Gobas, 2004; Condon, 2007).

Pelletier and Mohamedali (2009) performed initial Puget Sound modeling simulations with PCBs due to the relative abundance of data. Model input values were derived from actual data collected from Puget Sound to the extent possible, and supplemented with default values from the literature for parameters that could not be estimated from observed data.

A high degree of uncertainty was associated with some of the model inputs because regional toxics data were lacking or limited for a number of ecosystem components. These uncertainties limited the usability of the model for evaluating source control strategies. Pelletier and Mohamedali (2009) recommended that additional data on toxic contaminant concentrations in the marine water column, ocean boundary waters, various species of biota, and external loads to Puget Sound were needed to improve calibration of the model and to reduce uncertainty in the model predictions. Several projects were undertaken in Phase 3 of the PSTLA to collect regional toxics data to fill the identified critical data gaps.

Project Description

This project will update and expand existing numerical models for toxic contaminants in Puget Sound to provide a more effective tool for evaluating ecosystem responses to changes in contaminant loading. The PSRTM will be modified to:

- Provide the capability and apply the model to simulate contaminants of concern (COCs) beyond PCBs, including PBDEs, selected PAHs, copper, lead, and zinc.
- Incorporate newly collected regional data from Phase 3 of the PSTLA and other readily available sources to improve model inputs and reduce overall uncertainty in the model predictions.

The enhanced model will be used to predict concentrations of the selected COCs in the water, sediment, and biota of Puget Sound. Model simulations will be used to estimate numeric reductions in toxic contaminants loadings needed to meet environmental quality standards to protect Puget Sound biota, and will also yield estimates of time requirements to achieve those endpoints under various source control strategies. These results will be used to evaluate potential management actions to reduce threats to the health of the ecosystem, and will be critical to the development of a toxics reduction strategy for Puget Sound.

Goals and Objectives

The overall goals of this project are to build on the foundation of previous modeling of toxics in Puget Sound to (1) further develop a quantitative understanding of the long-term fate of toxic contaminants in the Sound, (2) provide quantitative estimates of loading reductions needed to achieve acceptable levels of these contaminants in the ecosystem, and (3) improve understanding of the response time of the ecosystem to contaminant loading reductions.

Specific objectives that will be accomplished in support of project goals are listed below. Unless specified otherwise, the term *concentrations* refers to contaminant concentrations in water, sediment, and biota.

- Compile regional data on concentrations of PCBs, PBDEs, selected PAHs, copper, lead, and zinc for model inputs and boundary conditions. Sources will include environmental databases, scientific literature, and recently collected data from Phase 3 of the PSTLA.
- Develop the capability to model PBDEs, PAHs, copper, lead, and zinc. This will involve updates to the PSRTM code and literature searches for model parameters specific to the selected contaminants. Modeling of PCBs and PBDEs will include fate, transport, and bioaccumulation to predict concentrations in water, sediment, and biota. Modeling of PAHs, copper, lead, and zinc will include fate and transport to predict concentrations in water and sediment.
- Calibrate the PSRTM to regional data for each of the selected contaminants. The model will be re-calibrated for PCBs if the incorporation of new data is found to significantly alter the model calibration used by Pelletier and Mohamedali (2009).
- Evaluate the sensitivity and uncertainty of model predictions to various input parameters and boundary conditions for each of the modeled contaminants.
- In consultation with collaborators and regional experts, identify and summarize *model scenario threshold concentrations*[2] (MSTCs) for PCBs, PBDEs, and selected PAHs and metals in Puget Sound.
- Execute model scenarios to investigate:
    - Numeric reductions in contaminant loadings needed to meet MSTCs.
    - Time required to meet MSTCs under different load reduction scenarios.

The results from this project will provide load reduction targets for the modeled COCs for use in evaluating management actions to control toxic contaminant inputs to Puget Sound.

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[2] For this project, a *model scenario threshold concentration* (MSTC) is a contaminant concentration in water, sediment, or biota below which aquatic resources and human health are considered to be adequately protected from toxic effects. Concentrations that exceed an MSTC impart harm to the health of the ecosystem or humans or both.

Organization and Schedule

Table 1 lists the individuals involved in this project. Except as noted, all are employees of the Washington State Department of Ecology, Environmental Assessment Program. Table 2 presents the proposed schedule for project milestones.

Table 1. Organization of project staff and responsibilities.

Staff (all are EAP except client)	Title	Responsibilities
Andrew Kolosseus Watershed Planning Unit Water Quality Program Phone: (360) 407-7543	EAP Client	Clarifies scopes of the project, provides internal review and approval of the QAPP.
Greg Pelletier MISU, SCS, EAP Phone: (360) 407-6485	Project Manager	Reviews and approves the QAPP, develops model code, performs calibration and sensitivity analyses, analyzes and interprets model output, co-authors the draft and final report.
David Osterberg TSU, SCS, EAP Phone: (360) 407-6446	Principal Investigator	Writes the QAPP, develops model input database, assists with model code development, performs calibration and sensitivity analyses, runs model scenarios, analyzes and interprets model output, co-authors the draft and final report.
Karol Erickson MISU, SCS, EAP Phone: (360) 407-6694	Unit Supervisor for the Project Manager	Reviews the project scope and budget, reviews and approves the QAPP, tracks project progress.
Dale Norton TSU, SCS, EAP Phone: (360) 407-6765	Unit Supervisor for the Principal Investigator	Defines the project scope and budget, reviews and approves the QAPP, tracks project progress.
Will Kendra SCS, EAP Phone: (360) 407-6698	Section Manager for the Project Manager	Reviews the project scope and budget, reviews and approves the QAPP, tracks project progress.
Brandon Sackmann MISU, SCS, EAP Phone: (360) 407-6684	Ecology Internal Peer Reviewer	Provides internal technical review of the QAPP and final report.
William Kammin Phone: (360) 407-6964	Ecology Quality Assurance Officer	Reviews and approves the QAPP.
Tom Gries SCS, EAP Phone: (360) 407-6327	NEP Quality Assurance Coordinator	Reviews and approves the QAPP.

EAP: Environmental Assessment Program.
MISU: Modeling and Information Support Unit.
NEP: National Estuary Program.
QAPP: Quality Assurance Project Plan.
SCS: Statewide Coordination Section.
TSU: Toxics Studies Unit.

Table 2. Proposed schedule for completing modeling work and reports.

Progress report (unpublished)	
Author lead / Support staff	Greg Pelletier / David Osterberg
Report due to client	September 2012
Final published report	
Author lead / Support staff	Greg Pelletier / David Osterberg
Schedule	
Draft due to supervisors	5/27/2013
Draft due to client/peer reviewer	6/24/2013
Draft due to external reviewer(s)	7/22/2013
Final (all reviews done) due to publications coordinator	9/30/2013
Final report due on web	10/31/2013

Puget Sound Regional Toxics Model (PSRTM)

Study Area and Model Domain

Puget Sound is the largest estuarine fjord system in the continental United States. Located between the Olympic and Cascade mountain ranges in Washington State, the estuary is an arm of the Pacific Ocean that extends inland where it meets 19 different river watersheds. The Puget Sound watershed covers more than 16,800 square miles (43,400 km^2) of land and water, with approximately 2,800 square miles (7,250 km^2) of inland marine waters bounded by 2,500 miles (4,025 km) of complex shorelines (Hart Crowser et al., 2007).

The hydrography of Puget Sound consists of a series of interconnected basins separated by relatively shallow ridges, or sills. The three major branches of Puget Sound include the Main Basin and South Sound (separated by a sill and constriction at the Narrows), Hood Canal, and Whidbey Basin. Admiralty Inlet links the three branches of the Sound together and serves as the primary outlet to the Straits of Juan de Fuca (SJF) and Georgia (SOG) and ultimately the Pacific Ocean. The only other outlet to SJF/SOG is the extremely shallow and narrow Deception Pass located at the northern end of Whidbey Basin.

The PSRTM domain includes the marine waters of Puget Sound south of the outlets at Admiralty Inlet and Deception Pass. The model domain is divided into ten regions based on the locations of sills and data stations (Figure 1). Seven of the regions correspond to the principal basins: Admiralty Inlet, Whidbey Basin, Main Basin, the Narrows, South Sound, northern Hood Canal, and southern Hood Canal. Three additional regions represent urban bays: Elliott Bay, Commencement Bay, and Sinclair/Dyes Inlets. The open boundary to the model domain consists of the U.S. portions of the Straits of Juan de Fuca and Georgia.

