Strategy for In-Bay Fate Modeling to Support Contaminant and Sediment Management in San Francisco Bay

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### ACRONYMS AND ABBREVIATIONS

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<tr>
<td>Bay</td>
<td>San Francisco Bay</td>
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<tr>
<td>CEC</td>
<td>contaminant of emerging concern</td>
</tr>
<tr>
<td>DFM</td>
<td>D-Flow Flexible Mesh</td>
</tr>
<tr>
<td>EPA</td>
<td>U.S. Environmental Protection Agency</td>
</tr>
<tr>
<td>NMS</td>
<td>Nutrient Management Strategy</td>
</tr>
<tr>
<td>PAH</td>
<td>polycyclic aromatic hydrocarbon</td>
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<tr>
<td>PCB</td>
<td>polychlorinated biphenyl</td>
</tr>
<tr>
<td>PFAS</td>
<td>per- and polyfluoroalkyl substances</td>
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<tr>
<td>PFOA</td>
<td>perfluorooctanoic acid</td>
</tr>
<tr>
<td>PFOS</td>
<td>perfluorooctane sulfonic acid</td>
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<tr>
<td>PMU</td>
<td>priority margin unit</td>
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<tr>
<td>RMP</td>
<td>Regional Monitoring Program for Water Quality in San Francisco Bay</td>
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<tr>
<td>SFEI</td>
<td>San Francisco Estuary Institute</td>
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<tr>
<td>SLB</td>
<td>San Leandro Bay</td>
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<tr>
<td>SPLWG</td>
<td>Sources Pathways and Loading Workgroup</td>
</tr>
<tr>
<td>SS/RC</td>
<td>Steinberger Slough/Redwood Creek</td>
</tr>
<tr>
<td>S&amp;T</td>
<td>Status and Trends</td>
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<tr>
<td>TMDL</td>
<td>total maximum daily load</td>
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1 INTRODUCTION

This report presents a strategy and multi-year workplan for modeling polychlorinated biphenyls (PCBs), contaminants of emerging concern (CECs), and sediment in San Francisco Bay (the Bay). Robust in-Bay fate modeling is needed to address priority management questions that have been identified for these constituents.

PCB contamination is a high priority concern for Bay water quality managers due to health risks for humans and wildlife. A total maximum daily load (TMDL) for PCBs was approved in 2009 (SFBRWQCB 2008) and has been in an implementation phase since that time. Management attention for PCBs is increasingly focused on the contaminated intertidal and shallow subtidal areas adjoining the Bay shoreline generally characterized as the margins. These areas have relatively severe contamination that is not showing clear signs of decline (Buzby et al. 2021; Davis and Buzby 2021). In addition, these are areas where management actions have relatively high potential for reducing PCB impairment, either through reduction of watershed inputs or remediation of contaminated sediment in the Bay. Simple preliminary fate models for three contaminated margin areas (Emeryville Crescent, San Leandro Bay [SLB], and Steinberger Slough/Redwood Creek) suggest that reduction of watershed inputs could accelerate recovery in some cases (Davis et al. 2017; Yee et al. 2019, 2021), but these one-box models, while useful as a first step, are based on simplistic assumptions and generate highly uncertain predictions.

More realistic and robust models are needed to support and guide the expensive management actions that are needed to reduce PCB impairment. Robust in-Bay fate modeling is also needed to assess how management of these contaminated margin areas will affect Bay PCB impairment at a regional scale. A review and potential revision of the PCBs TMDL is planned for 2028. Updated and enhanced modeling is needed to synthesize the PCB data that have been generated since 2009 and to support development of updated control plans.

Monitoring and management of CECs have also become a top priority for Bay water quality managers (Miller et al. 2020). As one major indication of this, the design of the Regional Monitoring Program for Water Quality in San Francisco Bay (RMP) Status and Trends (S&T) Program was updated in 2021 to include CEC management as a primary driver (Foley et al. in preparation). The new S&T design includes CEC monitoring in margin areas near stormwater and wastewater discharges, where the signal strength and impacts of these contaminants are expected to be greatest, as well as monitoring at a regional scale to assess broader impacts. Robust in-Bay fate modeling will be valuable in guiding S&T monitoring of CECs (e.g., placement of sampling stations and timing of sample collection) and in assessing the likely spatial distribution and temporal duration of potential water quality impacts.

The RMP has been monitoring suspended sediment in the Bay since the Program began in 1993. In recent years, sea level rise has increased interest in sediment supply to the Bay. The mass balance and transport pathways of Bay sediment are critical factors controlling the degree to
which mudflats, marshes, and other shoreline habitats receive the sediment supply needed to keep pace with sea level rise over the long-term. As the San Francisco Bay Restoration Authority decides how to allocate $500 million over the next 20 years, it is critical to know the amount and quality of sediment available for restored tidal habitats. Modeling for in-Bay sediment fate is therefore needed both for understanding the fate of particle-associated contaminants like PCBs and for understanding sediment movement between Bay segments and into mudflats and shoreline habitats. The RMP Sediment Workgroup is very interested in the whole-Bay sediment transport modeling effort, particularly at the margins (or baylands) (McKee et al. 2020). This workgroup is currently funding monitoring of sediment flux from shallows onto marshes at several locations around the Bay—these results could be used for this modeling effort.

The strategy for in-Bay modeling presented in this report is a major element of a broader, integrated strategy that is being developed across RMP Workgroups for modeling contaminants flowing from the Bay watersheds and other pathways into the Bay. The broader project is expected to yield an integrated strategy in 2022, followed by implementation of a pilot effort in 2023. Coordination of the in-Bay modeling effort with the broader integrated strategy and other modeling work (e.g., nutrient modeling under the Nutrient Management Strategy) will be critical to optimizing use of the funds allocated to modeling.
2 PRIORITY MANAGEMENT QUESTIONS

There are a number of areas in the Bay that are on the 303(d) List of impaired water bodies due to elevated concentrations of one or more contaminants (PCBs, mercury, polycyclic aromatic hydrocarbons [PAHs], selenium, and others) that have been well documented by the RMP. Studies conducted by the RMP help improve our understanding of the interaction of these contaminants with the physical, chemical, and biological processes in the Bay affecting contaminant transport and fate.

The goal of the RMP is to collect data and communicate information about water quality in the Bay in support of management decisions. The focus on management decisions is achieved through articulation and prioritization of specific questions that managers need answered. The PCB Workgroup of the RMP has articulated the following high-priority management questions, which the in-Bay modeling strategy will be of great value in addressing:

1. What are the rates of recovery of the Bay, its segments, and in-Bay contaminated sites from PCB contamination?
   a. What would be the impact of focused management of priority margin unit (PMU) watersheds?
   b. What would be the impact of management of in-Bay contaminated sites (e.g., removing and/or capping hotspots), both within the sites and at a regional scale?

“Recovery” refers to the reduction of PCBs in shiner surfperch (the key impairment indicator established by the TMDL) to concentrations below the TMDL target of 10 ppb. A good understanding of current and projected loads of PCBs from surrounding watersheds and other upland sources will be key to answering these questions. The Sources Pathways and Loading Workgroup (SPLWG) is currently overseeing the development of such a regional-scale watershed loading model with work on the PCB portion of that model beginning in 2022 (Wu and McKee 2019; Zi et al. 2021, 2022), but in-Bay modeling of PCB transport and fate is also needed that will link to this watershed model to predict the long-term outcomes of load reductions and other management actions.

