San Francisco Bay PCB Food Web Bioaccumulation Model

Final Technical Report

July 4, 2005

Prepared for the the Clean Estuary Partnership

by

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SCOPE

In response to the listing of the San Francisco Estuary as impaired by presence of PCBs, the San Francisco Regional Water Quality Control Board (Water Board) coordinated efforts on development of two models for use in interpreting effects of PCBs and identifying potential management actions required to address:

- a contaminant fate model to link PCB loading to the Bay to PCB concentrations in water and sediments;
- a food-web model to relate concentrations in water and sediment to levels in certain fish species.

The initial food web model was published as an RMP Technical Report in December 2003 (Gobas and Wilcockson, 2003). This original model included plankton, benthic detritovores, filter feeders and fish as ecological receptors.

In review of the original model, several potential refinements to the model were identified to increase its ecological relevance. The objective of these refinements is to provide the model with the capability to determine protective sediment PCB concentrations and to take into account effects on ecological as well as human receptors. Funding was provided by the Clean Estuary Partnership (CEP), a collaboration of the Bay Area Clean Water Agencies (BACWA), Bay Area Stormwater Management Agencies Association (BASMAA), and the Water Board, to add these refinements to the model and produce a peer-reviewed technical report documenting its usage. The ecological receptors that were incorporated into the model as part of the CEP effort are piscivorous birds (e.g. Double-crested Cormorant, *Phalacrocorax auritus*, and Forster's Terns, *Sterna forsterii*), and marine mammals (i.e. harbor seals, *Phoca vitulina*), as well as prey for each of the added species.

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ACKNOWLEDGEMENTS

The authors acknowledge the Clean Estuary Partnership (CEP) for their help and insights throughout the completion of the study as well as their financial support of the study.

We also would like to thank the many individuals who have provided crucial input. They include several members of the San Francisco Estuary Institute (SFEI) like Jay Davis, Bruce Thompson, Ben Greenfield, Jennifer Hunt and Sarah Lowe. They have contributed much advice and guidance as well as data and other information. We would particularly wish to acknowledge the comments and suggestions from Jay Davis and Andy Jahn. Their insights and direction were instrumental. We also acknowledge Rusty Fairey, Cassandra Roberts, and Marco Sigala from the Moss Landing Marine Institute for collecting and analyzing field data needed for parameterizing the model. We would also like to acknowledge data and information provided by Jim Harvey at Moss Landing Marine Laboratories, Myrto Petreas at the Hazardous Materials Laboratory, Kathy Hieb at the California Department of Fish and Game, Andy Jahn at the Port of Oakland, Barry Nickel at San Francisco State University as well as Emma Grigg and Jennifer Neale at University of California – Davis. Finally we acknowledge the work of Fred Hetzel of the Regional Water Quality Control Board, who was the overall manager of the PCB TMDL modeling process and Jay Johnson and Paul Salop from Applied Marine Sciences, Inc., for their assistance in the PCB food web modeling effort. We also thank Anissa Ip for her help with the layout of the report.

EXECUTIVE SUMMARY

The objective of this report is to document the development and evaluation of a food web bioaccumulation model for PCBs in San Francisco Bay. The purpose of this model is to estimate the concentrations of PCBs in a set of key species that reside in the Bay as a result of PCB concentrations in sediments and water in the Bay. The species that are the main focus of this study are the Double-crested Cormorant (*Phalacrocorax auritus*), the Forster's Tern (*Sterna Forsteri*), and the harbor seal (*Phoca vitulina richardsi)*, as well as three fish species that are frequently caught by fishermen in the Bay, i.e. shiner surfperch (*Cymatogaster aggregata*), jacksmelt (*Atherinopsis californiensis*) and white croaker (*Genyonemus lineatus*). The fish species are important end-points of the model because of their role in passing PCBs to fishermen. Double-crested Cormorants, Forster's Terns and harbor seals are included in the model because they have been identified as sensitive receptors of PCBs. The model can be used to determine what concentrations of PCBs in the water and sediments of the Bay need to be reached to achieve an adequate margin of safety in wildlife and humans exposed to PCBs in the Bay area. This information can be used as part of a Total Maximum Daily Loading (TMDL) characterization to formulate remedial actions to achieve desired water quality goals. This report also documents the application of the model with the goal to propose preliminary estimates of the total PCB sediment concentrations that are protective of the health of humans and wildlife consuming San Francisco Bay fish and shellfish.

