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A Food-Web Transfer Bioaccumulation Model for PCBs in San Francisco Bay in Support of Implementing Total Maximum Daily Loading (TMDL) Remediation Targets and Timelines for Recovery

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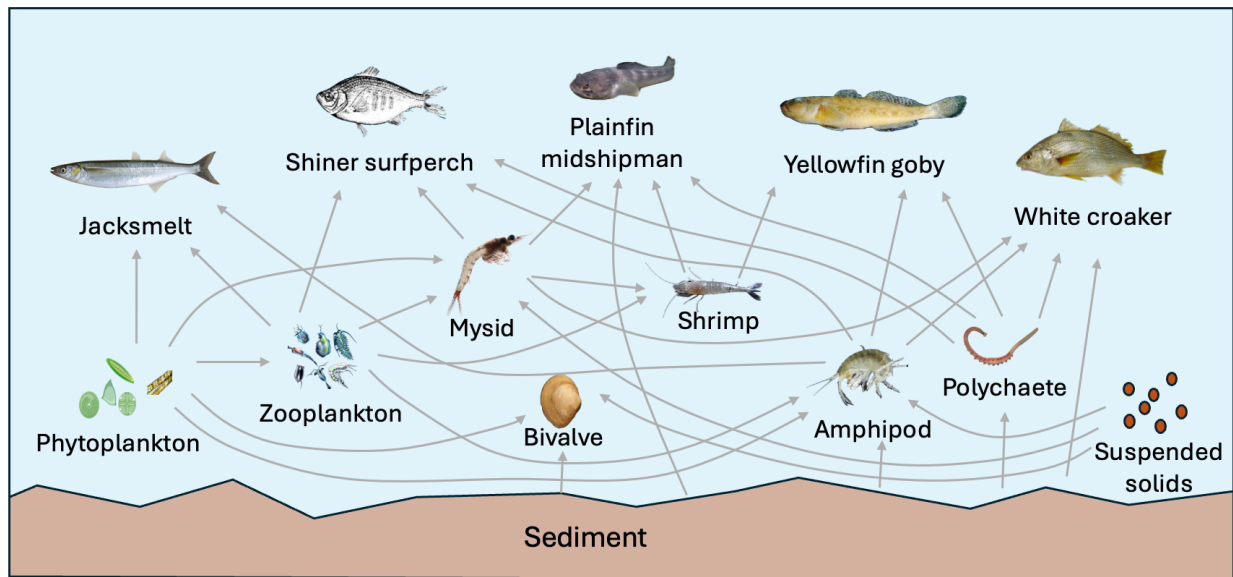
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Report

A Food-Web Transfer Bioaccumulation Model for PCBs in San Francisco Bay in Support of Implementing Total Maximum Daily Loading (TMDL) Remediation Targets and Timelines for Recovery

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Executive Summary

This study developed and tested a food web bioaccumulation model for PCBs in San Francisco Bay that can be used on a site specific basis at Priority Margin Units (PMUs) to predict how concentrations of PCBs in fish and other species of the aquatic food-web at PMUs can be expected to change over time in response to changes in PCB concentrations in water and sediments at PMUs resulting from remediation initiatives at the PMUs. This model is meant to be used in conjunction with an environmental fate model that can estimate the change in concentrations of PCBs in water and sediments over time in response to changes in loadings of PCBs into the PMU. The main goal of the model is to anticipate PCB concentrations in sport fish consumed by local fishers as a result of remediation efforts at the PMUs. The overall approach is to inform on (i) when PCB concentrations are going to be low enough to safely consume fish caught at the PMUs and the larger San Francisco Bay and what concentrations of PCBs in water and sediments are required to meet health advisories with regards to the consumption of sport fish.

Model testing at the San Leandro Bay and Steinberger Slough/Redwood Creek Complex PMUs and the larger San Francisco Bay shows that model predictions of PCB congeners in fish are in good agreement with observed concentrations. In most tests, observed $\sum$ PCB concentrations were found to be well within a factor of 2 of the predicted concentrations. The largest systematic overprediction of $\sum$ PCB concentrations in fish was equivalent to a factor of 2.3, the largest underprediction was by a factor of 1.09 or less than 10%. The mean and median for all mean model bias MB* for $\sum$ PCB were 1.54 and 1.59 respectively. This means that on average the model overpredicts concentrations of PCBs in fish by approximately 59%. This level of predictability is very good and a credit to the amount and excellence of research done on the bioaccumulation of PCBs in San Francisco Bay and other locations around the world. It should be emphasized that the uncertainty of the model expressed by the mean model bias and its 95% confidence intervals includes not only error in the model but also error in the empirical concentration data that were used for determining uncertainty. As a result, we feel that the model can be used to predict concentrations of PCBs in fish at the PMUs and can be expected to provide estimates of PCB concentrations in fish with a high level of confidence. We suggest that a factor of 2 is used to represent the uncertainty in model predictions of the concentrations of PCBs in fish. The model without further calibration can be expected to be slightly on the conservative side.

The ability of the model to predict concentrations of individual PCB congeners is similar to that for $\sum$ PCBs, but model uncertainty is somewhat larger than that for $\sum$ PCBs as evidenced by the 95% confidence intervals of the mean model bias. Model testing in the Steinberger Slough/Redwood Creek Complex PMU also showed a tendency for the model to overpredict concentrations in fish of lower molecular weight PCB congeners while underestimating concentrations in fish of higher molecular weight PCB congeners. We expect this to reflect some of the equilibrium assumptions that were made with regards to the distribution of PCBs

between water and particulate matter where field data were absent. Better field data on the equilibrium status of PCBs between water and particulate matter is expected to remedy this issue and further improve the accuracy of the model. The application of passive samplers in future studies of the fate of PCBs in San Francisco Bay will be of particular value in this regard.

Model simulations of the temporal response of PCB concentrations in fish over time showed considerable differences in response times to changes in concentrations in water and sediments among PCB congeners. We expect there to be similar PCB congener specific differences in the response times of PCB congener concentrations in water and sediments in response changes in PCB loadings. This means that PCB loading reductions will lead to a relatively quick decline of concentrations of lower molecular weight PCBs compared to a slower decline of concentrations of higher molecular weight PCB congeners. As a result, the composition of PCBs in water, sediments and fish can be expected to change over time in response to a PCB loading reduction. In fish, PCB mixtures will become “heavier”, containing a higher fraction of higher molecular weight PCBs. The change in composition of PCBs in fish as a result of PCB loading reductions can be relevant for the calculation of human health risks of PCBs associated with fish consumption. The change in PCB composition in fish may also provide a way to track progress of remediation efforts and associated changes in PCB loading rates., which are often difficult to measure. The decline of the contribution of lower molecular weight PCBs to the Σ PCB concentration in fish is an indicator of loading decline over time.

The PCB food-web bioaccumulation model for 3 PMUs (i.e., San Leandro Bay, Emeryville Crescent and the Steinberger Slough/Redwood Creek Complex) and the larger San Francisco Bay are presented in an Excel spreadsheet format and can be used with minimal training to evaluate the impact of remediation initiatives on concentrations of PCBs in fish. The model also acts as a record of the state of knowledge of the food-web bioaccumulation of PCBs in San Francisco Bay. The model includes knowledge gained from years of studies of San Francisco Bay. The model imbeds information on the chemistry and ecology of the Bay and presents this knowledge in a mathematical form such that it can be used as a management tool and serve as a hypothesis for further scientific and monitoring studies aimed at improving knowledge of the environmental fate of PCBs and informed decision making with regards the management of pollutants.

The model is developed for PCBs, but can be applied with some modification, to other organic chemical pollutants such as brominated flame-retardants, PFAS, pesticides and others. The model is not appropriate for metals and nutrients.

To improve the developed time-dependent food-web biotransformation models of PCBs and other organic chemical contaminants for specific PMUs and the larger San Francisco Bay and improve their use, we recommend to continue on-going monitoring efforts to obtain empirical PCB congener concentrations in key fish species (e.g., shiner surfperch and topsmelt) and environmental media (e.g., water, sediments, and suspended sediments). Such information can be used to refine the bioaccumulation models and used to gain confidence in the application of the model for management purposes. For the purpose of model development and testing, it is beneficial to coordinate sampling of sediments, water and fish to be spatially, temporally and

ecologically consistent. We also recommend the application of passive sampling methods, which are particularly useful for parameterizing the food-web bioaccumulation model as it can be used to measure the equilibrium status of concentrations of PCBs in sediments and water, which is a key factor controlling the degree to which PCBs are absorbed by fish via food-consumption vs. respiration and are transferred through the benthic vs. pelagic routes.

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Introduction

For many years, San Francisco Bay has been the subject of contamination of Polychlorinated Biphenyls or PCBs as a result of run-off from contaminated streams and urban areas (Gunther et al. 2001; Kinetic Laboratories 2002), effluent discharges (Yee et al. 2001; Yee et al. 2002), and atmospheric deposition (Tsai et al. 2002). Polychlorinated Biphenyls (PCBs) have been found in water, sediments and many wildlife species, including fish, birds and marine mammals throughout the Estuary (State Water Resources Control Board 2000) for many years and are still found to date. Tissue concentrations of PCBs in San Francisco Bay sport fish became an issue of public concern in the early 1990s and resulted in a fish consumption advisory issued by California's Office of Environmental Health Hazard Assessment. The USEPA placed San Francisco Bay on the 303(d) impaired water body list for PCBs and other contaminants (State Water Resources Control Board 2000). As required by the Clean Water Act, the Regional Water Quality Control Board (Regional Board) initiated a total maximum daily loading (TMDL) study of the Bay to better understand the relationships between sources and PCB concentrations in water, sediments and wildlife throughout the Bay and to facilitate and support management decisions protective of wildlife and humans.

As part of the TMDL study, an abiotic mass balance model was developed by Davis (2004) to describe the relationship between PCB inputs into the Bay and resulting PCB concentrations in water and sediments. Also, a food web bioaccumulation model was developed to assess concentrations of PCBs in fish and other wildlife species as a result of direct exposure to PCBs in water and sediments of San Francisco Bay and transfer through the food-web (Gobas and Arnot 2010). The main purpose of the model was to identify what PCB concentrations in the sediments and water of the Bay needed to be achieved before wildlife would no longer be at risk of PCB contamination and that people would be able to safely consume fish caught in San Francisco Bay. The model was used to derive a TMDL for PCBs in San Francisco Bay and this TMDL is still in place to date. The TMDL provides guidance to initiatives aimed at eliminating PCBs as a cause of concern for human and environmental health.

The modeling approach that was used to derive the TMDL was based on describing the relationship between sources of PCBs and concentrations of PCBs in wildlife species for the entire San Francisco Bay. In the following years, this whole-Bay approach to deriving a TMDL was revisited to make place for a more site-specific approach that focused on specific areas of concern because of the presence of significant sources of PCB contamination. These specific areas of concern were designated Priority Margin Units or PMUs. Examples of PMUs are San Leandro Bay, Steinberger Slough/Redwood Creek Complex, and Emeryville Crescent. One of the reasons for a focus on PMUs was that significant reductions in PCB emissions could be achieved at these sites through remediation initiatives, but that the impact of these reductions would be difficult to register when monitoring and modeling studies are conducted on a whole Bay basis rather than the PMUs themselves. A site-specific approach provides a more direct and simpler approach to follow the improvements in water quality achieved by remediation initiatives.

However, to better understand the relationship between changes in PCB emissions over time and resulting changes in concentrations of PCBs in water, sediments and wildlife on a site-specific basis, it is necessary to develop site-specific models for PCBs at the PMUs. Key questions that the model should be able to address is what changes in PCB concentrations in wildlife species can be expected on a site-specific basis as a result of remediation initiatives and are those changes sufficient for people to safely consume fish and protect local wildlife species at the PMUs and the larger San Francisco Bay. Also, the models should provide insights into how quickly changes in PCB concentrations in wildlife species can be expected to take place in the PMUs and how these site-specific changes in PCB inputs affect concentrations of PCBs in wildlife species throughout the Bay. The change in management from a whole Bay approach to a site-specific PMU approach and a focus on short term improvements in water quality in addition to longer term impacts on water quality meant that models needed to be developed that have better spatial and temporal resolution than the models developed previously.

The objective of this study is to develop and evaluate a food web bioaccumulation model for PCBs in San Francisco Bay that can be used on a site specific basis at PMUs and that can estimate how concentrations of PCBs in species of the aquatic food-web can be expected to change over time in response to remediation initiatives at the PMUs. This model is meant to be used in conjunction with hydrodynamic, sediment transport and environmental fate models to gain insights into the relationship between PCB emission reduction at PMUs and PCB concentrations in sport fish consumed by local fishers. While the model is specific to PCBs it can be useful to address other pollutants as well. The food-web bioaccumulation behavior of many neutral hydrophobic organic pollutants such as chlorinated dioxins, polybrominated biphenyls, ethers and ethanes can also be investigated by the model. Furthermore, we have shown that with appropriate accommodations for the chemical partitioning properties, the modeling approach is also useful for many polyfluoroalkyl substances (PFAS) (Kelly et al. 2024).

Methodology

Overview

The development and evaluation of the food-web trophic transfer model for PCBs in San Francisco Bay involves the following steps:

First, a mechanistic model of the uptake, depuration and trophic transfer of PCB congeners in plankton, benthic invertebrates, fish and sport fish is constructed. This model is a further development of a previously developed food-web bioaccumulation for San Francisco Bay (Gobas et al. 2010). The new attributes of the model are its site-specific focus and its time dependency to support the application of the model at various PMUs and to account for temporal changes in PCB concentrations in water and sediments. The model applies a congener specific approach recognizing the large variation in partitioning properties among PCB congeners and uses an additive approach to the masses of different PCB congeners to arrive at a combined or total PCB (Σ PCB) concentration.

Secondly, we parameterize the model with up-to-date information on the chemical properties of PCBs, environmental and ecological characteristics at 3 PMUs (i.e. Emeryville Crescent, San Leandro Bay and Steinberger/Redwood Creek complex) as well as the larger San Francisco Bay.

Thirdly, we compile measured concentrations of PCB congeners in water, sediments and fish species at the 3 PMUs and the larger San Francisco Bay on a site-specific basis and identify the concentrations of PCBs in water and sediments that are most suitable for testing the model. The testing of the model involves the calculation of concentrations of PCB congeners and Σ PCB in fish from the concentrations of the PCB congeners in water and sediments. To provide the best conditions for model testing, measured concentrations in water, sediments and fish collected in approximately the same locations and within approximately the same period of time were selected. Testing of the model includes a comparison of calculated and measured concentrations of both PCB congeners and Σ PCB.

Fourth, concentrations of PCB congeners in fish of the PMUs were calculated by the model from the measured concentrations of PCB congeners in water and sediments of the PMUs. Similar calculations were done for the larger San Francisco Bay. For the Emeryville PMU, there were not sufficient data to conduct model testing. Hence, the model testing was only done for the San Leandro Bay and Steinberger-Redwood Creek PMUs. Because the spatial and temporal overlap between measured concentrations of PCBs in water, sediments and fish for the larger San Francisco Bay area was poor, model calculations were conducted based on the range of PCB concentrations in water and sediments measured throughout the entire Bay. The range of PCB concentrations in water and sediments included the minimum and maximum observed concentrations. Model calculations therefore generated a range of model-calculated

concentrations of PCB congeners in fish that were then compared to the observed range of concentrations of PCB congeners in fish.

Fifth, model-calculated ($C_{P,i}$) and observed concentrations of PCB congeners ($C_{O,i}$) in various fish species were then compared to evaluate the performance of the model. The main metric used to express model performance is the mean model bias (MB), which is determined on a PCB congener specific basis and on a total PCB concentration for each individual fish species. The mean model bias (MB) on a congener-specific basis is calculated according to:

$$MB = 10^{(\sum_{i=1}^n (\log (C_{P,i}/C_{O,i}))/n)} \quad (1)$$

where MB is the geometric mean (assuming a log-normal distribution of the ratio $C_{P,i} / C_{O,i}$) of the ratio of model-calculated or predicted ($C_{P,i}$) and mean observed ($C_{O,i}$) concentrations for all PCB congeners from $i=1$ to n in a particular fish species.

To quantitatively express model performance for Σ PCBs, we used the model bias MB^* , which is derived for each individual fish species as:

$$MB^* = \frac{\sum_{i=1}^n C_{P,i}}{\sum_{i=1}^n C_{O,i}} \quad (2)$$

MB^* is the ratio of predicted and observed concentrations of Σ PCB in a specific fish species.

MB and MB^* are measures of the systematic over- ($MB > 1$) or under-prediction ($MB < 1$) of the concentrations of PCB congeners in fish (for MB) or the concentration of Σ PCBs (for MB^*) in fish. For example, if the MB or MB^* is 2, then, the model has a general tendency to overestimate concentrations in fish of PCB congeners (for MB) or Σ PCBs (for MB^*) by a factor of 2. An MB of 1 indicates a lack of model bias and therefore good agreement between model-calculated and observed concentrations. This metric also provides a simple way of calibrating the model predictions if this is considered appropriate. For example, if the model systematically overestimates concentrations of PCBs in fish by a factor of 2, then the model calculations can be adjusted by lowering the model calculated concentrations by a factor of 2 if this is considered appropriate. It is important to note that in the calculation of the mean model bias over- and under-estimations of concentrations of PCBs in fish tend to cancel out. Hence, MB tracks the central tendency of the ability of the model to predict PCB congener concentrations. However, the variability of over- and under-estimation of measured values can also be tracked by the standard deviation of the mean model bias and/or the 95% confidence interval of the mean model bias, i.e. $95\% \text{ CI} = \text{antilog}(\log MB \pm (t_{v, 0.05} \times \log \text{standard deviation}))$. The 95% confidence interval represents the range of model calculated concentrations of PCB congeners in fish that includes 95% of the observed concentrations. Due to the log-normal distribution of the ratio of predicted and observed concentrations, this variability can be expressed as a factor (rather than a term) of the geometric mean. The model's performance improves when MB and MB^* approach 1.0 and the standard deviation or 95% confidence intervals of the mean model bias become smaller. It is important to stress that MB (and its 95% confidence intervals) and MB^*

represent several sources of error including model parameterization errors and errors in model structure and philosophy but also analytical and sampling and analytical errors in the empirical data (e.g. chemical concentrations in water, sediment and biota) and natural, spatial and temporal variability in the empirical data used in the model performance analysis. The model bias therefore quantifies the uncertainty of the larger modeling and monitoring approach, not only the model equations.

Finally, we apply the model in an illustrative fashion to investigate the temporal response of the model and the importance of conducting model simulations on a congener specific basis.

Polychlorinated biphenyls (PCBs)

The food-web bioaccumulation models for PCBs at specific PMUs and the larger San Francisco Bay were performed on a congener-specific basis. 40 PCB congeners (i.e., PCB 8, 18, 28, 31, 33, 44, 49, 52, 56, 60, 66, 70, 74, 87, 95, 97, 99, 101, 105, 110, 118, 128, 132, 138, 141, 149, 151, 153, 156, 158, 170, 174, 177, 180, 183, 187, 194, 195, 201, and 203) were selected for model construction. These PCB congeners have been monitored in San Francisco Bay by the Regional Monitoring Program (RMP) for decades and provide the opportunity to test and evaluate the model.

Aquatic food webs

The aquatic food-web bioaccumulation models were constructed for 3 PMUs (i.e., San Leandro Bay, Steinberger Slough/Redwood Creek Complex, and Emeryville Crescent) and the larger San Francisco Bay, with specific food web structures containing key species at various trophic positions (e.g., phytoplankton, zooplankton, aquatic benthic invertebrates, and fish) in the aquatic ecosystem.

Figure 1 illustrates the food web structure for the San Leandro Bay PMU, including modeled species of phytoplankton, zooplankton, bivalve, polychaete, gammarid, topsmelt, shiner surfperch, and white croaker. The food web was constructed based on the conceptual model report for the San Leandro Bay PMU (Yee et al. 2019) and the study on gut content analyses for key fish species in San Leandro Bay (Jahn 2018). Topsmelt and shiner surfperch are considered indicator species that respond to changes in PCB concentrations from changes in PCB inputs at San Leandro Bay (Yee et al. 2019). Topsmelt is a key prey fish for fish that feed primarily on small epibenthic invertebrates and plays a key role in the benthic food-chain transfer of PCBs. Shiner surfperch is an important sport fish that consumes mainly small benthic invertebrates and a critical indicator species for the Bay.

Figure 2 illustrates the food web structure for the Steinberger Slough/Redwood Creek Complex PMU, including modeled species of phytoplankton, zooplankton, copepods and ostracods, small crustacean, large crustacean, crangon, insect, polychaete, bivalve, and philine,

topsmelt, shiner surfperch, and white croaker. The food web was constructed based on the conceptual model report for the Steinberger Slough/Redwood Creek Complex PMU (Yee et al. 2021) and the study on gut content analyses for key fish species in San Francisco Bay (Jahn 2008). Topsmelt and shiner surfperch are considered indicator species for PCB contamination in the Steinberger Slough/Redwood Creek PMU (Yee et al. 2021).

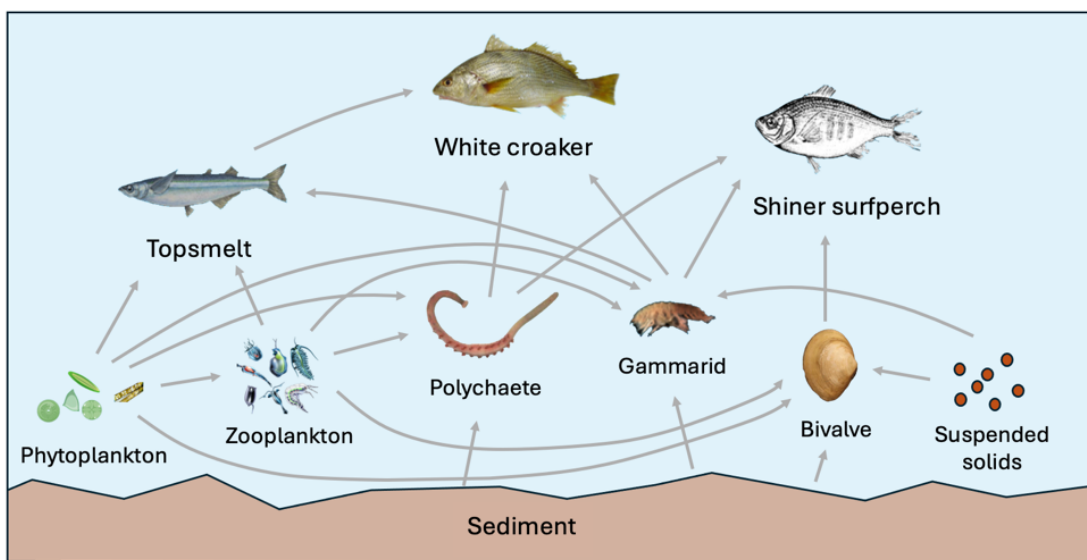


Figure 1. Conceptual diagram illustrating organisms included in the San Leandro Bay PMU food-web bioaccumulation model and their trophic interactions.

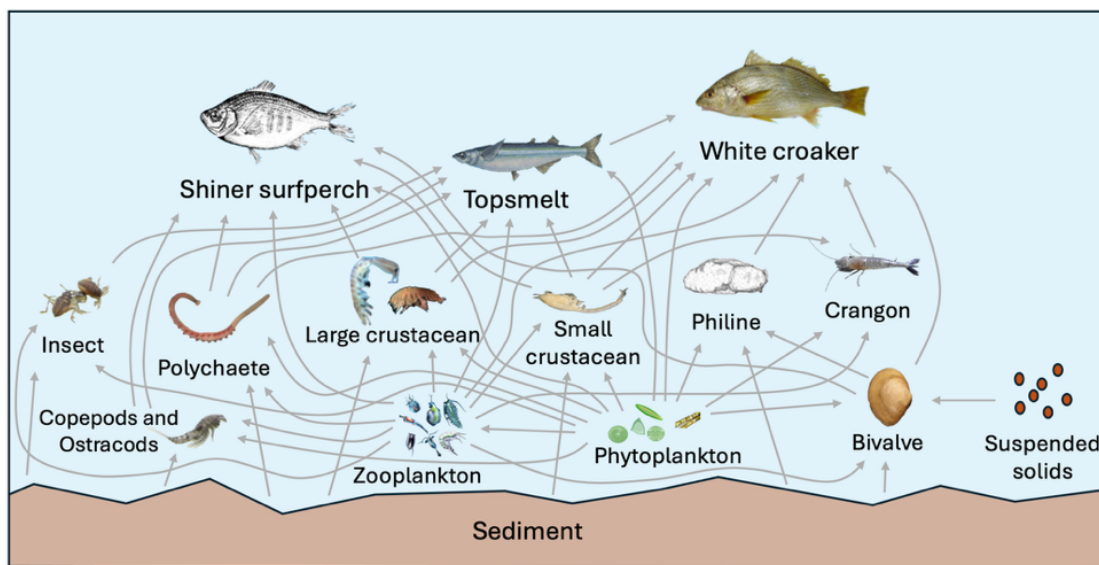


Figure 2. Conceptual diagram illustrating organisms included in the Steinberger Slough/Redwood Creek Complex PMU food-web bioaccumulation model and their trophic interactions.

The food web structure for the Emeryville Crescent PMU model, which is illustrated in Figure 3, includes phytoplankton, zooplankton, copepods and ostracods, small crustacean, large

crustacean, insect, polychaete, bivalve, Mississippi silverside, topsmelt, shiner surfperch, and striped bass. The food web was constructed based on the conceptual model report for the Emeryville Crescent PMU (Davis et al. 2017a) and the study on gut content analyses of key fish species in San Francisco Bay (Jahn 2008). Mississippi silverside and topsmelt are the key prey fish species and main indicator species for changes in PCB concentrations due to changes in PCB loads at Emeryville Crescent (Davis et al. 2017a). Shiner surfperch is also a key indicator species for the PCB TMDL in the Bay and serves as an additional indicator of changes in watershed inputs of PCBs (Davis et al. 2017a).