Similarly, the Emerging Contaminant Workgroup of the RMP has articulated a set of high-priority management questions:

1. Which CECs have the potential to adversely impact beneficial uses in the Bay?
2. What are the sources, pathways, and loadings leading to the presence of individual CECs or groups of CECs in the Bay?
3. What are the physical, chemical, and biological processes that may affect the transport and fate of individual CECs or groups of CECs in the Bay?
4. Have the concentrations of individual CECs or groups of CECs increased or decreased in the Bay?

5. **Are the concentrations of individual CECs or groups of CECs predicted to increase or decrease in the future?**

6. **What are the effects of management actions?**

Questions 3, 5, and 6 in particular require modeling of in-Bay processes to project likely impacts of CEC discharges. Additional management questions for CECs (specific elements of Question 3 above) have been identified in discussions related to the draft strategy for in-Bay contaminant fate modeling and the redesign of RMP S&T monitoring that occurred in 2021–2022.

- What is the predicted spatial and temporal extent of potential impact of CECs?
- What are areas of management interest where CECs should be monitored to assess S&T in water and sediment?

An understanding of CEC loading from various pathways is an important component to be provided by monitoring and models of watersheds, wastewater, and other local discharges. The subsequent fate of these discharges can then be modeled through inclusion of the processes of greatest importance for each given contaminant. Overall, it is apparent that any modeling strategy for the Bay needs to work for a spectrum of chemicals with varying chemical properties to support the multi-faceted management questions.

Sediment fate in the Bay is also of high management interest due to its nexus with nutrient impacts, wetland restoration, contaminants, and sediment transport. The following priority management questions have been articulated by the RMP Sediment Workgroup:

1. **What are the sources, sinks, pathways and loadings of sediment and sediment-bound contaminants to and within the Bay and subembayments?**

2. **How much sediment is passively reaching tidal marshes and restoration projects and how could the amounts be affected by management actions?**

3. **What are the concentrations of suspended sediment in the Estuary and its segments?**

Similar to the case for legacy and emerging contaminants, the sediment loads originating from upland sources are to be addressed through watershed models within the broader integrated strategy, while an in-Bay fate modeling can address management questions relating to long-term fate processes impacted by those discharges.

The overall goal of this document is to outline the strategic approach envisioned for developing quantitative in-Bay models for addressing these management questions and supporting management actions. The strategy provides the rationale for implementation of a multi-year
workplan for modeling PCBs, CECs, and sediment in the Bay. Further, this strategic approach will inform future monitoring strategies and programs that address the management questions.
3 PREVIOUS WORK AND CONCEPTUAL SITE MODEL

Overall, it is critical to develop a sound baseline from the significant work completed to date on contaminant transport in the Bay and a conceptual site model is a useful platform for this. A conceptual site model provides a general representation of the physical, chemical, and biological conditions of interest. While this document is not intended to provide a comprehensive overview of previous work, the conceptual site model here provides a brief description of contaminant distribution, fate and transport, and bioaccumulation as important background context in the development of a long-term modeling strategy. The following section provides a general summary of contaminant nature and extent in the Bay followed by a general review of the key fate and transport and bioaccumulation modeling to date. The conceptual site model laid out here follows the work conducted by Jones et al. (2012).

While there are biota with elevated concentrations of contaminants throughout the Bay, there are localized zones of particularly high concentrations in sediment and biota, where current or historical sources entered the Bay and contaminants were deposited, or historical activity contaminated a site (Jones et al. 2012; Davis and Buzby 2021). The majority of these locations are in the Bay margins—intertidal and shallow subtidal areas adjoining the Bay shoreline. In margin areas, wastewater, watershed, and shoreline contaminant sources and processes are primarily responsible for these higher contaminant concentrations. Urban and industrial development has generally occurred near the margins, with the margins accumulating contamination. Figure 1 shows examples of some of the margin sites in the Bay with higher contaminant concentrations. These regions of higher contamination subsequently provide a potential pathway for transport of contamination into the wider Bay environment. Productive and valuable ecosystems are also present in and rely upon the health of the margins, compounding the risk posed by entry or retention of contaminants in these areas. The margins, while limited in area, provide unique and diverse habitats that are often sensitive to both local and system-wide modifications.

The RMP is conducting fish monitoring in selected margin areas to track PCB impairment. Shiner surfperch are the key PCB indicator species for the Bay, and this species resides in these margin habitats. Long-term monitoring stations for PCBs in shiner surfperch, selected primarily based on fishing pressure, include Redwood Creek, Oakland Harbor, and San Francisco Waterfront. Recent shiner surfperch monitoring in the margins has also included SLB and Richmond Harbor, and could be expanded to other margin areas with historical or ongoing PCB contamination. Success in reducing PCB loads to the Bay should be reflected in reduced impairment, i.e., lower concentrations in shiner surfperch at these margin monitoring stations. For areas where surfperch are not found, other species, ambient sediment and water concentrations, or other proxies such as passive sampler uptake might be used as indicators of improvement.
For CECs, margins near the entry of urban stormwater and wastewater discharges are of particular concern due to the potential for higher contaminant concentrations, biotic exposure, and risk. Exposure to CECs is a concern not only for fish, but also other aquatic species in margin areas that may be sensitive to CECs. Quantitative modeling of contaminant transport and fate, subsequent processes resulting in exposure, and possible resultant direct effects, or contaminant accumulation in sediment and bioaccumulation in fish and other biota will be useful in understanding the linkages critical to effectively managing and mitigating the risks from CEC discharges.

3.1 FATE AND TRANSPORT MODELING

Previous modeling efforts provide important background on available data, process modeling capabilities, and present availability of suitable tools for supporting future contaminant modeling efforts. While this document is not intended to provide a comprehensive account of modeling efforts in the Bay, it does provide a high-level summary of some of the relevant efforts that can support the RMP strategic approach. It is important to note that all of these efforts rely on the large body of work not cited here that has been completed in the Bay.
Davis (2004) developed a simple one-box mass budget model as a first step toward a quantitative understanding of the long-term fate of PCBs in the Bay. Sensitivity analysis
indicated that in the short-term, among the most influential model parameters were average PCB concentrations in sediment and depth of the active sediment layer. Moderately influential parameters included organic carbon content of suspended solids, mass transfer coefficients, and other PCB physiochemical characteristics.

However, the ongoing loading of PCBs was shown to be most important to determining the ultimate long-term fate of the Bay. Significant findings included that eliminating external loading entirely would result in a halving of the mass of PCBs in the Bay every 20 years. With a sustained loading in the range of current estimates, the model predicted the total PCB mass in the active sediment layer would never fall below a level that is 10 to 25% of the initial mass. Therefore, the ongoing work to find and abate watershed sources, the existing estimates of watershed and regional scale loadings, and the ongoing development of the watershed dynamic loading model for PCBs, sediments, and CECs loads and trends will be essential inputs for the development of accurate in-Bay fate models.

One of the key limitations of the initial Davis (2004) model is that the Bay was treated as a single box, unable to represent the finer-scale processes occurring in different Bay segments, nor those on the Bay margins, where many of the highest concentrations of and risks due to contaminants exist, pointing to the need for more finely resolved, higher-fidelity modeling.