The PCB food web bioaccumulation model for San Francisco Bay (which is attached with this report) is presented in an Excel spreadsheet. It consists of two modules, i.e. a *science* module and a *management* module. The *science* module includes the actual model including the model's external and internal variables, functional relationships, sensitivity analyses and model performance evaluations. It calculates the Biota Sediment Accumulation Factor (BSAF) for individual PCB congeners and total PCBs (ΣPCBs). The BSAF is the main output of the model and represents the relationship between the PCB concentrations in biota (C_B) and that in the sediment (C_S), i.e. BSAF = C_B/C_S. The

management module, includes a simple worksheet to conduct two types of calculations, i.e. "forwards" calculations to estimate the concentrations of PCBs in biota of the Bay from PCB concentrations in the sediments of the Bay and "backwards" calculations to calculate the PCB concentrations in the sediments of the Bay that are required to meet PCB concentration based criteria in fish and wildlife for the Bay. The backwards calculation is designed to determine target PCB concentrations in sediments that meet ecological and/or human health criteria.

The behavior of the model was investigated by conducting sensitivity analyses, model performance evaluations and uncertainty analyses. Sensitivity analyses were conducted to determine key variables in the model. The particulate organic carbon content in the water and water temperature were found to be key abiotic state variables in the model. Lipid content (and organic carbon content in phytoplankton), lipid absorption efficiency and non-lipid organic matter absorption efficiency are sensitive biological state variables and their selection has an important effect on the model outcome. The growth rate (e.g. phytoplankton and seals) and the coefficients used to calculate the growth rate (in invertebrates and fish) are also sensitive model state variables.

The model performance analysis involved the comparison of model predicted BSAFs to observed BSAFs. Observed PCB concentrations in sediments, fish and wildlife of the Bay and corresponding observed BSAFs were not utilized in the construction of the model. The observed concentration data can therefore be used as an independent test of the performance of the model. The analysis showed that predicted BSAFs are well within the range of the observed values. The model reproduced the PCB "congener patterns" observed in organisms of the SFB food web. The mean Model Bias of the BSAF of PCB congeners (MB), which is the geometric mean of the ratio of predicted and observed BSAFs among the 40 PCB congeners included in the analysis, ranged between 0.86 for female harbor seals to 1.32 for the white croaker (ideal = 1). This means that *on average* observed BSAFs of PCB congeners in the various species investigated are within 2 to 32% (depending on the species) of the predicted mean values. This indicates that the

apparent systematic error in the BSAFs of PCBs is small. The 95% confidence intervals of the mean model bias ranged between a factor of 1.5 for male harbor seals to 4.7 for white croaker. This indicates that while on average observed and predicted BSAFs vary by less than 32%, BSAFs of certain PCB congeners were over- or under-estimated by the model by several fold. The mean Model Bias of the BSAF of _PCB (MB^*), which is the geometric mean of the ratio of predicted and observed BSAFs of _PCB, ranged between 0.71 for Pacific oysters to 1.22 for male harbor seals (ideal = 1). This means that *on average* observed BSAFs of PCB congeners in the various species investigated are within 29% (depending on the species) of the predicted mean values. This indicates that the apparent systematic error in the BSAFs of _PCBs is small. The 95% confidence intervals of the mean model bias ranged between a factor of 2.0 for California mussels to 10 for male harbor seals. This indicates that while on average observed and predicted BSAFs vary by less than 29%, BSAFs of certain PCB congeners were over- or under-estimated by the model by several fold. The small sample size of the harbor seal samples also contributed significantly to the magnitude of the 95% confidence intervals of the MB*.

The uncertainty in the calculations of the BSAF of ΣPCB in fish and wildlife of San Francisco Bay was assessed by two methods. The first method relied on the application of field monitoring data to characterize the uncertainty in the model calculations. This method enhances the credibility of the model as model calculations are compared to actual observations. However, the spatial and temporal scale of the monitoring data available for the analysis as well as methodological limitations of the sampling programs that collected the data limit characterizing uncertainty in this fashion. This method uses the 95% confidence intervals of the mean model bias MB* to characterize the uncertainty in model predicted BSAFs of ΣPCB. The 95% confidence intervals of predicted BSAFs range between a factor of 2.0 for California mussels to 10 for male harbor seals. The second method of uncertainty analysis involved a stochastic technique, Monte Carlo Simulation (MCS), to assess the effect of inherent variability and error associated with the model state variables on the model outcome (i.e. the BSAF). This methodology is based on representing model state variables by statistical distributions rather than point

estimates. The distribution represents the uncertainty in the value of the model variable selected for use in the model. The distribution expresses how the state variables may vary due to geographical location, time of the year, differences in behavior among individuals of a species and other factors. The 95% confidence intervals calculated by Monte Carlo simulations ranged between a factor of approximately 2.5 for white croaker to a factor of 10 for male harbor seals. Monte Carlo simulations and model bias (MB^*) were found to produce comparable estimates of model uncertainty. This implies that the selection of the methodology for estimating model uncertainty is of little consequence, i.e. both methods arrive at comparable estimates of the magnitude of model uncertainty.