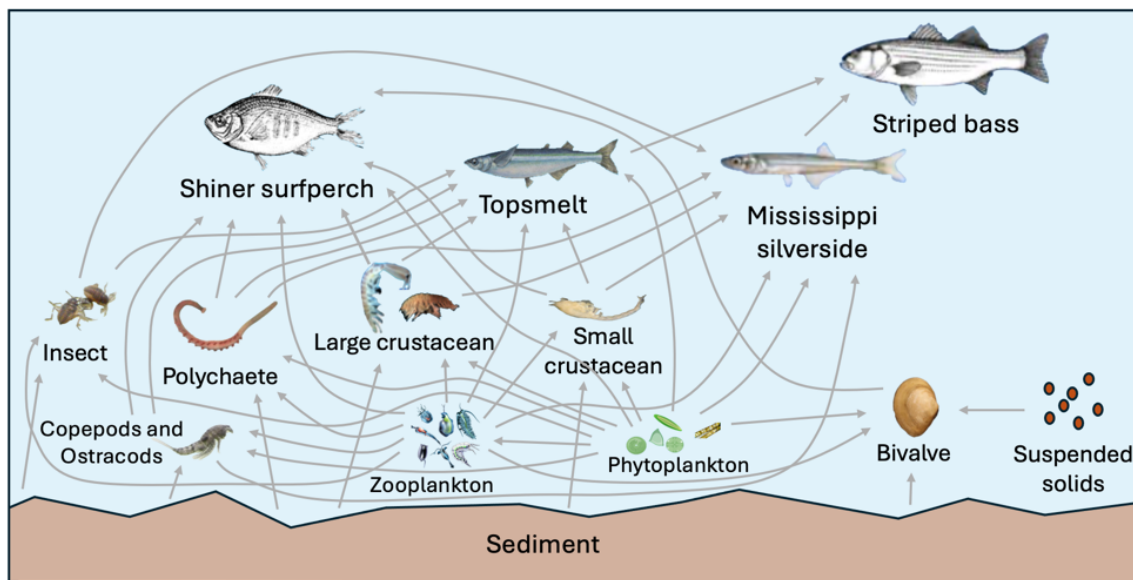


Figure 3. Conceptual diagram illustrating organisms included in the Emeryville Crescent PMU food-web bioaccumulation model and their trophic interactions.

Figure 4 illustrates the aquatic food web structure for the larger San Francisco Bay, including phytoplankton, zooplankton, polychaete, amphipod, bivalve, mysid, shrimp, shiner surfperch, jacksmelt, yellowfin goby, plainfin midshipman, and white croaker as the representative species included in the model. The aquatic food web was constructed based on previous modeling efforts for PCBs in San Francisco Bay (Gobas and Arnot 2010). Shiner surfperch, jacksmelt, and white croaker are sport fish species of primary management interest (Gobas and Arnot 2010).

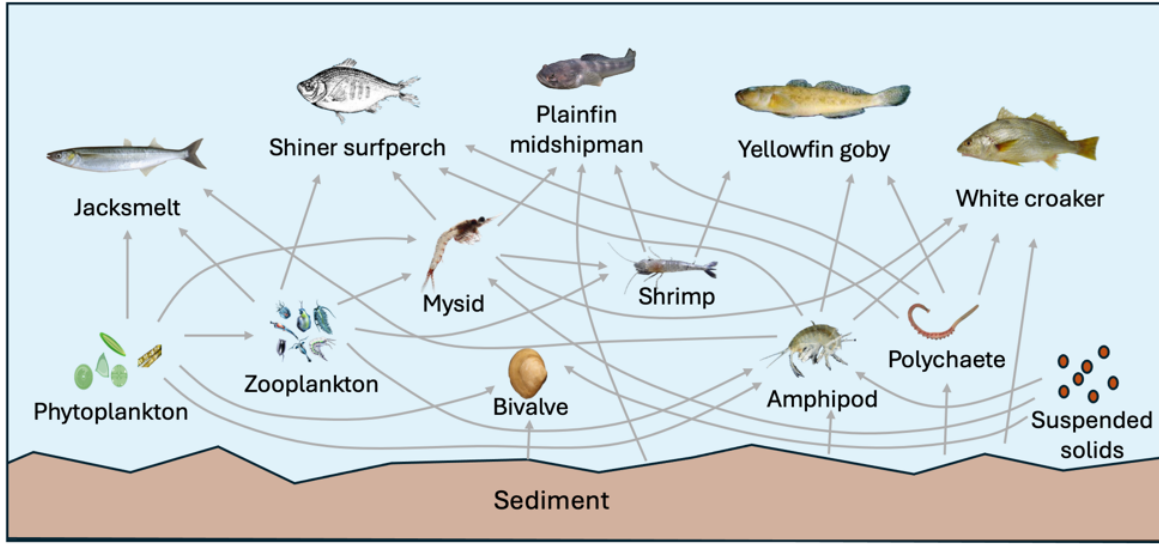


Figure 4. Conceptual diagram illustrating key organisms included in the San Francisco Bay food-web bioaccumulation model and their trophic interactions.

Time-dependent food-web bioaccumulation model

The aquatic food-web bioaccumulation model is a mechanistic model based on mass-balance principles that capture the various ways that PCBs are taken up and eliminated by species. Previous versions of the model included steady-state or time-independent formulations that were used in the development of the original TMDL for San Francisco Bay (Gobas and Arnot 2010) and the USEPA Kow based Aquatic Bioaccumulation Model (KABAM) used for pesticide risk assessment in the US (USEPA 1993). Key simplifying assumptions of the model are that organisms are viewed as single, well-mixed compartments and PCB congeners are distributed homogeneously within the lipids of the organism. The exchange of PCB congeners between the organism and its ambient environment can be described by a single general equation for a number of aquatic organisms. The general mathematical expression (Equation 3) describes the change in concentration of a PCB congener in a single organism over time, accounting for all major mechanisms of PCB congener uptake and elimination.

$$\frac{dC_B}{dt} = [k_1 \cdot (m_O \cdot \phi \cdot C_{WT,O} + m_P \cdot C_{WD,P}) + k_D \cdot \sum_{i=1}^n (P_i \cdot C_{D,i})] - (k_2 + k_E + k_G + k_M) \cdot C_B \quad (3)$$

where C_B is the wet-weight concentration of the PCB congener in the organism (g chemical/kg organism wet wt); k_1 is the clearance rate constant ($L \text{ water} \cdot \text{kg organism wet wt}^{-1} \cdot \text{d}^{-1}$) for chemical uptake via the respiratory surfaces (i.e., gills and skin); $C_{WT,O}$ is the total concentration (g chemical/L water) of the PCB congener in the overlying water above the sediments; $C_{WD,P}$ is the freely dissolved concentration (g chemical/L water) of the PCB congener in the sediment-associated porewater; m_O and m_P are the fractions (unitless) of the respiratory ventilation that involves overlying water and sediment-associated porewater, respectively; ϕ is the freely dissolved fraction (unitless) of the total chemical concentration in the overlying water that can

be absorbed via membrane diffusion; k_D is the clearance rate constant ($\text{kg diet} \cdot \text{kg organism wet wt}^{-1} \cdot \text{d}^{-1}$) for chemical uptake via ingestion of food and water; $C_{D,i}$ is the concentration of the PCB congener in prey item i ($\text{g chemical/kg prey item } i$); P_i is the fraction (unitless) of the diet consisting of prey item i ; k_2 is the rate constant (d^{-1}) for the elimination of the PCB congener via respiratory surfaces (i.e., gills and skin); k_E is the rate constant (d^{-1}) for the elimination of the PCB congener via fecal egestion; k_G is the rate constant (d^{-1}) for growth dilution, describing a pseudo elimination process for the dilution effect due to the increase in weight and volume of the organism during growth while no loss of the mass of the PCB congener occurs; and k_M is the rate constant (d^{-1}) for biotransformation of the PCB congener in the organism. The derivation and calculation of kinetic parameters (i.e., k_1 , k_2 , k_D , k_E , and k_G) and other model parameters are described in Appendix A.

In this modeling approach, the multiplication of ϕ and $C_{WT,O}$ represents the freely-dissolved concentration of the PCB congener in the overlaying water above the sediments ($C_{WD,O}$; $\text{g chemical/L water}$). $C_{WD,P}$ is the freely dissolved concentration of the PCB congeners in the pore water. In the model testing, we assume that the passive sampling technique applied to both the sediments and the overlaying water measures the freely dissolved concentrations of the PCB congeners rather than the overall combined concentration of freely dissolved and particulate bound PCBs.

The modeling approach includes two pathways of bioaccumulation of sediment bound PCBs into organisms. The first pathway is through equilibrium partitioning of the PCBs between sediment particles and pore water. In this approach, freely dissolved concentration of PCBs in pore water are estimated from the concentrations of PCBs in the sediment particulates using the organic carbon-water partition coefficients K_{OC} and the organic carbon contents of the sediment particles ($\phi_{OC,S}$):

$$C_{WD,P} = \frac{C_S}{K_{OC} \cdot \phi_{OC,S}} \quad (4)$$

PCBs dissolved in the pore water of sediments are then absorbed through the respiratory route in benthic dwelling organisms, which are consumed by predators.

The second pathway is dietary consumption of PCB contaminated sediment particles. The model then calculates how much of the PCB in ingested sediments is absorbed by sediment-consuming organisms. Both routes provide significant transfer of PCBs from the sediments to aquatic biota in San Francisco Bay and contribute to PCB concentrations in fish throughout the Bay.

The significance of the benthic route to deliver PCBs to fish is elevated when disequilibria between concentrations of PCBs in water and sediments exist. These disequilibria can originate from the faster time response of PCBs in the water column compared to that of the sediments and result in apparent sediment-water partition coefficients that are greater than sediment-water partition coefficients at equilibrium. If inputs of PCBs to the water column

would be instantly reduced to zero, then concentrations of PCBs in water can be expected to fall quickly due to the large water displacement that takes place in the PMUs on a daily basis. In contrast, concentrations of PCBs in sediments decrease more slowly in response to a zero PCB input as diffusion, net sediment transport and sediment burial are relatively slow processes. As a result, concentrations of PCBs in water can be expected to be below their equilibrium values with the sediments upon a reduction in loading and tend to follow the rate of temporal decline of the concentrations of PCBs in the sediments. This also means that upon reductions of PCB loadings to the PMU, the benthic food-chain can become the dominant source of PCBs in fish.

The concentration of the PCB congener in the organism at steady state (i.e., $dC_B/dt = 0$) can be derived from Equation 3 as:

$$C_B = \frac{k_1 \cdot (m_O \cdot \phi \cdot C_{WT,O} + m_P \cdot C_{WD,P}) + k_D \cdot \sum_{i=1}^n (P_i \cdot C_{D,i})}{k_2 + k_E + k_G + k_M} \quad (5)$$

To calculate the time-dependent concentration of the PCB congener in the organism, the mass-balance differential equation (Equation 3) is solved numerically using the Euler's approximation method. The concentration of the PCB congener in the organism at every time step ($C_{B,t=n+1}$) is estimated from the chemical concentration at the previous time step ($C_{B,t=n}$) as:

$$C_{B,t=n+1} = C_{B,t=n} + h \cdot (k_1 \cdot (m_O \cdot \phi \cdot C_{WT,O} + m_P \cdot C_{WD,P}) + k_D \cdot \sum_{i=1}^n (P_i \cdot C_{D,i}) - (k_2 + k_E + k_G + k_M) \cdot C_B) \quad (6)$$

where h is the incremental time step. The steady-state concentration of the PCB congener in the organism (calculated using Equation 5) is used as the initial concentration (i.e., $C_{B,t=0}$). Note that Equation 3 is used for time-dependent concentration simulation for species at a higher trophic level (i.e., fish) in the present study. To calculate concentrations of PCBs in lower trophic level species (e.g., phytoplankton, zooplankton, and benthic invertebrates), it is not necessary to conduct numerical integration as steady-state concentrations are reached quickly. As a result, the steady-state model is adequate. This approach greatly reduces computation time.

The time-dependent food-web bioaccumulation model was developed as a spreadsheet model in Microsoft Excel. The calculations of model parameters and time-dependent concentrations were performed within the spreadsheets.

Model parameterization

The aquatic time-dependent food-web bioaccumulation model were parameterized for specific PMUs (i.e., Emeryville Crescent, San Leandro Bay, and Steinberger Slough/Redwood Creek Complex) and the larger San Francisco Bay. Two types of input parameters are required to perform model calculations, including chemical (i.e., PCB congener) specific parameters and ecosystem related parameters.

The chemical specific input parameters include congener-specific chemical properties and biotransformation rate constants (k_M). The congener-specific chemical properties characterize the partitioning affinity of the PCB congener for binding to organic matters (e.g., lipids and organic carbon). These parameters include the logarithm of the octanol-water partition coefficient ($\log K_{OW}$), the logarithm of the organic carbon-water partition coefficient ($\log K_{OC}$), and the disequilibrium factors for particulate organic carbon (POC) partitioning (D_{POC} ; unitless) and for dissolved organic carbon (DOC) partitioning (D_{DOC} ; unitless). The D_{POC} and D_{DOC} are associated with the estimation of freely dissolved fraction of the total chemical concentration in the overlying water (ϕ), as described in Appendix A. In the present study, the $\log K_{OW}$ values of modeled PCB congeners were adjusted for temperature and salinity; the $\log K_{OC}$ values were estimated from the $\log K_{OW}$ values (Table B-1 in Appendix B). The model is meant to run based on concentrations of PCBs congeners in water and sediments that are provided by an independent PCB environmental fate model. This approach avoids the need for estimating D_{DOC} and D_{POC} . However, at the time of writing of this report, the PCB environmental fate model has not been fully developed. Hence, values for D_{DOC} and D_{POC} needed to be assumed and were assumed to be 1 (i.e., assuming that disequilibrium for PCB concentrations between POC or DOC in water and particulate matter is negligible). The biotransformation rates of all modeled PCB congeners in all modeled species were assumed to be negligible (i.e., $k_M = 0$).

Ecosystem related input parameters include biotic and abiotic components. The biotic input parameters include the wet weight of the organism (W_B ; kg wet wt), the contents of lipids (v_{LB} ; unitless), non-lipid organic matter (v_{NB} ; unitless), and water (v_{WB} ; unitless) of the organism, the fractions of the respiratory ventilation of the organism that involves overlying water (m_O ; unitless) and sediment-associated porewater (m_P ; unitless), and the fraction of the diet composition (P_i for the diet item i ; unitless) of the organism. Note that the sum of v_{LB} , v_{NB} , and v_{WB} approximates 1; the sum of m_O and m_P approximates 1; and the sum of P_i approximates 1. The abiotic input parameters include water temperature (T_W ; °C), the concentrations of dissolved oxygen (DO; mg/L) and suspended solids (SS; kg/L) in water, the concentrations of POC (χ_{POC} ; kg/L) and DOC (χ_{DOC} ; kg/L) in water, and the organic carbon content in sediments ($\phi_{OC,S}$; kg/kg dry wt). If freely dissolved PCB congener concentrations in sediment-associated porewater and overlying water are readily available as input values (e.g., when PCB congener concentration in water and sediments are measured using passive sampling techniques), some input parameters (e.g., POC, DOC, and OC) are not required for model calculations as the model calculations are used to calculate freely dissolved concentrations from bulk concentration measurements. Recent studies in San Francisco Bay have used passive sampling techniques for measurements of concentration of PCBs in water and sediments. Where such measurements were available, the model used the measurements of the freely dissolved concentrations of PCBs in water and sediments as input parameters, hence by-passing some of the calculations for assessing freely dissolved concentrations in water and sediments. The input parameters for the 3 PMU models and the larger San Francisco Bay model are summarized in Appendix B.

Model testing and performance evaluation

The food-web bioaccumulation model was tested and evaluated for two PMUs (i.e., San Leandro Bay and Steinberger Slough/Redwood Creek Complex) and the larger San Francisco Bay. For these two PMUs, both measured concentrations of PCB congeners in water, sediments and fish species of interest were available. For the Emeryville PMU there was insufficient data for model testing. Model testing involved calculating concentrations of PCBs using measured concentrations of PCBs in water and sediments of the PMU, followed by a comparison of calculated and empirically observed concentrations of PCB congeners. An effort was made to focus the model testing on concentrations in water, sediments and biota measured at the same locations and time periods. Geospatial analysis using the QGIS Geographic Information System (Version 3.34) was performed to accomplish this. PCB congener concentrations measured within the “active” sediment layer (i.e., within top 10 cm) were used in model testing. These are sediments believed to be in exchange with the water column.

San Leandro Bay PMU model testing

At San Leandro Bay, fish sampling data used in model testing included shiner surfperch data collected in 2019 (Buzby et al. 2021) and 2016 (Davis et al. 2017b) and topsmelt data collected in 2016 (Davis et al. 2017b). The congener-specific PCB concentration data in shiner surfperch and topsmelt were downloaded from the San Francisco Estuary Institute (SFEI) Contaminant Data Display and Download (CD3) database. The geometric mean of composite samples and its standard error was calculated.

To compare model calculated and observed concentrations of PCBs in shiner surfperch collected in 2019, model calculation was performed using input values for measured PCB congener concentrations in sediments collected in 2016 (Davis et al. 2017b) and the dissolved concentrations of PCB congeners in the water column and sediment-associated porewater measured using passive sampling devices in 2021 (Cho et al. 2024). Figure 5 shows the sampling locations for shiner surfperch (2019), sediment (2016), and water (2021 passive sampling) for model testing at San Leandro Bay. Data from the sediment sampling site (site code: SLBsub1) and passive sampling site (site code: SLBsub1) near the only shiner surfperch sampling site in 2019 (site name: San Leandro Bay) were used in model testing. The measured congener-specific PCB concentration data in sediments were obtained from the SFEI CD3 database. Sediment samples were collected at 0.5 and 3 cm depths. Measured data were pooled across sampling depths for each congener to calculate the geometric mean value, representing the PCB congener concentration in the active sediment layer. The freely-dissolved concentrations of PCB congeners measured using passive sampling devices in the overlaying water (at 0.5 and 7.5 cm above the sediment-water interface) and sediment-associated porewater (at 0.5, 3, and 7.5 cm depth below the sediment-water interface) were obtained from Y.-M. Cho via personal communication. Data with duplicate sampling were pooled across sampling depths for each PCB congener and geometric means and their standard errors were calculated.

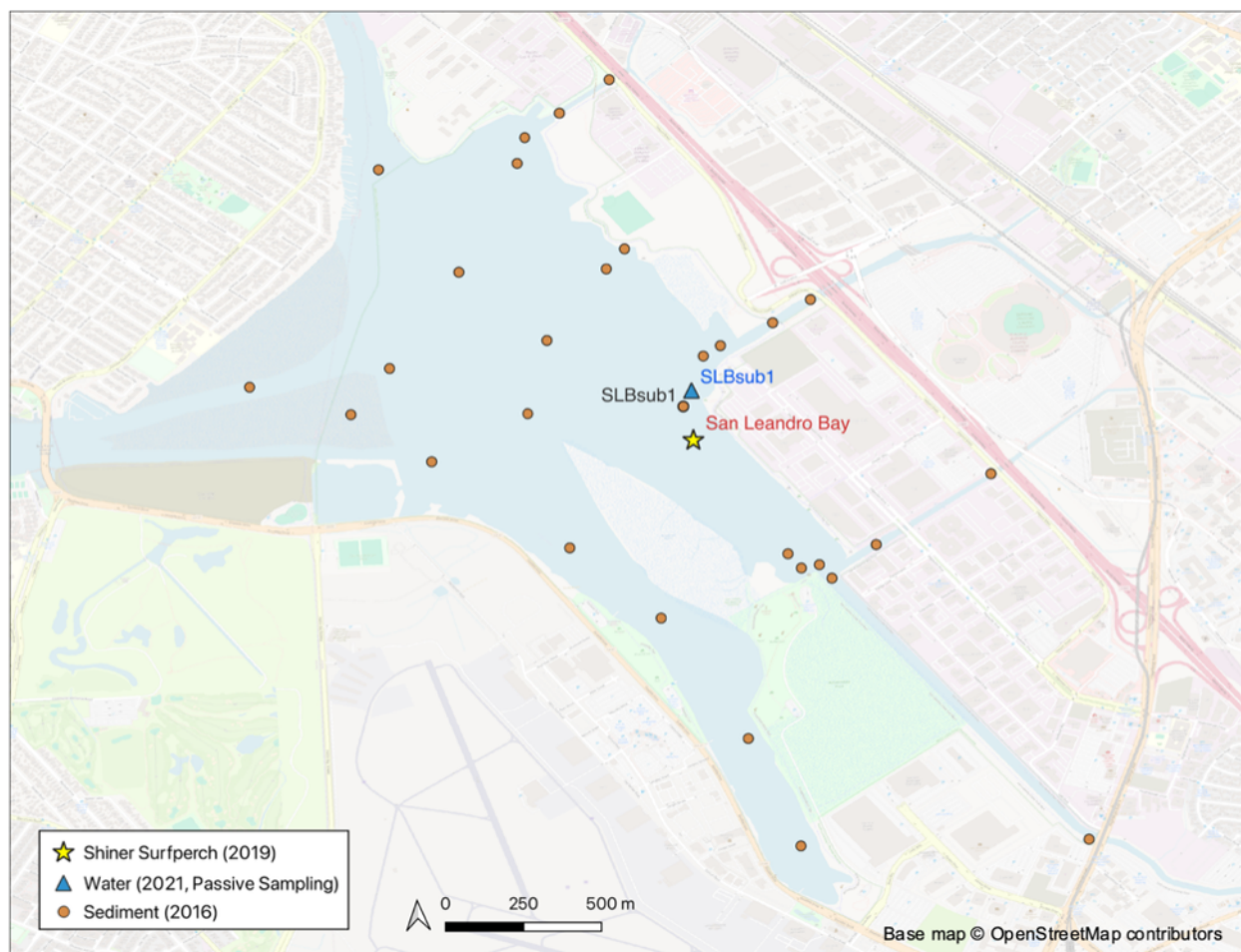


Figure 5. Sampling locations of shiner surfperch (2019 sampling), water (2021 passive sampling), and sediments (2016 sampling) for testing the San Leandro Bay PMU food-web bioaccumulation model.

To compare model calculated and observed concentrations of PCBs in shiner surfperch and topsmelt, model calculations were performed using measured concentrations of PCB congeners in sediments collected in 2016 (Davis et al. 2017b) and freely-dissolved concentrations of PCB congeners in the water column and sediment-associated porewater measured using passive sampling devices in 2016 (Cho et al. 2024). The measured congener-specific PCB concentration data in sediments (2016) were obtained from the SFEI CD3 database. The congener-specific, freely-dissolved PCB concentrations in water measured using passive sampling devices deployed in 2016 were obtained from Y.-M. Cho via personal communication.

The spatial locations of the sampling sites at San Leandro Bay for shiner surfperch (2016), sediments (2016), and water (2016 passive sampling) are shown in Figure 6. Shiner surfperch were collected at two locations (i.e., San Leandro Bay Main and Airport Lagoon) in 2016. For shiner surfperch sampled at San Leandro Bay Main, data from nearby sediment sampling sites (DSM20m, DSM100m, SLBsub1, SLCM100m, SLCM20m, and ELM20m) and passive sampling site (SLBsub1) were used in model testing. For shiner surfperch sampled at

Airport Lagoon, data from nearby sediment sampling sites (E8g and G4g) and passive sampling site (G4g) were used in model testing. Sediment samples were collected at 0.5 and 3 cm depth at sites DSM20m, SLBsub1, SLCM20m and ELM20m, and at 2.5 cm depth at sites DSM100m, SLCM100m, E8g, and G4g. The freely-dissolved concentrations of PCB congeners were sampled in duplicates in the overlaying water (at 0.5 and 7.5 cm above the sediment-water interface) and sediment-associated porewater (at 0.5, 3, and 7.5 cm depth below the sediment-water interface) using passive sampling devices. The measured data were pooled across sampling depths for each PCB congener. Geometric mean concentrations and their standard errors were calculated when multiple measurements were available.

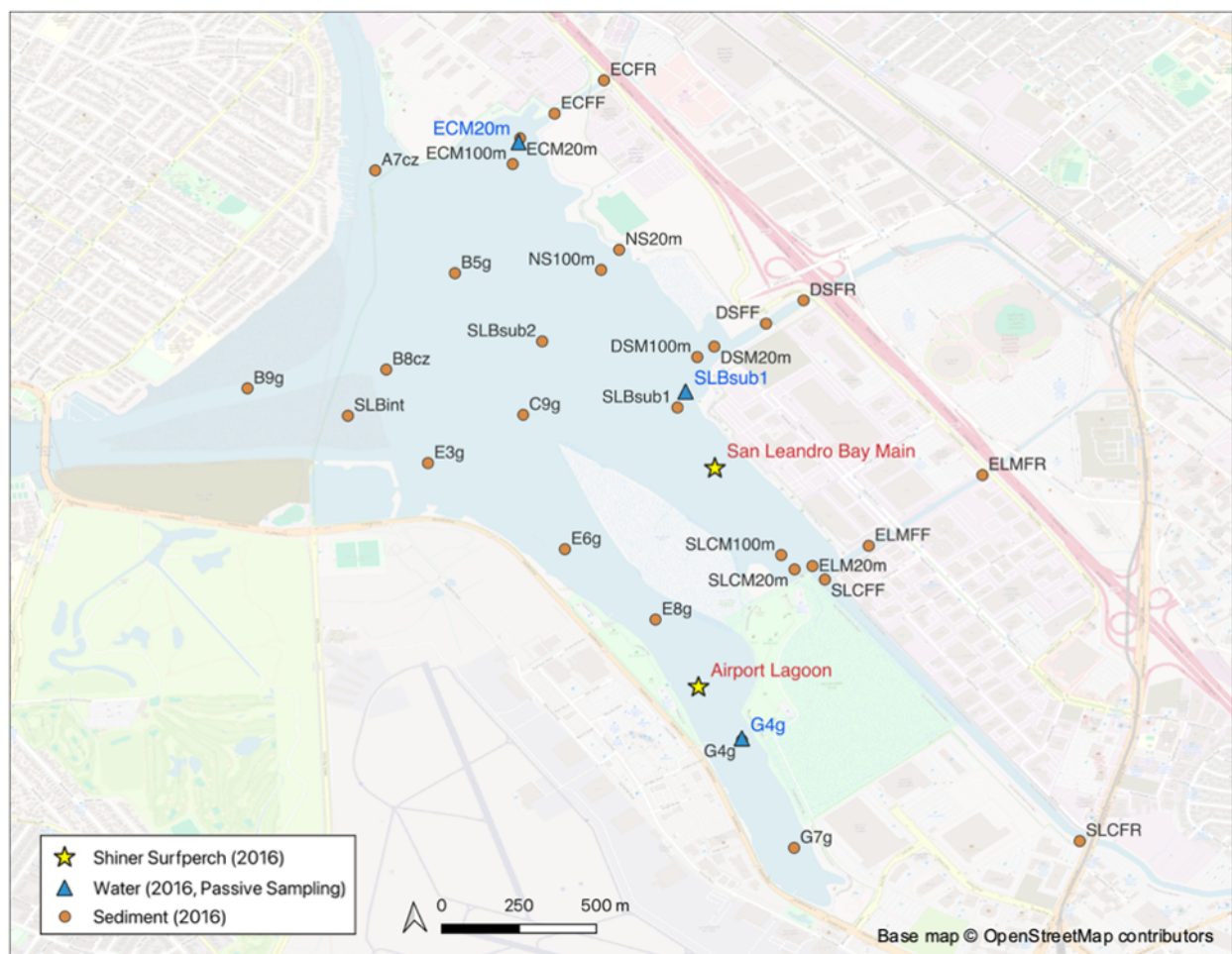


Figure 6. Sampling locations of shiner surfperch (2016 sampling), water (2016 passive sampling), and sediments (2016 sampling) for testing the San Leandro Bay PMU food-web bioaccumulation model.