Oram and Davis (2008) developed a higher-fidelity multi-box model of the Bay (Figure 2). The model was built upon two existing models: 1) a tidally averaged hydrodynamic model previously used to interpret daily to decadal variability in salinity, and 2) a sediment transport model used to estimate long-term bathymetric change. After initial development, the PCB model was calibrated to PCB concentrations observed in water and sediment. Despite uncertainties in historical PCB load estimates and other influential parameters, the model was found to reasonably simulate observed patterns of PCB distribution between segments. However, the highest concentration and risk areas on the margins were still not adequately resolved, as the model treated each cross-sectional box (with both deep channel and shoal areas) uniformly. A key finding of that study was that a model better resolved in three dimensions would be needed to reproduce sediment bed concentration profiles throughout all areas of the Bay.
Recently completed conceptual model reports for several PMUs (Davis et al. 2017; Yee et al. 2019, 2021) have applied simple box models similar to those used in Davis (2004) and Oram and Davis (2008) at a much smaller scale, illustrating the processes and resultant responses and ambient concentrations of PCBs in PMUs much better than could be resolved by the Bay- and segment-scale models of the prior efforts. Nonetheless, even within the scale of a specific PMU, simple one- or two-box models used for these conceptual models are unable to recreate finer-scale contaminant gradients observed in the local empirical data. Thus, they are most useful as general and uncertain illustrative models of system responses on this smaller scale, rather than as precise or accurate quantitative projections of likely outcomes of management action and long-term recovery.

The simple box model approach of Davis (2004) has also recently been applied to the CECs perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) by Sanchez-Soberon et al. (2020), who provided an intermediate degree of spatial fidelity by using three boxes (for North, Central, and South Bay). They also modeled bioaccumulation of these contaminants in shiner surfperch using a food chain model, following the methods of Larson et al. (2018). There
were large uncertainties in many input parameters for the model (such as historical and ongoing inputs of PFOS and PFOA), but similar to the case for PCBs, long half-lives in sediment resulted in slow recovery from contamination even after new loads had been reduced.

The Bay Nutrient Management Strategy (NMS) Science Program is charged with developing the scientific foundation to inform decisions related to managing nutrient loads to the Bay. While the loading and biogeochemical processes for nutrients differ from those for many toxic contaminants, many of the physical transport mechanisms of interest are the same. Since a major focus of the NMS is developing numerical models to simulate hydrodynamics and biogeochemical processes in the Bay, much of these ongoing efforts can be directly leveraged for the PCB, CEC, and sediment fate modeling efforts. The NMS modeling work is guided by a 5-year modeling workplan (2019–2024; King 2020). Importantly, the process-based, numerical model is being used to improve quantitative understanding of processes that shape present conditions and evaluate potential effectiveness of nutrient management actions.

The Bay hydrodynamic model used by the NMS is built on the open-source modeling platform D-Flow Flexible Mesh (DFM). DFM is a finite-volume, three-dimensional, unstructured hydrodynamic model (Martyr-Koller et al. 2017). The unstructured nature of the grid allows for efficient and flexible resolution of flow features ranging from small perimeter sloughs and ponds up to a regional representation of the coastal ocean. This range of features is resolved without explicit seams or nesting boundaries as would be required for a structured grid model applied to the same area.

The NMS DFM model inputs include tides, direct precipitation, evaporation, stormwater runoff, wastewater discharges, Delta outflow, and wind. From these inputs, the DFM calculates water levels, salinity, temperature, currents, and the force of the currents on the bed throughout the Bay. Presently, simulations cover water years 2013 through 2018 plus 2003 and 2006, where water year is defined as the period spanning October 1 through September 30, with the first three months in the previous year. There is good agreement between the model results and observations, including water level, salinity, and velocity. The good comparison proves the suitability of the hydrodynamic model for simulating fundamental physical processes in the Bay (King et al. 2020). While the NMS DFM modeling efforts have included some preliminary efforts at investigating sediment transport, at present, the model does not include a direct simulation of sediment transport.
High-resolution models have already been used to some extent in modeling contaminant fate in the Bay. Sutton et al. (2019) developed and applied numerical models to estimate the dispersal and fate of microparticles and microplastics in the Bay and the adjacent National Marine Sanctuaries. This model differed from many Bay applications in that it seamlessly allowed transport between the Bay and the coastal environment, capturing the tide- and river-driven dynamics within the Bay, as well as inertial- and wind-driven currents in the coastal ocean. To this end, the study used the SUNTANS hydrodynamic model, which had been successfully used in previous Bay model applications as well as coastal domains (Fringer et al. 2006). This three-dimensional hydrodynamic model is unique in its spatial coverage from small-scale sloughs and mudflats within the Bay, to shelf-scale dynamics in the coastal ocean. A particle tracking model was used to simulate the transport of microparticles in the Bay and coastal ocean. The FISH-PTM model (Ketefian et al. 2016) was chosen for this application due to its speed, flexibility, track record of successful application in the Bay, and compatibility with SUNTANS hydrodynamic data.
Detailed hydrodynamic models have also been used in preliminary evaluations of PCB fate in PMUs (Davis et al. 2017; Yee et al. 2019, 2021). In the Steinberger Slough/Redwood Creek PMU, exploratory analyses were carried out using a two-dimensional flexible mesh hydrodynamic model, which includes tidal forcing in the coastal ocean, outflows from major rivers, and a simplified wind field. Based on these inputs, the model predicts sea surface height and depth-averaged current velocity. The model is an adaptation of the early NMS DFM model (Nuss et al. 2018). The model output was analyzed for several specific purposes: 1) extracting local tidal datums for each PMU, 2) characterizing tidal velocities and transport, and 3) characterizing the extent and degree of influence for various stormwater runoff inputs (each considered in isolation). Given the goal of capturing bulk transport processes at the PMU scale, the adapted model was run in two-dimensional mode rather than the more computationally intensive three-dimensional mode. The modeling efforts were preliminary and only offered information regarding the general footprint associated with tributary inputs. Key mechanisms not directly addressed in that high-resolution modeling work were sediment input, transport, and fate processes.

3.2 BIOACCUMULATION MODELING

To support development of the PCBs TMDL, a food web model for PCB bioaccumulation in the Bay was developed by Gobas and Arnot (2010). The model was supported by field studies funded by the RMP and the San Francisco Bay Regional Water Board. The model is based on a deterministic understanding of the processes that control the bioaccumulation of PCBs in the food web. The model combines the toxicokinetics of chemical uptake and elimination in individual organisms and trophic interactions between organisms of the Bay to estimate PCB concentrations in biota. For example, the model uses data on the size and lipid content of fish as well the fish’s feeding behavior, the chemical properties of PCBs, and data on the characteristics of the Bay to estimate the quantitative relationships between concentrations of PCBs in water, sediment, and biota. The model calculates spatial distributions of PCB concentrations in a range of invertebrate, fish, avian, and mammalian organisms, including shiner surfperch, harbor seals, double-crested cormorants, and Forster’s terns (Figure 4). The performance of the model was evaluated against independent empirical PCB concentrations and showed good agreement. The model was applied to produce Bay-wide PCB concentration distributions in modeled biota. This modeling was performed at a Bay-wide scale due to a lack of empirical data to support modeling at a finer spatial resolution. Gobas and Arnot (2010) chose to employ a steady-state simulation for the model, due to the long response times of sediment relative to biota; with this formulation, PCB concentrations in biota are directly proportional to concentrations in sediment.

Examining bioaccumulation at finer spatial scales, Greenfield and Allen (2013) provided empirical evidence of the direct proportionality of PCB concentrations in biota and sediment. In spite of using datasets for sediment contamination and prey fish that were collected in different
studies, PCB concentrations in topsmelt and silverside from locations throughout the Bay were positively correlated to concentrations in nearby sediment samples, suggesting the possibility of localized recovery through prioritizing the improvement of the most highly contaminated areas.