The model was applied in a *forwards* manner to calculate estimates of PCB concentrations in key species of the San Francisco Bay food web based on current concentrations of PCBs in San Francisco Bay. To accomplish this, PCB sediment concentration data from Regional Monitoring Program (RMP) monitoring stations were analyzed to represent the spatial distribution of PCB concentrations in the Bay. The ΣPCB concentration in the sediments of the Bay was found to be highly variable. Concentrations of ΣPCB in sediments sampled ranged by 3 orders of magnitude. ΣPCB concentrations in the Northern section of the Bay are lower than those in the Central and Southern sections of the Bay. A compilation of all sediment concentration data showed that a single log-normal distribution provides a satisfactory representation of the Bay wide distribution of ΣPCB concentrations in the sediments. This distribution has a geometric mean of 11.6 μg/kg dry sediment. The 95% confidence intervals of the geometric mean are equivalent to a factor of 7.4. This indicates that fish and wildlife in the Bay are exposed to PCB concentrations that vary substantially throughout the Bay.

Forwards calculations of the concentrations of PCB congeners and ΣPCB in fish and wildlife of the Bay, based on current distributions of PCB concentrations in the sediments of the Bay, showed a good agreement with the distributions of observed PCB concentrations. The geometric means of observed and predicted PCB concentrations were essentially identical (i.e. within 29% of the model predicted geometric mean). The

distributions of observed PCB concentrations fell within the distribution of predicted concentrations. The observation that the range of observed PCB concentrations in fish and wildlife species was in most cases smaller than the range of predicted PCB concentrations in the Bay can be expected to be due to differences in the spatial coverage of the sample collection programs. Sediment samples were taken from many more areas of the Bay than fish, bird egg and harbor seal samples. As a result, the PCB concentrations in some of the fish and wildlife species of the Bay may not represent the full spatial variation in _PCB concentrations that is expected by the model. It is also possible that the PCB concentration distribution for the Bay derived from the RMP monitoring data does not provide an accurate description of the actual distribution of the PCB concentrations in the sediments of the Bay or the PCB concentrations distribution experienced by the biota of the Bay. Perhaps, areas that are very contaminated with PCBs and areas that are devoid of PCB contamination are over presented in the sediment concentration database. To further explore this possibility it is important to further explore the spatial distribution of PCB concentrations in the Bay.

A comparison of the model predicted PCB concentration distributions to human health and ecological risk criteria shows that there is a substantial probability that various human health and ecological risk criteria are currently exceeded in the Bay (Table 4.8). Based on current PCB concentrations in the sediments of the Bay, the probability that PCB concentrations exceed threshold effects concentration in harbor seals is approximately 70 to 73% (for male harbor seals) and 56% (for female harbor seals). The probability of exceeding the excess human cancer risk of one in a hundred thousand (1.10^{-5}) is 82% and 84% in shiner surfperch and white croaker respectively. The shape of the PCB concentration distributions in biota has a large effect on the calculated incidence of exceeding ecological and human health criteria.

The model was also applied in a *backwards* manner to calculate recommended target PCB concentrations in the sediment that can be expected to meet various human health and ecological risk criteria. Geometric mean concentrations of ΣPCB in the sediments

that are expected to result in Bay wide geometric mean concentrations in biota that meet various human health and ecological criteria in San Francisco Bay were calculated and are presented in Table 4.9. One of the consequences of this approach is that at any calculated geometric mean PCB concentration in the sediments, it can be expected that PCB concentrations will exceed the criterion value in approximately half the population of the Bay while the PCB concentration in the other half of the population will be less than the criterion value. For this reason, we explored the application of the model to calculate the geometric mean PCB concentration in the Bay sediments that is expected to result in a 5% exceedence of certain criterion values. For male and female harbor seals, which appear to be the most sensitive ecological receptors explored in this study, we calculated the geometric mean PCB concentration in the Bay that is expected to result in a distribution of PCB concentrations in Bay harbor seals in which the PCB concentration in only 5% of the Bay harbor seals exceed the threshold effect concentration.