The spatial locations of the sampling sites at San Leandro Bay for topsmelt (2016), sediments (2016), and water (2016 passive sampling) are shown in Figure 7. PCB concentration data for topsmelt collected from multiple locations (i.e., Damon Slough, Airport Lagoon, Alameda Channel, and East Creek) were used for model testing. For model testing of PCB concentrations in topsmelt sampled at Damon Slough, PCB concentration data from nearby

sediment sampling sites (DSFR and DSFF) and passive sampling site (SLBsub1) were used. For topsmelt sampled at Airport Lagoon, PCB concentration data from nearby sediment sampling sites (E8g and G4g) and passive sampling site (G4g) were used for model testing. For topsmelt sampled at Alameda Channel, PCB concentration data from nearby sediment sampling site (A7cz) and passive sampling site (ECM20m) were used for model testing. For topsmelt sampled at East Creek, PCB concentration data from nearby sediment sampling sites (ECFR and ECFF) and passive sampling site (ECM20m) were used. Sediment samples were collected at 0.5 and 3 cm depth at sites DSFF and ECFF and at 2.5 cm depth at sites DSFR, E8g, G4g, A7cz, and ECFR. The freely-dissolved concentrations of PCB congeners were sampled in duplicates in the overlaying water (at 0.5 and 7.5 cm above the sediment-water interface) and sediment-associated porewater (at 0.5, 3, and 7.5 cm depth below the sediment-water interface) using the passive sampling devices. The measured data were pooled across sampling depths for each PCB congener. Geometric mean concentrations and their standard errors were calculated when multiple measurements were available.

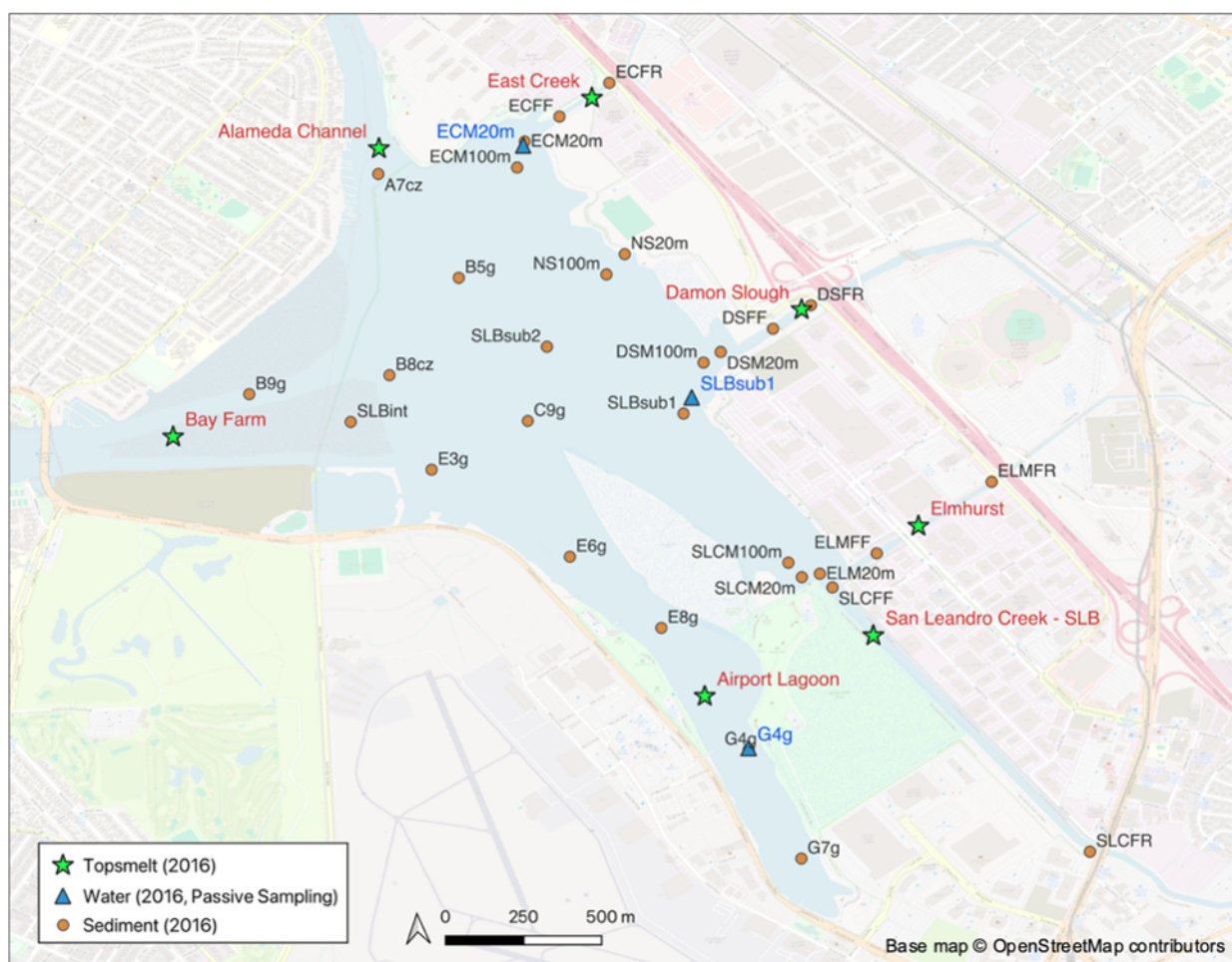


Figure 7. Sampling locations of topsmelt (2016 sampling), water (2016 passive sampling), and sediments (2016 sampling) for testing the San Leandro Bay PMU food-web bioaccumulation model.

The geometric mean measured concentrations of PCBs in sediments and the freely dissolved concentration of PCBs in the overlaying water and sediment-associated porewater were used as input values in the San Leandro Bay PMU food-web model to calculate the concentrations of PCB congeners in shiner surfperch and topsmelt. The input concentrations of PCB congeners in suspended solids were assumed to be the same as those in bottom sediments. Uncertainty in model-calculated concentrations of PCB congeners in shiner surfperch and topsmelt was estimated using the lower bound (i.e., the ratio of geometric mean and its standard error) and upper bound (i.e., the product of geometric mean and its standard error) input values for model calculations. Model bias values (MB in Equation 1 and MB* in Equation 2) were calculated to compare the model-calculated and observed PCB congener concentrations in fish for model performance evaluations.

Steinberger Slough/Redwood Creek Complex PMU model testing

For model testing at the Steinberger Slough/Redwood Creek Complex, we used measured PCB concentration data in (i) topsmelt collected in 2022; (ii) shiner surfperch collected in 2019 (Buzby et al. 2021); and white croaker collected in 2019 (Buzby et al. 2021). The congener-specific PCB concentration data in topsmelt collected in 2022 were obtained from J. A. Davis via personal communication. The congener-specific PCB concentration data in shiner surfperch and white croaker collected in 2019 were obtained from the SFEI CD3 database. Geometric mean concentrations for composite samples and corresponding standard errors were calculated.

The spatial locations of the sampling sites at Steinberger Slough/Redwood Creek Complex for topsmelt (2022) and sediments (2022) are shown in Figure 8. Topsmelt was collected at multiple locations (site codes: RCFSHLWR, RCFSHMID, RCFSHUP, SSFSHMID, and SSFSHUP) in 2022. The PCB concentrations in sediment data collected in 2022 were used for model testing. The sediment samples were collected at approximately 3-5 cm depth and the congener-specific PCB concentration data were obtained from J. A. Davis via personal communication. For topsmelt sampled at site RCFSHLWR, PCB concentrations in sediments from nearby sampling sites (RCWPTC and RCPTLD) were used for model testing. For topsmelt sampled at site RCFSHMID, measured PCB concentration data in sediments from nearby sampling site (RCMRNA) were used. For topsmelt sampled at site RCFSHUP, measured PCB concentrations in sediments from nearby sampling site (RCDKTB) were used for model testing. For topsmelt sampled at site SSFSHMID, measured PCB concentrations in sediments from nearby sampling site (SSFIRE) were used for model testing. For topsmelt sampled at site SSFSHUP, measured PCB concentrations in sediments from nearby sampling sites (SSPOND and BAIRIN) were used.

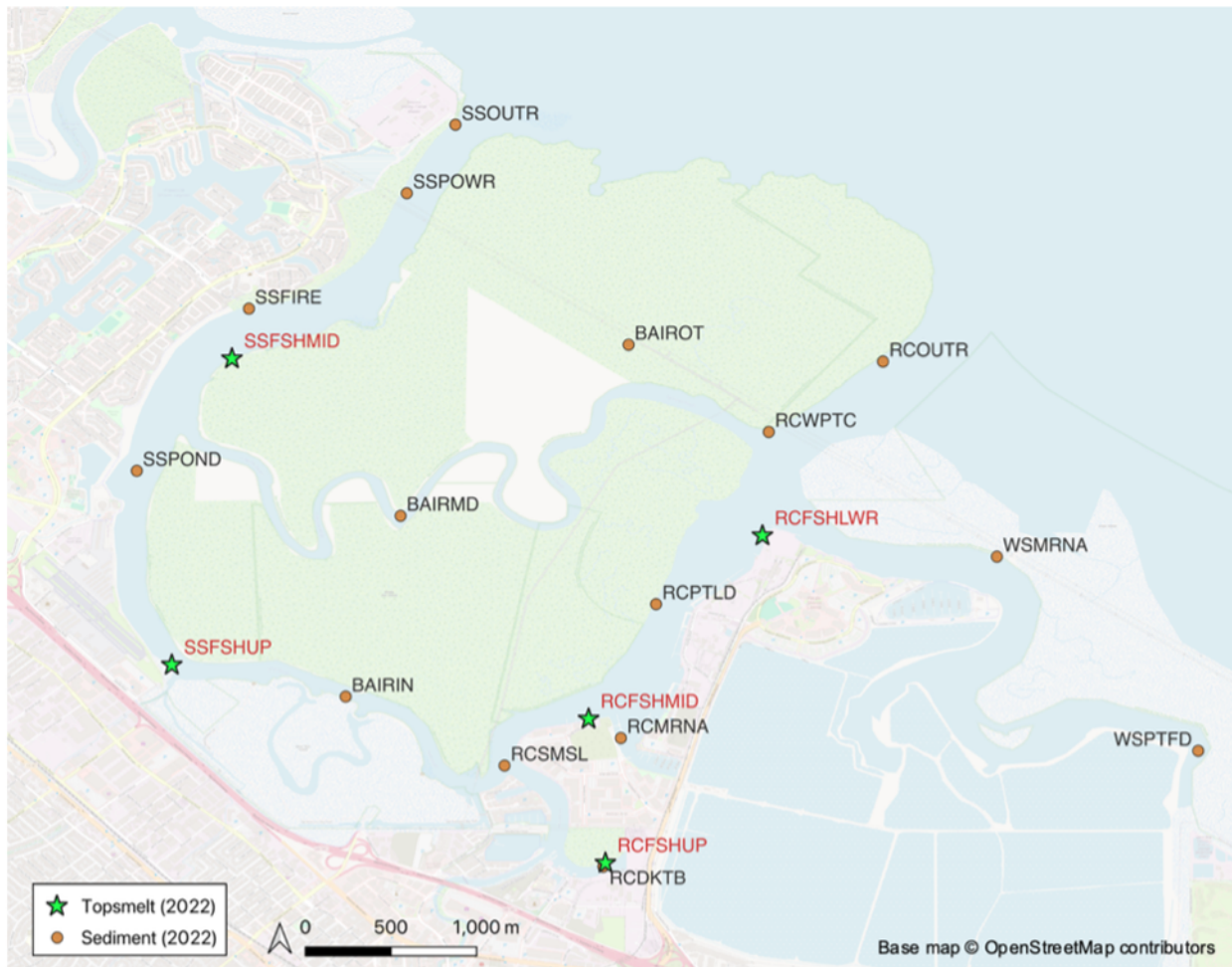


Figure 8. Sampling locations of topsmelt (2022 sampling) and sediments (2022 sampling) for testing the Steinberger Slough/Redwood Creek Complex PMU food-web bioaccumulation model.

For model testing at Steinberger Slough/Redwood Creek Complex using observed shiner surfperch and white croaker data, the sampling locations for shiner surfperch (collected in 2019) and sediments (collected in 2022) are shown in Figure 9, and the sampling locations for white croaker (collected in 2019) and sediments (collected in 2022) are shown in Figure 10. For both fish species, only one sampling site (i.e., South Bay) was involved in the 2019 sampling. The best available measured PCB concentration sediment data collected in 2022 from a nearby sampling site (RCPTLD) were used for model testing. The sediment samples were collected at approximately 3-5 cm depth and the congener-specific PCB concentration data were obtained from J. A. Davis via personal communication.

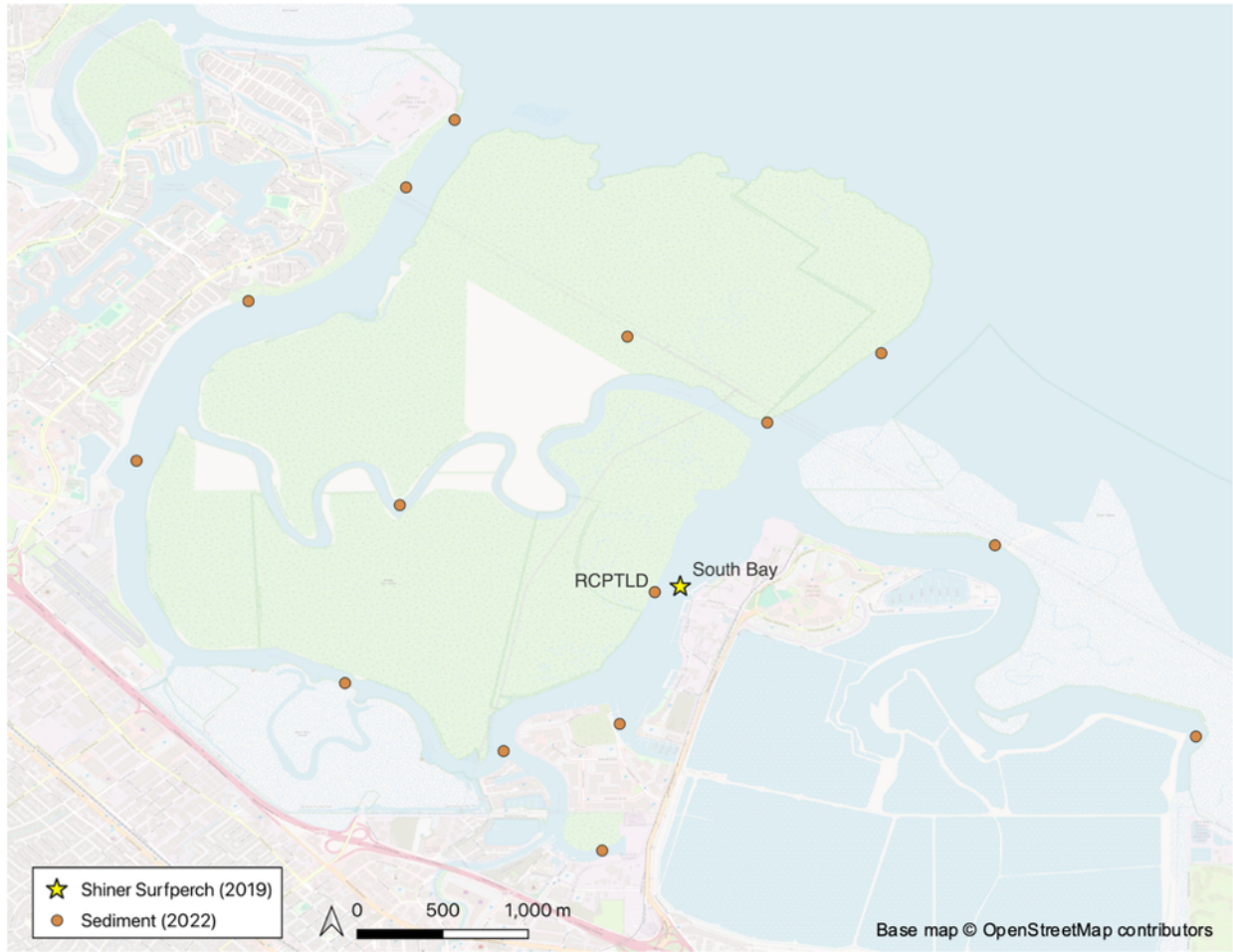


Figure 9. Sampling locations of shiner surfperch (2019 sampling) and sediments (2022 sampling) for testing the Steinberger Slough/Redwood Creek Complex PMU food-web bioaccumulation model.

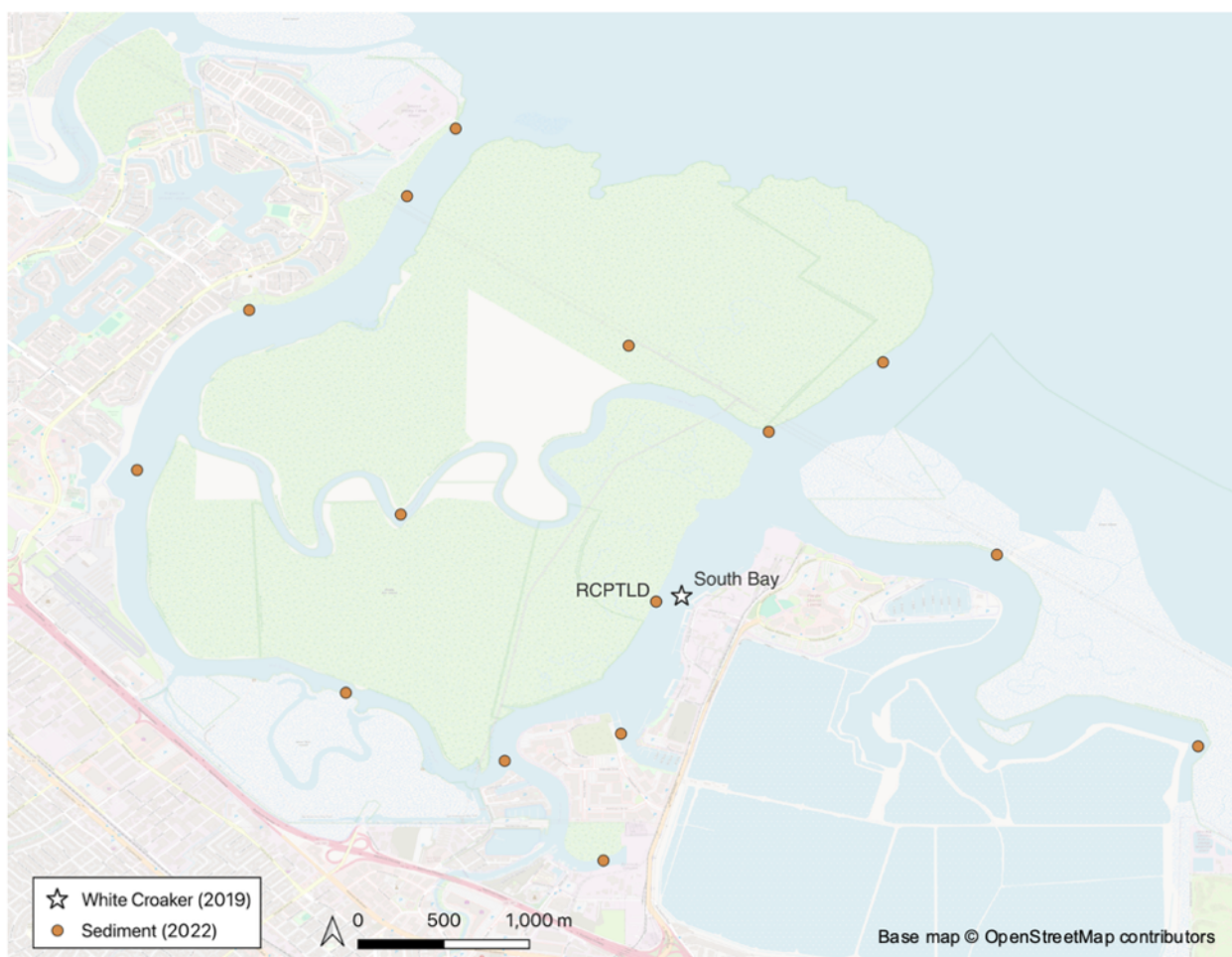


Figure 10. Sampling locations of white croaker (2019 sampling) and sediments (2022 sampling) for testing the Steinberger Slough/Redwood Creek Complex PMU food-web bioaccumulation model.

The geometric mean of measured PCB congener concentrations in sediments and their standard errors was calculated when multiple measurements were available. The geometric mean concentrations of PCB congeners in sediments were used as input values to calculate the concentrations of PCB congeners in topsmelt, shiner surfperch, and white croaker using the Steinberger Slough/Redwood Creek Complex PMU model. The input values for dissolved PCB congener concentrations in the sediment-associated porewater were estimated from measured PCB concentrations in sediments (using Equation 4). The input values of dissolved PCB congener concentrations in the overlaying water were assumed to be the same as those in the sediment-associated porewater, and the input concentrations of PCB congeners in suspended solids were assumed to be the same as those in sediments. Uncertainty in the concentrations of PCB congeners in fish was estimated using the lower bound (i.e., the ratio of geometric mean and its standard error) and upper bound (i.e., the product of geometric mean and its standard error) input values for model calculations if multiple measurement data were available. Model bias values (MB in Equation 1 and MB* in Equation 2) were calculated to compare model-calculated and observed PCB congener concentrations for model performance evaluation.

San Francisco Bay model testing

The testing of the food-web model for the entire San Francisco Bay is challenging as there is no good spatial and temporal overlap of concentrations of PCBs in water, sediments and fish. Also, available data for model testing are concentrated in “hotspots” and do not provide a means to correctly assess concentrations of PCBs in sediments, water and fish on a whole Bay basis. The geographical distribution of measured PCB concentration data is therefore not suitable for the method of model testing that is applied to the PMUs. For this reason, we determined the range of PCB concentrations in water, sediments and several fish species. The range of concentrations is the spread of concentrations between the lowest and highest concentrations measured. The lowest and highest concentrations of PCBs in water and sediments were then used by the model to calculate the lowest and highest concentration of PCBs in fish. The model-calculated range of concentrations of PCBs in various fish species were then compared to the range of observed PCB concentrations in the same fish species. The goal of the test is to determine if the model is able to predict the range of concentrations of PCBs in fish that is actually observed in the Bay.

The observed data of PCB congener concentrations in shiner surfperch and white croaker collected in 2019 (Buzby et al. 2021) were used for testing the larger San Francisco Bay food-web bioaccumulation model. Measured PCB congener concentrations in sediments collected in 2018 and in water (total concentration) collected in 2011 were identified as the best available data for model testing. The congener-specific PCB concentration data measured in sediments, water, and fish tissues were obtained from the SFEI CD3 database. Figure 11 shows the sampling locations of shiner surfperch (6 sites), sediments (20 sites), and water (14 sites) for model testing at San Francisco Bay. The sediment samples were collected at 5 cm depth in the active layer. The minimum and maximum values of the measured PCB congener concentrations in sediments and water were used as input values for the San Francisco Bay model. The input concentrations of PCB congeners in suspended sediments were assumed to be the same as those in sediments. Model-calculated concentrations of PCB congeners in shiner surfperch were compared to the range (i.e., minimum and maximum values) of the observed PCB congener concentrations in shiner surfperch for model evaluation. Figure 12 shows the sampling locations of white croaker (4 sites), sediments (20 sites), and water (14 sites) for model testing at San Francisco Bay. As the measured sediment and water data were shared for model testing with white croaker and shiner surfperch, the same input concentrations were used in both model tests. The model-calculated concentrations of PCB congeners in white croaker were compared to the range (i.e., minimum and maximum values) of observed PCB congener concentrations in white croaker for model evaluation.

Due to the lack of measured concentrations of PCB 74 and PCB 97 in shiner surfperch (2019), topsmelt (2022), white croaker (2019), and sediments (2016, 2018, and 2022), these two congeners were excluded from all model testing and performance analyses in the present study.

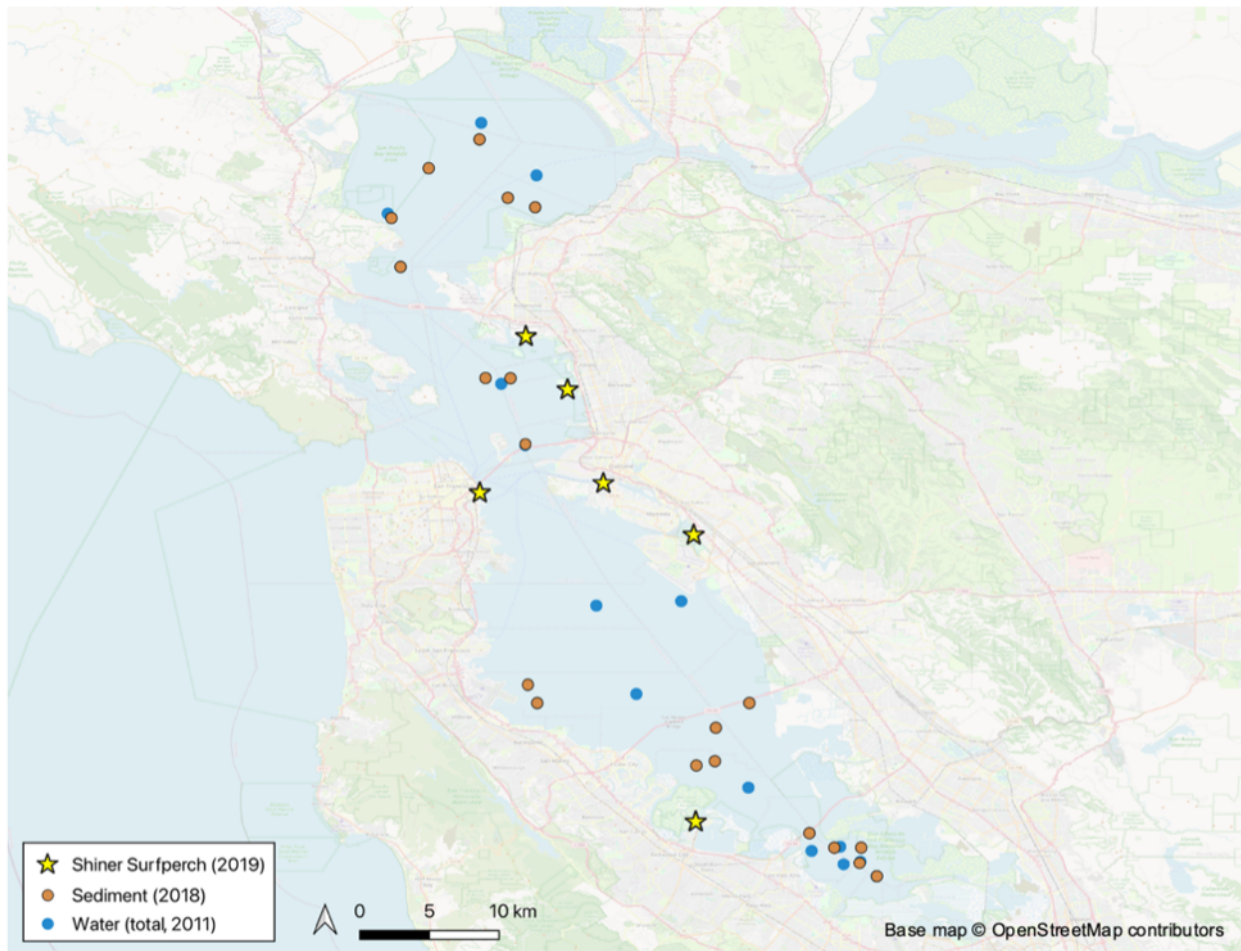


Figure 11. Sampling locations of shiner surfperch (2019 sampling), sediments (2018 sampling), and water (2011 sampling) for testing the San Francisco Bay food-web bioaccumulation model.