Another recent effort modeled bioaccumulation of per- and polyfluoroalkyl substances (PFAS) in shiner surfperch, as mentioned above, as part of a broader assessment of the long-term abiotic and biotic fate of PFAS in the Bay (Sanchez-Soberon et al. 2020). Predicted concentrations in sediment and water obtained from a water and sediment fate box model were used to calculate levels of PFOA and PFOS in fish tissue by using a bioaccumulation model described in Larson et al. (2018). The model calculates the concentrations of PFAS in fish tissue based on its dietary pattern and water intake.

For PCBs and PFAS, the same or similar models can be used with updated information on contaminant distributions and food web structure as available. Similar models can be developed and applied for other CECs, by identifying and characterizing the primary pathways of contaminant uptake and removal for the species of interest.

![Conceptual diagram illustrating organisms included in the PCB food web model and their trophic interactions (Gobas and Arnot 2010).](image)
3.3 SUMMARY

Studies of PCBs to date support a management focus on contaminated margin areas. Previous PCB monitoring and modeling have demonstrated the need for a higher-fidelity understanding of contaminant trends through monitoring and for higher-resolution modeling to provide quantitative information for management decisions. For many CECs, concentrations and health risks may also be relatively high in margin areas where inputs from stormwater and wastewater enter the Bay via channels and sloughs in margin areas. However, some CECs or other contaminants may be discharged from deep-water outfalls, directly deposited through atmospheric deposition, or enter from the Delta, so any modeling framework adopted should have flexibility to incorporate these loads as inputs as needed. To date, no comprehensive fate and transport modeling effort has been undertaken in the Bay that can answer the management questions for contaminants and sediment. The NMS hydrodynamic modeling framework is the highest fidelity modeling framework available, with tens to hundreds of cells within the PMUs of interest; this may be sufficient to reproduce some of the spatial gradients observed in the empirical data for these locations and other sites in Bay margin areas, particularly for characterizing processes of contaminants primarily occurring in the water column. However, at present it does not include a mechanistic sediment transport model, which is important for fate and transport modeling of PCBs and other sediment-associated contaminants.
4 MODEL CAPABILITY REQUIREMENTS

Previous work by SFEI through the RMP and other efforts provides important information for identifying and quantifying the key processes important to addressing priority management questions for contaminants in the Bay. Quantitative modeling provides a computational framework to describe those key processes. A model provides a mechanistically linked description of processes so that the system being modeled can be better understood. Figure 5 from the U.S. Environmental Protection Agency (EPA) shows a simple, but comprehensive, view of the most common processes involved in the fate of contaminants in surface water ecosystems (USEPA 2009). While modeling frameworks are available that consider all of these processes, full application of these models requires significant resources in terms of expertise, data, time, and cost. Further, increasing model complexity can often increase model uncertainty. Most importantly though, in effectively addressing site management questions, many processes may be secondary or negligible to the larger management goals. The following section briefly considers the physical, chemical, and biological processes important to the management questions for this effort and provides a brief assessment of their importance for consideration in the present contaminant fate modeling strategy.

Figure 5. Overview of contaminant fate and transport processes (USEPA 2009).
4.1 PHYSICAL

The contaminants of interest for this modeling strategy (i.e., PCBs and various CECs) are transported in the water in a dissolved phase, in or on particles, or some combination of the two. Therefore, the physical processes of concern are associated with the hydrodynamics (e.g., tides and currents) and subsequent sediment transport in the Bay. Since contaminant sources are a primary concern for PCBs and some CECs, one of the first physical processes to characterize is the plumes associated with tributaries, wastewater discharges, and other input locations. Freshwater plumes enter the Bay and dilute, often depositing sediment throughout their area of influence that may be reworked by tides later. Any modeling framework must be able to approximate a freshwater dilution field for both tributaries and wastewater discharges across seasons. Additionally, the subsequent transport and fate of the water and sediment discharged into the Bay due to tides and other receiving water circulation must be simulated for both near- and far-field transport, as well as over event and seasonal scales, ultimately extending to the annual and decadal scales needed to anticipate long-term effects of management actions for persistent contaminants.

In addressing contaminant sources and distribution in Bay sediment, the model must track sediment associated with local tributaries and far-field sediment delivery from the whole Bay. By tracking these primary sources of sediment to and from the bed, both reduction in bioavailable contaminants due to burial and degradation (i.e., recovery) and recontamination due to erosion, mixing, and transport can be investigated. The modeling framework should be able to simulate the local deposition and subsequent erosional processes that act on the contaminant distribution profiles of sediment in areas of interest.

For PCBs and other persistent bioaccumulative contaminants, the ability to forecast the recovery of surface sediment (i.e., generally the top 10–15 cm) over long periods of time is critical to addressing the effectiveness of management options. The surface water modeling can address the transport, deposition, and erosion of sediment to and from the sediment bed, but a sound mechanistic description of contaminant transport and fate (e.g., bioturbation, burial) within the sediment bed is required to address management options for sediment recovery. A model capable of generating results such as those in Oram and Davis (2008) (Figure 6) are necessary for supporting management options.

The physical modeling needs to highlight the importance of sediment transport at both the PMU and larger segment scales in the Bay. To adequately address the physical transport and fate of contamination at all scales requires a robust foundational understanding of sediment transport. Therefore, the model must be able to adequately resolve important sediment transport processes in the Bay.

Remediation of contaminated hotspot areas within PMUs and other margin areas is a type of management action that will receive consideration. This could occur through removal, capping,
or sequestration (e.g., activated carbon amendments). The model should be able to assess the projected impacts of these actions on contamination at local (within PMUs or other specific sites) and regional (segment) scales. While management attention for contaminants will have an initial focus on PMUs, forecasting impairment at a regional scale is also of interest. The model should be able to forecast the net regional (segment scale) impact of focused management of PMUs and other contaminated sites along with broader regional actions that reduce inputs from stormwater and wastewater.

4.2 CHEMICAL

As mentioned previously, the contaminants of greatest interest for this modeling strategy (PCBs and various CECs) are transported in the water in a dissolved phase, in or on particles, or some combination of the two. The proportion of contaminant concentration in water or solids (e.g., sediment) can be described by equilibrium partitioning or dynamically modeled through simulation of process kinetics. Initially, the classes of contaminants that will be investigated in this effort will focus on those either dominantly in a phase sorbed to solids (e.g., PCBs) or dissolved (e.g., some CECs), to reduce the number of factors needed to calibrate and validate the physical processes in the model. Thus, mechanisms for dynamic partitioning will not need to be initially simulated; even in cases where dynamic processes are important, equilibrium assumptions may provide a first order illustration of the bounds. However, eventual inclusion of dynamic processes should be considered as a future need in the modeling and could affect both short-term fate after discharge as well as long-term recovery. Chemical transformation and degradation are also processes that affect contaminant concentrations over time. The need for explicit simulation of these processes is not anticipated for PCBs, but is anticipated for some CECs, as the impacts of many CECs may be linked to degradation to more toxic products or other dynamic transformation or transport processes.

Ideally, the modeling should be able to reproduce distributions such as dilution gradients in the short to long term for water column constituents (e.g., using behavior of a conservative tracer as one bounding scenario, and exploring a range of parameterizations for transformation and/or partitioning to predict the possible fate of chemicals for which these characteristics are currently poorly known). Similarly, for hydrophobic or other sediment-bound contaminants, reproducing gradients (both lateral and vertical extent) of contaminants in surface sediment at both local (PMU and other tributary discharge points) and regional (Bay segment) scales would be desirable for evaluating the likely long-term fate of pollutants under different loading and management scenarios.
Figure 6. Segment-scale sediment recovery profiles over time produced from the Oram and Davis (2008) multi-box modeling work.