The backwards calculations illustrate that at the current geometric mean concentrations of ΣPCB in the sediments of the Bay can be expected to meet several human health and ecological risk criteria. Non-cancer risk hazard indices for the consumption of all three fish species of primary interest in the Bay are less than 1 based on a geometric mean ΣPCB concentration of 11.6 μg/kg dry weight in sediments of the Bay. Also, the 1.10^{-5} excess human cancer risk criterion is not exceeded for Bay residents consuming jacksmelt under these conditions. In addition, current ΣPCB concentrations in sediments of the Bay can be expected to cause geometric mean ΣPCB concentrations in female harbor seals that are below the LOAEL, but not the NOAEL or threshold effect concentration. However, a ΣPCB concentration of 11.6 μg/kg dry weight in sediments of the Bay can be expected to produce geometric mean ΣPCB concentrations in fish and wildlife that do not meet all other criteria investigated in this study.

The human excess lifetime cancer risk criterion of 1.10^{-5} for Bay fish consumption can be expected to be met in all three fish species investigated if the geometric mean ΣPCB concentrations in sediments is reduced to a value of 3.5 mg/kg dry weight. The geometric

mean ΣPCB concentrations in adult male and female harbor seals can be expected to fall below the threshold effects concentration if the geometric mean ΣPCB concentrations in sediments drops to a value of 4.5 mg/kg dry weight. As explained earlier, a geometric mean ΣPCB concentration in sediments of the Bay of 4.5 mg/kg dry weight still implies that approximately half the population of male harbor seals can be expected to exceed the threshold effect concentration. The geometric mean for ΣPCB concentrations in sediments that is required to produce only a 5% probability of exceeding the threshold effect concentration in male and female harbor seals are 1.4 and 1.6 mg/kg dry weight, respectively. Target mean ΣPCB concentration in sediments of the Bay that meet other human health and ecological criteria are included in Table 4.9. With the help of the model, it is possible to explore other future scenarios for the PCB concentration in the Bay. We encourage this as we developed the model with this purpose in mind.

Finally, it is important to recognize that the PCB concentrations derived through back calculation are geometric mean values. They are the Bay wide means of logarithmic distributions of PCB concentrations in the sediments. Theoretically, there can be many different distributions that have the same mean. This implies that different PCB sediment concentration distributions in San Francisco can meet the ecological and human health criteria illustrated in Table 4.9 (as long as they exhibit the same mean). This also means that there may be different management options that can be considered to meet the same ecological and human health goals.

1. INTRODUCTION

San Francisco Bay is the largest estuary on the Pacific coast of both North and South America. It includes numerous productive wetlands and has traditionally supported an abundant and diverse wildlife community. The influence of human activity became first apparent in the 19th century when mining activities increased the heavy metal and silt loading to the Estuary. Since this time, human development in the area has transformed wetlands and introduced numerous anthropogenic contaminants into the ecosystem [San Francisco Estuary Project 1990]. A group of contaminants that are of particular concern in the San Francisco Estuary are Polychlorinated Biphenyls (PCBs). PCBs are man-made substances that have been used extensively in the Bay area and elsewhere in the world. They were used as dielectric fluids in electrical transformers and in carbon-less copy paper, ink, machine oils and many other products. PCBs are no longer produced. They were banned from production in 1978. However, run-off from PCB contaminated streams and urban areas continue to deliver these pollutants to the Bay. PCBs are known to be present in Delta outflow, local watersheds and their outflows to the Bay [Gunther et al. 2001, Kinetic Laboratories Inc. 2001], effluent discharges [Yee et al. 2001, 2002], and atmospheric deposition [Tsai et al. 2002].

Since PCBs are persistent and hydrophobic pollutants, they have a tendency to bioaccumulate in tissues of biological organisms. PCBs can biomagnify in aquatic and terrestrial food webs [e.g. Connolly and Pedersen 1988, Kelly and Gobas 2001], causing lipid concentrations in fat tissues of organisms to increase with increasing trophic level. As a result, PCB concentrations reach high levels in fish, wildlife and humans. This is of

considerable concern as PCBs are potent toxins. PCBs are probable human carcinogens and can also cause non-cancer health effects, such as reduced ability to fight infections, low birth weights, and learning and developmental disabilities [US EPA 1999]. It is believed that the risks and hazards associated with PCBs are related to the types of PCBs an individual is exposed to as well as the degree of an individual's exposure. The decline in the abundance and the health of a number of bird and mammalian species around the world, including cormorants and seals, has been associated with elevated PCB concentrations [Fairbrother et al. 1999, Ross et al. 1996, Ross et al. 2000].