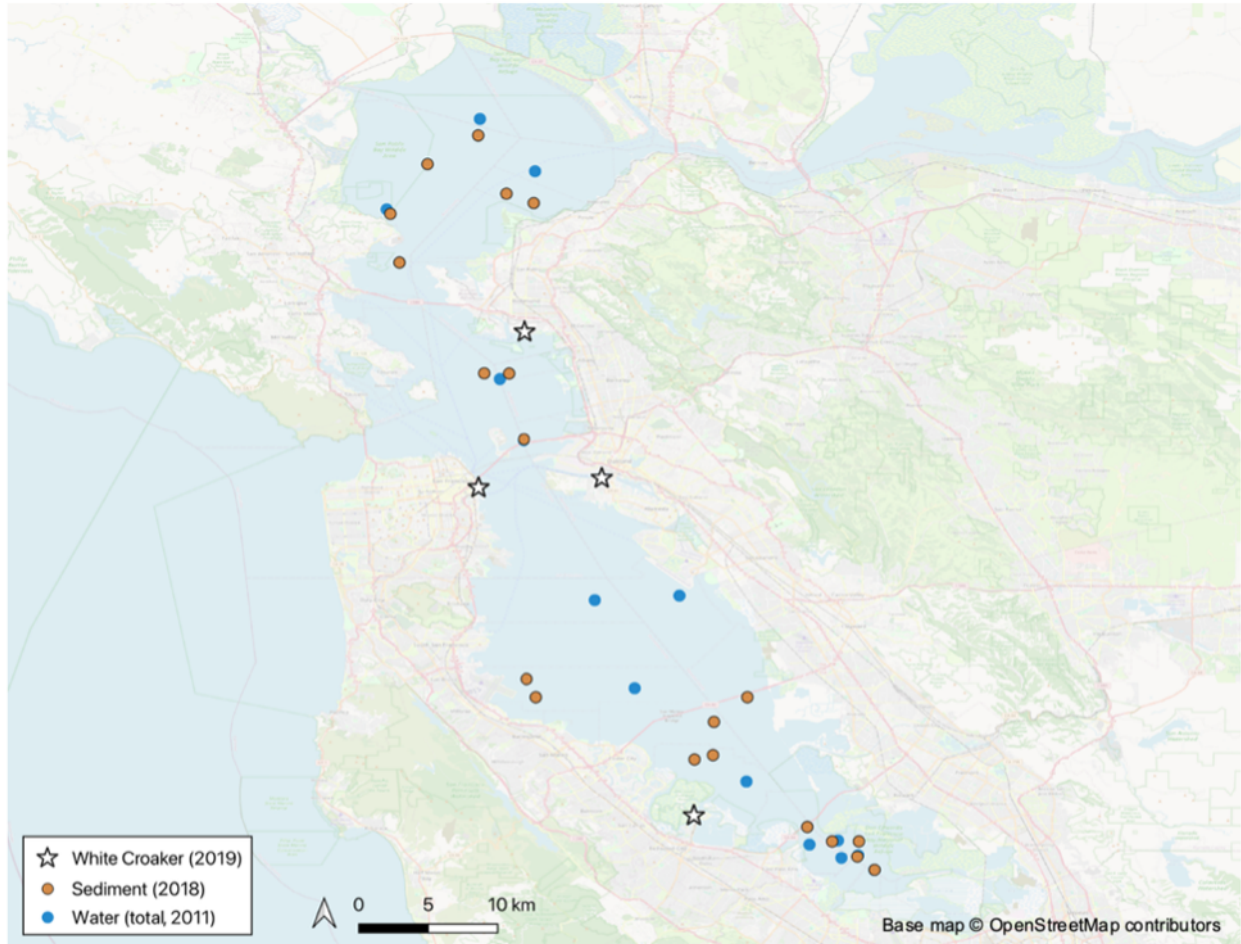


Figure 12. Sampling locations of white croaker (2019 sampling), sediments (2018 sampling), and water (2011 sampling) for testing the San Francisco Bay food-web bioaccumulation model.

Temporal response

The time-dependent trophic transfer model was applied to demonstrate the expected temporal changes in the concentrations of PCB congeners in fish in response to reductions in PCB concentrations in water and sediments (e.g., due to remediation efforts). The San Leandro Bay PMU model was used to illustrate the temporal response of the food-web to a hypothetical scenario where PCB congener concentrations in sediments and water fall immediately to drop to zero to simulate a clean environment scenario. To express the temporal response, we used the time to reach 95% of steady-state $t_{95\%}$, which mathematically is the inverse of the combined first order elimination rate constant of the PCB congener in fish times 3 (or 4.33 times the half-life time). It is the approximate time required for the PCB congener concentration to reach its new steady-state concentration after a change in the concentrations of the PCB congener in water and/or sediment. It is also the time for the concentration of the PCB congener to drop to 5% of its original concentration in a hypothetical scenario where the exposure concentrations of the PCB congener in water and sediment drop to zero instantaneously. It is important to note

that the $t_{95\%}$ is not the time required for the PCB concentrations in the fish to respond to changes in PCB loading. The $t_{95\%}$ only measures the response of the concentrations of PCBs in the fish to changes in the concentrations of PCBs in water and sediments and not to changes in inputs of PCBs into the PMUs. The response time of PCB concentration in fish to changes in inputs of PCBs to the PMU is longer than that due to the changes in PCB concentrations in water and sediments.

To illustrate the effect of time on the composition of PCBs in the fish, we also used the model to calculate the mass contribution of each PCB congener to the total mass of PCBs in the fish over time in response to an immediate decline in PCB concentrations in the sediments and water to zero. This approach illustrates the change in “*PCB fingerprints*” due to remediation. These *fingerprints* illustrate the change in the composition of PCBs and only reflect the contribution of the food-web to the compositional changes of the PCB mixtures in the fish. Differences in response times of the various PCB congener concentrations in water and sediments to changes in PCB loadings causes additional temporal changes in the composition of PCBs in the fish. A congener specific environmental fate model is able to calculate the change in PCB composition as a result of changes in PCB loadings.

Results and Discussion

Model testing and performance evaluation

San Leandro Bay PMU model

Figure 13 shows that model-calculated PCB congener concentrations in shiner surfperch were in good agreement with measured PCB congener concentrations in shiner surfperch collected in 2019 at San Leandro Bay. The calculated mean model bias (MB) for PCB congener concentrations was 0.939, with a 95% confidence interval (CI) ranging between 0.738 and 1.20. This suggests a slight but insignificant systematic underestimation of model-calculated concentrations of PCB congeners in fish. The mean model bias (MB*) value based on total PCB concentrations was calculated to be 1.00, indicating excellent overall agreement between model-calculated and observed concentrations. The 95% CI of the model calculations is equivalent to a factor of 1.28 or roughly 30%.

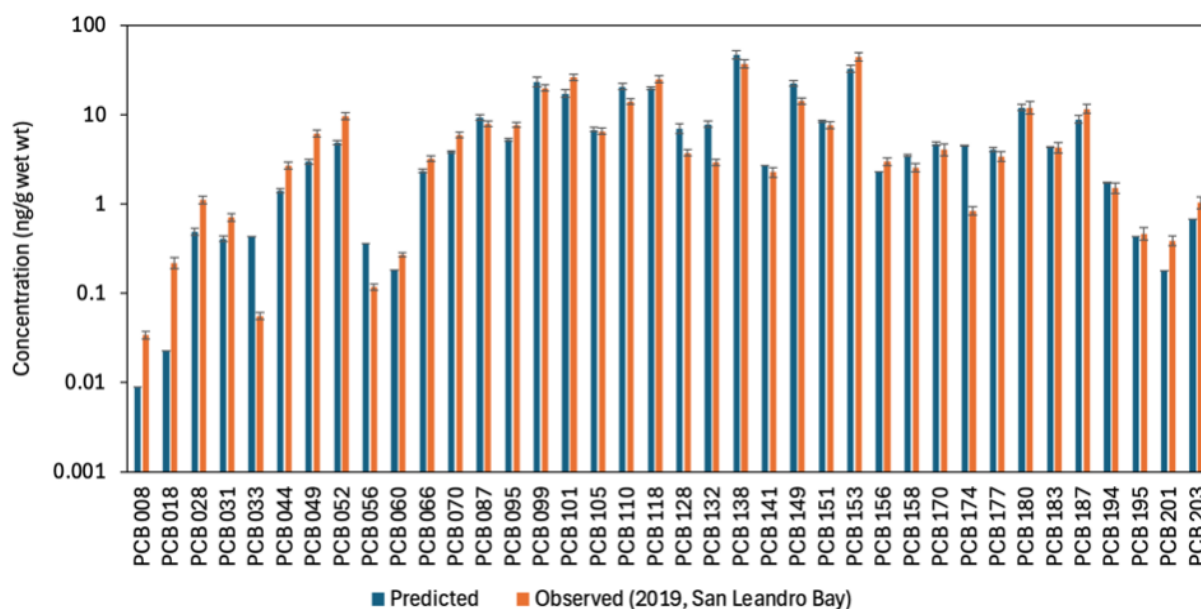


Figure 13. Geometric mean concentrations of PCB congeners in shiner surfperch calculated using the San Leandro Bay PMU food-web bioaccumulation model (blue bars) and observed in the 2019 at San Leandro Bay (red bars). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard error of the geometric mean of observed PCB concentrations in fish.

Model-calculated PCB congener concentrations in shiner surfperch were also in good agreement with measured PCB congener concentrations in shiner surfperch collected in 2016 at the sampling sites of San Leandro Bay Main (Figure 14) and Airport Lagoon (Figure 15). It is

important to stress here that there was a lack of measured data for certain PCB congeners especially for those with a lower molecular weight. At San Leandro Bay Main, the calculated mean model bias MB based for PCB congener concentrations was 1.47 (95% CI: 1.10–1.97), and the calculated model bias MB* based on total PCB concentrations was 1.52, indicating an approximate 50% systematic overestimation of PCB congener and Σ PCBs concentrations in fish by the model. The uncertainty of the mean model bias as expressed by the 95% CI is also approximately 50%. At Airport Lagoon, the calculated MB was 1.85 (95% CI: 1.37–2.50) and the calculated MB* was 1.98. The results suggest an overprediction of model calculations within a factor of 2.

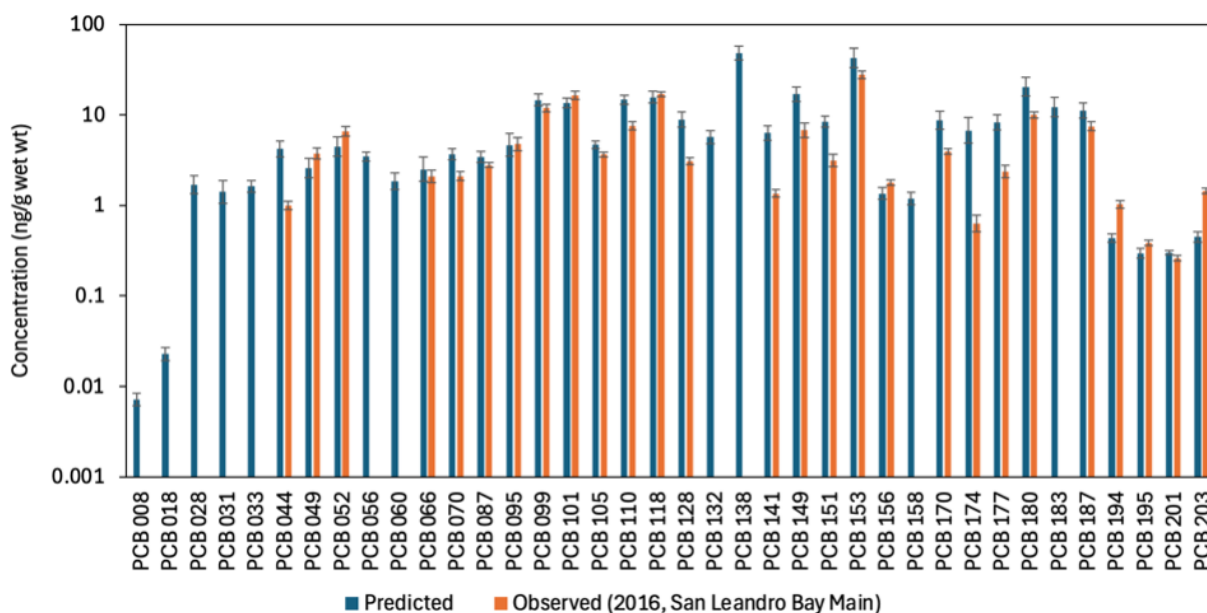


Figure 14. Geometric mean concentrations of PCB congeners in shiner surfperch calculated using the San Leandro Bay PMU food-web bioaccumulation model (blue bars) and observed in 2016 at the San Leandro Bay Main sampling site (red bars). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard error of the geometric mean of observed PCB concentrations in fish.

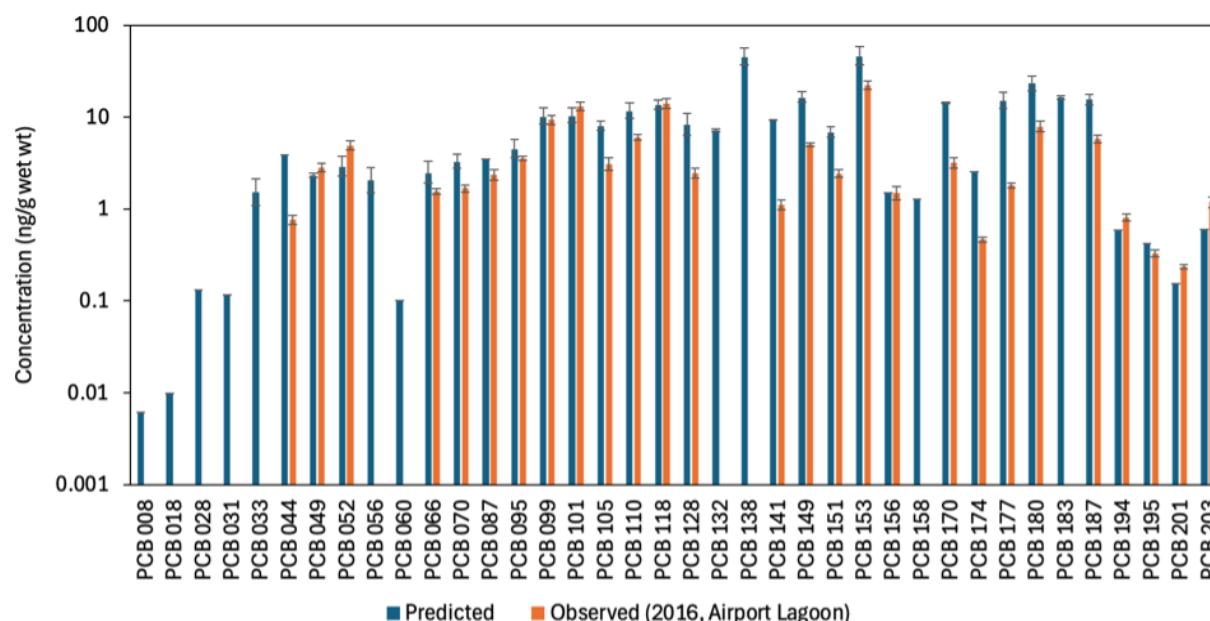
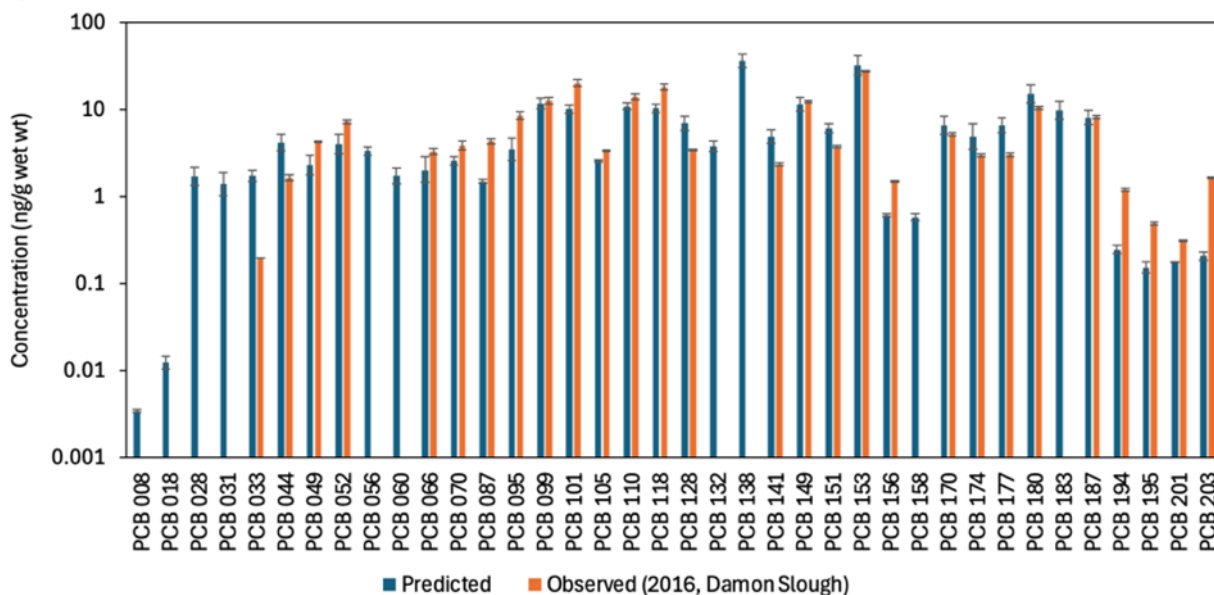


Figure 15. Geometric mean concentrations of PCB congeners in shiner surfperch calculated using the San Leandro Bay PMU food-web bioaccumulation model (blue bars) and observed in 2016 at the Airport Lagoon sampling site (red bars). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard error of the geometric mean of observed PCB concentrations in fish.

Figures 16A, 17A, 18A, and 19A illustrate the comparison of model-calculated and measured PCB congener concentrations in topsmelt collected in 2016 at the sampling sites of Damon Slough, Airport Lagoon, Alameda Channel, and East Creek, respectively. The model-calculated concentrations were generally in good agreement with the observed data at Damon Slough (Figure 16A), Airport Lagoon (Figure 17A), and Alameda Channel (Figure 18A), despite some relatively large discrepancies exhibited for certain PCB congeners. However, the model-calculated PCB concentrations in topsmelt were generally greater than those observed at East Creek (Figure 19A). The calculated mean model bias (MB) values based on PCB congener concentrations at Damon Slough, Airport Lagoon, Alameda Channel, and East Creek were 0.839 (95% CI: 0.601–1.14), 1.02 (95% CI: 0.732–1.43), 0.986 (95% CI: 0.555–1.75), and 2.04 (95% CI: 1.37–3.04), respectively. The calculated model bias (MB*) values based on total PCB concentrations at Damon Slough, Airport Lagoon, Alameda Channel, and East Creek were 0.921, 1.24, 1.46, and 2.31, respectively. The MB and MB* suggest a slight underprediction at Damon Slough and a slight overprediction at Airport Lagoon, but the difference between model predictions and field observations was not significant at both sites (95% CI of MB includes 1). At Alameda Channel, the calculated MB suggests a slight underprediction but the difference between predicted and observed concentrations was not significant (95% CI for MB includes 1), and the calculated MB* suggests an overprediction within a factor of 1.5. Note that the wider 95% CI of MB estimated at Alameda Channel compared to other sites indicates a greater

variability in observed PCB congener concentrations. At East Creek, both calculated MB and MB* suggest a 2 to 2.3 fold systematic overprediction of concentrations of PCBs in topsmelt.

(A)



(B)

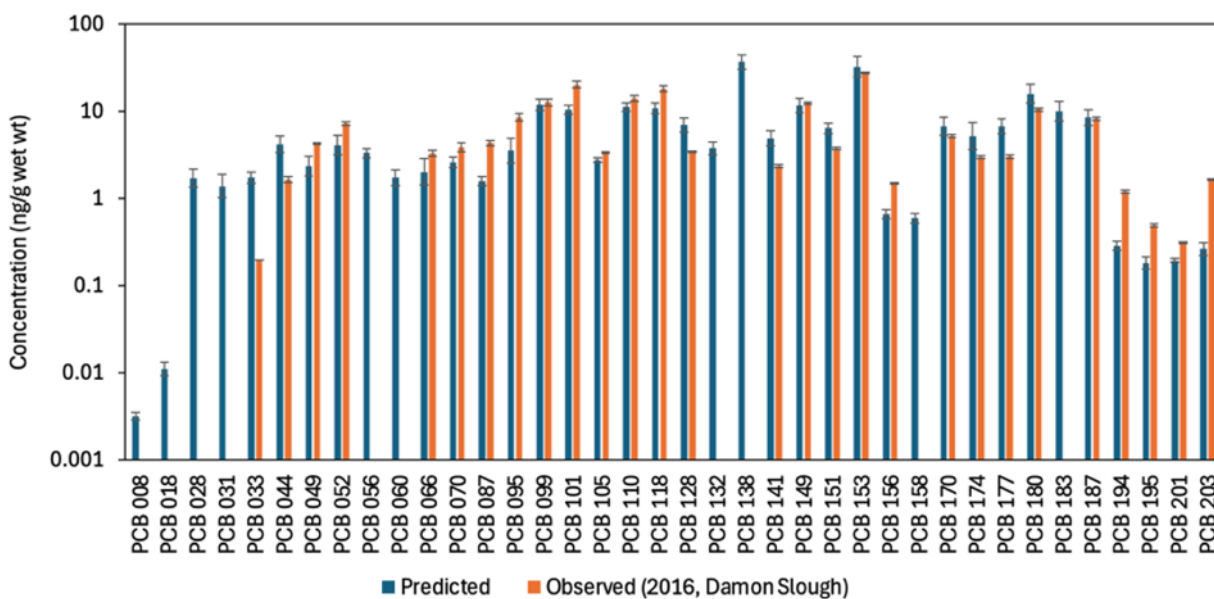


Figure 16. Geometric mean concentrations of PCB congeners in shiner surfperch calculated using the San Leandro Bay PMU food-web bioaccumulation model (blue bars) and observed in 2016 at the Damon Slough sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

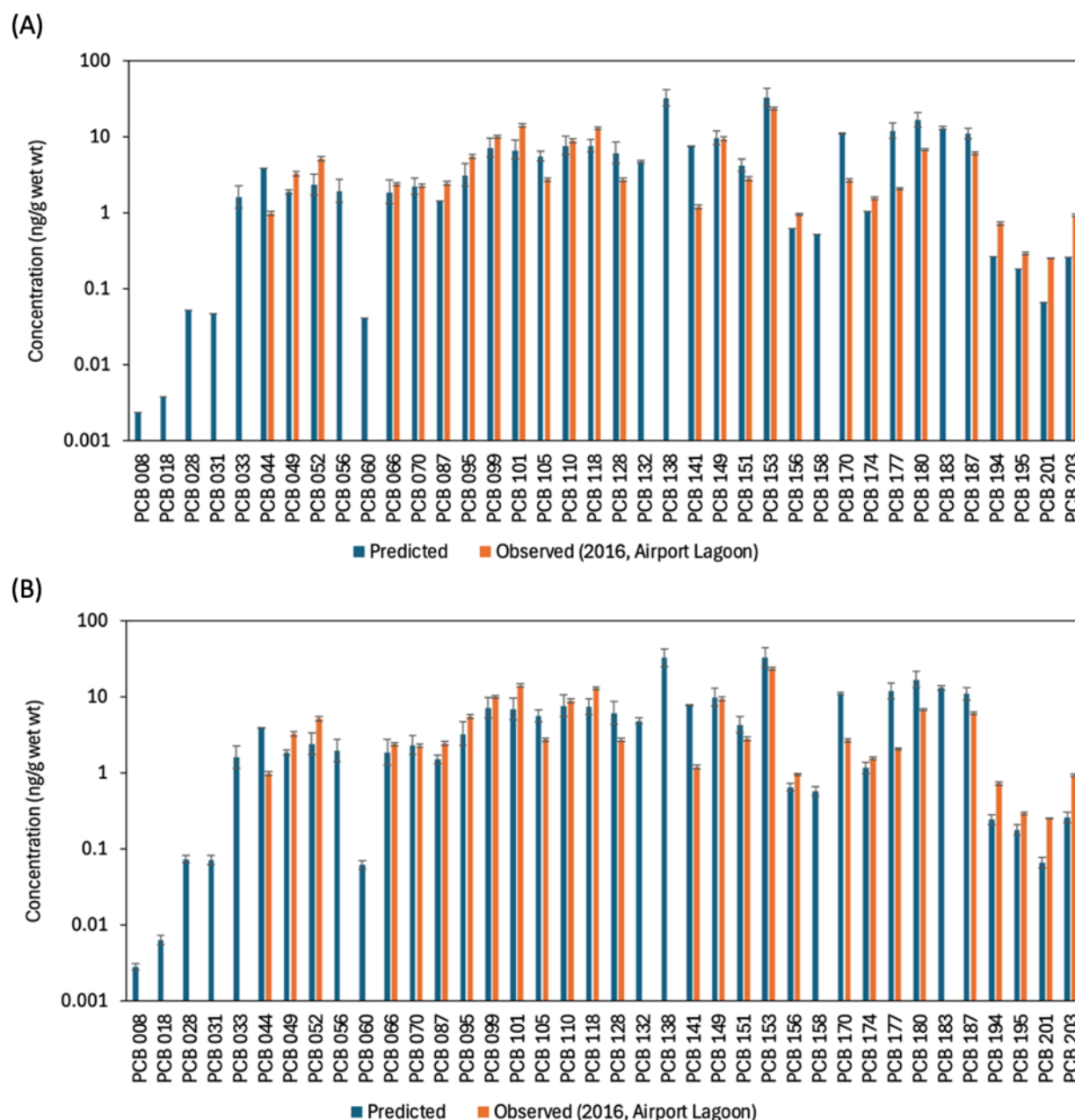


Figure 17. Geometric mean concentrations of PCB congeners in shiner surfperch calculated using the San Leandro Bay PMU food-web bioaccumulation model (blue bars) and observed in 2016 at the Airport Lagoon sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