### 4.3 BIOLOGICAL

For PCBs and some CECs, accumulation in fish will be a key endpoint of concern, so the exposures of interest will include the foraging areas of fish and their principal prey items, at seasonal to decadal time scales. Sediment PCB concentrations are known to vary over moderate to small spatial scales; concentrations at legacy contaminated sites such as Hunters Point and
Seaplane Lagoon decrease by orders of magnitude within a few hundred meters of the most contaminated points. Depending on the motility and foraging characteristics of resident biota, tissue concentrations might mirror sediment distributions on these small spatial scales, or integrate exposure from a wider spatial extent. Even within a species, behavior may differ on seemingly small spatial scales. In the Port of Redwood City, small fish may be able to remain within a small area due to the continuous availability of hard structures and deep-water refuge, whereas in nearby Steinberger Slough, the same small fish species might need to transit a greater distance to deeper water refuge on ebb tides. Thus, the spatial extent of exposure integration may differ in these areas, even for the same species. Other PMUs and margin areas might similarly include fish with different foraging habits and thus different exposure characteristics. The modeling should allow for identification of hotspots within the foraging ranges of fish that may contribute disproportionately to bioaccumulation; this could support targeted management actions that have a relatively high impact on reducing bioaccumulation.

For bioaccumulation in fish, despite the possibility of spatial differences in habitat use, a simple exposure model integrating sediment pollutant concentrations across fixed spatial extents for a given species should be attempted first, and may be sufficient for most cases. Most available open Bay and margin data report composite concentrations from the top 5–10 cm of sediment for each site, but there may be cases where deeper or shallower burrowing benthic organisms comprise important components of fish diets. More complex models can be considered and developed as needed.

For many CECs, bioaccumulation may not be the most important exposure pathway. For example, for 6PPD-quinone toxicity to salmonids, it is the immediate exposure to the chemical for a short period that causes mortality (or unpublished, other effects). Similarly, pulses of stormwater runoff have been shown to affect herring roe, potentially related to PAHs. For CECs like these, a pulse of contamination or pseudo-persistence (continuous presence due to constant inputs) in combination with toxicity may lead to adverse impacts. These types of exposures are also often important for other species, such as aquatic invertebrates. For CECs where these shorter-term modes of toxicity are important, a relatively fine-scale (both spatial and temporal) understanding of exposure may be needed to characterize zones of significant risk.

In summary, the model should be capable of representing the exposure fields and durations for species of concern in a manner that supports cost-effective management actions to reduce exposure. The dimensions of exposure that should be considered include three-dimensional characterization of contaminant distribution in water and sediment (addressing lateral gradients as well as vertical gradients in sediment), as well as changes in these distributions over time (from daily to decadal time scales).
4.4 DESIRED OUTPUTS

One of the principles of developing and using models at contaminated sites from USEPA (2005) is to determine what model output data are needed to facilitate decision-making. In other words, what information can the model provide to help address the management questions and inform decisions. In identifying outputs, it is recognized that even detailed and complex models only represent an approximation of the system, and given inherent simplifications, data gaps, and uncertainties, their outputs should be considered as an estimated range of potential outcomes and their relative probabilities. Overall, there are six key areas of anticipated model outputs that will assist with addressing the contaminant management questions. These are:

1. **Distribution fields (water column and sediment concentrations, three-dimensional) for contaminant loads from tributaries and other pathways over time.** The model must have the ability to investigate the dilution and potential depositional footprint of ongoing sources of contaminants to the Bay (past example provided in Figure 7). This information can guide assessment of risk, monitoring, and management. The model should allow assessment of exposure times of organisms in water and sediment, especially in areas directly downstream of inputs of stormwater, wastewater, river inflow, and other pathways.

2. **Rates of sediment accumulation in areas of interest on the margins and Bay segments.** The model must be able to address the erosion and deposition of sediment in areas of interest starting with the individual PMUs. Eventually, a robust model of sediment accumulation rates throughout Bay segments will support regional and whole Bay contaminant management questions.

3. **Surface sediment and contaminant distributions.** Investigation of the nature (e.g., concentration) and spatial extent of contamination. The linkage of modeled processes and site data allow for a deeper understanding of the processes governing sediment recovery and therefore can better inform management decisions.

4. **Sediment recovery depth profiles.** Recovery depth profiles similar to the Oram and Davis (2008) multi-box model (past example provided in Figure 6), for both margin areas and at the regional scale, provide not only an integration of the physical, chemical, and biological processes responsible for sediment recovery; they provide an intuitive method for evaluating the trajectory of sediment recovery at given locations. Further, the profiles must be grounded with field-collected sediment data. The profiles directly support the evaluation of present-day recovery as well as the outcomes of potential management actions.

5. **Recovery of sediment contaminant concentrations over time.** Simulations of not only the horizontal and vertical distribution of contaminants as described above, but how those distributions change site-wide over time all for management actions need to be evaluated in terms of spatial impacts (past example provided in Figure 8). This requires
a model that addresses the quality and quantity of incoming sediment accumulating in areas of interest.

6. *Biota contaminant exposure and concentrations.* Although simple equilibrium correlation models of ambient sediment to biotic concentrations of bioaccumulative contaminants may suffice for PCBs and other legacy pollutants, the capability to add more dynamic simulations of exposure for CECs with acute or short-term chronic modes of toxicity is desirable.

Figure 7. Example of a model-forecasted distribution field for microplastic particles near the sediment bed in wet weather (Sutton et al. 2019).
Figure 8. Hypothetical forecasted recovery of surface (top 5 cm) sediment concentrations for the foraging area of shiner surfperch within a PMU under different load reduction scenarios. Adapted from Yee et al. (2019).

4.5 SUMMARY TABLE OF MODEL REQUIREMENTS

In summary, based on review of all of the management questions, previous modeling efforts, and modeling needs, a capabilities matrix has been developed (Table 1). The table follows the general guidelines for model development and use from USEPA (2005, 2017). The general requirement areas include a peer-reviewed platform, user technical expertise, institutional support, and mechanistic processes. This is not intended to be a comprehensive list, but an overview of the key capabilities needed for the present studies.

It should be noted that this model only covers in-Bay fate processes. The model will be able to incorporate time-variable inputs from all pathways in a spatially explicit manner. Fate processes upstream of the Bay will need to be addressed, as needed, by watershed models.
Table 1. Summary of modeling capabilities needed for addressing contaminant management questions.

<table>
<thead>
<tr>
<th>Requirement</th>
<th>Capabilities</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peer-reviewed platform</td>
<td>● Established history of peer-reviewed applications in similar management scenarios</td>
</tr>
</tbody>
</table>
| User technical expertise and available resources | ● Accessible to capable technical staff  
● Available training resources  
● Freely available and open-source software |
| Community/institutional support    | ● Ties into and leverages existing model development efforts  
● Long-term developer training support  
● Long-term developer support for model improvements and upgrades  
● Local Bay Area community acceptance and support |
| Mechanistic processes              | ● Hydrodynamics and sediment transport processes:  
  - Spatially and temporally explicit inputs of water and sediment  
  - Scalable grid  
  - Local plume dynamics  
  - Tidal circulation  
  - Basic deposition and erosion processes with multiple sediment grain size classes  
  - Tracer studies  
● Chemical processes:  
  - Spatially and temporally explicit inputs of contaminants  
  - Tracking sediment-bound and dissolved contaminant transport in water column  
  - Contaminant tracking in sediment bed at vertical scales of interest (centimeter)  
  - Contaminant fluxes and phase changes at the sediment water interface  
  - Partitioning and transformation  
● Biological processes:  
  - Sediment bed physical mixing  
  - Tracking concentrations in water and sediment for exposure pathway quantification |
5 STRATEGIC AND TECHNICAL APPROACH

The overall goal of this strategy is to outline an approach for developing and applying quantitative in-Bay models to support addressing management questions and evaluating management actions for PCBs, various CECs, and fine sediment. The workplan addresses, or contributes to addressing, current and future management questions articulated in the RMP strategies for these constituents. Table 3 provides an overview of the workplan activities developed herein.