PCBs are found in water and sediments throughout the Estuary [SWRCB 2000]. PCB concentrations in San Francisco Bay have exceeded water quality guidelines at the majority of sampling stations throughout the Bay for the entire duration that samples were collected. Tissue concentrations of PCBs in San Francisco Bay sport fish became an issue of public concern when a fish tissue monitoring study in the early 1990s resulted in a fish consumption advisory issued by California's Office of Environmental Health Hazard Assessment. As a result of the advisory, EPA placed San Francisco Bay on the 303(d) impaired water body list for PCBs and other contaminants [SWRCB 2000]. As required by the Clean Water Act, the Regional Water Board of California (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, the Regional Board has coordinated the assembly of several studies with the objective to develop a mass balance model for PCBs in the Bay. As part of this effort, an abiotic mass balance model was developed to describe the relationship between PCB inputs into the Bay and resulting PCB concentrations in water and sediments [Davis 2004]. This study estimated current PCB loadings to the Bay of approximately 20 kg per year. The study further pointed out that reductions in PCB loadings are expected to result in lower PCB concentrations in water and sediments in the

Bay in the future. The second phase of the mass balance model development includes the construction of a food web bioaccumulation model. The purpose of this model is to investigate the relationship between PCB concentrations in water and sediments and resulting PCB concentrations in organisms of the San Francisco Bay food web. This model can be used to identify what PCB concentrations in the sediments and water of the Bay need to be achieved before PCB concentrations in biota of the Bay will fall below acceptable levels. The two models combined can be used to determine what reduction in PCB loadings needs to be accomplished to achieve a situation where organisms are no longer at risk of PCB contamination and people can safely consume fish caught in San Francisco Bay. Other goals of the San Francisco Bay mass balance and food web bioaccumulation model are: (i) to integrate existing information on the behavior of PCBs in San Francisco Bay and to improve our understanding of this pollution problem, (ii) to identify data and knowledge gaps and direct future research efforts, and (iii) to assist in the communication of RMP findings to the scientific community and general public.

The objective of this report is to document the development and evaluation of a food web bioaccumulation model for PCBs in San Francisco Bay. The purpose of this model is to estimate the concentrations of PCBs in a set of key species that reside in the Bay due to PCB concentrations in sediments and water in the Bay. The model can then be used to determine what concentrations of PCBs in the water and sediments of the Bay need to be reached to achieve an acceptable level of risk of PCB to wildlife and humans living in the Bay area. This information can be used to formulate remedial actions to achieve the desired water quality goals.

This report also documents the application of the model with the goal to propose preliminary estimates of the total PCB sediment concentrations that are protective of the health of human and wildlife consuming San Francisco Bay fish and shellfish. Since this effort involves a risk assessment, which is subject to judgment and interpretation, we have presented the PCB food web bioaccumulation model in a format that allows various scenarios regarding acceptable human health and ecological risks to be evaluated.

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 San Francisco Bay to estimate PCB concentrations in different organisms of the food web. 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 of the characteristics of the San Francisco Bay estuary to estimate what the relationship is between concentrations of PCBs in water, sediments and biota. The model is then tested against field observations of the concentrations of PCBs in San Francisco Bay to ensure that the model predictions are consistent with current empirical data regarding PCBs in San Francisco Bay.

In the second chapter of the report the model development is documented. It includes a description of the model's architecture, the model parameterization and the implementation of the model in an Excel spreadsheet. The third chapter of the report discusses the methods used to evaluate the behavior and the performance of the model. This includes a description of the methodology used for sensitivity and uncertainty analyses. The fourth chapter documents and discusses the results of the analyses carried out to analyze the behavior and performance of the model. The fifth chapter includes a discussion of the application of the model to develop sediment based target concentrations for PCBs in San Francisco Bay.