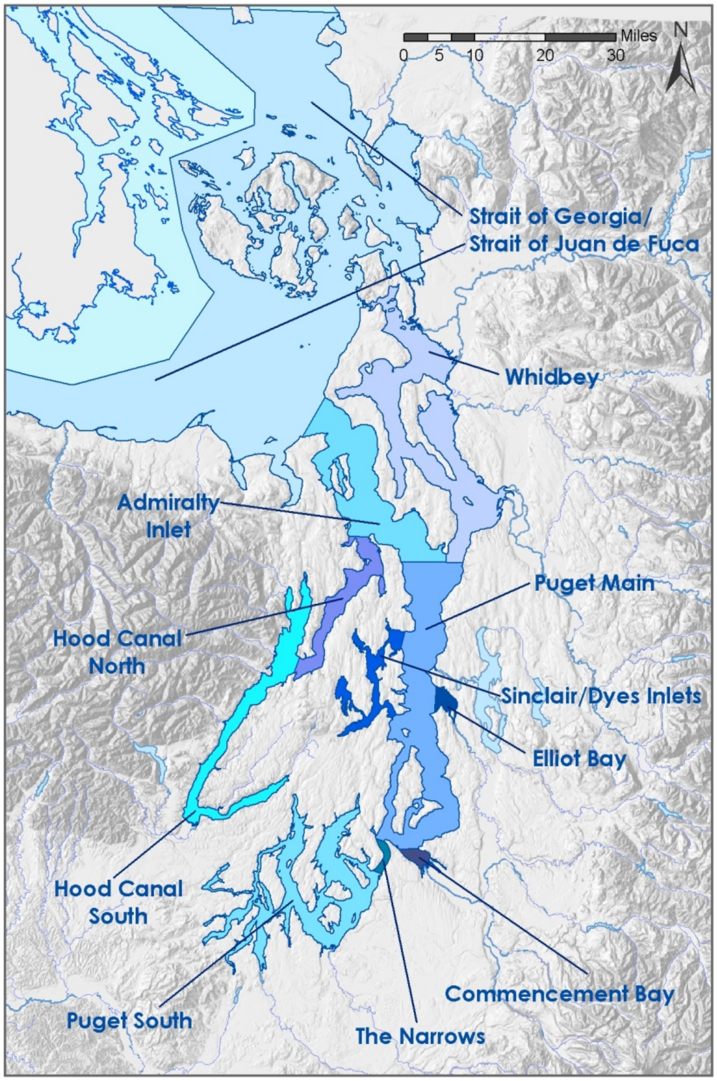

Figure 1. Map of Puget Sound showing PSRTM regions.

Model Components (Modules)

Building on the work of Pelletier and Mohamedali (2009), the numerical modeling approach for this project will be comprised of three integrated parts, or modules.

Circulation and Transport of Water

A previously published box model of circulation and transport of water in Puget Sound (Babson et al., 2006) was used by Pelletier and Mohamedali (2009) and will be adapted for the present study. The model is capable of predicting seasonal and interannual variations of water residence times, as well as transports and exchanges of water between model boxes (i.e., regions and water column layers).

The theory of the circulation and transport model is described in detail by Babson et al. (2006). Briefly, equations are based on conservation of mass and salt, as well as advection, mixing, and forcing functions. The model estimates salinity for each box and transports of salt and water between boxes due to vertical mixing and horizontal and vertical advection.

Circulation in Puget Sound is driven primarily by density differences between freshwater river inputs and salty marine water at the Puget Sound seaward boundaries. The model approximates this circulation as two-layer exchange flow, with mean flow seaward at the surface and landward at depth. Thus, the water column in each region of the model is divided vertically into a surface layer and a deep layer, resulting in a total of twenty “boxes.” The thickness of the surface layer varies by region and is determined by the depth of no motion, where the tidally averaged velocity crosses zero between an outgoing surface layer and an incoming deep layer (Babson et al., 2006). A schematic of the circulation box model is presented in Figure 2.

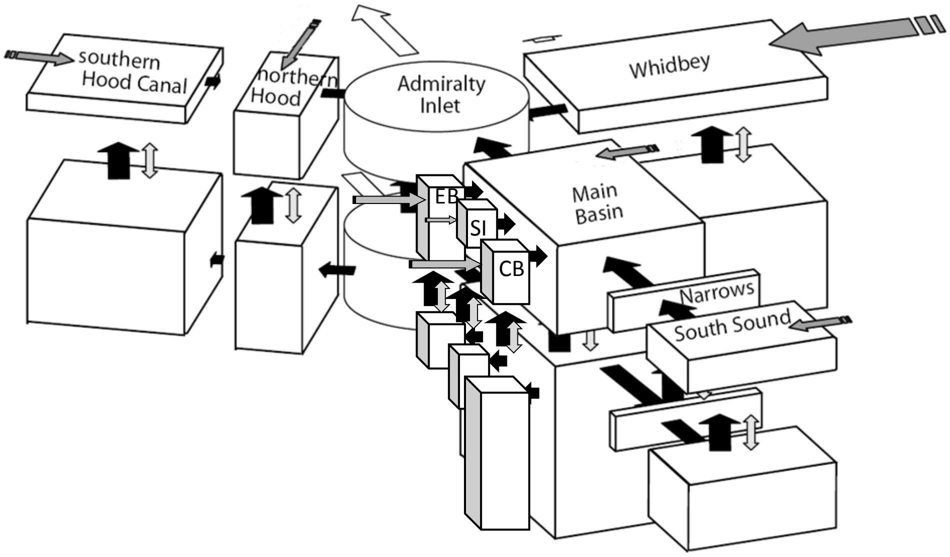

Figure 2. Schematic diagram of the box model of circulation and transport of water in Puget Sound (after Babson et al., 2006).

Boxes have been scaled to show relative volumes, and arrows have been scaled to show transports. Black arrows represent advection, two-way gray arrows represent mixing, and white arrows are boundary exchanges. Gray arrows with dashed ends represent river inputs and are proportional on a log scale.

The three boxes separated from the Main Basin represent urban bays (EB = Elliott Bay, CB = Commencement Bay, and SI = Sinclair/Dyes Inlets). EB and CB are located on the eastern side of the Main Basin, but their boxes are shown on the western side for visualization purposes.

Contaminant Fate and Transport

A process-based mass balance model of contaminant fate and transport of non-ionic hydrophobic organic contaminants (HOCs) is joined with the circulation module. The mass balance model was originally developed by Davis (2004) for PCBs in San Francisco Bay and was incorporated into the PSRTM by Pelletier and Mohamedali (2009). The combined model is capable of predicting seasonal and interannual variations of HOC concentrations in water and sediment in response to external loading and internal processes.

The model theory for PCB fate and transport is explained in detail by Davis (2004), and is applicable to other HOCs (e.g., Oram et al., 2008). The model estimates inputs, outputs, and changes of HOC concentrations in water and sediment compartments. Sediments are divided conceptually into an active sediment layer and buried, deep sediment. The active sediment layer is the mass of sediment that is actively exchanging HOCs with the water column and the biota of the aquatic food web. The major processes that add or remove HOCs from water or sediment include (Figure 3):

- External loading (e.g., atmospheric deposition, surface runoff wastewater discharges, erosion of buried sediment).
- Partitioning of dissolved and particulate forms.
- Volatilization.
- Diffusion (water-to-sediment and sediment-to-water).
- Solids settling and resuspension.
- Degradation in water and in sediment.
- Burial of deep sediments.
- Transport exchanges between basins and layers, including inflow and outflow at the model boundaries.

In the PSRTM the fate and transport module is integrated with the circulation module. Thus, horizontal and vertical exchanges occur between the ten regions and two water column layers of the model domain. Pelletier and Mohamedali (2009) updated the fate and transport module to allow simulation of the transport of sediment from the shallow margins to deeper areas, classifying two sub-areas of active sediment (Figure 4): (1) sediments that are below the surface water layer, and (2) sediments that are below the deep water layer.

An alternative mass balance modeling tool, the EPA WASP model (Wool et al., 2003), will be considered for this project if it is determined that the ability to simulate more complex kinetic processes is required. The WASP model is widely used and is capable of simulating a broad range of contaminants, including non-ionic and ionic organic contaminants, mercury, and other metals. Pelletier and Mohamedali (2009) developed a linkage between the circulation module and the WASP model through output of an external hydrodynamic file, but it was not used. If selected for the present study, the external linkage may be utilized or the kinetic processes in the WASP model may be incorporated into the PSRTM code.