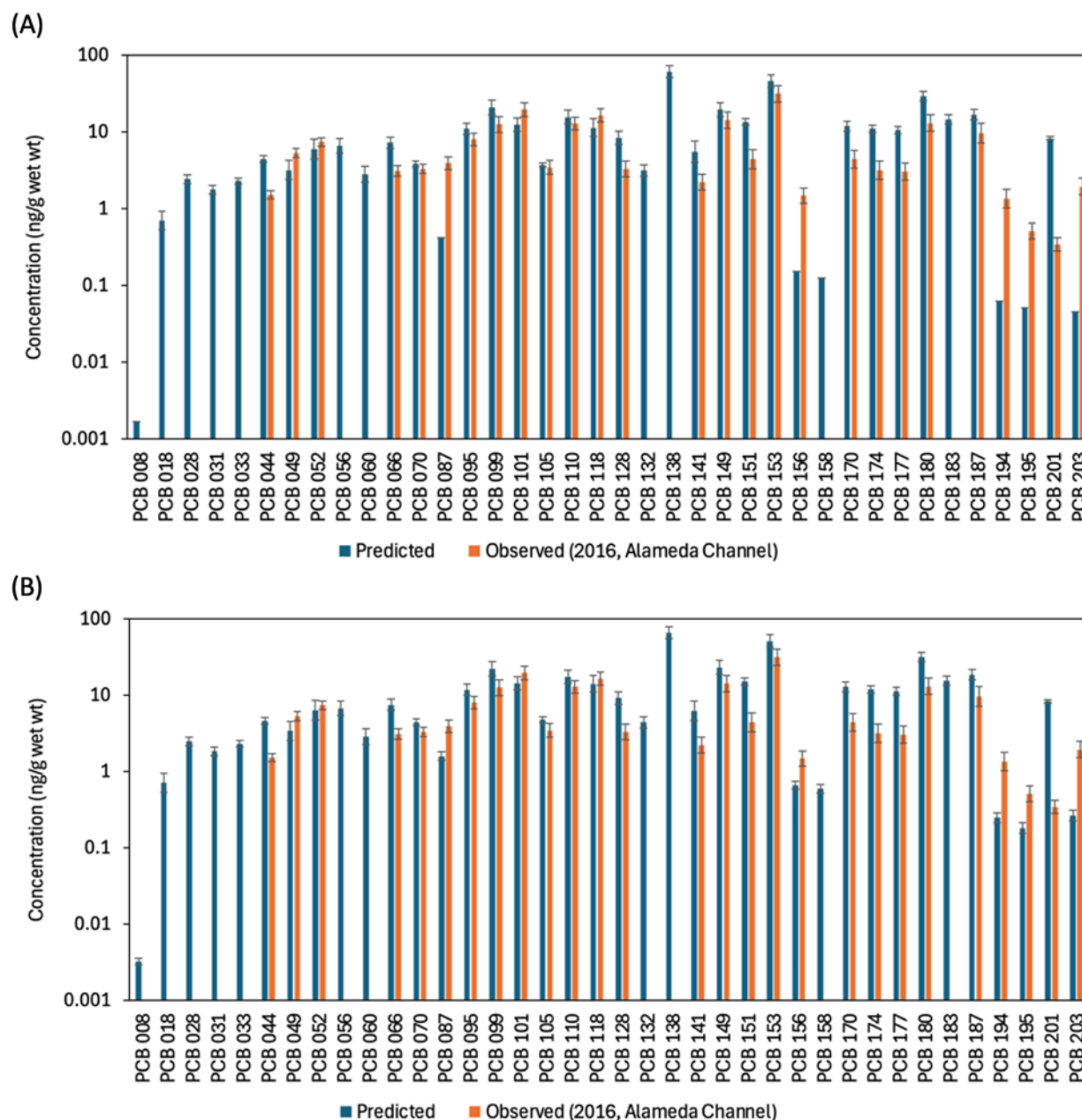


Figure 18. Geometric mean concentrations of PCB congeners in shiner surfperch calculated using the San Leandro Bay PMU food-web bioaccumulation model (blue bars) and observed in 2016 at the Alameda Channel sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

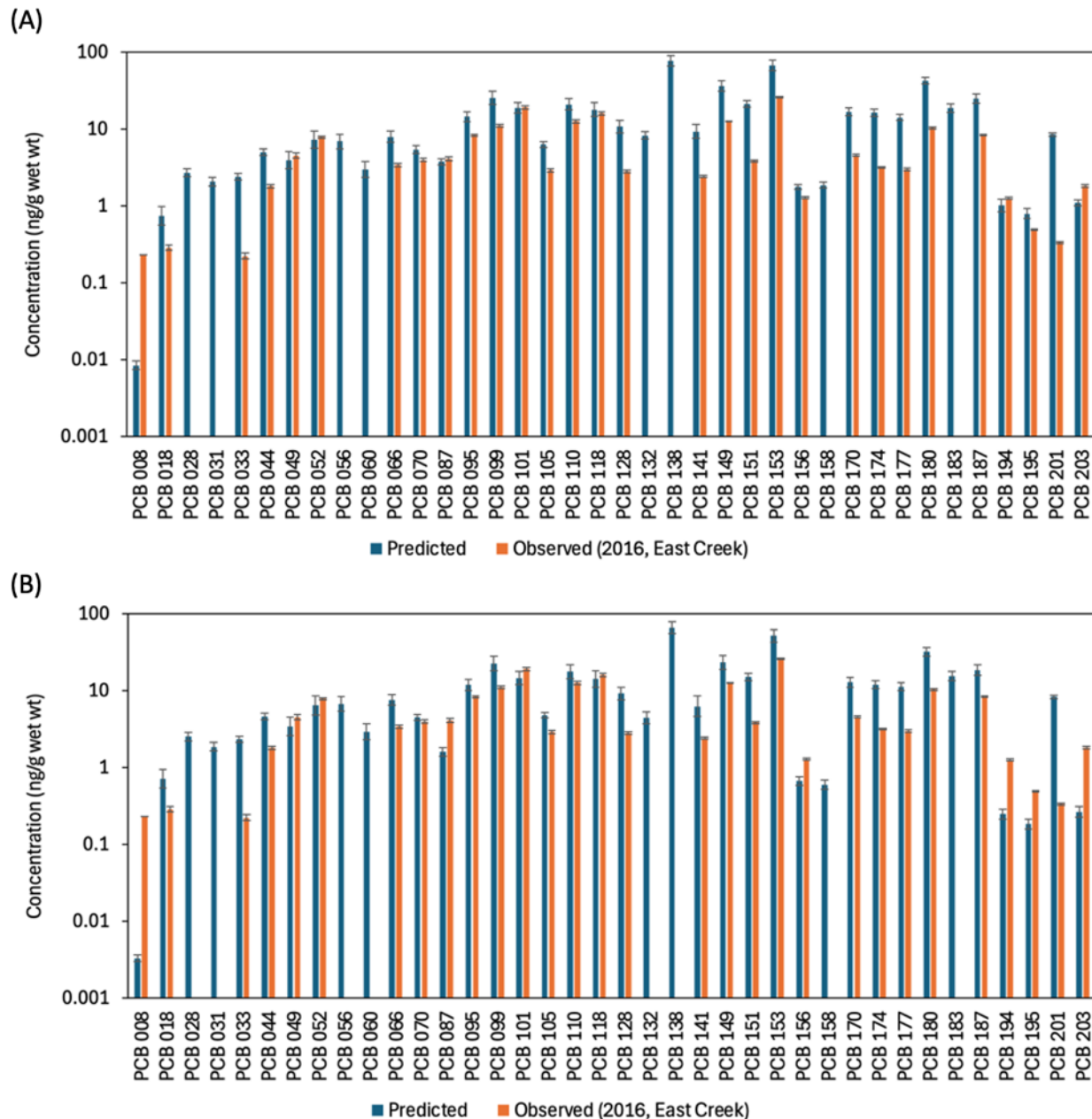


Figure 19. Geometric mean concentrations of PCB congeners in shiner surfperch calculated using the San Leandro Bay PMU food-web bioaccumulation model (blue bars) and observed in 2016 at the East Creek sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

It is important to note that a large spatial variation was observed in measured PCB concentrations in sediments collected in 2016 at San Leandro Bay, as shown in Figure C-1

(Appendix C) using PCB 153 as an example. Much higher sediment concentrations were observed near East Creek, which is located near the old industrial (General Electric) site known to be highly contaminated historically. Interestingly, the spatial variation in measured PCB concentrations in topsoil seemed to be smaller than that in sediments. This could explain the overprediction of PCB concentrations in fish at East Creek because of the high input concentrations of PCB congeners in sediments used in the model calculations. These findings suggest that the selection of sites is critical for model testing especially when a high spatial variation of measured concentrations is evident.

To investigate the significance of the high variation in measured PCB concentrations in sediments at some locations on model testing, we also conducted model calculations using PCB concentrations in sediments from all sampling sites in San Leandro Bay. The results are illustrated in Figures 16B, 17B, 18B, and 19B for Damon Slough, Airport Lagoon, Alameda Channel, and East Creek, respectively. The calculated mean model bias (MB) values based on PCB congener concentrations at Damon Slough, Airport Lagoon, Alameda Channel, and East Creek were 0.870 (95% CI: 0.639–1.18), 1.04 (95% CI: 0.741–1.45), 1.40 (95% CI: 0.936–2.09), and 1.37 (95% CI: 0.839–2.24), respectively. The calculated mean model bias (MB*) values based on total PCB concentrations at Damon Slough, Airport Lagoon, Alameda Channel, and East Creek were 0.945, 1.25, 1.63, and 1.78, respectively. These results indicate only minor improvements in model performance and suggest only minor impacts of the selection of spatial concentration data on the overall performance of the model in San Leandro Bay. On average, model predictions of PCB concentrations in fish are within a factor of 2. The results suggest that fish may occupy a foraging area that is larger than the area they were collected in and that environmental concentrations from a larger geographical area within the PMU can act as a reliable indicator of exposure of PCBs to fish. A summary of the results of model testing at San Leandro Bay are summarized in Table 1.

Table 1. Calculated mean model bias values (MB and MB) for model testing at San Leandro Bay. An MB or MB* of 1 indicate a lack of model bias and good agreement between model-calculated and observed concentrations of PCBs in fish.*

Fish species (sample year)	Fish site (sample year)	Water (passive sampling) site (sample year) ^a	Sediment site (sample year) ^a	MB (n) 95% CI ^b	MB* ^c
Shiner surfperch (2019)	San Leandro Bay (2019)	SLBsub1 (2021)	SLBsub1 (2016)	0.939 (38) 0.738–1.20	1.00
Shiner surfperch (2016)	San Leandro Bay Main (2016)	SLBsub1 (2016)	DSM20m, DSM100m, SLBsub1, SLCM100m, SLCM20m, ELM20m (2016)	1.47 (27) 1.10–1.97	1.52
	Airport Lagoon (2016)	G4g (2016)	E8g, G4g (2016)	1.85 (27) 1.37–2.50	1.98
Topsmelt (2016)	Damon Slough (2016)	SLBsub1 (2016)	DSFR, DSFF (2016)	0.839 (28) 0.601–1.14	0.921
			All stations (2016)	0.870 (28) 0.639–1.18	0.945
	Airport Lagoon (2016)	G4g (2016)	E8g, G4g (2016)	1.02 (27) 0.732–1.43	1.24
			All stations (2016)	1.04 (27) 0.741–1.45	1.25
	Alameda Channel (2016)	ECM20m (2016)	A7cz (2016)	0.986 (27) 0.555–1.75	1.46
			All stations (2016)	1.40 (27) 0.936–2.09	1.63
	East Creek (2016)	ECM20m (2016)	ECFR, ECFF (2016)	2.04 (30) 1.37–3.04	2.31
			All stations (2016)	1.37 (30) 0.839–2.24	1.78

^a The locations of sampling sites are shown in Figures 5–7.

^b Mean model bias MB determined based on PCB congener concentrations and calculated using Equation 1.

n = number of comparisons. 95% confidence interval (CI) = antilog (log MB ± [$t_{v,0.05}$ × standard deviation]).

^c Model bias MB* determined based on total PCB concentrations and calculated using Equation 2

Steinberger Slough/Redwood Creek Complex PMU model

Figures 20A, 21A, 22A, 23A, and 24A illustrate the model-calculated and measured PCB congener concentrations in topsmelt collected in 2022 at the sampling sites RCFSHLWR, RCFSHMID, RCFSHUP, SSFSHMID, and SSFSHUP, respectively. Three sampling sites (i.e., RCFSHLWR, RCFSHMID, and RCFSHUP) were located on the Redwood Creek side and two sampling sites (i.e., SSFSHMID and SSFSHUP) were located on the Steinberger Slough side of the Steinberger Slough/Redwood Creek Complex PMU (Figure 8). For sites RCFSHLWR (Figure 20A), RCFSHMID (Figure 21A), and SSFSHUP (Figure 24A), similar levels of model-calculated and measured PCB congener concentrations were obtained, but model-calculated concentrations seemed to be higher than the observed concentrations for lower molecular weight congeners. For sites RCFSHUP and SSFSHMID, model-calculated concentrations were higher than observed concentrations for all PCB congeners. The calculated mean model bias (MB) values based on PCB congener concentrations at sites RCFSHLWR, RCFSHMID, RCFSHUP, SSFSHMID, and SSFSHUP were 2.05 (95% CI: 1.55–2.70), 1.81 (95% CI: 1.46–2.24), 7.14 (95% CI: 5.74–8.88), 4.11 (95% CI: 3.26–5.17), and 1.56 (95% CI: 1.23–1.97), respectively. The calculated model bias (MB*) values

based on total PCB concentrations at sites RCFSHLWR, RCFSHMID, RCFSHUP, SSFSHMID, and SSFSHUP were 1.63, 1.53, 5.69, 3.04, and 1.15, respectively. The results suggest a minor overprediction of the concentrations of PCBs in fish, except for sites RCFSHUP and SSFSHMID where a greater overprediction was observed. This suggests that the fish collected from RCFSHUP and SSFSHMID may occupy areas that are larger than the areas where they were collected. As a result, we also used the geometric mean concentrations of PCB congeners in sediments collected from all sampling sites to further test the model. The results are illustrated in Figures 20B, 21B, 22B, 23B, and 24B for sites RCFSHLWR, RCFSHMID, RCFSHUP, SSFSHMID, and SSFSHUP, respectively. For sites RCFSHUP (Figure 22) and SSFSHMID (Figure 23), model-calculated concentrations of PCBs in fish derived using PCB concentrations in water and sediments from the larger PMU area were in better agreement with observed concentration data than those derived specifically from the RCFSHUP and SSFSHMID sampling sites where fish were collected. Using a broader geographical approach generated mean model bias (MB) values for PCB congener concentrations at sites RCFSHLWR, RCFSHMID, RCFSHUP, SSFSHMID, and SSFSHUP of 2.75 (95% CI: 2.19–3.47), 1.40 (95% CI: 1.17–1.66), 2.01 (95% CI: 1.64–2.45), 3.05 (95% CI: 2.29–4.08), and 2.32 (95% CI: 1.87–2.87), respectively. The calculated model bias (MB*) values based on total PCB concentrations at sites RCFSHLWR, RCFSHMID, RCFSHUP, SSFSHMID, and SSFSHUP were 2.12, 1.21, 1.68, 2.13, and 1.83, respectively. The calculated MB and MB* values for fish collected at sites RCFSHUP and SSFSHMID were reduced as a result of using a broader geographical approach and indicate an approximate 2-fold overprediction of the PCB concentrations in fish from these sites. Using all measured environmental concentration data collected in the entire PMU for model testing appeared to improve model performance for fish collected at “hot spots” within the PMU. This suggests that fish at this PMU track PCBs and other contaminants in the larger PMU.

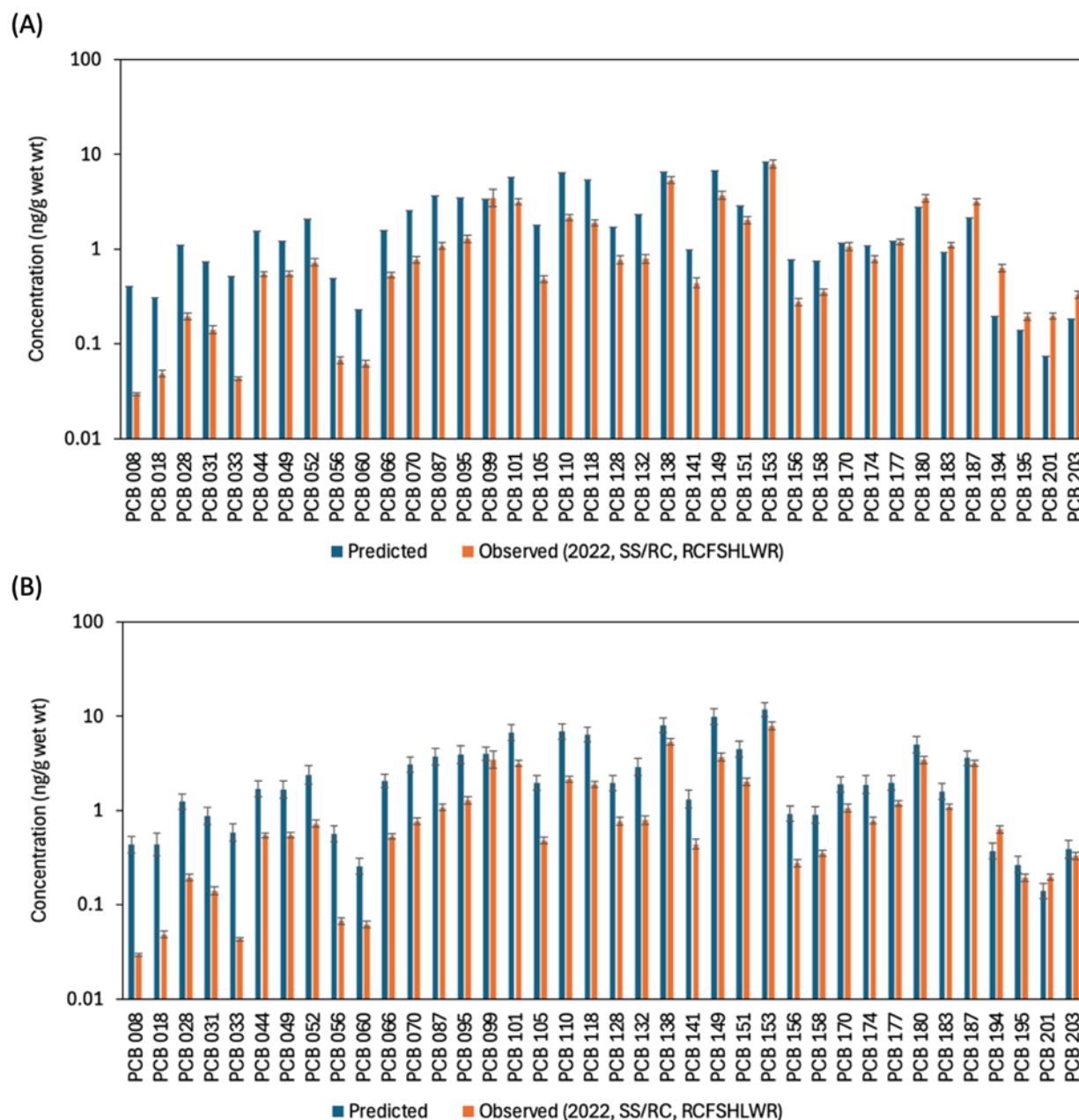


Figure 20. Geometric mean concentrations of PCB congeners in topsmelt calculated using the Steinberger Slough/Redwood Creek (SS/RC) PMU model (blue bars) and observed in 2022 at the RCFSHLWR sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

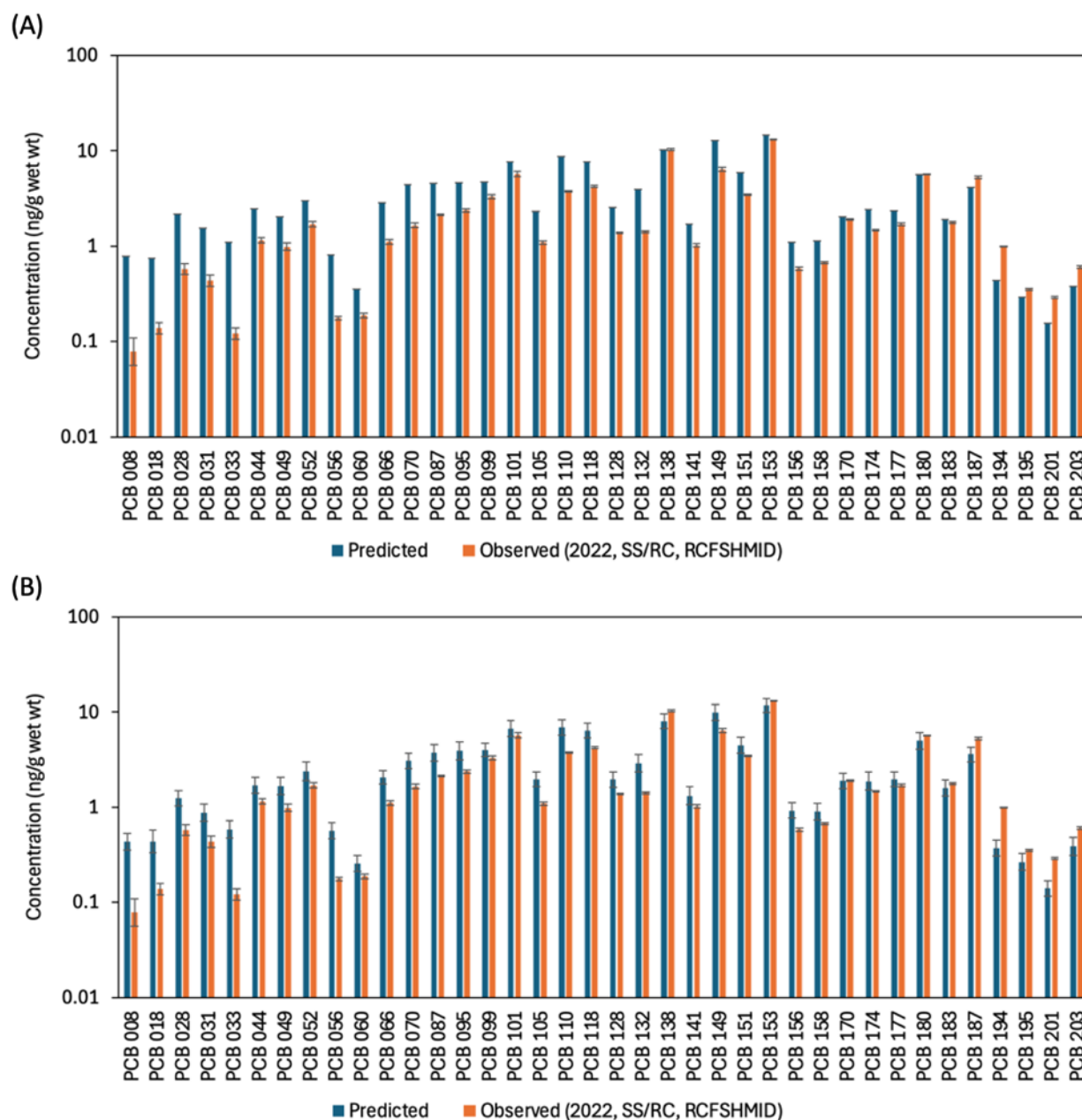


Figure 21. Geometric mean concentrations of PCB congeners in topsmelt calculated using the Steinberger Slough/Redwood Creek (SS/RC) PMU model (blue bars) and observed in 2022 at the RCFSHMID sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