Based on current information needs, the approach will initially focus primarily on the PMU scale where major contaminant inputs of PCBs and CECs occur and the most concentrated reservoirs of sediment contamination are located. While there are similarities in the PMUs that have been outlined in the margins conceptual model report (Jones et al. 2012) and the PMU conceptual model reports (Davis et al. 2017; Yee et al. 2019, 2021), all PMUs have unique characteristics requiring individual study.

While the PMUs are unique, they provide excellent case studies for small-scale model development that reduce complexity. The lessons learned from the smaller-scale studies can be applied to the development of a large-scale modeling framework to address Bay-wide management questions. As outlined in previous sections, a high-fidelity (resolution) description of local hydrodynamics is required to quantify transport and recovery processes in an individual PMU. Fortunately, much of the groundwork for this has been developed as part of the NMS efforts (King et al. 2020). Further, only local sediment transport processes, and minimal chemical and biological process descriptions are required to begin to answer the management questions. Table 2 summarizes how modeling components at various scales can address the management questions. The majority of the management questions are addressed at the scale of local geomorphic features. The footnotes at the end of the table provide definitions of the scales consistent with the NMS work.

Whole-Bay modeling for assessing the fate of PCBs, various CECs, potentially other contaminants, and fine sediment is also needed by managers. While the complexity of this model is high, the lessons learned from the PMU modeling efforts can be used to help reduce complexity where appropriate and reduce overall uncertainty as opposed to starting with a Bay-wide effort. An overarching workplan that includes development of PMU and whole-Bay models is provided in Table 3. The key modeling phases of the workplan are outlined further in the sections below.
Table 2. Summary of management questions addressable by an in-Bay fate model and the relevant spatial and temporal scales of modeling needed.

<table>
<thead>
<tr>
<th>Question</th>
<th>Notes</th>
<th>Relevant Spatial Scales&lt;sup&gt;1&lt;/sup&gt;</th>
<th>Relevant Temporal Scales&lt;sup&gt;1&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCB1: What are the rates of recovery of the Bay, its segments, and in-Bay contaminated sites from PCB contamination?</td>
<td>Sediment recovery is dependent on stable net deposition of clean sediment.</td>
<td>Coincident with region in question. Key risk points for shiner surfperch are on the scale of priority management units geomorphic features.</td>
<td>Recovery occurs over decades; but seasonal processes (e.g., wet seasons) are generally responsible for the majority of recovery</td>
</tr>
<tr>
<td>PCB1a: What would be the impact of focused management of PMU watersheds?</td>
<td>The key assumption is that recovery of local PMUs is reduced by continued PCB delivery from local watersheds.</td>
<td>Local PMU geomorphic features with consideration of Bay segments</td>
<td>Seasonal, tidal, and storm event scale</td>
</tr>
<tr>
<td>PCB1b: What would be the impact of management of in-Bay contaminated sites, both within the sites and at a regional scale?</td>
<td>Bay segment scale is best investigated by looking at average PCB trends.</td>
<td>Bay segment with consideration of local PMUs and geomorphic features</td>
<td>Seasonal to interannual</td>
</tr>
<tr>
<td>CEC1: Which CECs have the potential to adversely impact beneficial uses in the Bay?</td>
<td>Need to estimate distributions of concentrations in space and time.</td>
<td>All spatial scales</td>
<td>All temporal scales</td>
</tr>
<tr>
<td>CEC3: What are the physical, chemical, and biological processes that may affect the transport and fate of individual CECs or groups of CECs in the Bay?</td>
<td>CECs will generally need to be considered on the basis of their individual chemistry and primary sources.</td>
<td>Geomorphic features, Bay segments, and whole Bay</td>
<td>Event to interannual</td>
</tr>
<tr>
<td>CEC5: Are the concentrations of individual CECs or groups of CECs predicted to increase or decrease in the future?</td>
<td>CECs will generally need to be considered on the basis of their individual chemistry and primary sources</td>
<td>Geomorphic features, Bay segments, and whole Bay</td>
<td>Seasonal to interannual</td>
</tr>
<tr>
<td>CEC6: What are the effects of management actions?</td>
<td>Forecasting distributions of concentrations in space and time in response to changes in loading.</td>
<td>All spatial scales</td>
<td>All temporal scales</td>
</tr>
</tbody>
</table>
Table 2. Summary of management questions addressable by an in-Bay fate model and the relevant spatial and temporal scales of modeling needed.

<table>
<thead>
<tr>
<th>Question</th>
<th>Notes</th>
<th>Relevant Spatial Scales</th>
<th>Relevant Temporal Scales</th>
</tr>
</thead>
<tbody>
<tr>
<td>CEC: What is the predicted spatial and temporal extent of potential impact of CECs?</td>
<td>More explicit statement of CEC1</td>
<td>All spatial scales</td>
<td>All temporal scales</td>
</tr>
<tr>
<td>CEC: What are areas of management interest where CECs should be monitored to assess S&amp;T in water and sediment?</td>
<td></td>
<td>Local geomorphic features to Bay segment</td>
<td>Event to seasonal</td>
</tr>
<tr>
<td>Sed3: What are the sources, sinks, pathways and loadings of sediment and sediment-bound contaminants to and within the Bay and subembayments?</td>
<td>Question encompasses movement within the Bay</td>
<td>Local geomorphic features to Bay segment</td>
<td>Seasonal to decadal</td>
</tr>
<tr>
<td>Sed4: How much sediment is passively reaching tidal marshes and restoration projects and how could the amounts be affected by management actions?</td>
<td></td>
<td>Local geomorphic features</td>
<td>Occurs over decades, but strongly driven by annual wet season processes</td>
</tr>
<tr>
<td>Sed5: What are the concentrations of suspended sediment in the Estuary and its segments?</td>
<td></td>
<td>Bay segment</td>
<td>Seasonal to interannual</td>
</tr>
</tbody>
</table>

Notes:

1 The approximate distance ranges of spatial scales are as follows:

- Bay (100+ km)—Areas within the Bay do not need to be distinguished at this scale.
- Segment (10+ km)—Differences among Bay segments (Suisun, San Pablo, etc.) are needed.
- Sub-segment (1–10 km)—Areas within segments (e.g., east vs. west shoreline) need to be distinguished.
- Local (0.1–1 km)—Geomorphic features (intertidal mudflats, margins mudflats, main channel, etc.) are differentiated. Generally consistent with PMU scales.

Temporal scales to be considered include:

- Decadal (10+ years)—Needed for persistent contaminant fate, long-term geomorphic change.
- Interannual (1+ years)—To distinguish wet vs. dry year processes and responses.
- Seasonal (weeks to months)—To distinguish wet vs. dry season processes and responses.
- Tidal (days to weeks)—Differentiation between portions of tidal (spring/neap) cycles.
- Event (hours to days)—Periods during and around discharge events (for acute or chronic toxicity of CECs or other pollutants).
Table 3. Details of five-phase workplan.