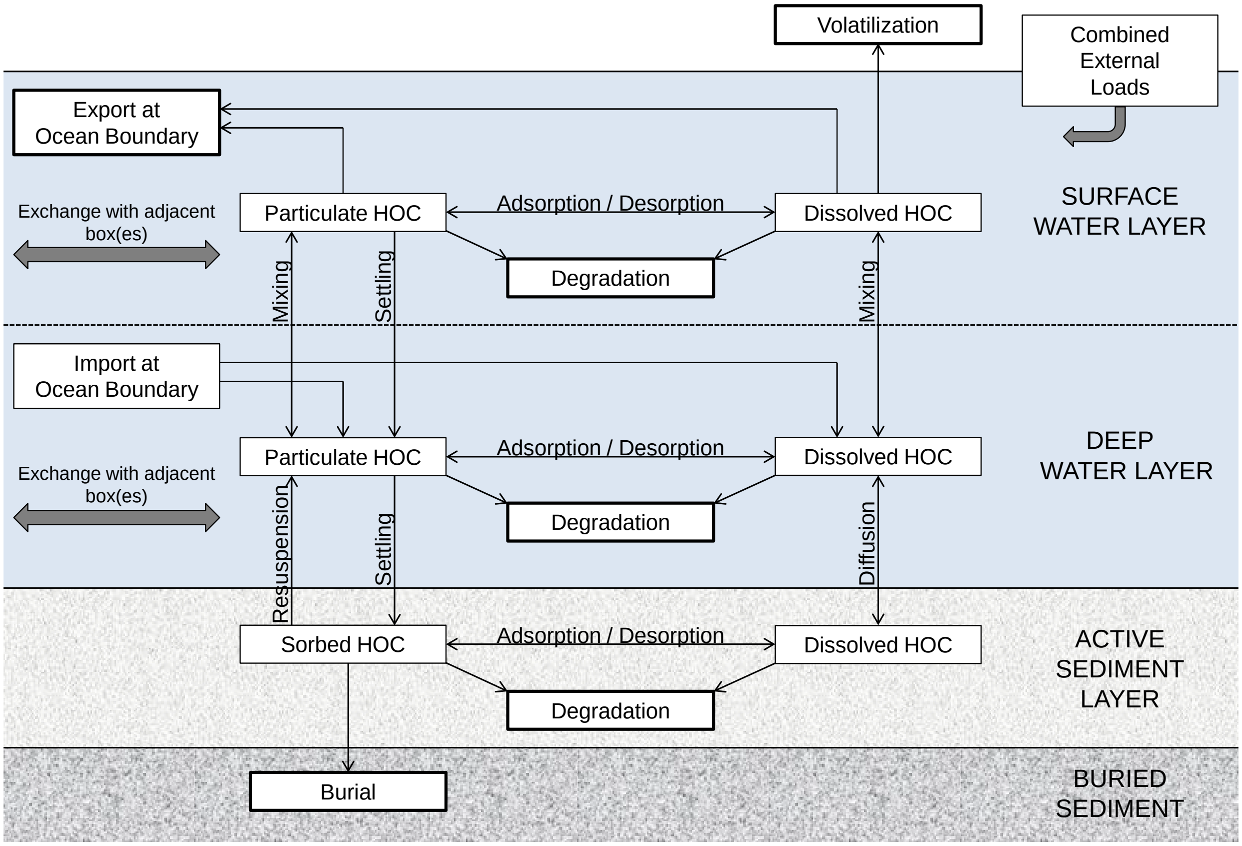

Figure 3. Diagram of the fate and transport component of the PSRTM (after Davis, 2004) for hydrophobic organic contaminants (HOCs).

Arrows represent mass fluxes; thick gray arrows are mass fluxes of both particulate and dissolved forms; heavy outlines indicate sinks (i.e., removal from the system). The fate and transport of metals is identical except degradation and volatilization processes are omitted. In shallow areas the deep water layer is absent and the surface water layer is in direct contact with the active sediment layer (see Figure 4).

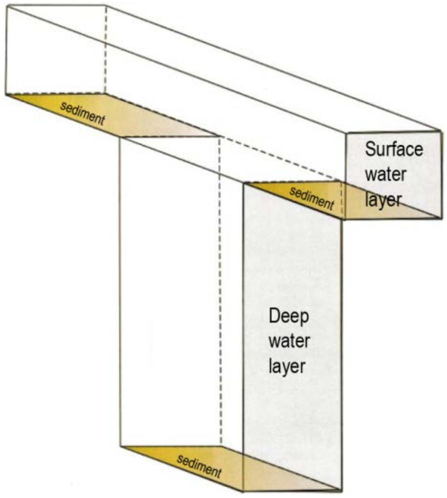

Figure 4. Conceptual representation of water column layers for the fate and transport module showing areas of active sediment.

Food Web Bioaccumulation

A generalized bioaccumulation model for aquatic ecosystems was developed by Arnot and Gobas (2004) to simulate uptake and bioaccumulation of HOCs from sediment to biota and the food web. Condon (2007) applied the Arnot and Gobas (2004) model in the Pacific Northwest, evaluating concentrations of PCBs in the biota at various trophic levels of the Strait of Georgia. Pelletier and Mohamedali (2009) linked the Condon (2007) model to the fate and transport module of the PSRTM and incorporated additional species to simulate fluxes of PCBs from sediments to biota in Puget Sound. The work of Pelletier and Mohamedali (2009) will be adapted for the present study.

The theory for the food web bioaccumulation module is given in detail in Condon (2007) and Arnot and Gobas (2004). The model describes the principal feeding relationships of the aquatic food web and simulates the movement of HOCs through sediments, primary producers (phytoplankton and other plants), secondary producers (herbivores), forage species (carnivores), and top predators via bioaccumulation[3]. Each representative organism or species is described as a single compartment in terms of exchange with the surrounding environment. Tissue concentrations of HOCs in the biota at various trophic levels are predicted by simulation of the fluxes into and out of each organism, including:

- Direct uptake from water
- Uptake from feeding
- Uptake and loss from respiration
- Loss due to metabolism
- Dilution due to growth
- Loss due to diffusion
- Loss due to fecal egestion (excretion)
- Loss due to reproduction and nursing

A diagram of the selected species and trophic linkages in the Puget Sound aquatic food web used by Pelletier and Mohamedali (2009) is presented in Figure 5 (after Condon, 2007). Additional organisms may be incorporated into this food web based on recent bioaccumulation modeling of central Puget Sound by King County (Townes-Witzel and Ryan, 2007; Stern et al., 2009; Nairn et al., 2011). The top predators selected for the PSRTM include harbor seals, double-crested cormorants, and great blue herons. Despite their iconic regional status, orcas (or “killer whales”) are not used as top predators in the model; fish-eating harbor seals occupy the same trophic position and have a similar diet compared with orcas, and they are more amenable to prediction of bioaccumulation because they have a much smaller feeding range (Pelletier and Mohamedali, 2009).

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[3] *Bioaccumulation* is the process by which the chemical concentration within an organism achieves a level that exceeds that in its environment as a result of chemical uptake through all possible routes of exposure (e.g., dietary, dermal, respiratory) (Gobas and Morrison, 2000).

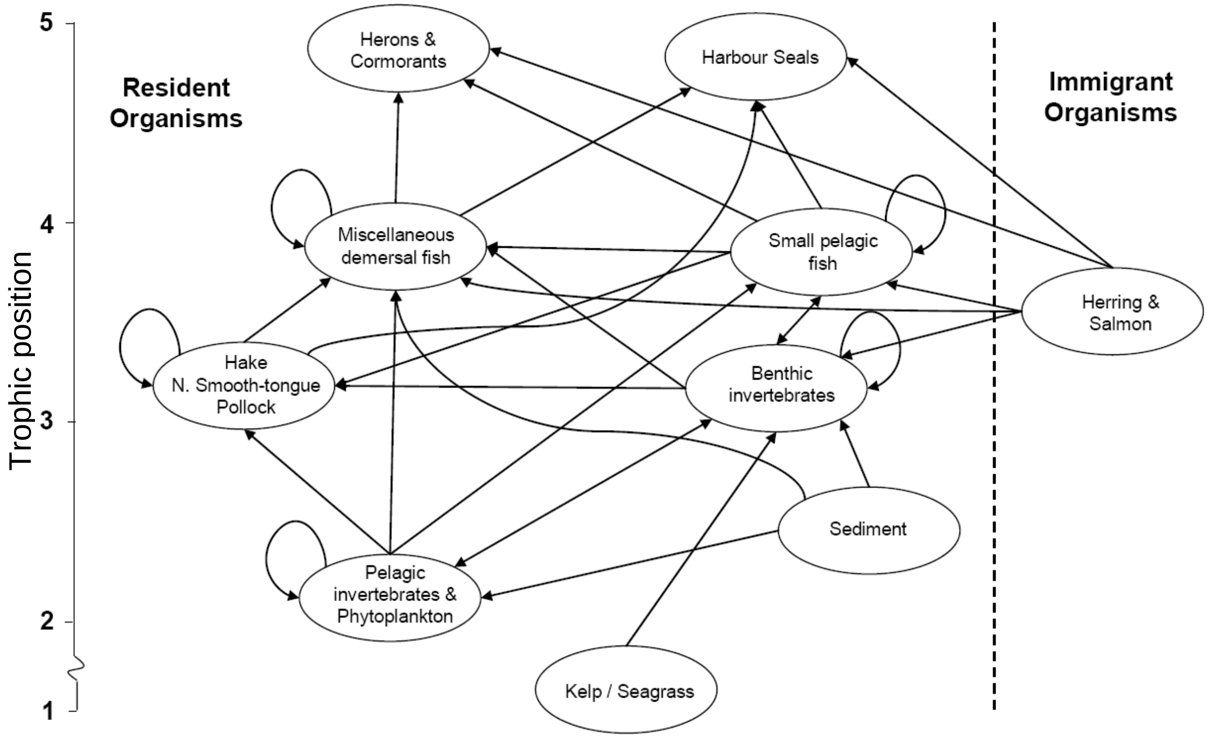

Figure 5. Diagram of trophic linkages for the major feeding groups in the food web bioaccumulation module (after Condon, 2007).