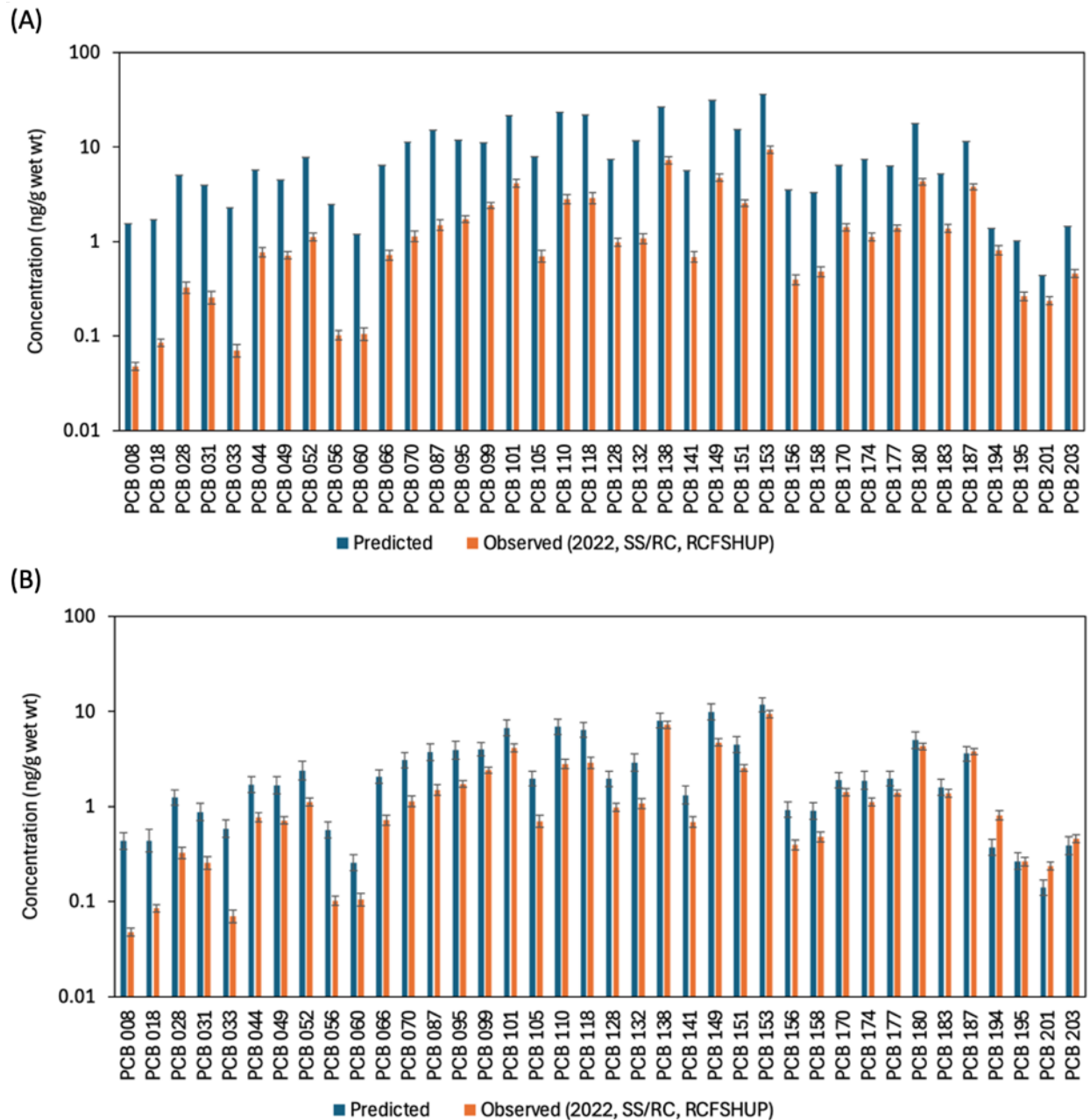


Figure 22. Geometric mean concentrations of PCB congeners in topsmelt calculated using the Steinberger Slough/Redwood Creek (SS/RC) PMU model (blue bars) and observed in 2022 at the RCFSHUP sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

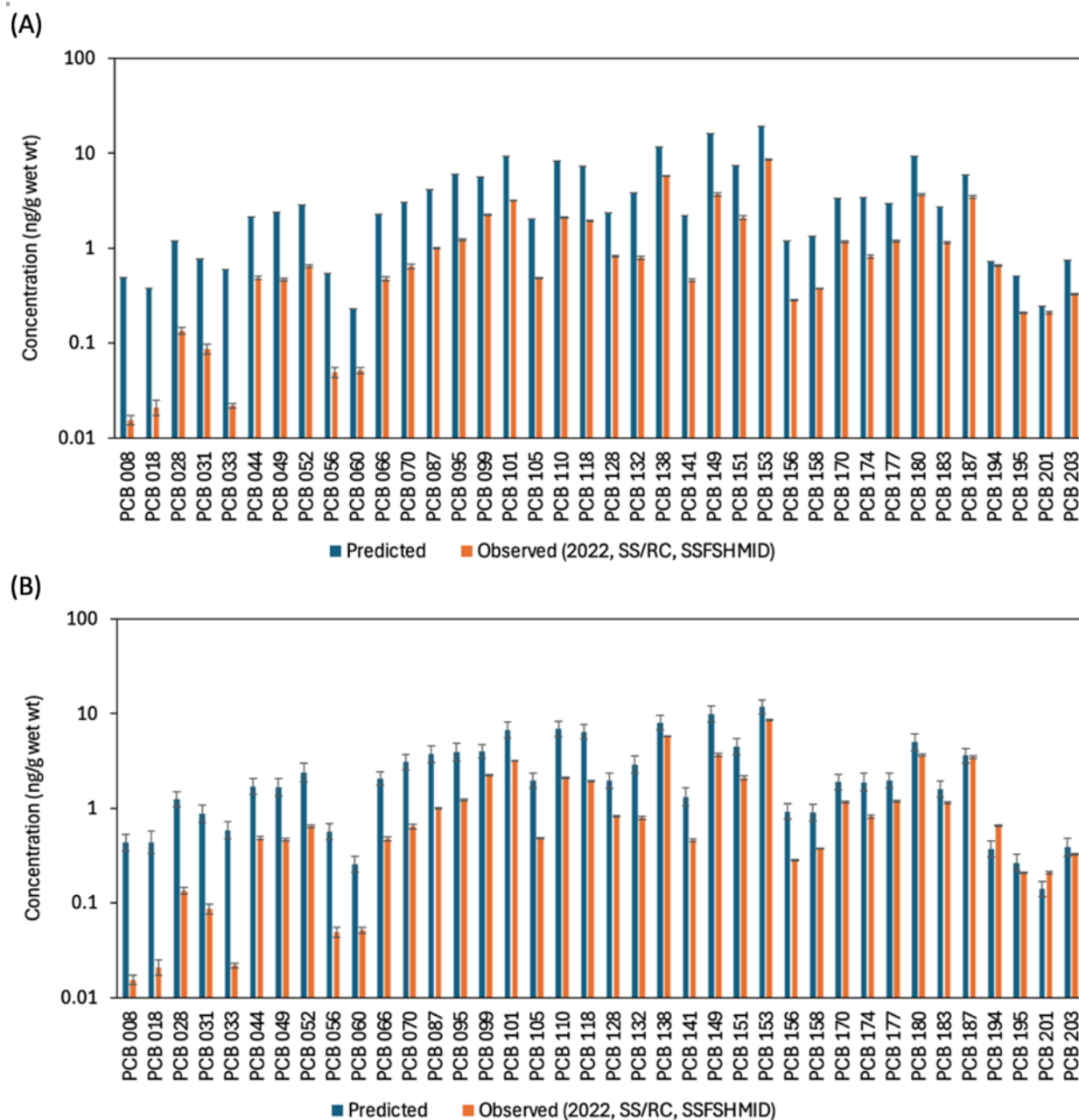


Figure 23. Geometric mean concentrations of PCB congeners in topsmelt calculated using the Steinberger Slough/Redwood Creek (SS/RC) PMU model (blue bars) and observed in 2022 at the SSFSHMID sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

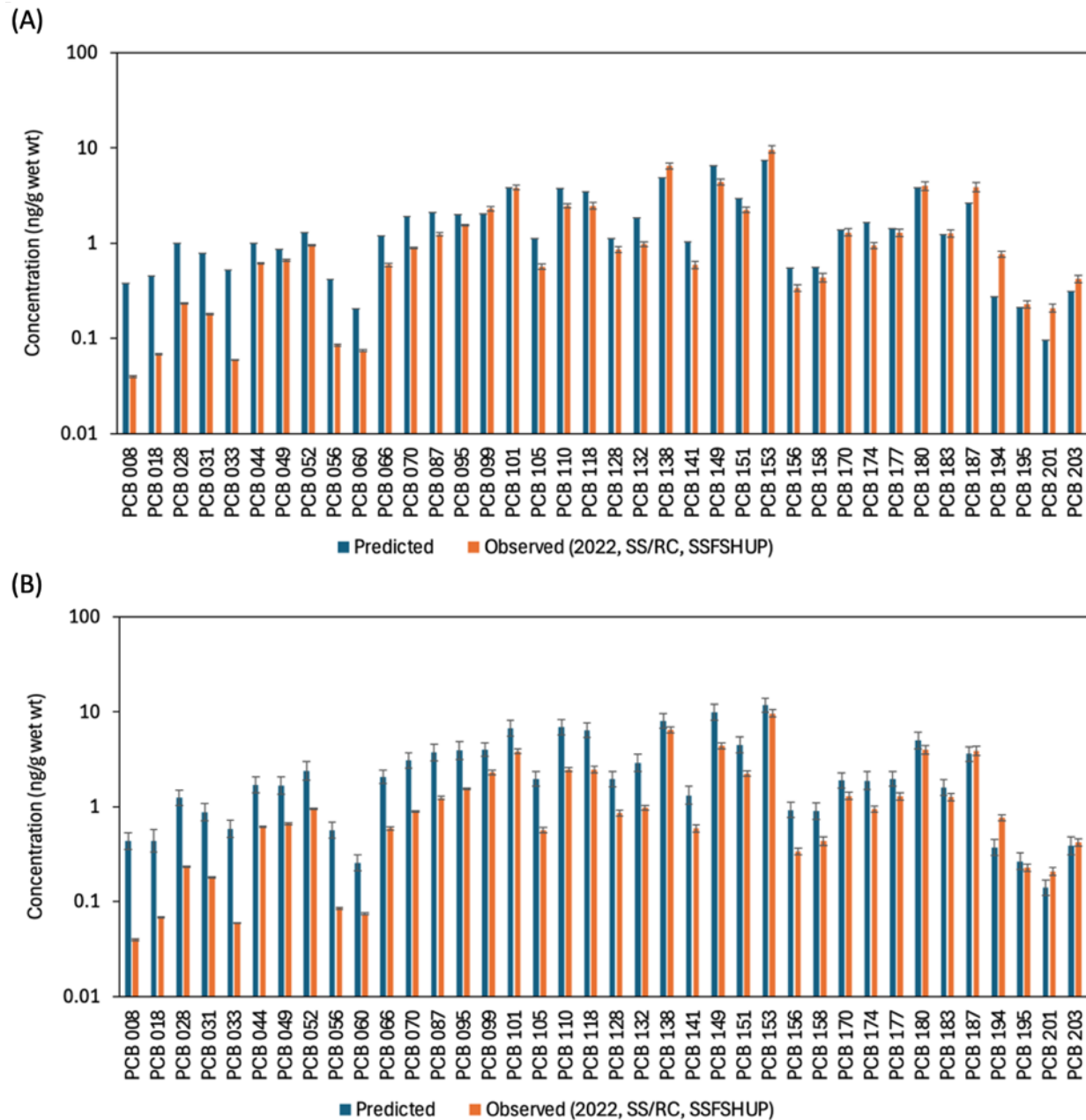


Figure 24. Geometric mean concentrations of PCB congeners in topsmelt calculated using the Steinberger Slough/Redwood Creek (SS/RC) PMU model (blue bars) and observed in 2022 at the SSFSHUP sampling site (red bars). Input PCB concentrations in sediments were collected from adjacent sites (A) or all sediment sampling sites (B). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

Figure 25 shows that the model-calculated PCB concentrations in shiner surfperch were generally in good agreement with the measured PCB concentrations in shiner surfperch

collected at South Bay in 2019. South Bay was the only fish sampling site in the Steinberger Slough/Redwood Creek Complex PMU in the 2019 sport fish sampling program. Also, it is important to note that for the model testing with shiner surfperch and white croaker at Steinberger Slough/Redwood Creek, measured concentrations in fish and sediment were not perfectly matched temporally. The fish samples were collected in 2019 while the sediment samples were collected in 2022. These were best available data sets for model testing. Future monitoring efforts may generate PCB concentration data that are better matched temporally and spatially and useful for testing and refining the model.

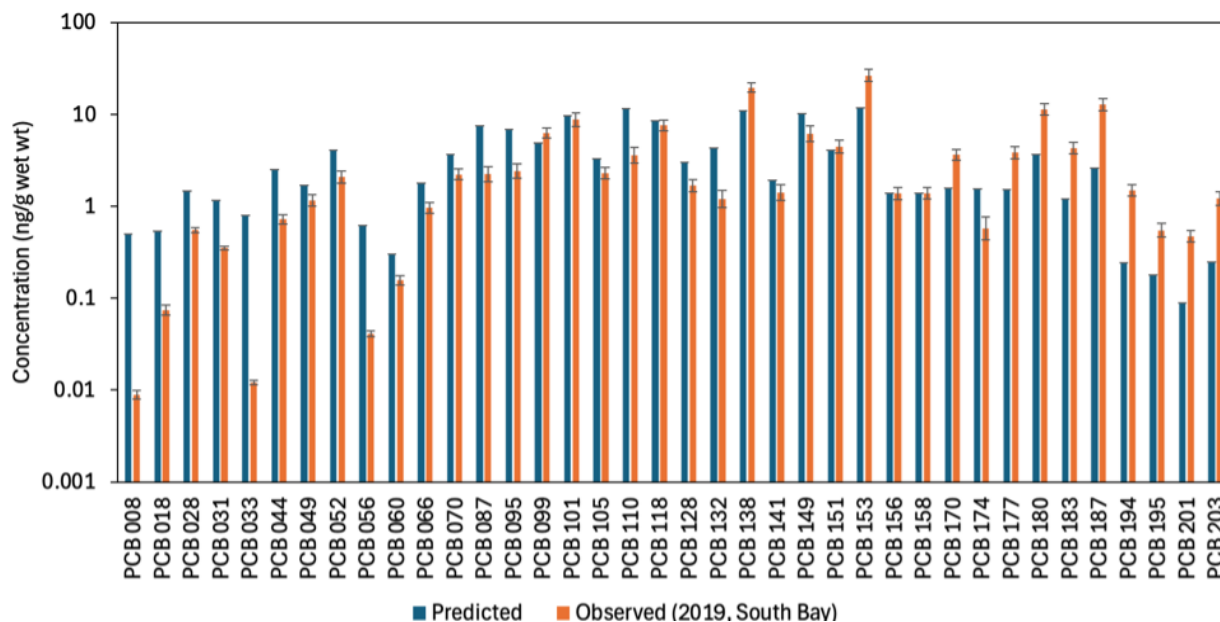


Figure 25. Geometric mean concentrations of PCB congeners shiner surfperch calculated using the Steinberger Slough/Redwood Creek (SS/RC) PMU model (blue bars) and observed in 2022 at the South Bay sampling site (red bars). Error bars of predicted concentrations in shiner surfperch represent uncertainty in PCB congener concentrations in sediments and water. Error bars of the observed concentrations represent standard errors of the geometric mean of observed PCB concentrations in fish.

Model calculated concentrations of PCB congeners in shiner surf perch were greater than observed concentrations for the lower molecular weight PCB congeners; but lower for the highest molecular weight PCB congeners; and in good agreement with observed concentrations for PCB congeners with a molecular weight in the mid-range (Figure 25). The calculated mean model bias MB for PCB congener concentrations were 1.41 (95% CI: 0.909–2.20), suggesting an overall 41% overprediction but the difference between model-calculated and observed concentrations was not significant (95% CI covers 1). The calculated mean model bias MB* based on total PCB concentrations was 0.918, suggesting a slight underprediction of the model. In general, the model-calculated PCB congeners were in good agreement with observed concentrations.

Figure 26 illustrates the model-calculated PCB congener concentrations in white croaker in comparison to the observed PCB concentrations in white croaker collected in 2019 at the South Bay sampling site. The observed white croaker concentration data were obtained from just one composite sample collected in 2019 and did not include an uncertainty estimate. Model-calculated PCB concentrations were generally in good agreement with observed concentrations for PCB congeners with medium to higher molecular weights, but model-calculated concentrations tended to be higher than the observed data for the congeners with lower molecular weights. The calculated mean model bias MB based on PCB congener concentrations was 2.64 (95% CI: 1.57–4.44) and the calculated model bias MB* based on total PCB concentrations was 1.59. The results indicate a general overprediction of PCB congener concentrations in the white croaker. However, the overprediction of total PCB concentrations is relatively modest at about 59%. The results of the Steinberger Slough/Redwood Creek Complex PMU model testing are summarized in Table 2.

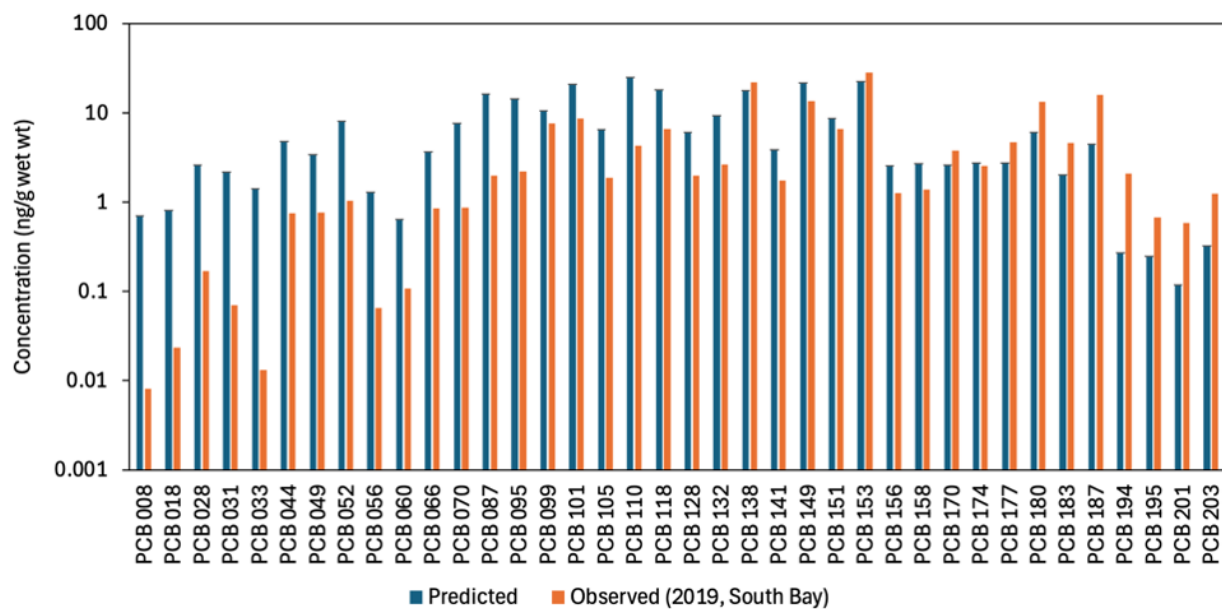


Figure 26. Concentrations of PCB congeners in white croaker calculated using the Steinberger Slough/Redwood Creek PMU model (blue bars) and observed in the 2019 sampling collected at the South Bay sampling site (red bars).

Table 2. Calculated model bias values (MB and MB*) for model testing at Steinberger Slough/Redwood Creek Complex. An MB or MB* of 1 indicate a lack of model bias and good agreement between model-calculated and observed concentrations of PCBs in fish.

Fish species (sample year)	Fish site (sample year)	Sediment site (sample year) ^a	MB (n) 95% CI ^b	MB* ^c
Topsmelt (2022)	RCFSLWR (2022)	RCWPTC, RCPTLD (2022)	2.05 (38) 1.55, 2.70	1.63
		All stations (2022)	2.75 (38) 2.19, 3.47	2.12
	RCFSHMID (2022)	RCMRNA (2022)	1.81 (38) 1.46, 2.24	1.53
		All stations (2022)	1.40 (38) 1.17, 1.66	1.21
	RCFSHUP (2022)	RCDKTB (2022)	7.14 (38) 5.74, 8.88	5.69
		All stations (2022)	2.01 (38) 1.64, 2.45	1.68
	SSFHSHMID (2022)	SSFIRE (2022)	4.11 (38) 3.26, 5.17	3.04
		All stations (2022)	3.05 (38) 2.29, 4.08	2.13
	SSFHSHUP (2022)	SSPOND, BAIRIN (2022)	1.56 (38) 1.23, 1.97	1.15
		All stations (2022)	2.32 (38) 1.87, 2.87	1.83
Shiner surfperch (2019)	South Bay (2019)	RCPTLD (2022)	1.41 (38) 0.909, 2.20	0.918
White croaker (2019)	South Bay (2019)	RCPTLD (2022)	2.64 (38) 1.57, 4.44	1.59

^a The locations of sampling sites are shown in Figures 8–10.

^b Mean model bias MB determined based on PCB congener concentrations and calculated using Equation 1.
n = number of comparisons. 95% confidence interval (CI) = antilog (log MB ± [$t_{v,0.05}$ × standard deviation]).

^c Model bias MB* determined based on total PCB concentrations and calculated using Equation 2

San Francisco Bay model

It is important to re-emphasize here that the model testing for the larger San Francisco Bay is different from that for the PMUs. The model testing for the PMUs involved matching observed concentrations of PCBs in water, sediments and fish both temporally and spatially as best as possible with the available data. This approach could not be carried out for model testing in the entire San Francisco Bay despite much data being available. Instead, the available empirical concentration data for PCBs in San Francisco Bay from all sampling locations were used to calculate the range of expected concentrations of PCB congeners in various fish species and then compared to the observed range of concentrations.

Figure 27 shows that PCB congener concentrations in shiner surfperch calculated by the San Francisco Bay model were in line with measured concentrations in shiner surfperch collected in 2019. Similar ranges between model-calculated and observed concentrations were obtained for PCB congeners with lower to medium molecular weights, while the ranges of model-calculated concentration were generally greater than the ranges of the observed concentrations for PCB congeners with a higher molecular weight. The greater ranges of model-

calculated concentrations may be attributed to the greater variability in measured environmental concentrations used as model input values.

Figure 28 shows that model-calculated PCB concentrations in white croaker were generally in line with measured concentrations in white croaker collected in 2019 for PCB congeners with a medium to higher molecular weight. For lower molecular weight congeners, the model-calculated concentrations were higher than the observed concentrations; and the ranges of model-calculated concentrations tended to be greater than the ranges of observed concentrations, potentially due to greater variability in measured concentrations in environmental media. Note that the measured PCB concentration data for sediments were collected in 2018 and the measured PCB concentration data for water were collected in 2011 and not temporally matched with the measured PCB concentration data for fish collected in 2019. The model could be better tested and refined if monitoring programs conduct water, sediment and fish sampling at the same time. Also, for the development and testing of a general San Francisco Bay food-web model a broader geographical distribution of sampling locations could be considered in addition to the more spatially refined monitoring approach applied to the PMUs.

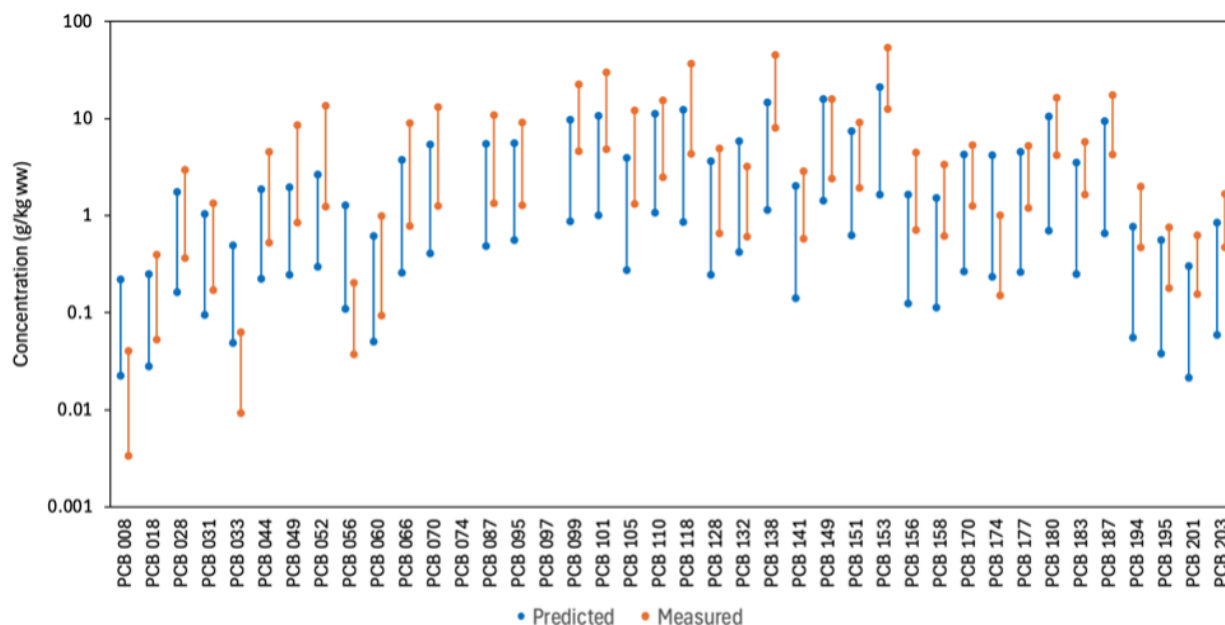


Figure 27. Ranges of concentrations of PCB congeners in shiner surfperch calculated using the San Francisco Bay model (blue lines) and observed in the 2019 sampling collected at San Francisco Bay (red lines).

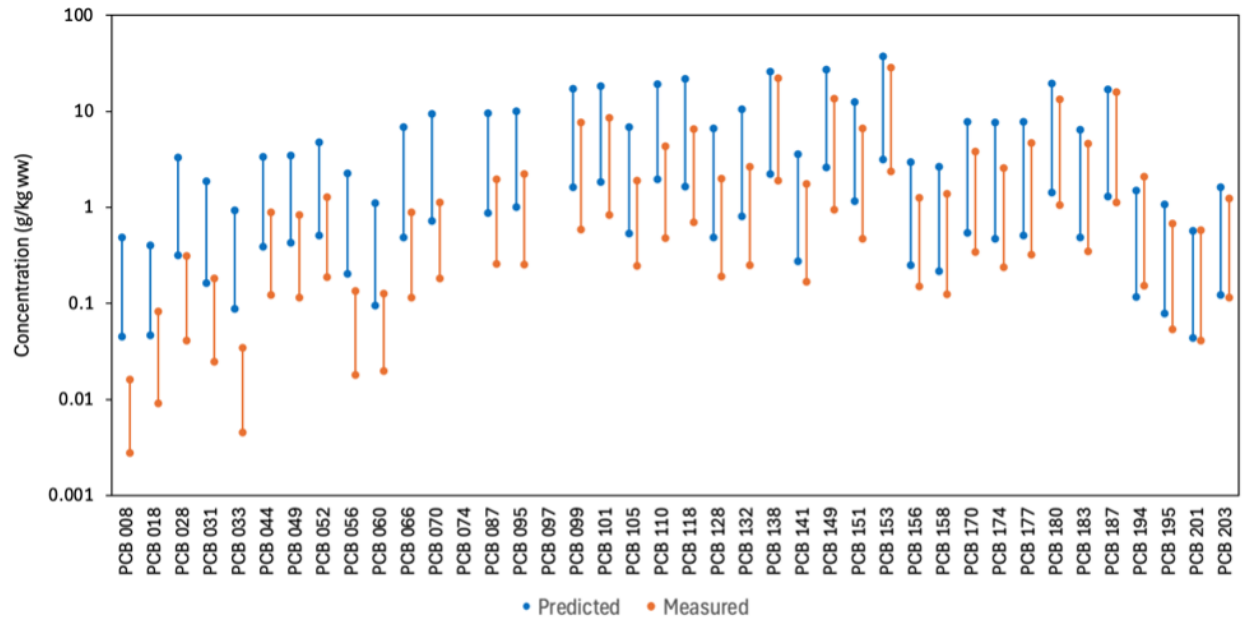


Figure 28. Ranges of concentrations of PCB congeners in white croaker calculated using the San Francisco Bay model (blue lines) and observed in the 2019 sampling collected at San Francisco Bay (red lines).