<table>
<thead>
<tr>
<th>Task/Phase</th>
<th>Sub-tasks</th>
<th>Description</th>
<th>Duration</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>San Leandro Bay (SLB) Model Development and Evaluation</td>
<td>1 Year Starting Q3 2022</td>
<td>$150k</td>
<td></td>
</tr>
<tr>
<td>1.1</td>
<td>Define local model goals and tasks in terms of management questions (focus on PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.2</td>
<td>Compile sediment boundary conditions for tributaries and local sediment evaluation data (focus on PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.3</td>
<td>Evaluate NMS model grid</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.4</td>
<td>Setup diagnostic model for local SLB simulations for dry and wet conditions scenarios (focus on sediment associated PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>Conduct diagnostic model simulations and compare with available sediment data (e.g., accumulation rates, sediment chemistry) and iteratively refine parameters (e.g., boundary conditions) to refine model</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.6</td>
<td>Develop additional scenarios for CEC model evaluation and diagnostics (focus on dissolved phase transport)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.7</td>
<td>Reporting on model analysis and lessons learned for larger scale model</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Steinberger Slough/Redwood Creek (SS/RC) Model Development</td>
<td>1 year starting Q4 2022</td>
<td>$150k</td>
<td></td>
</tr>
<tr>
<td>2.1</td>
<td>Define local model goals and tasks in terms of management questions (focus on PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.2</td>
<td>Compile sediment boundary conditions for tributaries and local sediment evaluation data (focus on PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.3</td>
<td>Evaluate NMS model grid</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Task/Phase</td>
<td>Sub-tasks</td>
<td>Description</td>
<td>Duration</td>
<td>Cost</td>
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<td>--------</td>
</tr>
<tr>
<td>2.4</td>
<td>Setup diagnostic model for local SLB simulations for dry and wet conditions scenarios (focus on sediment associated PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>Conduct diagnostic model simulations and compare with available sediment data (e.g., accumulation rates, sediment chemistry) and iteratively refine parameters (e.g., boundary conditions) to refine model</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.6</td>
<td>Develop additional scenarios for CEC model evaluation and diagnostics (focus on dissolved phase transport)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.7</td>
<td>Reporting on model analysis and lessons learned for larger scale model</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Whole-Bay Model Development</td>
<td>2 years starting in 2023</td>
<td>$500k</td>
<td></td>
</tr>
<tr>
<td>3.1</td>
<td>Evaluate model goals and tasks in terms of management questions (focus on PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.2</td>
<td>Develop Boundary Conditions</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Compile baywide sediment boundary conditions for tributaries and delta (focus on PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Compile model evaluation data for sediment and contaminant accumulation rates</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Develop 3D description of SF Bay sediment bed</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.3</td>
<td>Diagnostic Sediment transport modeling</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Setup diagnostic model for bay wide sediment transport simulations for dry and wet conditions scenarios (focus on sediment associated PCBs)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 3. Details of five-phase workplan.

<table>
<thead>
<tr>
<th>Task/Phase</th>
<th>Sub-tasks</th>
<th>Description</th>
<th>Duration</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4</td>
<td>Conduct diagnostic model simulations and compare with available sediment data (e.g., accumulation rates, sediment chemistry) and iteratively refine parameters (e.g., boundary conditions) to refine model</td>
<td>Conduct model calibration and validation with metrics of primary interest (Subtask 3.1)</td>
<td>3.4</td>
<td>TBD</td>
</tr>
<tr>
<td>3.5</td>
<td>Conduct prognostic model analysis</td>
<td>3.5</td>
<td>TBD</td>
<td></td>
</tr>
<tr>
<td>3.6</td>
<td>Develop additional scenarios for CEC model evaluation and diagnostics (focus on dissolved phase transport)</td>
<td>Reporting on model analysis and lessons learned for future modeling</td>
<td>3.6</td>
<td>TBD</td>
</tr>
<tr>
<td>4</td>
<td>Bioaccumulation Model Development</td>
<td>2 years starting Q1 2023</td>
<td>4</td>
<td>TBD</td>
</tr>
<tr>
<td>4.1</td>
<td>Develop and validate a bioaccumulation model suitable for application with the PMU models.</td>
<td>4.1</td>
<td>TBD</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>Model Maintenance and Future Application</td>
<td>Ongoing</td>
<td>5</td>
<td>$150k/yr</td>
</tr>
<tr>
<td>5.1</td>
<td>Investigate long-term scenarios, maintain the model, and provide model applications to other management challenges in the Bay.</td>
<td>5.1</td>
<td>TBD</td>
<td></td>
</tr>
</tbody>
</table>

5.1 MODELING STRATEGY STEPS

The approach to quantitative modeling will include the following general steps. The work will be conducted at scales appropriate to the phases outlined above (e.g., specific PMU scale, whole Bay)

1. Develop a conceptual site model that identifies contamination nature and extent and processes relevant to ongoing contamination and recovery. Use the conceptual model to generally address the management questions.
2. **Identify data needs and gaps.** Using the management questions, develop a matrix of where adequate information exists and where the highest uncertainty exists. Identify key areas of uncertainty so that both empirical and modeling needs and gaps can be identified.

3. **Determine model output needed.** Outline the desired model outputs that are necessary to address the management questions.

4. **Conduct a complete modeling study.** Utilize modeling tools to conduct a complete modeling study (as described in USEPA [2017] and summarized here), including model calibration and validation where applicable.

5. **Use modeling results in conjunction with empirical data to refine the conceptual model.** Using the best available information, refine the conceptual model and address the site management questions and consider uncertainty.

Steps 2 and 5 includes refining the conceptual site model to identify the key areas of uncertainty where additional information and assessment may be needed. A conceptual site model should be developed that identifies the processes and the major sources of uncertainty that may affect the effectiveness of potential management actions. Model assumptions, limitations, and the results of the sensitivity and uncertainty analyses should be clearly documented and presented to decision-makers (USEPA 2009).

### 5.2 SAN LEANDRO BAY WORKPLAN

The SLB PMU offers a prime opportunity to develop and validate a quantitative contaminant process model to inform management. Significant progress has already been made on Modeling Strategy Steps 1, 2, and 3, as documented in a conceptual model report (Yee et al. 2019), and a relatively substantial body of field data is also available. This work is considered Phase 1 of the modeling workplan.

Distributions of PCBs and other pollutants are available at fairly fine spatial scales for different time periods in SLB. Data exist from an extensive subtidal survey in 1998 (Daum et al. 2000), a core from a wetland adjoining SLB in 2006 providing hints of system response to the ban of PCBs (Yee et al. 2011), and a subsequent survey in 2016 (Davis et al. 2017) repeating some of the subtidal sites in the 1998 study and including samples from some of the tributaries discharging to SLB. The latter study also included fish collection from various areas in SLB and adjacent tributary channels, indicating significant spatial variation in biota for some sites.

In addition to the relatively abundant sediment and biota contamination data, there are recent and ongoing PCB remediation sites in the watersheds upstream of SLB. One site formerly occupied by Union Pacific Railroad adjacent to the Oakland Coliseum, and locations in the channel up and downstream, showed extensive contamination by PCBs, with concentrations up to 46,000 µg/kg in sediment (GHD 2017). Other historical land uses and inputs upstream along the channel may have also contributed to the observed contamination. Remediation actions for
the site are in the planning stages. Damon Slough was recently dredged from Lion Creek to the mouth of the Slough. In another watershed discharging to SLB, a contaminated General Electric site was closed, with remediation actions (capping) completed. The remediation actions taken at these sites are expected to decrease emissions and thus reduce loading to SLB. Impacts on loads to their respective tributaries may be difficult to quantify, but illustrative scenarios (e.g., using average discharges from regional urban watersheds not containing source sites as projected post remediation loads) may be useful to estimate the degree of recovery that might be expected. Water quality managers are very interested in assessing the impact of these cleanup actions on PCB concentrations in fish in SLB.