Arrows point from prey to predators.

Selected Contaminants of Concern

The PSTLA studies analyzed a core group of contaminants of concern (COCs) based on their (1) documented history of presence in Puget Sound, (2) capacity to harm or threaten the ecosystem, and (3) potential to represent, or serve as an indicator for, a particular class of chemicals in different pathways (Ecology, 2011). In general, these contaminants are highly persistent in the environment and can have toxic effects on aquatic organisms, and some have high bioaccumulation potential. The COCs chosen for this project are a subset of the PSTLA analytes:

- Total PCBs
- Total PBDEs
- Selected PAHs
- Copper (Cu)
- Lead (Pb)
- Zinc (Zn)

"Total PCBs" consists of 209 possible compounds, or congeners, which vary in degree of chlorine substitution and arrangement on the biphenyl molecule. Similarly, "Total PBDEs" represents 209 individual congeners, each with different numbers (1 to 10) and placement of bromine atoms attached to a diphenyl ether molecule. The chemical properties, fate, and toxicity of different PCB and PBDE congeners vary widely[4]. Following Pelletier and Mohamedali (2009), model simulations for PCBs and PBDEs will involve a subset of congeners that will be selected based on prevalence in Puget Sound samples (i.e., high frequency of detection and representing a majority of the total mass), their importance in terms of toxicity, and the inclusion of a broad range of chemical properties. These subsets of PCB and PBDE congeners will be determined after all data and model inputs have been compiled, and the rationale for their selection will be documented in the final report.

PAHs are also a class of hundreds of compounds, with individual PAHs characterized by two or more fused aromatic rings composed of carbon and hydrogen. As with PCBs and PBDEs, chemical properties and toxicity range widely among PAHs[5]. Most studies and environmental criteria focus on the 16 PAH compounds designated as "priority pollutants" in the federal Clean Water Act[6]. For the PSRTM, PAHs will either be addressed as single compounds or as subgroups of compounds (Table 3), such as low molecular weight (LPAHs; fewer than four rings), high molecular weight (HPAHs; four or more rings), and carcinogenic (cPAHs). Special consideration will be given to the seven PAH compounds used by Greenfield and Davis (2004) for fate and transport modeling in San Francisco Bay, as these compounds cover a broad range of molecular weights and chemical properties and their parameters could be applied to Puget Sound

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[4] The persistence of PCBs (e.g., resistance to metabolization, degradation, and volatilization) increases with the degree of chlorination, as do bioconcentration and adsorption (Mabey et al., 1982). For PBDEs, heavier congeners tend to be less volatile and bind more strongly to solids; once in the environment they may degrade to lighter, lower-brominated congeners that are more toxic (Kelley et al., 2008).

[5] Solubility, volatilization, and biodegradation tend to decrease with increasing molecular weight for PAHs. Low molecular weight PAHs tend to be more toxic but less carcinogenic than high molecular weight PAHs.

[6] See Appendix A to 40 CFR Part 423. The current list of 126 "priority pollutants" is available from EPA at water.epa.gov/scitech/methods/cwa/pollutants.cfm.

with only minor modifications. Final selection will be made after data compilation, based on the same factors listed above for PCBs and PBDEs, and documented in the final report.

Table 3. Classification of “priority pollutant” PAHs by molecular weight.

LPAHs	HPAHs
• Naphthalene • Acenaphthylene • Acenaphthene • Fluorene • Phenanthrene • Anthracene	• Fluoranthene • Pyrene • Benz(a)anthracene* • Chrysene • Benzo(b)fluoranthene* • Benzo(k)fluoranthene* • Benzo(a)pyrene* • Indeno(1,2,3–c,d)pyrene* • Dibenzo(a,h)anthracene* • Benzo(g,h,i)perylene

* Designated as probable human carcinogen (cPAH) by EPA.

Environmental Data Sources

Regional environmental data will serve as inputs and boundary conditions for the PSRTM. While no data collection is planned for this study, relevant information on concentrations of the selected COCs in Puget Sound water, sediment, and biota will be compiled from a variety of sources.

Phase 3 of the PSTLA included several studies specifically targeted to fill important data gaps that had caused previous model inputs to be highly uncertain. The data from these recent studies will be obtained from Ecology’s Environmental Information Management (EIM) database. The Phase 3 studies that will contribute the most to the present work include:

- **Loadings via Surface Runoff** (Herrera, 2011). Pelletier and Mohamedali (2009) found that external loading of contaminants (PCBs) in surface runoff from watersheds was the main driver of model-predicted concentrations in water, sediment, and biota in Puget Sound. Model inputs used loading estimates from Phases 1 and 2 of the PSTLA that relied on existing values which in a number of cases were taken from outside the Puget Sound basin and represented a combination of conveyance samples and in-stream data to estimate loadings. The Phase 3 surface runoff study provided regional monitoring results that used methods with very low detection limits to significantly improve loading estimates.
- **Air Deposition** (Brandenberger et al., 2010). The Phase 1 loading study found very little data to assess atmospheric deposition loads and found that the existing data was two decades old. The report suggested that atmospheric loads may be comparable or even greater than loads from surface runoff. The Phase 3 study collected bulk samples (dry and wet deposition) from a network geographically dispersed around Puget Sound and developed seasonal loading estimates for model regions.

- **Ocean Exchange and Major Tributary Loadings** (Gries and Osterberg, 2011). The scarcity of marine water column data using methods that were capable of detecting low concentrations of toxic contaminants was a major data gap identified in the initial modeling effort. Marine waters data were collected to improve calibration and better evaluate boundary conditions (i.e., exchange with ocean waters). Additional data on concentrations in the freshwater and suspended sediment delivered by the largest rivers discharging to the Sound was also targeted.

- **Priority Pollutant Scans for Ten Publicly Owned Treatment Works** (Ecology and Herrera, 2010). Studies from Phases 1 and 2 of the PSTLA found a limited amount of data that could be used to calculate reliable loading estimates from publicly owned treatment works (POTWs). The POTWs study used methods with very low detection limits to characterize loadings from a range of treatment facilities.

- **Toxic Contaminants in Selected Biota** (West et al., 2011a and 2011b; Noel et al., 2011). Data gaps existed for concentrations of contaminants in several species within the Puget Sound food web. These missing links in the food chain limited the predictive capability of the model to translate target concentrations in biota to reductions in loadings needed to meet the targets. Phase 3 studies collected concentration data for low trophic level species (plankton) and harbor seal prey (hake and pollock), and improved spatial coverage for harbor seals, which are used as the sentinel species for the PSRTM.

Data from existing repositories (e.g., government and public databases) will be queried to supplement the PSTLA information. When available, regional data will also be obtained from peer-reviewed literature and direct communications with experts. Below is a description of a few such sources:

- **Ecology's EIM database**. EIM is the central database for environmental monitoring data collected by multiple entities including Ecology and other state agencies, private consultants, counties, cities, and local governments. Queries and spatial joins allow data for toxic contaminants to be referenced to the different regions of the model.

- **Washington Coastal EMAP (Environmental Monitoring and Assessment Program)**. EMAP is a large-scale assessment of all of Washington's coastal areas funded by the U.S. Environmental Protection Agency (EPA) and jointly conducted by Ecology, NOAA, and EPA. EMAP surveys measured sediment concentrations for a variety of toxic contaminants throughout the Puget Sound area in 2000, 2004, and 2010.

- **Fisheries and Oceans Canada (DFO)**. DFO and collaborators have conducted a number of studies on toxic contaminant concentrations in the Straits of Juan de Fuca and Georgia (e.g., Noel, 2007; Johannessen et al., 2008). Published and unpublished data from recent studies will be useful for regional comparisons and for characterizing boundary conditions.

- **King County Department of Natural Resources (KCDNR)**. King County's Marine and Sediment Assessment Group supports a comprehensive, long-term marine monitoring program in central Puget Sound. Their data sets consist of near- and off-shore water quality and sediment variables from routine monitoring and targeted studies.