Temporal response

Figure 29 illustrates changes in PCB congener concentrations over time in response to a drop in PCB concentrations in water and sediments to zero. Figure 29 shows that concentrations of higher molecular weight PCB congeners respond to changes in exposure concentrations more slowly than lower molecular weight PCB congeners. The $t_{95\%}$ of the PCB congeners varies from approximately 42 days to 210 days and is approximately the same for shiner surfperch and white croaker. This means that concentrations of PCBs in fish can respond to changes in exposure concentrations in the course of weeks to months, not years or decades. The relatively quick response times of the PCB concentrations in fish also means that the temporal response of PCB concentrations in water and especially the sediments (which are controlled to a large degree by PCB inputs) become the rate limiting step in the temporal response of PCB concentrations in fish to changes in PCB inputs. In many estuarine systems, water is relatively quickly replaced due to tidal movements and therefore concentrations of PCB in water can respond relatively quickly to changes in PCB loadings. However, the sediment is replaced more slowly than the water and therefore often becomes the compartment controlling the temporal response of PCB concentrations in the food-web to changes in PCB inputs. The environmental fate modeling that is currently being carried out is likely to shed more light on this. The temporal response of the concentrations of PCBs in water and sediment due to changes in loading is important for the transfer of PCBs through the food-web. Reductions in PCBs loads to the PMUs can be expected to increase PCB mass transport via the benthic food-chain relative to the pelagic food-chain. Also, the dietary route will become a more important source of PCBs to

the fish than direct respiratory uptake as a result of loading reductions. The main implication of this is that real-world response times for PCB concentrations to changes in PCB loadings into the PMU can be expected to be longer than the $t_{95\%}$ values we are reporting here. The combination of environmental fate and food-web bioaccumulation models can provide the most accurate assessment of the temporal response of PCB concentrations in fish to PCB loading reductions.

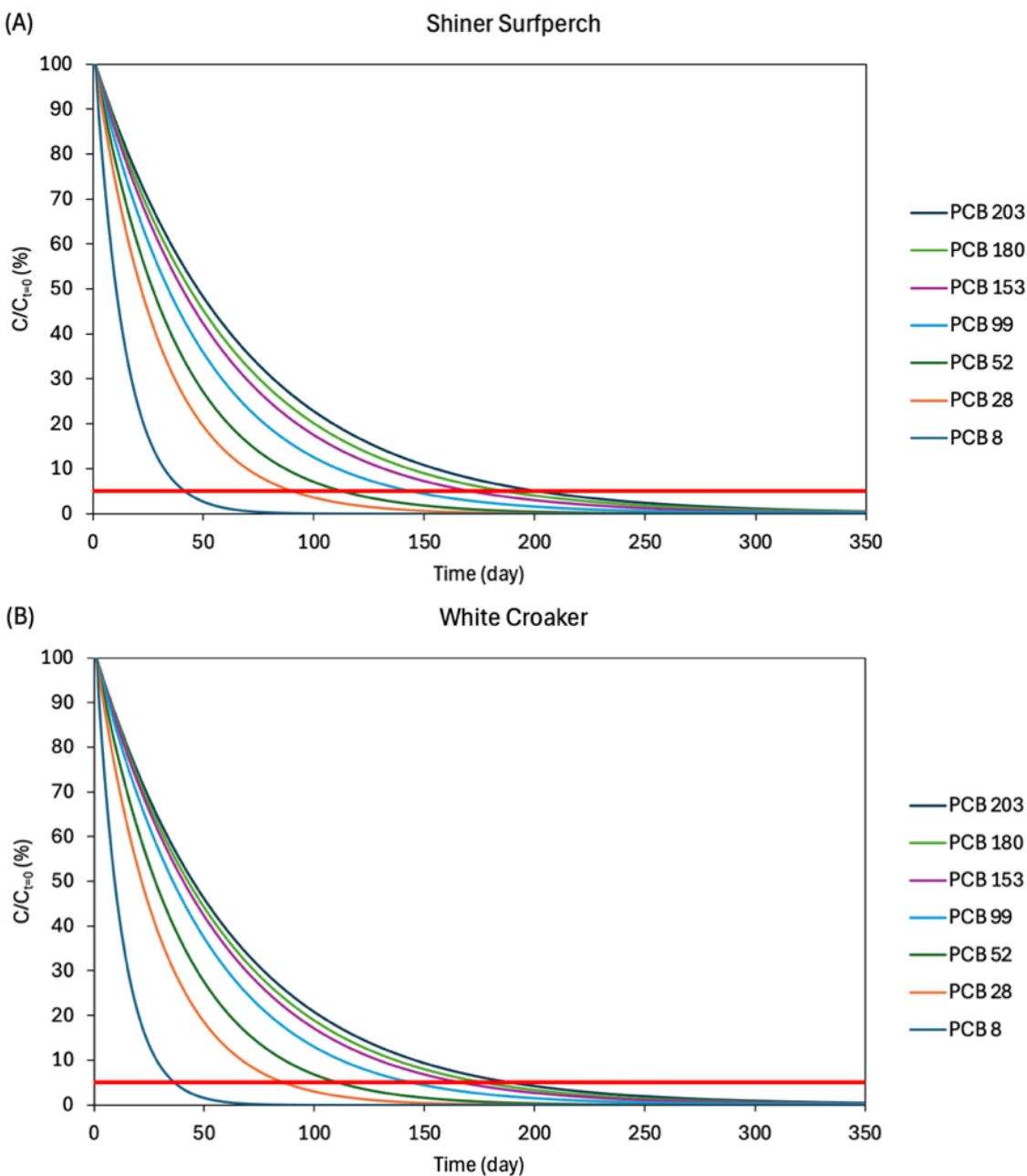


Figure 29. Demonstration of relative changes in representative PCB congener concentrations in shiner surfperch (A) and white croaker (B) over time using the San Leandro Bay PMU food-web bioaccumulation model under a hypothetical scenario where PCB concentrations in sediments

and water drop to zero at day 0. The red line represents 95% reduction in the initial PCB congener concentration in fish.

Figure 30 illustrates the change in the composition of PCBs in fish over time as a result of an instantaneous drop in the PCB concentration in water and sediments to zero. As a result of the differences in response times of the PCB congeners that make up the total combined concentration of PCBs (Σ PCBs) in fish, the contribution of lower molecular weight PCB congeners to the total PCB concentration in the fish falls more quickly over time than higher molecular weight PCBs. This causes the PCB composition in the fish to change to a heavier molecular weight mixture over time. Changes in PCB composition can have an effect on how human health risks of PCBs due to fish consumption are calculated.

It is important to note that the dependence of the response time of PCB concentrations in fish on the molecular weight of PCB congeners is likely to extend to the response time of PCB concentrations in water and sediments. This is due to the large variation in physical-chemical properties among PCB congeners. As a result, there can be considerable differences in the clean-up rates among PCB congeners in response to PCB loading reductions at the PMUs. This can manifest itself in terms of changes in PCB composition and “fingerprints” and may impact how measured concentrations of PCBs in fish and other media are reported. The combination of an environmental fate model and the food-web bioaccumulation model can reveal the change in PCB composition (and PCB fingerprint) as a result of changes in PCB loadings. The change in PCB composition in sediments and fish over time presents a useful way to track the change in PCB loadings to PMUs over time. For example, the change in the ratio of mass fractions of a higher and a lower molecular weight PCB in sediments or fish can provide information on whether PCB loadings are falling or not and may even provide a loading decline rate.

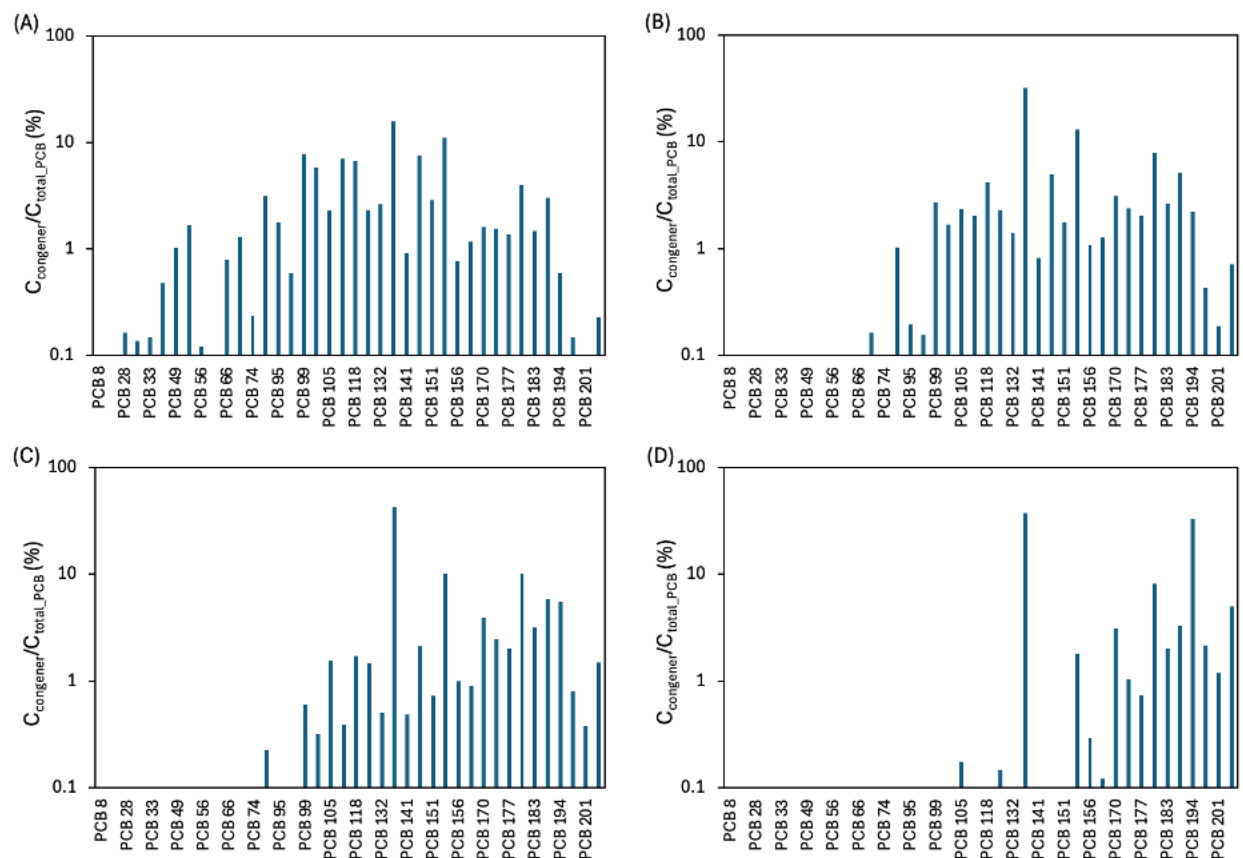


Figure 30. Demonstration of changes in PCB congener profiles in shiner surfperch at day 0 (A), 1 year (B), 2 years (C), and 5 years (D) using the San Leandro Bay PMU model under a hypothetical scenario that input PCB concentrations in sediments and water are dropped to zero at day 0.

Conclusions

This study developed a food web bioaccumulation model for PCBs in San Francisco Bay that can be used on a site specific basis at PMUs to predict how concentrations of PCBs in fish and other species of the aquatic food-web at PMUs can be expected to change over time in response to changes in PCB concentrations in water and sediments at PMUs resulting from remediation initiatives at the PMUs. This model is meant to be used in conjunction with an environmental fate model that can estimate the change in concentrations of PCBs in water and sediments over time in response to changes in loadings of PCBs into the PMU. The main goal of the model is to anticipate PCB concentrations in sport fish consumed by local fishers as a result of remediation efforts at the PMUs. The overall approach is to inform on when PCB concentrations are going to be low enough to safely consume fish caught at the PMUs and the larger San Francisco Bay.

The PCB food-web bioaccumulation model, which is presented in an Excel spreadsheet, can be used with minimal training to evaluate the impact of remediation initiatives on concentrations of PCBs in fish. The model also acts as a record of the state of knowledge of the food-web bioaccumulation of PCBs in San Francisco Bay. The model includes knowledge gained from years of studies of San Francisco Bay. The model imbeds information on the chemistry and ecology of the Bay and presents this knowledge in a mathematical form such that it can be used as a management tool and serve as a hypothesis for further scientific and monitoring studies aimed at improving knowledge of the environmental fate of PCBs and informed decision making with regards to pollutants.

The model is developed for PCBs, but can be applied with some modification, to other organic chemical pollutants such as brominated flame-retardants, PFAS, pesticides and others. The model is not appropriate for metals and nutrients.

Model testing at the San Leandro Bay and Steinberger Slough/Redwood Creek Complex PMUs and the larger San Francisco Bay shows that model predictions of PCB congeners in fish are in good agreement with observed concentrations. In most tests, observed $\sum$ PCB concentrations were found to be well within a factor of 2 of the predicted concentrations. The largest systematic overprediction of $\sum$ PCB concentrations in fish was equivalent to a factor of 2.3, the largest underprediction was by a factor of 1.09 or less than 10%. The mean and median for all mean model bias MB* for $\sum$ PCB were 1.54 and 1.59 respectively. This means that on average the model overpredicts concentrations of PCBs in fish by approximately 59%. This level of predictability is very good and a credit to the amount and excellence of research done on the bioaccumulation of PCBs in San Francisco Bay and other locations around the world. It should be emphasized that the uncertainty of the model expressed by the mean model bias and its 95% confidence intervals includes not only error in the model but also error in the empirical concentration data that were used for expressing model uncertainty. As a result, we feel that the model can be used to predict concentrations of PCBs in fish at the PMUs and can be expected to provide estimates of PCB concentrations in fish with a high level of confidence. We

suggest that a factor of 2 is used to represent the uncertainty in model predictions of the concentrations of PCBs in fish. The model without further calibration can be expected to be slightly on the conservative side.

The ability of the model to predict concentrations of individual PCB congeners is similar to that for Σ PCBs, but model uncertainty is somewhat larger than that for Σ PCBs as evidenced by the 95% confidence intervals of the mean model bias. Model testing in the Steinberger Slough/Redwood Creek Complex PMU also showed a tendency for the model to overpredict concentrations in fish of lower molecular weight PCB congeners while underestimating concentrations in fish of higher molecular weight PCB congeners. We expect this to reflect some of the equilibrium assumptions that were made with regards to the distribution of PCBs between water and particulate matter where field data were absent. Better field data on the equilibrium status of PCBs between water and particulate matter is expected to remedy this issue and further improve the accuracy of the model. The application of passive samplers in future studies of the fate of PCBs in San Francisco Bay will be of particular value in this regard.

Model simulations of the temporal response of PCB concentrations in fish over time showed considerable differences in response times to changes in concentrations in water and sediments among PCB congeners. We expect there to be similar PCB congener specific differences in the response times of PCB congener concentrations in water and sediments in response changes in PCB loadings. This means that PCB loading reductions will lead to a relatively quick decline of concentrations of lower molecular weight PCBs compared to a slower decline of concentrations of higher molecular weight PCB congeners. As a result, the composition of PCBs in water, sediments and fish can be expected to change over time in response to a PCB loading reduction. In fish, PCB mixtures will become “heavier”, containing a higher fraction of higher molecular weight PCBs. The change in composition of PCBs in fish as a result of PCB loading reductions can be relevant for the calculation of human health risks of PCBs associated with fish consumption. The change in PCB composition in fish may also provide a way to track progress of remediation efforts and associated changes in PCB loading rates., which are often difficult to measure. The decline of the contribution of lower molecular weight PCBs compared to higher molecular weight PCBs to the Σ PCB concentration in fish is an indicator of loading decline over time.

While the model is specific to PCBs it can be useful to address other pollutants as well. The food-web bioaccumulation behavior of many neutral hydrophobic organic pollutants such as chlorinated dioxins, polybrominated biphenyls, ethers and ethanes can also be investigated by the model. Furthermore, we have shown that with appropriate accommodations for the chemical partitioning properties, the modeling approach is also useful for many polyfluoroalkyl substances (PFAS) (Kelly et al. 2024).

To improve the developed time-dependent food-web biotransformation models for specific PMUs and the larger San Francisco Bay and improve their use, we have the following recommendations:

First, it is crucial to continue on-going monitoring efforts to obtain empirical PCB congener concentrations in key fish species (e.g., shiner surfperch and topsmelt) and environmental media (e.g., water, sediments, and suspended sediments). Such information can be used to refine the bioaccumulation models and used to gain confidence in the application of the model for management purposes. For the purpose of model development and testing, it is beneficial to coordinate sampling of sediments, water and fish to be spatially and temporally consistent.

Secondly, the application of passive sampling methods are particularly useful for the food-web bioaccumulation model as it can be used to measure the equilibrium status of concentrations of PCBs in sediments and water, which is a key factor controlling the degree to which PCB is absorbed by fish via food-consumption vs. respiration and reaches fish via benthic vs. pelagic routes.

Thirdly, the food-web trophic transfer model can be used in conjunction with other models, such as hydrodynamic and sediment transport models, to provide an integrated approach to investigate the relationship between PCB emission reduction and PCB concentrations in sport fish to protect human health.

Fourth, the time-dependent food-web biotransformation model developed specifically to PCBs can be applied to other pollutants of interest (e.g., PFAS of emerging concern) to better protect human and environmental health at the Bay region.

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Appendix A. Model description

The calculation of model parameters is described below, following the previous study on food web bioaccumulation modeling for PCBs in San Francisco Bay (Gobas and Arnot 2010) with minor modifications.

Clearance rate constant for chemical uptake via the respiratory area (k_1)

The parameter k_1 describes the rate at which the PCB congener is taken up into the organism from the water via the respiratory surface (e.g., gills and skin). For fish, aquatic benthic invertebrates, and zooplankton, k_1 is characterized by the clearance rate of the PCB congener in the organism, that is, the volume of water cleared of chemical by the organism over time (in the units of L water·kg organism wet wt⁻¹·d⁻¹). For those organisms, k_1 is calculated as a function of the organism's ventilation rate (G_V ; L water/d) and the diffusion rate of the chemical across the respiratory surface area using the following equation:

$$k_1 = \frac{E_W \cdot G_V}{W_B} \quad (\text{A1})$$

where E_W is the gill chemical uptake efficiency (unitless) and W_B is the wet weight of the organism (kg organism wet wt). E_W is a function of the K_{OW} of the PCB congener and is approximated based on empirical observations in fish as:

$$E_W = \frac{1}{A_{EW} + (B_{EW}/K_{OW})} \quad (\text{A2})$$

where K_{OW} is the octanol-water partition coefficient of the PCB congener, and A_{EW} and B_{EW} are constants (with default values of 1.85 for A_{EW} and 155 for B_{EW}).

G_V is calculated using an allometric relationship (Equation A3) between the wet weight and oxygen consumption of the organism based on observations from over 200 fish species.

$$G_V = 1400 \cdot \frac{W_B^{0.65}}{DO} \quad (\text{A3})$$

where DO is the dissolved oxygen concentration in water (mg O₂/L).

For phytoplankton, a biphasic relationship for k_1 is used based on a two-phase (i.e, aqueous and organic phases of the organism) resistance model (Equation A4).

$$k_1 = \frac{1}{A_p + (B_p/K_{OW})} \quad (A4)$$

where A_p and B_p are constants representing the resistance to PCB uptake through respectively the aqueous and organic phases of the organism, with default values of $6.0 \cdot 10^{-5}$ for A_p and 5.5 for B_p .

Rate constant for chemical elimination via the respiratory area (k_2)

The chemical elimination rate constant via the respiratory area (k_2 ; d^{-1}) is fundamentally related to the uptake clearance rate k_1 as the respiratory exchange of hydrophobic organic chemicals in aquatic organisms is passive in nature, involving the same processes of water ventilation and membrane permeation for both k_1 and k_2 . For all aquatic organisms, k_2 is calculated using Equation A6:

$$k_2 = \frac{k_1}{K_{BW}} \quad (A5)$$

where K_{BW} (L/kg organism wet wt) is the organism-water partition coefficient. The partitioning of PCBs between the water and organism is viewed to occur into the lipids, non-lipid organic matter (NLOM, such as proteins and carbohydrates), and water phases of the organism. Therefore, K_{BW} is calculated as:

$$K_{BW} = \frac{v_{LB} \cdot K_{OW}}{d_L} + \frac{v_{NB} \cdot \beta \cdot K_{OW}}{d_N} + \frac{v_{WB}}{d_W} \quad (A6)$$

where v_{LB} is the lipid content of the organism (kg lipid/kg organism wet wt), v_{NB} is the NLOM content of the organism (kg NLOM/kg organism wet wt), v_{WB} is the water content of the organism (kg water/kg organism wet wt), d_L is the density of lipids (g/mL), d_N is the density of NLOM (g/mL), d_W is the density of water (g/mL), and β is the proportionality constant expressing the sorption capacity of NLOM to that of octanol. Note that for phytoplankton, v_{NB} represents the non-lipid organic carbon (NLOC) content (kg NLOC/kg organism wet wt), and β represents the proportionality constant expressing the sorption capacity of NLOC to that of octanol. The default values of β are 0.35 for phytoplankton and 0.035 for fish, aquatic benthic invertebrates, and zooplankton. The default values of d_L , d_N , and d_W are 0.90, 1.22, and 1.0 g/mL, respectively.

Clearance rate constant for chemical uptake via ingestion of food and water (k_D)

The rate at which PCBs are absorbed from the diet via the gastrointestinal tract is expressed by the dietary uptake clearance rate k_D (kg diet·kg organism wet wt⁻¹·d⁻¹) and calculated as:

$$k_D = \frac{E_D \cdot G_D}{W_B} \quad (A7)$$

where E_D is the dietary chemical transfer efficiency (unitless) and G_D is the feeding rate of the organism (kg diet/d). E_D is highly variable in empirical observations, but empirical data show a general trend of decreasing efficiency with increasing K_{OW} for high K_{OW} chemicals. For modeling purposes, E_D for a PCB congener is calculated based on the lipid-water two-phase resistance model as:

$$E_D = \frac{1}{A_{ED} \cdot K_{OW} + B_{ED}} \quad (A8)$$

where A_{ED} and B_{ED} are constants, with default values of $8.5 \cdot 10^{-8}$ and 2.0, respectively, for fish, aquatic benthic invertebrates, and zooplankton.

The feeding rate G_D is estimated using Equation A9 based on a general bioenergetic relationship, except for filter feeders.

$$G_D = 0.022 \cdot W_B^{0.85} \cdot e^{0.06 \cdot T_W} \quad (A9)$$

where T_W is the water temperature ($^{\circ}\text{C}$). For filter feeders, G_D is estimated using Equation A10:

$$G_D = G_V \cdot SS \cdot \sigma \quad (A10)$$

where G_V is the gill ventilation rate (L/d), SS is the concentration of suspended solids in water (kg/L), and σ is the scavenging efficiency of particles absorbed from the water (unitless). G_V can be calculated using Equation A4. The default value of σ is 1 for filter feeders.

Rate constant for chemical elimination via excretion into egested feces (k_E)

The rate at which PCBs are eliminated by the egestion of fecal matter is expressed by the fecal elimination rate constant k_E (d^{-1}) and calculated as:

$$k_E = \frac{G_F \cdot E_D \cdot K_{GB}}{W_B} \quad (A11)$$

where G_F is the fecal egestion rate ($\text{kg fecal matter} \cdot \text{kg organism}^{-1} \cdot \text{d}^{-1}$), and K_{GB} is the partition coefficient of the chemical between the digesta (i.e., contents of the gastrointestinal tract) and the organism. G_F is a function of the feeding rate (G_D) and the digestibility of the diet, which is calculated based on the fractions of lipids, NLOM, and water in the diet and their respective absorption efficiencies (Equation A12).

$$G_F = [(1 - \varepsilon_L) \cdot v_{LD} + (1 - \varepsilon_N) \cdot v_{ND} + (1 - \varepsilon_W) \cdot v_{WD}] \cdot G_D \quad (\text{A12})$$

where v_{LD} is the lipid content of the diet (kg lipid/kg diet), v_{ND} is the NLOM content of the diet (kg NLOM/kg diet), v_{WD} is the water content of the diet (kg water/kg diet), ε_L is the dietary assimilation efficiency of lipids, ε_N is the dietary assimilation efficiency of NLOM, and ε_W is the dietary assimilation efficiency of water. The default values of ε_L , ε_N , and ε_W are 0.72, 0.72, and 0.55, respectively for zooplankton; 0.80, 0.75, and 0.75, respectively for aquatic benthic invertebrates, and 0.92, 0.50, and 0.55, respectively for fish species.

K_{GB} expresses the changes in phase partitioning properties that occur as the results of the digestion of the diet after ingestion and is calculated as:

$$K_{GB} = \frac{(v_{LG} \cdot K_{OW}/d_L + v_{NG} \cdot \beta \cdot K_{OW}/d_N + v_{WG}/d_W) \cdot d_G}{(v_{LB} \cdot K_{OW}/d_L + v_{NB} \cdot \beta \cdot K_{OW}/d_N + v_{WB}/d_W) \cdot d_B} \quad (\text{A13})$$

Where v_{LG} is the lipid content of the digesta (kg lipid/kg digesta), v_{NG} is the NLOM content of the digesta (kg NLOM/kg digesta), v_{WG} is the water content of the digesta (kg water/kg digesta), d_G is the density of the digesta (g/mL), and d_B is the density of the organism (g/mL). The default value is 1.0 g/mL for both d_G and d_B .