2. THEORY: MODEL DEVELOPMENT & PARAMETERIZATION

2.1 MODEL DEVELOPMENT

This section documents the selection of a conceptual framework that forms the basis for the internal mechanics of the model. The food web bioaccumulation model for PCBs in San Francisco is an attempt to represent key aspects of the behavior of PCBs in the Bay with the goal to address several management issues. To accomplish this, the behavior of PCBs in the model is simplified to a set of key processes that control the fate of PCBs in the food web of the Bay. In the construction of the model, the management objectives of the model are of overriding importance as they determine the reasons for developing the model. The model objectives are therefore defined in section 2.2 of this report. Secondly, a set of simplifying assumptions is made to make it possible to develop the model. These assumptions are geared to the model objectives. It is important to stress that the model can only be used to address the issues for which it is constructed. Hence, certain assumption that are justifiable for the management objectives related to the relationship between concentrations of PCBs in sediments and biota of the Bay may not be appropriate to address other aspects related to PCBs in the Bay. The most important assumptions in the development and their rationale are discussed in section 2.3. Thirdly, a set of functional relationships is proposed in section 2.4 to describe the transfer mechanics of PCBs from the sediments, water and air of the Bay into a number of species in the Bay. These relationships are based on current understanding of the distribution of PCBs in aquatic food webs. The relationships and their scientific basis are discussed in section 2.4. To ensure that these relationships are representative of the environmental

conditions in the Bay, the functional relationships in section 2.4 are parameterized. This is documented in section 2.5. The end result of the model development is a model of the transfer of PCBs in the San Francisco Bay food web. This model is based on the best available information on the trophodynamics of PCBs in the food web and on considerable information on biological, physical and geochemical conditions of the Bay. The model development does not involve the use of measured concentrations of PCBs in biota or sediments of the Bay. The existing empirical PCB concentration data is used to test and evaluate the model and to assess the accuracy of the model predictions of the PCB concentration in biota of the Bay. The methodology for doing this is explained in section 3 and the results are reported in section 4. The testing results of the model are crucial as the purpose of the model is to make estimates of PCB concentrations in fish and wildlife of the Bay resulting from PCB concentrations in the sediments under new conditions.

2.2 MODEL OBJECTIVES

The objectives of the PCB food web bioaccumulation model are:

- To estimate, with reasonable confidence, the Bay-wide concentrations of individual PCB congeners as well as total PCB concentrations in several key species of San Francisco Bay food web resulting from PCB concentrations in water and sediment of the Bay. The species that are the main focus of this study are the Double-crested Cormorant (*Phalacrocorax auritus*), the Forster's Tern (*Sterna Forsteri*), and the harbor seal (*Phoca vitulina richardsi)*, as well as three fish species that are frequently caught by fishermen in Bay, i.e. shiner surfperch (*Cymatogaster aggregata*), jacksmelt (*Atherinopsis californiensis*) and white croaker (*Genyonemus lineatus*).
- To determine the performance of the model by comparing model predictions to available independent empirical measurements.
- To determine the uncertainty in the model predictions of the PCB concentrations in biota.

- To illustrate the application of the model to (i) assess Bay-wide PCB concentrations in several species in the Bay as a result of PCB concentrations in sediments under various management scenarios and (ii) to aid in the selection of a target PCB sediment concentration for the Bay based on human health and ecological risk assessment.
- To develop a model which can be applied to contaminants other than PCBs. There are several recognized chemical contaminants in the Bay. They include: polyaromatic hydrocarbons (PAHs), diazinon, dieldrin, heptachlorepoxide and possibly polychlorinated dibenzo-*p*-dioxins (PCDDs) and polychlorinated dibenzofurans (PCDFs), Polybrominated diphenyethers (PBDEs). Some of these chemicals exhibit a mode of toxicity that is similar to that of PCBs and tend to act in an "additive" mode. The concentrations of PBDEs in harbor seals in the San Francisco Bay have increased dramatically over the past decade, with current levels among the highest reported for this species [She et al. 2002]. In the future it may become important to evaluate the fate of some of these chemicals in relation to that of PCBs. The objective of the model development is to construct the model such that it can be adapted in a simple manner to evaluate the behavior of other chemical substances and mixtures of chemicals.

2.3 GUIDING PRINCIPLES

Guiding principles are key considerations in the conceptual development of the PCB food web bioaccumulation model for San Francisco Bay. The objective of any model is to simplify the enormous complexity found in nature. How the simplifications are made depends on the nature of the question the model is to address. The model developed as part of this study specifically deals with the relationship between PCB concentrations in sediments and those in a number of key species in the larger San Francisco Bay Estuary. The model conceptualization is targeted to this specific question. While the model deals with the distribution of PCBs in the San Francisco Bay food web, the model is not

expected to be able to address food web related questions not directly related to PCBs. The major guiding principles are described below.