- **Lower Duwamish Waterway (LDW) Remedial Investigation**. Work by EPA and Ecology to clean up contaminated sediment and control sources of additional contamination involved development of a bioaccumulation model for the site (LDW, 2010). The Condon (2007) model was the foundation for the LDW model, and food web parameters used for the LDW model may inform parameterization for the present study.

Environmental data for ancillary model input variables will also be compiled. Such information will include temperature and salinity data, total and dissolved organic carbon (TOC and DOC) concentrations in water and sediment, total suspended solids (TSS) in water, percent solids in sediment, and sediment accumulation rates from Pb-210 studies.

Acceptance Criteria and Data Rules

The following acceptance criteria will be applied to all data used for model calibration and scenario evaluation purposes:

- *Data Reasonableness*. The quality of existing data will be evaluated where available. Statistical tests will be used to identify erroneous or outlier data; if there is a known reason to doubt their validity, these observations will be removed from the data set.
- *Data Representativeness*. Data will be used that are reasonably complete and representative of typical conditions at the location under consideration (e.g., model region, water column layer, watershed). Data from highly contaminated "hot spots" will be included if it is representative of current conditions; however, data collected prior to a known or suspected cleanup action will not be used.
- *Data Comparability*. Long-term water quality monitoring programs often collect, handle, preserve, and analyze samples using methodologies that evolve over time, particularly for highly regulated or recently banned chemicals. Advances in analytical methods in recent decades have improved the capability of detecting extremely low concentrations of contaminants such as metals and organic compounds. Best professional judgment will be used to determine whether data from the various sources are comparable. The final project report will detail any caveats or assumptions that were made when using data collected with differing sampling or analysis techniques.

In addition to these general criteria, data will only be accepted for use in the present study if the analytical result is unqualified (detected) or "J" qualified (estimated). Results that are qualified as "N" (tentative), "B" (possible contamination in the blank), or "rejected" will not be used. It is anticipated that inconsistent rules for blank qualification/correction will have been applied in the various data sources; however, no attempt will be made to re-calculate or "normalize" the results according to a common set of rules.

Non-detects

Non-detect data (qualified as “U” or “UJ”) are results below the detection limit (DL) of the analytical method used to measure the concentration of the chemical. The reported values for non-detect data cannot directly be used for analysis since they do not represent a quantified concentration. However, numerous substitution methods are available in which non-detect values are replaced with a substitute value and then used in further analyses. Different substitution methods can bias the results in different ways, so a method that is appropriate for the data set and the purposes of the project must be selected.

It is anticipated that a significant subset of the data for PCB, PBDE, and PAH concentrations in Puget Sound will be non-detects. Pelletier and Mohamedali (2009) tested several substitution methods for PCBs and determined that the least biased method was as follows: (1) non-detect congeners are substituted with a value of zero for samples with at least one detected congener, and (2) the sample is omitted altogether for samples with all congeners reported as non-detects. These rules are applicable to other HOCs and for this project will be used for Total PBDEs and PAHs (either individual compounds or the sub-groups LPAHs, HPAHs, and cPAHs) in addition to Total PCBs.

For metals data, the following substitution methods will be explored to determine the least biased method: non-detect results are substituted with a value of (1) zero, (2) half the quantitation limit, or (3) the full quantitation limit of the analytical method. The evaluation process and selection of the appropriate substitution method will be presented in the final report.

Summation for “Total” Values

Concentrations of organic compounds for this project will be expressed as “total” values, meaning the sum of all congeners for PCBs and PBDEs, or the sum of various compounds for LPAHs, HPAHs, and cPAHs. “Total” values will be calculated by *summing the detected values as reported for individual addends (congeners or compounds) in the group*. As mentioned above, non-detect results will be assigned a value of zero for the summing process when the addends being summed consist of both detected and non-detected results. When all results for individual addends are reported as non-detects, the sample will not be used (as opposed to assigning the “total” a value of zero, or half the reporting limit, or the reporting limit). These rules are adapted from Ecology internal guidance (Ecology, 2008) and will apply to all media (i.e., water, sediment, and tissue).

Pelletier and Mohamedali (2009) found that different data sources summed different subsets of PCB congeners for “total” concentrations, and acknowledged this as a source of uncertainty in the analysis. For the present study such inconsistencies are expected for both PCB and PBDE data. Following the precedent of Pelletier and Mohamedali (2009), congener subsets will not be adjusted to extrapolate to all 209 congeners. The handling of PCB Aroclors[7] will also be guided by Pelletier and Mohamedali (2009), with Total PCB concentrations approximated from the sum of Aroclors using a linear regression of paired samples for which congeners and Aroclors were detected.

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[7] The trade name Aroclor refers to various commercial mixtures of PCB congeners.

Model Adaptation to Additional COCs

Re-configuration Approach

The PSRTM is presently configured to predict Total PCB concentrations in Puget Sound water, sediment, and biota. However, "Total PCBs" encompass 209 congeners that vary widely in their chemical and toxicological properties. To simulate Total PCBs, the framework of the fate/transport and bioaccumulation modules allow for either (1) use of the properties of a single congener to represent the entire chemical class, or (2) separate simulations of a number of different congeners which are then summed to determine the "total" result for the entire class.

For the fate and transport module, Davis (2004) and Pelletier and Mohamedali (2009) used the first strategy to simulate mass fluxes of Total PCBs according to the chemical properties of a single congener, PCB-118. Selection of PCB-118 as the "representative" congener was based on its intermediate chemical properties and level of chlorination, abundance in the ecosystem, similarity to a highly toxic congener, and data availability. In contrast, the bioaccumulation module as employed by Condon (2007) and Pelletier and Mohamedali (2009) used the second strategy, simulating the movement of 57 different PCB congeners through the food web and then summing to get "total" concentrations for the various organisms. The modeled congeners were chosen due to their presence in regional sediment and biota data and because those congeners were known to comprise the majority of the Total PCB mass (and were thus considered to be reasonably representative of the behavior of the entire family of PCB congeners).

As the model is expanded to include the capacity to simulate additional organic contaminants, the option of simulating either an individual representative compound or a suite of compounds will be maintained. For example, an intermediate PBDE congener can be chosen to simulate Total PBDEs, or a number of individual PAH compounds can each be simulated and then the results summed to determine end concentrations of PAH subgroups (e.g., LPAHs, HPAHs, and cPAHs). If data are sufficient to support the simulation of individual congeners or compounds, that will be the preferred method. Absent sufficient data, the default approach will be to use the chemical characteristics of a representative congener or compound to simulate the "total" concentration of the class or subgroup. Determination of which strategy is most appropriate for the various organic contaminants will be made on an individual (i.e., chemical by chemical) basis, and may vary by module as in Pelletier and Mohamedali (2009).

Modeled processes for copper, lead, and zinc will use partition coefficients to account for particulate and dissolved forms of each metal.

Model Framework

The computer code used to execute the calculations for each of the three modules of the PSRTM is written in Microsoft Excel's Visual Basic for Applications (VBA) programming language. Excel worksheets serve as the user interface for entering data and viewing output results.

Adaptation of the model code to the selected organic contaminants will not involve major modifications since the present framework for PCBs is applicable to other HOCs such as PBDEs.

PAHs are also readily simulated, but the food web bioaccumulation module will not be used because these compounds generally do not bioaccumulate (while they concentrate in many species of aquatic invertebrates, they can be metabolized by fish and vertebrates and so do not accumulate in higher trophic level organisms).

The processes that govern the fate and transport of metals in the ecosystem differ from those dictating the movement of organic contaminants. For example, most metals are conservative and do not have a gaseous phase, and so degradation mechanisms (e.g., biodegradation, photolysis) and volatilization processes do not apply (Chapra, 1997). Thus, changes to the fate and transport module code will be required to simulate only those processes that are applicable to metals. The EPA WASP model, which is capable of simulating metals kinetics, will provide guidance for modifications to the PSRTM code. The kinetic processes for metals simulation in WASP may be embedded in the PSRTM VBA code as an additional module or a modification of the existing fate and transport module. Alternatively, the WASP framework may be used via an external linkage (i.e., bypassing the current fate and transport module). As with PAHs, the food web bioaccumulation module will not be used for metals modeling because they do not bioaccumulate.

Model Inputs and Parameters

The input data for the model are used to describe the chemical properties of the selected COCs, derive the rate constants for modeled processes, and describe the concentrations in various media throughout the model domain and at the model boundary. Some attributes are independent of the contaminant modeled, allowing for efficient re-application to other contaminants (e.g., sediment deposition and burial rates in the fate and transport module). However, many model inputs and parameters are chemical-specific and will require updates as the model is expanded to simulate new contaminants.