The fractions of v_{LG} , v_{NG} , and v_{WG} are estimated depending on the absorption efficiency for each component of the diet and calculated using Equations A14, A15, and A16, respectively.

$$v_{LG} = \frac{(1 - \varepsilon_L) \cdot v_{LD}}{(1 - \varepsilon_L) \cdot v_{LD} + (1 - \varepsilon_N) \cdot v_{ND} + (1 - \varepsilon_W) \cdot v_{WD}} \quad (\text{A14})$$

$$v_{NG} = \frac{(1 - \varepsilon_N) \cdot v_{ND}}{(1 - \varepsilon_L) \cdot v_{LD} + (1 - \varepsilon_N) \cdot v_{ND} + (1 - \varepsilon_W) \cdot v_{WD}} \quad (\text{A15})$$

$$v_{WG} = \frac{(1 - \varepsilon_W) \cdot v_{WD}}{(1 - \varepsilon_L) \cdot v_{LD} + (1 - \varepsilon_N) \cdot v_{ND} + (1 - \varepsilon_W) \cdot v_{WD}} \quad (\text{A16})$$

Rate constant for growth dilution (k_G)

Growth rates may vary considerably within and among species. For modeling purposes, generalized allometric equations are used to estimate the rate constant for growth dilution (k_G ; d^{-1}). For fish, k_G is approximated using Equation A17.

$$k_G = F_{GR} \cdot W_B^{-0.2} \quad (\text{A17})$$

where F_{GR} is a constant, with a default value of 0.006. For zooplankton and benthic invertebrates, k_G is approximated using Equation A18.

$$k_G = I_{GR} \cdot W_B^{-0.2} \quad (A18)$$

where I_{GR} is a constant, with a default value of 0.00035.

Rate constant for biotransformation (k_M)

The rate at which a parent compound can be eliminated via metabolic transformation is represented by the biotransformation rate constant k_M (d^{-1}). PCBs are poorly metabolized in many species, and it is assumed that k_M is negligible in the present study.

Freely dissolved fraction of the total chemical concentration in the overlying water (ϕ)

PCBs are hydrophobic chemicals and have a high affinity for binding to organic matter, such as particulate organic carbon (POC) and dissolved organic carbon (DOC) in the water column. When bound, PCBs are generally considered unavailable for uptake via diffusion into organisms. For a PCB congener, the freely dissolved fraction of the total chemical concentration in the overlying water (ϕ , unitless) can be estimated using Equation A19.

$$\phi = \frac{C_{WD}}{C_{WT}} = \frac{1}{1 + \chi_{POC} \cdot D_{POC} \cdot \alpha_{POC} \cdot K_{OW} + \chi_{DOC} \cdot D_{DOC} \cdot \alpha_{DOC} \cdot K_{OW}} \quad (A19)$$

where C_{WD} is the freely dissolved concentration (g chemical/L water) of the PCB congener in the water column; C_{WT} is the total concentration (g chemical/L water) of the PCB congener in the water column; χ_{POC} is the concentration of POC in water (kg POC/L water); χ_{DOC} is the concentration of DOC in water (kg DOC/L water); D_{POC} is the disequilibrium factor for POC partitioning (unitless); D_{DOC} is the disequilibrium factor for DOC partitioning (unitless); α_{POC} is the proportionality constant describing the similarity in phase partitioning of POC in relation to that of octanol (unitless); and α_{DOC} is the proportionality constant describing the similarity in phase partitioning of DOC in relation to that of octanol (unitless). The default values of α_{POC} and α_{DOC} are 0.35 and 0.08, respectively.

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Appendix B. Model parameters

Table B-1. Default values of chemical-specific input parameters, including the logarithm of the octanol-water partition coefficient ($\log K_{OW}$), the logarithm of the organic carbon-water partition coefficient ($\log K_{OC}$), and the disequilibrium factors for particulate organic carbon partitioning (D_{POC} ; unitless) and for dissolved organic carbon partitioning (D_{DOC} ; unitless).

PCB congener	$\log K_{OW}^a$	$\log K_{OC}^b$	D_{POC}^c	D_{DOC}^c
PCB 8	5.42	3.35	1	1
PCB 18	5.62	3.49	1	1
PCB 28	5.99	3.76	1	1
PCB 31	6.11	3.84	1	1
PCB 33	5.98	3.75	1	1
PCB 44	6.16	3.88	1	1
PCB 49	6.30	3.97	1	1
PCB 52	6.26	3.95	1	1
PCB 56	6.39	4.03	1	1
PCB 60	6.49	4.11	1	1
PCB 66	6.36	4.02	1	1
PCB 70	6.46	4.09	1	1
PCB 74	6.46	4.09	1	1
PCB 87	6.72	4.27	1	1
PCB 95	6.43	4.06	1	1
PCB 97	6.64	4.22	1	1
PCB 99	6.73	4.28	1	1
PCB 101	6.68	4.24	1	1
PCB 105	7.20	4.61	1	1
PCB 110	6.68	4.24	1	1
PCB 118	6.97	4.45	1	1
PCB 128	7.18	4.60	1	1
PCB 132	6.90	4.40	1	1
PCB 138	7.59	4.89	1	1
PCB 141	7.13	4.57	1	1
PCB 149	6.99	4.46	1	1
PCB 151	6.96	4.44	1	1
PCB 153	7.28	4.67	1	1
PCB 156	7.37	4.73	1	1
PCB 158	7.23	4.63	1	1
PCB 170	7.56	4.87	1	1
PCB 174	7.43	4.78	1	1
PCB 177	7.41	4.76	1	1
PCB 180	7.57	4.87	1	1
PCB 183	7.52	4.84	1	1
PCB 187	7.49	4.82	1	1
PCB 194	8.18	5.31	1	1
PCB 195	7.87	5.09	1	1
PCB 201	7.92	5.12	1	1
PCB 203	7.95	5.14	1	1

^a Corrected for salt-water at 14.9 °C (Gobas and Arnot 2010).

^b Calculated using $\log K_{OC} = 0.71 * \log K_{OW} - 0.05$ (Burkhard 2000).

^c Assumed.

Table B-2. Diet composition of modeled species in the San Leandro Bay PMU model.

Diet item	Modeled species						Shiner Surfperch ^b	White Croaker ^b
	Phytoplankton	Zooplankton ^a	Bivalve ^a	Polychaete ^a	Gammarid ^a	Topsmelt ^b		
Sediment	N/A	0	0.15	0.9	0.15	0	0	0
Suspended solids	N/A	0	0.15	0	0.15	0	0	0
Phytoplankton	N/A	1	0.65	0.05	0.35	0.294	0	0
Zooplankton	N/A	0	0.05	0.05	0.35	0.089	0	0
Bivalve	N/A	0	0	0	0	0	0.178	0
Polychaete	N/A	0	0	0	0	0	0.113	0.095
Gammarid	N/A	0	0	0	0	0.618	0.709	0.762
Topsmelt	N/A	0	0	0	0	0	0	0.143

^a Assumed.

^b Obtained from Jahn 2018 (rescaled to a summed value of 1 for modeling purposes).

Table B-3. Representative input values of the body weight (W_B), fraction of the respiratory ventilation involving sediment-associated porewater (m_p), lipid content (v_{LB}), non-lipid organic matter content (v_{NB}), and water content (v_{WB}) of modeled species in the San Leandro Bay PMU model.

Modeled species	W_B^a (kg wet wt)	m_p^b (unitless)	v_{LB}^c (unitless, w/w)	v_{NB}^d (unitless, w/w)	v_{WB}^e (unitless, w/w)
Phytoplankton	N/A	N/A	0.0012	0.060	0.939
Zooplankton	7.10E-08	0	0.01	0.200	0.790
Bivalve	1.00E-02	0.05	0.0086	0.100	0.891
Polychaete	1.00E-04	0.05	0.01	0.200	0.790
Gammarid	1.00E-06	0.05	0.01	0.200	0.790
Topsmelt	3.44E-03	0	0.0245	0.220	0.756
Shiner surfperch	1.79E-02	0	0.02	0.213	0.767
White croaker	2.92E-01	0	0.02	0.224	0.756

^a Topsmelt and shiner surfperch: from SFEI CD3 database; zooplankton: from Gobas and Arnot 2010; others: assumed.

^b Assumed.

^c Topsmelt: from Davis et al. 2017; shiner surfperch and white croaker: from Buzby et al. 2021; phytoplankton, zooplankton, and bivalve: from Gobas and Arnot 2010; others: assumed.

^d Topsmelt, shiner surfperch, and white croaker: calculated using $v_{LB} + v_{NB} + v_{WB} = 1$; others: assumed.

^e Topsmelt: from Davis et al. 2017; shiner surfperch and white croaker: from Buzby et al. 2021; others: calculated using $v_{LB} + v_{NB} + v_{WB} = 1$.

Table B-4. Diet composition of modeled species in the Steinberger Slough/Redwood Creek Complex PMU model.

Diet item	Modeled species												
	Phytoplankton	Zooplankton ^a	Copepods and Ostracods ^a	Small Crustacean ^a	Large Crustacean ^a	Crangon ^a	Insect ^a	Polychaete ^a	Bivalve ^a	Philine ^a	Topsmelt ^b	Shiner Surfperch ^b	White Croaker ^b
Sediment	N/A	0	0.34	0.34	0.34	0	0.34	0.9	0.15	0.3	0	0	0
Suspended solids	N/A	0	0	0	0	0	0	0	0.15	0	0	0	0
Phytoplankton	N/A	1	0.33	0.33	0.33	0.3	0.33	0.05	0.65	0.3	0.002	0.001	0.026
Zooplankton	N/A	0	0.33	0.33	0.33	0.3	0.33	0.05	0.05	0	0.106	0.017	0.012
Copepods and ostracods	N/A	0	0	0	0	0	0	0	0	0	0.094	0.107	0
Small crustacean	N/A	0	0	0	0	0.4	0	0	0	0	0.077	0.150	0.068
Large crustacean	N/A	0	0	0	0	0	0	0	0	0	0.564	0.308	0.042
Crangon	N/A	0	0	0	0	0	0	0	0	0	0	0	0.285
Insect	N/A	0	0	0	0	0	0	0	0	0	0.066	0	0
Polychaete	N/A	0	0	0	0	0	0	0	0	0	0.091	0.300	0.046
Bivalve	N/A	0	0	0	0	0	0	0	0	0.4	0	0.116	0.093
Philine	N/A	0	0	0	0	0	0	0	0	0	0	0	0.148
Topsmelt	N/A	0	0	0	0	0	0	0	0	0	0	0	0.280

^a Assumed.

^b Obtained from Jahn 2008 (rescaled to a summed value of 1 for modeling purposes).

Table B-5. Representative input values of the body weight (W_B), fraction of the respiratory ventilation involving sediment-associated porewater (m_p), lipid content (v_{LB}), non-lipid organic matter content (v_{NB}), and water content (v_{WB}) of modeled species in the Steinberger Slough/Redwood Creek Complex PMU model.

Modeled species	W_B^a (kg wet wt)	m_p^b (unitless)	v_{LB}^c (unitless, w/w)	v_{NB}^d (unitless, w/w)	v_{WB}^e (unitless, w/w)
Phytoplankton	N/A	N/A	0.0012	0.060	0.939
Zooplankton	7.10E-08	0	0.01	0.200	0.790
Copepods and ostracods	1.00E-07	0.05	0.01	0.200	0.790
Small crustacean	1.70E-10	0.05	0.01	0.200	0.790
Large crustacean	7.00E-09	0.05	0.01	0.200	0.790
Crangon	3.72E-04	0	0.02	0.200	0.780
Insect	1.00E-04	0.05	0.01	0.200	0.790
Polychaete	1.00E-04	0.05	0.01	0.200	0.790
Bivalve	1.00E-02	0.05	0.0086	0.100	0.891
Philine	1.00E-02	0.05	0.01	0.200	0.790
Topsmelt	3.44E-03	0	0.0245	0.220	0.756
Shiner surfperch	2.54E-02	0	0.02	0.213	0.767
White croaker	2.92E-01	0	0.02	0.224	0.756

^a Topsmelt, shiner surfperch, and white croaker: from SFEI CD3 database; zooplankton and crangon: from Gobas and Arnot 2010; others: assumed.

^b Assumed.

^c Topsmelt: from Davis et al. 2017; shiner surfperch and white croaker: from Buzby et al. 2021; phytoplankton, zooplankton, crangon, and bivalve: from Gobas and Arnot 2010; others: assumed.

^d Topsmelt, shiner surfperch, and white croaker: calculated using $v_{LB} + v_{NB} + v_{WB} = 1$; others: assumed.

^e Topsmelt: from Davis et al. 2017; shiner surfperch and white croaker: from Buzby et al. 2021; others: calculated using $v_{LB} + v_{NB} + v_{WB} = 1$.

Table B-6. Diet composition of modeled species in the Emeryville Crescent PMU model.

Diet item	Modeled species											
	Phytoplankton	Zooplankton ^a	Copepods and Ostracods ^a	Small Crustacean ^a	Large Crustacean ^a	Insect ^a	Polychaete ^a	Bivalve ^a	Topsmelt ^b	Mississippi Silverside ^b	Shiner Surfperch ^b	Striped Bass ^a
Sediment	N/A	0	0.34	0.34	0.34	0.34	0.9	0.15	0	0	0	0
Suspended solids	N/A	0	0	0	0	0	0	0.15	0	0	0	0
Phytoplankton	N/A	1	0.33	0.33	0.33	0.33	0.05	0.65	0.002	0.078	0.001	0
Zooplankton	N/A	0	0.33	0.33	0.33	0.33	0.05	0.05	0.106	0.044	0.017	0
Copepods and ostracods	N/A	0	0	0	0	0	0	0	0.094	0.184	0.107	0
Small crustacean	N/A	0	0	0	0	0	0	0	0.077	0.080	0.150	0
Large crustacean	N/A	0	0	0	0	0	0	0	0.564	0.526	0.308	0
Insect	N/A	0	0	0	0	0	0	0	0.066	0.084	0	0
Polychaete	N/A	0	0	0	0	0	0	0	0.091	0.004	0.300	0
Bivalve	N/A	0	0	0	0	0	0	0	0	0	0.116	0
Topsmelt	N/A	0	0	0	0	0	0	0	0	0	0	0.5
Mississippi silverside	N/A	0	0	0	0	0	0	0	0	0	0	0.5
Shiner surfperch	N/A	0	0	0	0	0	0	0	0	0	0	0

^a Assumed.

^b Obtained from Jahn 2008 (rescaled to a summed value of 1 for modeling purposes).

Table B-7. Representative input values of the body weight (W_B), fraction of the respiratory ventilation involving sediment-associated porewater (m_p), lipid content (v_{LB}), non-lipid organic matter content (v_{NB}), and water content (v_{WB}) of modeled species in the Emeryville Crescent PMU model.

Modeled species	W_B^a (kg wet wt)	m_p^b (unitless)	v_{LB}^c (unitless, w/w)	v_{NB}^d (unitless, w/w)	v_{WB}^e (unitless, w/w)
Phytoplankton	N/A	N/A	0.0012	0.060	0.939
Zooplankton	7.10E-08	0	0.01	0.200	0.790
Copepods and ostracods	1.00E-07	0.05	0.01	0.200	0.790
Small crustacean	1.70E-10	0.05	0.01	0.200	0.790
Large crustacean	7.00E-09	0.05	0.01	0.200	0.790
Insect	1.00E-04	0.05	0.01	0.200	0.790
Polychaete	1.00E-04	0.05	0.01	0.200	0.790
Bivalve	1.00E-02	0.05	0.0086	0.100	0.891
Topsmelt	1.33E-03	0	0.0245	0.220	0.756
Mississippi Silverside	7.10E-04	0	0.02	0.200	0.780
Shiner Surfperch	2.46E-02	0	0.02	0.213	0.767
Striped Bass	1.00E+00	0	0.02	0.200	0.780

^a Topsmelt, Mississippi silverside, and shiner surfperch: from Jahn 2010; zooplankton: from Gobas and Arnot 2010; others: assumed.

^b Assumed.

^c Topsmelt: from Davis et al. 2017; shiner surfperch: from Buzby et al. 2021; phytoplankton, zooplankton, and bivalve: from Gobas and Arnot 2010; others: assumed.

^d Topsmelt and shiner surfperch: calculated using $v_{LB} + v_{NB} + v_{WB} = 1$; others: assumed.

^e Topsmelt: from Davis et al. 2017; shiner surfperch: from Buzby et al. 2021; others: calculated using $v_{LB} + v_{NB} + v_{WB} = 1$.

Table B-8. Diet composition of modeled species in the San Francisco Bay model (obtained from Gobas and Arnot 2010).

Diet Item	Modeled species									
	Phytoplankton	Zooplankton	Polychaete 1 ^a	Amphipod	Cumacea	Mysis	Bivalve 1 ^b	Bivalve 2 ^c	Polychaete 2 ^d	Shrimp
Sediment	N/A	0	0.90	0.15	0.075	0.05	0.15	0.15	0.90	0
Suspended solids	N/A	0	0	0.15	0.075	0.05	0.15	0.15	0	0
Phytoplankton	N/A	1	0.05	0.35	0.65	0.45	0.65	0.65	0.05	0.30
Zooplankton	N/A	0	0.05	0.35	0.20	0.45	0.05	0.05	0.05	0.30
Polychaete 1 ^a	N/A	0	0	0	0	0	0	0	0	0
Amphipod	N/A	0	0	0	0	0	0	0	0	0
Cumacea	N/A	0	0	0	0	0	0	0	0	0
Mysis	N/A	0	0	0	0	0	0	0	0	0.40
Bivalve 1 ^b	N/A	0	0	0	0	0	0	0	0	0
Bivalve 2 ^c	N/A	0	0	0	0	0	0	0	0	0
Polychaete 2 ^d	N/A	0	0	0	0	0	0	0	0	0
Shrimp	N/A	0	0	0	0	0	0	0	0	0
Shiner surfperch 1 ^e	N/A	0	0	0	0	0	0	0	0	0
Jacksmelt 1 ^e	N/A	0	0	0	0	0	0	0	0	0
Northern anchovy 1 ^e	N/A	0	0	0	0	0	0	0	0	0

^a Generic polychaete (e.g., *Neanthes succinea*)

^b Generic bivalve (e.g., *Mytilus californianus*)

^c Generic bivalve (e.g., *Crassostrea gigas*)

^d Generic polychaete (e.g., *Harmothoe imbricata*)

^e Age-0 (juveniles or young-of-the-year)

^f Age > 0 (one year old or older)

Diet Item	Modeled species (cont'd)									
	Shiner Surfperch 1 ^e	Jacksnelt 1 ^e	Northern Anchovy 1 ^e	White Croaker 1 ^e	Northern Anchovy 2 ^f	Shiner Surfperch 2 ^f	Jacksnelt 2 ^f	Yellowfin Goby	Plainfin Midshipman	White Croaker 2 ^f
Sediment	0.05	0	0	0.05	0	0.05	0	0	0.05	0.05
Suspended solids	0	0	0	0	0	0	0	0	0	0
Phytoplankton	0.10	0.80	0.20	0.05	0.20	0.10	0.65	0	0	0
Zooplankton	0.20	0.20	0.35	0.20	0.20	0.10	0.20	0	0	0
Polychaete 1 ^a	0.05	0	0	0.15	0	0.10	0.05	0.20	0.10	0.20
Amphipod	0.25	0	0.20	0.10	0.15	0.20	0.05	0.15	0.15	0.20
Cumacea	0.25	0	0.15	0.10	0.20	0.20	0.05	0.15	0.15	0.20
Mysis	0.05	0	0.10	0.10	0.25	0.15	0	0	0.20	0.10
Bivalve 1 ^b	0	0	0	0	0	0	0	0	0	0
Bivalve 2 ^c	0	0	0	0	0	0	0	0	0	0
Polychaete 2 ^d	0.05	0	0	0.15	0	0.10	0	0.20	0.05	0.20
Shrimp	0	0	0	0.10	0	0	0	0.25	0.20	0.05
Shiner surfperch 1 ^e	0	0	0	0	0	0	0	0.05	0.05	0
Jacksnelt 1 ^e	0	0	0	0	0	0	0	0	0	0
Northern anchovy 1 ^e	0	0	0	0	0	0	0	0	0.05	0

^a Generic polychaete (e.g., *Neanthes succinea*)

^b Generic bivalve (e.g., *Mytilus californianus*)

^c Generic bivalve (e.g., *Crassostrea gigas*)

^d Generic polychaete (e.g., *Harmothoe imbricata*)

^e Age-0 (juveniles or young-of-the-year)

^f Age > 0 (one year old or older)

Table B-9. Representative input values of the body weight (W_B), fraction of the respiratory ventilation involving sediment-associated porewater (m_p), lipid content (v_{LB}), non-lipid organic matter content (v_{NB}), and water content (v_{WB}) of modeled species in the San Francisco Bay model.

Modeled species	W_B^g (kg wet wt)	m_p^h (unitless)	v_{LB}^i (unitless, w/w)	v_{NB}^i (unitless, w/w)	v_{WB}^i (unitless, w/w)
Phytoplankton	N/A	N/A	0.0012	0.060	0.939
Zooplankton	7.10E-08	0	0.0100	0.200	0.790
Polychaete 1 ^a	1.10E-04	0.05	0.0075	0.200	0.793
Amphipod	3.13E-06	0	0.0100	0.200	0.790
Cumacea	5.00E-06	0	0.0100	0.200	0.790
Mysis	1.50E-05	0	0.0100	0.200	0.790
Bivalve 1 ^b	1.12E-02	0.05	0.0086	0.100	0.891
Bivalve 2 ^c	1.05E-02	0.05	0.0083	0.100	0.892
Polychaete 2 ^d	1.00E-07	0.05	0.0075	0.200	0.793
Shrimp	3.72E-04	0	0.0200	0.200	0.780
Shiner surfperch 1 ^e	1.31E-03	0	0.0200	0.200	0.780
Jacksmelt 1 ^e	4.00E-03	0	0.0120	0.200	0.788
Northern anchovy 1 ^e	3.70E-03	0	0.0200	0.200	0.780
White croaker 1 ^e	1.50E-02	0	0.0180	0.200	0.782
Northern anchovy 2 ^f	2.15E-02	0	0.0250	0.200	0.775
Shiner surfperch 2 ^f	2.17E-02	0	0.02	0.213	0.767
Jacksmelt 2 ^f	2.06E-01	0	0.0160	0.200	0.784
Yellowfin goby	3.00E-02	0	0.0300	0.200	0.770
Plainfin midshipman	1.30E-01	0	0.0300	0.200	0.770
White croaker 2 ^f	2.51E-01	0	0.02	0.224	0.756

^a Generic polychaete (e.g., *Neanthes succinea*)

^b Generic bivalve (e.g., *Mytilus californianus*)

^c Generic bivalve (e.g., *Crassostrea gigas*)

^d Generic polychaete (e.g., *Harmothoe imbricata*)

^e Age-0 (juveniles or young-of-the-year)

^f Age > 0 (one year old or older)

^g Shiner surfperch and white croaker: from SFEI CD3 database; others: from Gobas and Arnot 2010.

^h Assumed.

ⁱ Shiner surfperch and white croaker: from Buzby et al. 2021; others: from Gobas and Arnot 2010.

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Appendix C. Supplemental information for model testing

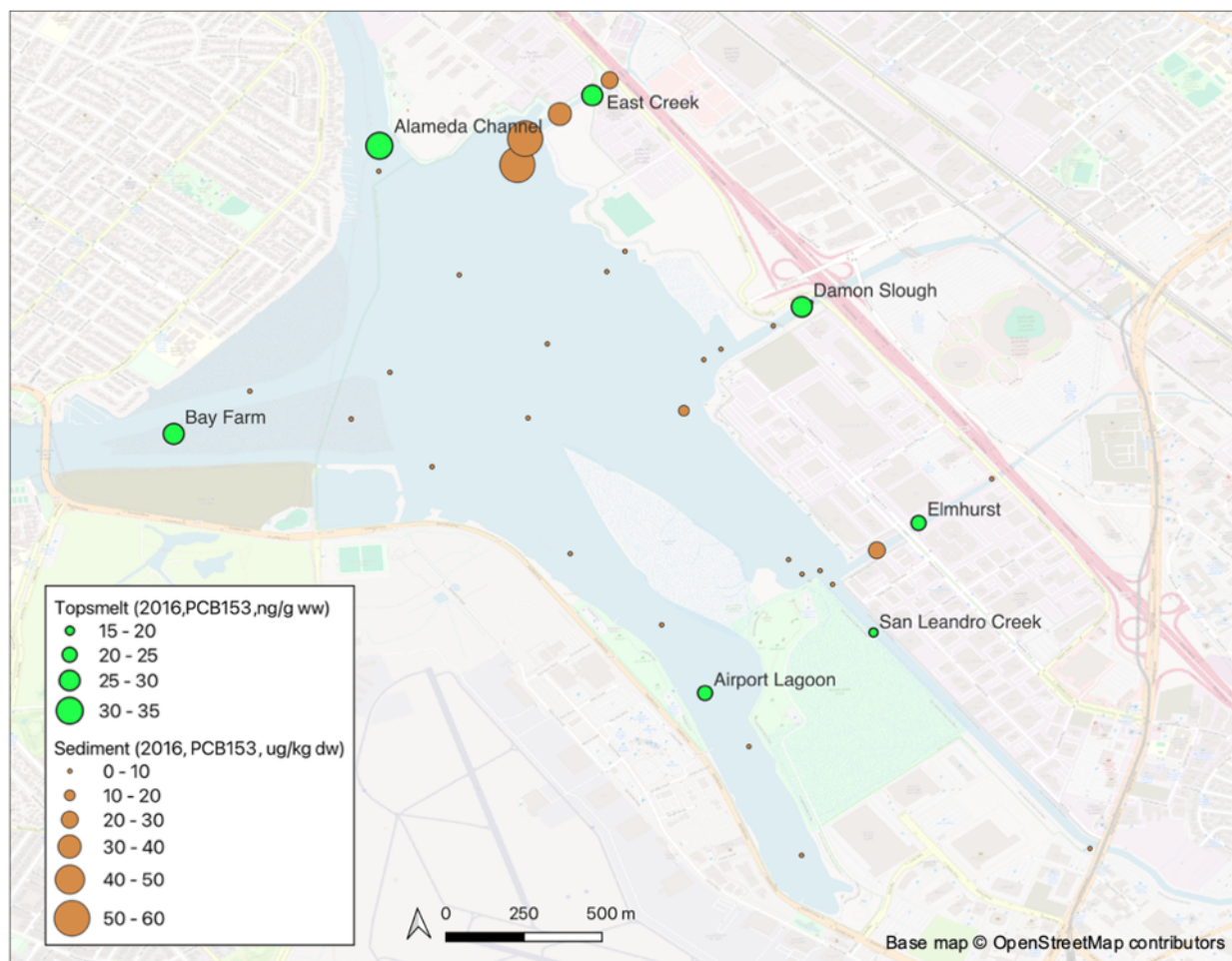


Figure C-1. Spatial distribution of measured PCB 153 concentrations in topsmelt and sediments collected in 2016 at San Leandro Bay. Geometric mean values are presented.