2.3.1 Representation of the Composition of the PCB Mixture

PCB oils, used in commerce, consist of many different types (or congeners) of PCBs. There are 209 possible PCB congeners, but depending on the type of PCB oil, some PCB congeners are much more prevalent than others. Each congener has its own specific properties, which control its distribution in the Bay and toxicity in biota. Differences in partitioning properties and toxicity among the congeners can be very large. As a result, it is important to know what PCBs are present in San Francisco Bay and how to represent this mixture in the model.

The majority of PCB analyses in the Bay have been reported for approximately 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. Because the majority of chemical analyses were initiated and documented by the San Francisco Estuary Institute (SFEI), we will refer to these PCBs as the RMP40. The majority of these congeners are non-coplanar. Toxic Equivalency Factor (TEF) values are available for only three of the 40 PCB congeners (i.e. PCB 101, 118 and 156) and the TEFs are low compared to those of coplanar PCBs such as PCBs 77, 126 and 169. A limited number of concentrations for the coplanar PCBs 77, 126 and 169, which have high TEFs, are also available for white croaker and shiner surfperch. However, there are no corresponding sediment concentrations for these congeners. Hence, the model could not be tested or applied to these congeners.

In the model, we will only consider the 40 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) that have actually been analyzed in environmental samples. Each PCB congener is

evaluated individually. After model calculations for all PCB congeners are completed, a total PCB (ΣPCB) concentration is calculated as the sum of the concentrations of the 40 congeners.

In addition to the total PCB concentration, the model also calculates the total toxic equivalent PCB concentration (TEQ), which is derived as the sum of taxon and PCB specific toxic equivalent concentrations (TEQs) based on Toxic Equivalency Factors TEFs derived from several sources:

$$TEQ = \Sigma(TEC_i) = \Sigma(TEF_i \cdot C_i) \qquad (2.1)$$

The latter is often used to represent the body burden or dose of chemicals that exhibit a "dioxin" like mode of toxic action. There is an increasing body of literature that relates the TEQ to toxic effects in fish and mammals. Total toxic equivalent concentrations are very useful to express the toxicological significance of the actual PCB mixtures found in the Bay. It should be stressed that a number of halogenated organic chemicals other than PCB (e.g. chlorinated dibenzo-p-dioxins, dibenzofurans and brominated diphenyl-ethers) can contribute to the TEQ because their mode of toxic action is similar to that of PCBs. Hence, TEQs calculated based on PCBs alone have the potential to underestimate the actual TEQ in the environment. It is possible to add these chemicals in future model analyses as more information about the presence of these other chemicals becomes available. It should be stressed that the majority of PCB concentration data available for this study include only a few congeners that have significant TEFs. As a result, the TEF calculations conducted in this study are likely to be underestimates of the actual TEQ in biota of San Francisco Bay. For that reason, we have not used TEQs calculated in this study by the model to assess probabilities of exceeding TEQ based threshold concentrations.

2.3.2 Representation of the Food Web Structure

The food web structure of San Francisco Bay is highly complex. The food web includes many different species which occupy a variety of habitats. Species composition varies between locations in the Bay and between different times of the year. Feeding relationships also vary between species, life-stages of species, abundance of the various species, location, time of the year and other factors. It is not possible or necessary to include all species in the San Francisco Bay food web in the model or to represent all possible trophic interactions. Because the objective of the model is to focus on a limited number of key species, it is sufficient to include only the most relevant trophic interactions relating to these species. Also, because PCB concentrations in organism lipid tissues tend to increase significantly between trophic positions but considerably less between organisms that occupy a similar trophic level, it is possible to "lump" species of comparable trophic guilds. The latter should be done with caution as certain species may exhibit very specific feeding behaviors that cannot be generalized to other organisms.

In the development of a food web structure for modeling the bioaccumulation of PCBs in SFB, we applied the following criteria:

1. Include species of primary management interest. On recommendation of the Technical Steering Committee, the Double-crested Cormorant (*Phalacrocorax auritus*), the Forster's Tern (*Sterna Forsteri*), the harbor seal (*Phoca vitulina richardsi)*, shiner surfperch (*Cymatogaster aggregata*), jacksmelt (*Atherinopsis californiensis*) and white croaker (*Genyonemus lineatus*) were included in the model. Harbor seal, Forster's Terns and Double-crested Cormorant were included in the model because they represent species of higher trophic levels in the SFB aquatic food web. PCBs are known to biomagnify in aquatic food webs [Connolly and Pedersen 1988, Macintosh et al. 2004] and biomagnification results in an increase in PCB concentrations with increasing trophic level. Hence the target species selected can be expected to be subject to a high degree of PCB exposure in SFB. Actual measurements of PCB concentrations confirm this. Elevated PCB

concentrations pose a risk to these species, which can be mediated by management actions. The white croaker, shiner surfperch and jacksmelt were included in the model because they are caught and consumed by local fishermen. Consumption of these fish species provides a route of PCB exposure to humans.