Anticipated sources of regional environmental data for the various contaminants were described earlier in this document. Model parameters for chemical properties and processes will be derived from Puget Sound data when possible, or obtained from closely related modeling studies found in the peer-reviewed literature. Potentially useful sources of parameterization information include Mackay and Hickie (2000), Greenfield and Davis (2004), and Oram et al. (2008) for the fate and transport module, and Townes-Witzel and Ryan (2007), Ecology and Environment (2009), Stern et al. (2009), LDW (2010), and Gobas and Arnot (2010) for the bioaccumulation module.

If data or published guidance for a particular parameter value is not available for Puget Sound (or a region thereof), then published values from similar aquatic systems will be considered. In all cases, best professional judgment will be used for the final determination of what data are used to calibrate and evaluate the model for each contaminant, and the process will be documented in the final report.

Model Calibration

Once initial conditions have been established and the model setup is completed, the model will be calibrated for each of the selected contaminants through comparison of model predictions to data collected in Puget Sound. The term *calibration* describes the process of adjusting model parameters within physically defensible ranges until the resulting predictions give the best possible match with observed data (EPA, 2009). Model calibration for this project will be an iterative procedure involving a combination of best professional judgment and quantitative goodness-of-fit statistics.

Accuracy refers to the closeness of model predictions to measured values, which are assumed to represent true values. Calibration will give highest priority to accurately representing chemical masses in sediment, followed by water and biota, because a substantial portion of the mass of each contaminant is anticipated to be contained in the sediments (for example, Pelletier and Mohamedali [2009] found that 97% of the total mass of PCBs in the aquatic ecosystem of Puget Sound was predicted to be in the active sediment layer). The overall goal will be to describe the bulk of the data, and short-term effects of ephemeral events may not be represented. During the calibration process, the accuracy of model predictions will be measured by the root mean square error (RMSE) of paired predicted-observed values.

Bias describes the systematic deviation between model predictions and true values (i.e., measured results). Bias will be measured by the mean and standard deviation of residuals for paired predicted-observed values.

Numeric targets for accuracy and bias are not specified, but the accepted calibrations will minimize the discrepancies between modeled and observed values as much as possible. For the new COCs there is no modeling precedent and the attainable accuracy cannot be anticipated; therefore, the goal will be to minimize the RMSE. The final report will detail the goodness-of-fit statistics of the final calibration for each modeled contaminant.

Pelletier and Mohamedali (2009) calibrated the current version of the PSRTM for PCBs using concentrations and loading estimates from the initial phases of the PSTLA. As part of the present project the model will be run incorporating the updated PCB results from Phase 3 studies. If necessary, the model calibration will be adjusted in consideration of the new data to achieve comparable or better accuracy than the earlier modeling work.

Sensitivity and Uncertainty Analyses

Sensitivity and uncertainty analyses will be conducted to evaluate model performance, informing both the credibility and applicability of model results. These analyses will follow methodologies consistent with standard practices for similar modeling studies (EPA, 2009).

Model *sensitivity* describes the degree to which results are affected by changes in a selected input. Sensitivity analyses can help improve understanding of the relative importance of model parameters, identifying which parameters do not significantly affect model outputs and which parameters and processes strongly influence results.

For sensitivity evaluations, the model will be executed with +/- 10% of a specific parameter's default median ("best estimate") value. Using this standard variation (+/- 10%) will allow comparison of the relative influence of each parameter on model results. The final report will describe the degree of relative influence of the tested parameters, and will discuss any implications for the interpretation of model results.

The term *uncertainty* is used to describe incomplete or imperfect knowledge about parameters, data, and assumptions. Uncertainty can arise from many sources, including measurement and analytical errors for model input data and imprecise estimates for key parameters. Uncertainty analyses investigate how the model results are affected by this lack of knowledge about the true values of certain inputs and parameters.

For this project, uncertainty analyses will follow the procedures employed by Pelletier and Mohamedali (2009). Key model inputs will be selected for each of the modeled contaminants to evaluate the effect of their uncertainty on the predicted concentrations of COCs in water, sediment, and biota. At a minimum, the model inputs selected for uncertainty analysis by Pelletier and Mohamedali (2009) will be tested. These include chemical specific parameters and processes (e.g., octanol-water partition coefficient, Henry's law constant, degradation rate), loads and initial conditions (e.g., external loads from watershed sources, initial concentration in the active sediment layer), boundary conditions (e.g., salinity and COC concentrations in the SJF/SOG), and ancillary inputs (e.g., sediment burial and resuspension velocities, active sediment layer thickness, and TSS and DOC in the water column).

To evaluate the uncertainty of a specific parameter, the model will be executed using the low and the high values from the interquartile range of estimated values (i.e., 25th and 75th percentiles, respectively) as input to the model. Meanwhile, all of the other model inputs will be held at their default median best estimate values. Model predictions using the low and high estimates will yield a range of possible outcomes and will help reveal whether uncertainty in the true value of the parameter has a significant effect on predictions of COC concentrations in water, sediment, or biota. The final report will document the parameters that are tested and will identify any parameters that have great uncertainty.

Model Output Quality (Usability) Assessment

Final assessment of model performance will be conducted to determine whether the model, despite its uncertainty, can be appropriately used to inform decision making. This determination will be based on assessment of the quality of the data used, evaluation of how well the model predictions correspond to the natural system, and analyses of sensitivity and uncertainty. The project team will make an overall recommendation for the appropriate use and application of the model and will summarize any important limitations in the final report.

Model Scenarios: Environmental Quality Targets

Model predictions of concentrations of COCs in the water, sediment, and biota of Puget Sound will allow estimation of loading reductions and time requirements to achieve specific environmental quality targets.

The targets of interest to this project concern the protection of ecosystem health. *Model scenario threshold concentrations* (MSTCs) will be defined for each of the modeled contaminants, describing concentrations above which there are harmful effects to exposed organisms or ecosystem processes. For PCBs and PBDEs, MSTCs will be concentrations in water, sediment, or biota; the bioaccumulation module is not used for PAHs and metals, so MSTCs for these contaminants will be concentrations in water or sediment. MSTCs will be set in consideration of a variety of ecological risks, such as acute and chronic toxic effects on indicator species, impacts on the dependencies and interactions among species (e.g., alterations to food web relationships, impairment of predator avoidance behaviors), human health effects associated with exposure or dietary consumption of aquatic organisms, and various impairments of ecosystem functions.

The development of MSTCs for this project will be made in consultation with regional experts and collaborators, including the Toxics Workgroup of the Puget Sound Ecosystem Monitoring Program (PSEMP) and "Indicator Champions" from the Puget Sound Partnership (PSP). To a large degree, selection will be informed by the Ecosystem Recovery Targets for Dashboard Indicators specified in the 2011 update to the Action Agenda (PSP, 2011). Guidance will also be taken from existing environmental statutes (e.g., Washington State water quality and sediment standards[8], National Toxics Rule criteria[9]) and the peer-reviewed literature. MSTCs will be summarized in the final report, along with the rationale for their selection. In cases where the selected MSTC is more restrictive than the corresponding regulatory criteria, model scenarios will evaluate both endpoints.

Once MSTCs have been defined, modeling scenarios will be executed to investigate (1) loading reductions required to meet the desired endpoints (i.e., the MSTCs), and (2) the response time of the ecosystem to meet the selected endpoints under various reduction strategies. For load reduction scenarios, the system loads will be incrementally reduced to determine the overall load (kg/yr) at which the MSTCs are achieved. For the response time scenarios, the system loads will be varied to estimate the overall loads at which MSTCs are met for planning periods of 10 years, 20 years, and 50 years. In all scenarios, the current inter-basin proportions of loads (i.e., relative magnitudes) will be maintained as the overall system load is varied.

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[8] Water quality and sediment standards for the State of Washington are found in WAC 173-201A and WAC 173-204, respectively. These standards are available from Ecology at www.ecy.wa.gov/laws-rules/ecywac.html.

[9] National Toxics Rule criteria are available from Ecology at www.ecy.wa.gov/programs/wq/swqs/toxics.html.

These simple scenarios will demonstrate the utility of the PSRTM for informing broad management concerns. With this tool, future scenarios can be developed to explore more specific management questions, such as the system response to basin-specific and/or pathway-specific loading reductions. The outcomes of such scenarios can help managers identify and prioritize the most effective strategies to aid the recovery of the Puget Sound ecosystem.

Project Deliverables

The following deliverables will be completed for this project according to the schedule presented in Table 2:

- Interim report summarizing progress (to date) in acquiring regional data, implementing model code changes, setting model inputs and parameters, and calibration.
- Final report documenting enhancements to the PSRTM and presenting the outcomes of modeling exercises. The report will include, at a minimum, the following:
    - Summary of regional contaminant data (data sources, loads, summary statistics).
    - Details of the model setup, such as physical characteristics of the boxes, initial and boundary conditions, and parameterizations for the modeled contaminants.
    - Qualitative and quantitative discussion of model calibration.
    - Analyses of model sensitivity and uncertainty.
    - Overview of MSTCs selected for each of the modeled contaminants.
    - Description of model scenarios and discussion of model estimates of required load reductions, response times, etc.
    - Recommendations for future uses and further model developments.
- Compilation of regional toxics data used for this project, accessible on the Ecology publication webpage (in Microsoft Excel spreadsheet format).
- A public domain model for simulating the fate/ transport and, where appropriate, bioaccumulation of PCBs, PBDEs, and selected PAHs and metals in Puget Sound.