The hydrodynamic model for the NMS already includes a mesh within SLB; this is likely sufficient to resolve transport processes to yield reasonable estimates of PCB gradients from the discharging tributaries. Additional data to calibrate and validate discharge flows and sediment transport during storm events, and resuspension processes and tidal flows during dry season periods, will be collated for developing a quantitative mechanistic model.

The SLB area is also of interest for CECs, due to its semi-enclosed morphology (restricting tidal exchange and dilution by water from the open Bay), and the proximity of extensive urban land uses and associated impervious surfaces. SLB was included in a pilot, non-targeted-analysis of CECs in water that indicated a large number and high abundances of compounds associated with urban stormwater (Overdahl et al. 2021), and played a significant role in directing increased attention to stormwater as a source of CECs to the Bay. For these reasons, SLB has been selected as a location for near-field stormwater monitoring as part of the newly revised RMP S&T monitoring design. SLB was also among the sites with the highest abundance of anthropogenic microparticles (much of it likely tire wear particles) in stormwater (Sutton et al. 2019), which is not surprising given the proximity of heavily trafficked I-880, Oakland Airport, and other urban development in the adjoining watersheds.

Even with sparse data, especially for some contaminants such as CECs, the model framework can provide a basis for hypothesis testing and other exploration to identify the most sensitive parameters affecting the fate of CECs and biotic exposure. From that information, monitoring plans can be devised or revised to advance understanding of contaminant processes, and iteratively improve projections of outcomes for various management alternatives.

### 5.3 STEINBERGER SLOUGH/REDWOOD CREEK (SS/RC) WORKPLAN

A module for the SS/RC PMU, another area of particular interest to managers, will be developed in Phase 2. Similar to SLB, a recent conceptual model report (Yee et al. 2021) has synthesized much of the available information for the Modeling Strategy Steps 1, 2, and 3. The Redwood Creek PMU presents another prime opportunity for model development for similar
reasons as outlined for SLB. To briefly summarize, reasons to prioritize work on this PMU include:

- An existing and increasing body of field data (currently consisting of historical sampling of sediment and fish, long-term monitoring of sport fish in one location, monitoring of stormwater runoff from several watersheds discharging to the area, a PMU-wide survey of sediment cores and passive samplers in 2021, and plans for PMU-wide sampling of surface sediment and prey fish in 2022)
- Ongoing and planned remediation of contaminated source areas in the watershed
- Hydrodynamics and other physical characteristics that may tend to retain contaminants and thus exacerbate the possibility of localized ecosystem effects and allow stronger linkages between management intervention and system response at temporal and spatial scales of interest
- A preliminary hydrodynamic modeling framework from the NMS
- Inclusion of a near-field CEC monitoring site for RMP S&T.

5.4 WHOLE-BAY MODELING WORKPLAN

A whole-Bay model for assessing the fate of PCBs, various CECs, potentially other contaminants, and fine sediment is also needed by managers. As part of Phase 1, a whole-Bay model will start with a relatively simple tracer analysis building on the work for SLB using the NMS model. The focus of the model would be to investigate dissolved-phase CEC transport and investigate how CECs dilute as they are transported from discharge areas. Similar to the prior work on microplastics (Sutton et al. 2019) and PFAS (Sedlak et al. 2018), projections of transport and dilution of concentrations can be readily produced based on hypothetical loading scenarios. The NMS hydrodynamic model is ideal for investigating CEC discharges in Bay margin areas and their subsequent transport throughout the Bay. The primary work in Phase 1 will be to utilize the NMS model with conservative tracers introduced as loadings at locations of interest into the model. The transport and fate of these discharges will provide quantitative information on the transport patterns and areas of influence, addressing management questions as well as informing the needs in the long-term modeling plan implemented in Phases 3 and 4.

An overarching workplan that includes development of PMU and whole-Bay models is provided in Table 3. Development of a whole-Bay dilution model will be a straightforward extension of the flow modeling that has been done by the NMS, and will be included in Phase 1 of the overall modeling workplan. Further development of the whole-Bay model will be completed in Phases 3 and 4. A module for the SS/RC PMU, another area of particular interest to managers, will be developed in Phase 2. An updated bioaccumulation model will be developed in Phase 4 to synthesize biota data collected in the past 20 years to link
concentrations in sediment and water to the endpoints of regulatory interest, and as a necessary component of a TMDL.

5.5 LONG-TERM MODELING WORKPLAN

As presented in Table 3, an overarching five-phase workplan will guide the future progression of model development.

While the modeling Phases 1 and 2 can rely upon the existing NMS modeling work for specific PMUs and baseline whole-Bay transport, future modeling must also incorporate sediment transport processes for fine-grained sediment to support the management questions for PCBs and other hydrophobic contaminants. While the DFM model used for the NMS efforts may be appropriate, a model and data gaps assessment will need to be conducted through the development of a conceptual model to ensure the model selected for the whole-Bay model can answer the management questions.

In Phase 3, a whole-Bay conceptual model of fine sediment and contaminant (PCBs and CECs) fate and transport will be developed to highlight key processes and further develop key modeling capabilities identified here. Fortunately, much of this work has been conducted (particularly for PCBs), but this effort will include an expert review of existing models to determine their suitability for contaminant and sediment fate and transport. Based upon that work, early in Phase 3 the team will select an existing numerical modeling framework and include key processes (e.g., sediment transport, chemical partitioning) important to contaminant transport in the Bay. For PCBs, the model will initially be focused on hotspot contributions to the Bay and then be expanded to investigate all primary sources and sinks of contamination in the Bay. Additional PMUs (beyond SLB and SS/RC) can be readily incorporated as study areas in Phase 3, not only to address specific management questions, but to also further calibrate and validate the model for whole-Bay use. While the PMUs are unique, the whole-Bay modeling approach in Phase 3 will provide the most robust support for addressing management questions in a long-term modeling strategy. For CECs, the modeling will initially be focused on informing, and being informed by, CEC monitoring in stormwater and in the Bay as part of the new design of RMP S&T monitoring (which includes near-field stations and wet season sampling). The modeling will be useful in identifying areas of potential concern given knowledge and assumptions about loading from stormwater, wastewater, and other pathways.

Once a whole-Bay model is calibrated and validated for addressing the management questions in Phase 3, broader contaminant profiles from the RMP will be included into the model so that future Bay recovery can be evaluated under different scenarios including, for example, individual PMU remedial activities and modifications in uses and loading of various CECs.
The model will additionally be developed to support bioaccumulation modeling in Phase 4 to fully support Bay management and TMDL goals. The development will necessarily include long-term model scenarios over decades, which include the effects of climate change on local watershed inputs (water and sediment) and sea level rise that may impact long-term contaminant recovery. The long-term scenarios, general model maintenance, and application to other management challenges in the Bay can be incorporated into an ongoing Phase 5 of the long-term strategy.

The modeling strategy laid out here is developed to be the basis of an overall monitoring and modeling strategy for the Bay. Maintained into future years, the modeling framework can be used for broader long-term goals, such as evaluating the trends in annual status and trends data. A modeling framework, as laid out here, can provide a platform that can be continually updated and refined as future data and modeling tools come available.
6 REFERENCES