The improved Puget Sound Regional Toxics Model will give managers a tool for evaluating responses of the Puget Sound ecosystem to changes in loadings for a variety of important contaminants. It will offer the capability of evaluating the outcomes of different source control options so as to direct recovery resources to the most effective strategies.

The results of the various model scenarios explored for this project will be summarized and provided to the Puget Sound Partnership, Ecology programs, and other state, federal, and local partners to help inform an overall control strategy for toxic contaminants entering Puget Sound.

References

Arnot, J.A. and F.A.P.C. Gobas. 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. Environmental Toxicology and Chemistry. 23(10): 2342-2355.

Babson, A.L., M. Kawase, and P. MacCready. 2006. Seasonal and interannual variability in the circulation of Puget Sound, WA: A box model study. Atmosphere-Ocean, 44(1): 29-45.

Brandenberger, J.M., P. Louchouarn, L-J. Kuo, E.A. Crecelius, V. Cullinan, G.A. Gill, C. Garland, J. Williamson, and R. Dhammapala. 2010. Control of Toxic Chemicals in Puget Sound, Phase 3: Study of atmospheric deposition of air toxics to the surface of Puget Sound. Prepared by Battelle Marine Sciences Laboratory for Washington State Department of Ecology, Olympia, WA. Publication No. 10-02-012. www.ecy.wa.gov/biblio/1002012.html.

Chapra, S.C. 1997. Surface Water-Quality Modeling. WCB/McGraw-Hill, Boston, MA.

Condon, C.D. 2007. Development, evaluation, and application of a food web bioaccumulation model for PCBs in the Strait of Georgia, British Columbia. Thesis: Master of Resource Management. School of Resource and Environmental Management. Simon Fraser University. Barnaby, B.C., Canada.

Davis, J.A. 2004. The long-term fate of polychlorinated biphenyls in San Francisco Bay (USA). Environmental Toxicology and Chemistry. 23(10): 2396-2409.

Dexter, R.N., D.E. Anderson, E.A. Quinlan, L.S. Goldstein, R.M. Strickland, S.P. Pavlou, J.R. Clayton, R.M. Kocan, and M. Landolt. 1981. A summary of knowledge of Puget Sound related to chemical contaminants. National Oceanic and Atmospheric Administration, Office of Marine Pollution Assessment. NOAA Technical Memorandum OMPA-13.

Ecology. 2008. Guidance for calculating “total” values of selected analytes for the EAP Toxics Studies Unit and EIM parameter names to use. Environmental Assessment Program, Washington State Department of Ecology, Olympia, WA.

Ecology. 2011. Control of Toxic Chemicals in Puget Sound Phase 3: Assessment of selected toxic chemicals in the Puget Sound basin, 2007-2011. Washington State Department of Ecology, Olympia, WA. Publication No. 11-03-055. www.ecy.wa.gov/biblio/1103055.html.

Ecology and Environment, Inc. 2009. Control of Toxic Chemicals in Puget Sound Phase 2: Sediment flux / Puget Sound sediments bioaccumulation model – Derived concentrations for toxics final summary technical report. Prepared by Ecology and Environment, Inc. for Washington State Department of Ecology, Olympia, WA. Publication No. 09-09-069. www.ecy.wa.gov/biblio/0909069.html.

Ecology and Herrera Environmental Consultants, Inc. 2010. Control of Toxic Chemicals in Puget Sound Phase 3: Loadings from POTW discharge of treated wastewater. Washington State Department of Ecology, Olympia, WA. Publication No. 10-10-057. www.ecy.wa.gov/biblio/1010057.html.

EPA (U.S. Environmental Protection Agency), 2009. Guidance on the Development, Evaluation and Application of Environmental Models. Council for Regulatory Environmental Modeling, Washington D.C. EPA Publication No. EPA/100/K-09/003.

Gobas, F.A.P.C. and J.A. Arnot. 2010. Food web bioaccumulation model for polychlorinated biphenyls in San Francisco Bay, California, USA. Environmental Toxicology and Chemistry. 29(6): 1385-1395.

Gobas, F.A.P.C. and H.A. Morrison. 2000. Bioconcentration and biomagnifications in the aquatic environment. Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences. Eds. R.S. Boethling and D. Mackay. Lewis Publishers, Boca Raton, FL.

Greenfield, B.K. and J.A. Davis. 2004. A simple mass balance model for PAH fate in the San Francisco Estuary. RMP Technical Report: SFEI Contribution 115. San Francisco Estuary Institute, Oakland, CA, USA.

Gries, T. and D. Osterberg. 2011. Control of Toxic Chemicals in Puget Sound Phase 3: Characterization of toxic chemicals in Puget Sound and major tributaries, 2009-10. Washington State Department of Ecology, Olympia, WA. Publication No. 11-03-008. www.ecy.wa.gov/biblio/1103008.html.

Hart Crowser, Inc., Washington State Department of Ecology, U.S. Environmental Protection Agency, and Puget Sound Partnership. 2007. Control of Toxic Chemicals in Puget Sound Phase 1: Initial estimate of toxic chemical loadings to Puget Sound. Washington State Department of Ecology, Olympia, WA. Publication No. 07-10-079. www.ecy.wa.gov/biblio/0710079.html.

Herrera. 2011. Control of Toxic Chemicals in Puget Sound Phase 3: Data and load estimates. Herrera Environmental Consultants, Inc. Ecology Publication No. 11-03-010. www.ecy.wa.gov/biblio/1103010.html.

Johannessen, S.C., R.W. Macdonald, C.A. Wright, B. Burd, D.P. Shaw, A. van Roodselaar. 2008. Joined by geochemistry, divided by history: PCBs and PBDEs in Strait of Georgia sediments. Marine Environmental Research. 66: S112-S120.

Kelley, B., M. Ikonomou, J. Blair, and F.A.P.C. Gobas. 2008. Bioaccumulation behavior of polybrominated diphenyl ethers (PBDEs) in a Canadian Arctic marine food web. Science of the Total Environment. 401(1): 60-72.

LDW (Lower Duwamish Waterway Group). 2010. Lower Duwamish waterway remedial investigation. Remedial investigation report. Appendix D: Food web model. Prepared by Windward Environmental, LLC. for the Lower Duwamish Waterway Group for submittal to the U.S. Environmental Protection Agency and the Washington State Department of Ecology. July 9, 2010, Final.

Mabey, W.R., J.H. Smith, R.T. Podoll, H.L. Johnson, T. Mill, T.W. Chou, J. Gates, I. Waight Partridge, H. Jaber, and D. Vandenberg. 1982. Aquatic fate process data for organic priority pollutants. Prepared by SRI International for U.S. Environmental Protection Agency, Office of Water Regulations and Standards, Washington, D.C. EPA Publication No. EPA 440/4-81-014.

Mackay, D. and B. Hickie. 2000. Mass balance model of source apportionment, transport and fate of PAHs in Lac Saint Louis, Quebec. Chemosphere. 41: 681-692.

Nairn, B., J. Stern, and K. Schock. 2011. The role of plankton in a PCB bioaccumulation model for Puget Sound's central basin. Poster presented at the 2011 Salish Sea Ecosystem Conference, Vancouver, B.C., Canada.

Noel, M. 2007. PCBs and PBDEs deposited onto coastal waters via rain, dry particulate, and gaseous deposition. 2007 Georgia Basin Puget Sound Research Conference. Sponsored by Environment Canada and the Puget Sound Action Team. Vancouver, BC, Canada.

Noel, M., P. Ross, S. Jeffries, and M. Lance. 2011. Control of Toxic Chemicals in Puget Sound Phase 3: Toxic Contaminants in harbor seal (*Phoca vitulina*) pups from Puget Sound. Washington Department of Fish and Wildlife, Olympia, WA. Ecology Publication No. 11-10-001. www.ecy.wa.gov/biblio/1110001.html.

Oram, J.J., L.J. McKee, C.E. Werme, M.S. Connor, D.R. Oros, R. Grace, and F. Rodigari. 2008. A mass budget of polybrominated diphenyl ethers in San Francisco Bay, CA. Environment International. 34: 1137-1147.

Pelletier, G., and T. Mohamedali. 2009. Control of Toxic Chemicals in Puget Sound Phase 2: Development of simple numerical models – The long-term fate and bioaccumulation of polychlorinated biphenyls in Puget Sound. Washington State Department of Ecology, Olympia, WA. Publication No. 09-03-015. www.ecy.wa.gov/biblio/0903015.html.

PSAT (Puget Sound Action Team). 2003. Status, trends, and effects of toxic contaminants in the Puget Sound environment. Prepared for the Puget Sound Action Team, Olympia, WA by EVS Environment Consultants, North Vancouver, BC, Canada.

PSP (Puget Sound Partnership). 2006. Sound Health, Sound Future: Protecting and restoring Puget Sound. Puget Sound Partnership, Olympia, WA.

PSP (Puget Sound Partnership). 2008. Puget Sound Action Agenda. Puget Sound Partnership, Olympia, WA.

PSP (Puget Sound Partnership). 2011. Update to the Puget Sound Action Agenda. Draft (December 9, 2011): In review. Puget Sound Partnership, Tacoma, WA. Accessed February 25, 2012 from agency website: www.psp.wa.gov/action_agenda_2011_draft-content.php.

PTI (PTI Environmental Services, Inc.). 1991. Pollutants of concern in Puget Sound. Prepared for U.S. Environmental Protection Agency, Office of Puget Sound, Region 10, Seattle, WA by PTI Environmental Services, Inc. EPA Publication No. EPA-910/9-91-003.
Redman, S., A. Criss, J. Dohrmann, and R. Schultz. 2006. Toxics in Puget Sound: Review and analysis to support toxic controls. Puget Sound Action Team, Olympia, WA.

Romberg, G.P., S.P. Pavlou, R.F. Shokes, W. Horn, E.A. Crecelius, P. Hamilton, J.T. Gunn, R.D. Muench, and J. Vinelli. 1984. Toxicant Pretreatment Planning Study Technical Report C1: Presence, distribution and fate of toxicants in Puget Sound and Lake Washington. Municipality of Metropolitan Seattle, Water Quality Division. Metro Toxicant Program Report No. 6A.

Stern, J., B. Nairn, K. Schock, and A. Ryan. 2009. Development of a PCBs bioaccumulation model for the Puget Sound ecosystem. Presentation given at the 2009 Puget Sound Georgia Basin Ecosystem Conference, Seattle, WA.

Townes-Witzel, S. and A. Ryan. 2007. Puget Sound food web bioaccumulation model for polychlorinated biphenyls: final intern report. King County Department of Natural Resources and Parks, Wastewater Treatment Division, Seattle, WA.

West, J.E., J. Lanksbury, and S.M. O'Neill. 2011a. Persistent organic pollutants in marine plankton from Puget Sound. Washington Department of Fish and Wildlife, Olympia, WA. Ecology Publication No. 11-10-002. www.ecy.wa.gov/biblio/1110002.html.

West, J.E., J. Lanksbury, S.M. O'Neill, and A. Marshall. 2011b. Persistent bioaccumulative and toxic contaminants in pelagic marine fish species from Puget Sound. Washington Department of Fish and Wildlife, Olympia, WA. Ecology Publication No. 11-10-003. www.ecy.wa.gov/biblio/1110003.html.

Wool, T.A., R.B. Ambrose, J.L. Martin, E.A. Comer. 2003. Water quality analysis simulation program (WASP). Version 6.0. Draft: User's manual. U.S. Environmental Protection Agency, Region 4, Atlanta, GA, and Environmental Research Laboratory, Athens, GA; U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, MS; and Tetra Tech, Inc., Atlanta, GA.

Appendix. Glossary, Acronyms, and Abbreviations

Glossary

Acute conditions: Changes in the physical, chemical, or biological environment which are expected or demonstrated to result in injury or death to an organism as a result of short-term exposure to the substance or detrimental environmental condition.

Bioaccumulation: The process by which the chemical concentration within an organism achieves a level that exceeds that in its environment as a result of chemical uptake through all possible routes of exposure (e.g., dietary, dermal, respiratory).

Carcinogen: A chemical or chemical group that has been identified as "carcinogenic to humans" or "likely to be carcinogenic to humans" by the Environmental Protection Agency, as a Group 1, 2A, or 2B carcinogen by the International Agency for Research on Cancer, or as a "known to be human carcinogen" or "reasonably anticipated to be a human carcinogen" by the National Toxicology Program.

Chemical: A naturally occurring element, mixture, or group of organic and inorganic compounds that is produced by or used in a chemical process. Chemical "groups" share a common chemical structure.

Chronic conditions: Changes in the physical, chemical, or biological environment which are expected or demonstrated to result in injury or death to an organism as a result of repeated or constant exposure over an extended period of time to a substance or detrimental environmental condition.

Degradation: The process by which organic chemicals are transformed into derivative chemicals and ultimately broken down.

Interquartile: A measure of the statistical dispersion of a data set, equal to the difference between the upper and lower quartiles (75th and 25th percentiles, respectively).

Media (or medium): A component of the environment (air, water, soil, or sediment) in which a contaminant is measured and from which an organism can accumulate contaminants.

Median: A statistical measure of central tendency, equal to the numerical value separating the higher half of a data set from the lower half. The median is the same as the second quartile, or 50th percentile.

Model scenario threshold concentration (MSTC): Project-specific term used to describe a chemical concentration in water, sediment, or biota below which exposed aquatic organisms and ecosystem processes are considered to be adequately protected from toxic effects.

Parameter: A physical, chemical, or biological property whose values determine environmental characteristics or behavior.

Persistence: The tendency of a chemical to remain in the environment without transformation or breakdown into another chemical form. It refers to the length of time a chemical is expected to reside in the environment and be available for exposure.

Point source: Sources of pollution that discharge at a specific location from pipes, outfalls, and conveyance channels to a surface water. Examples of point source discharges include municipal wastewater treatment plants, municipal stormwater systems, industrial waste treatment facilities, and construction sites that clear more than 5 acres of land.

Pollution: Contamination or other alteration of the physical, chemical, or biological properties of any waters of the state. This includes change in temperature, taste, color, turbidity, or odor of the waters. It also includes discharge of any liquid, gaseous, solid, radioactive, or other substance into any waters of the state. This definition assumes that these changes will, or are likely to, create a nuisance or render such waters harmful, detrimental, or injurious to (1) public health, safety, or welfare, or (2) domestic, commercial, industrial, agricultural, recreational, or other legitimate beneficial uses, or (3) livestock, wild animals, birds, fish, or other aquatic life.

Stormwater: The portion of precipitation that does not naturally percolate into the ground or evaporate but instead runs off roads, pavement, and roofs during rainfall or snow melt. Stormwater can also come from hard or saturated grass surfaces such as lawns, pastures, playfields, and from gravel roads and parking lots.

Total suspended solids (TSS): Dry weight measure of the portion of solids retained by a filter.

Toxicity: The degree to which a substance or mixture of substances can harm humans, plants, or wildlife.

Volatilization: The mass transfer process whereby a dissolved substance is vaporized.

Watershed: A drainage area or basin in which all land and water areas drain or flow toward a central collector such as a stream, river, or lake at a lower elevation.

25th percentile: A statistical number obtained from a distribution of a data set, above which 75% of the data exists and below which 25% of the data exists.

75th percentile: A statistical number obtained from a distribution of a data set, above which 25% of the data exists and below which 75% of the data exists.

Acronyms, Abbreviations, and Units of Measurement

COC	Contaminant of concern
cPAH	Carcinogenic PAH
DOC	Dissolved organic carbon
e.g.	For example
EAP	Environmental Assessment Program (Ecology)
Ecology	Washington State Department of Ecology
EIM	Environmental Information Management database
EMAP	Environmental Monitoring and Assessment Program (EPA)
EPA	U.S. Environmental Protection Agency
et al.	And others
i.e.	In other words
HOC	Hydrophobic organic contaminant
HPAH	High molecular weight PAH
KCDNR	King County Department of Natural Resources
LDW	Lower Duwamish Waterway
LPAH	Low molecular weight PAH
MSTC	Model scenario threshold concentration (See Glossary above)
PAH	polycyclic aromatic hydrocarbons
PBDE	polybrominated diphenyl ethers
PCB	polychlorinated biphenyls
POTW	Publicly owned treatment works
PSEMP	Puget Sound Ecosystem Monitoring Program
PSP	Puget Sound Partnership
PSRTM	Puget Sound Regional Toxics Model
PSTLA	Puget Sound Toxics Loading Analysis
QA	Quality Assurance
QAPP	Quality Assurance Project Plan
RMSE	Root mean square error
SJF	Strait of Juan de Fuca
SOG	Strait of Georgia
TOC	Total organic carbon
TSS	Total suspended solids (See Glossary above)
USGS	U.S. Geological Survey
VBA	Visual Basic for Applications (Microsoft)
WAC	Washington Administrative Code
WASP	Water Quality Analysis Simulation Program (EPA)
cms	cubic meters per second, a unit of flow
km	kilometer, a unit of length equal to 1,000 meters