2. Include species that can be considered residents of SFB. The receptors included in the model predominantly forage in SFB and can therefore be considered resident species. PCB concentrations in these organisms are expected to be affected by remediation.
3. Include species representing trophic guilds that are of key relevance to the food web transfer and accumulation of PCBs in the species of interest. Relevant trophic guilds include phytoplankton and algae, zooplankton, filter feeding invertebrates, benthic detritovores, juvenile and adult fish, male and female fish eating birds and male, female and juvenile marine mammals.
4. Minimize the number of species included in the model by representing key trophic guilds by one or two species. This is done to simplify the model and make the calculations more transparent.
5. Include species for which empirical concentration data are available. This provides the opportunity to test and ground-truth the model's calculations. Concentration data were available for Pacific oysters (*Crassostrea gigas*), California mussels (*Mytilus californianus*), shiner surfperch (*Cymatogaster aggregata*), jacksmelt (*Atherinopsis californiensis*), white croaker (*Genyonemus lineatus*), Double-crested Cormorant (*Phalacrocorax auritus*), and the harbor seal (*Phoca vitulina richardsi)* to test and evaluate the model.

This approach produced a food web model that included one category for phytoplankton, one category for zooplankton, 8 invertebrate species (including detritovores and filter feeders), 2 bird species (including male and female birds as well as eggs for each avian species) and male, female, juvenile and newborn harbor seals. The species that were included in the model and their feeding relationships are listed in Table 2.8.

The key species of management interest in the model are the Double-crested Cormorant (*Phalacrocorax auritus*), the Forster's Tern (*Sterna Forsteri*), the harbor seal (*Phoca vitulina richardsi)*, shiner surfperch (*Cymatogaster aggregata*), jacksmelt (*Atherinopsis californiensis*) and white croaker (*Genyonemus lineatus*). The species were included in the model for several reasons:

Double-crested Cormorant (*Phalacrocorax auritus*) are fish-eating birds that due to their relatively high trophic positions are subject to elevated concentrations of PCBs [Davis et al. 2004]. PCB concentrations in Double-crested Cormorant eggs are considered to be an excellent monitoring tool and biomarker since bird embryos are among the most sensitive life stages to the adverse effects of PCBs [Davis et al. 2004]. Empirical analyses of Double-crested Cormorant eggs from locally breeding birds are part of a long-term monitoring program for SFB conducted by the Coastal Intensive Sites Network (CISNet) Environmental Stress Indicators program. The eggs are collected from year-round colony residents that eat fish from the Bay [Davis et al. 2004]. Past monitoring data can be used to test the performance of the model. Future monitoring data will aid in measuring the effectiveness of management actions and provide further feedback on the ability of the model to anticipate future trends of PCB concentrations.

A number of studies have identified marine mammals as some of the most susceptible organisms to contamination of PCBs and other hydrophobic substances [Ross et al. 1996]. Bioaccumulation of PCBs in the food web and the high trophic position of the harbor seal in the aquatic food web have resulted in elevated PCB concentrations in several seal populations around the world. It is suspected that high PCB concentrations can produce immunotoxic effects in harbor seals [Ross et al. 1996]. These immunotoxic effects can lead to a diminished resistance to pathogens and an increased incidence and severity of infectious diseases, which puts harbor seal populations at risk. Studies show there are a number of harbor seal haul out sites located throughout SFB [Kopec and Harvey 1995, Torok 1994, Grigg 2003]. Based on historical counts (1970-2002) the three largest haul out sites in SFB are Mowry Slough (South Bay), Yerba Buena Island

(Central Bay) and Castro Rocks (North Bay). Nickel and Grigg [2002] also reported that most tagged seals use localized foraging areas within 20 km of a known haul out site and most foraging occurred within 1-5 km of the site, however they noted individual differences. Variation from these observations included some individuals moving 50-100 km between inshore foraging locations and a few observations of long-distance trips outside of SFB. Overall most seals are year-round SFB residents and most foraging is conducted within SFB [Grigg 2003]. Fish selected for the food web model comprise the vast majority of prey items for this species in SFB (i.e. yellowfin goby, white croaker, plainfin midshipmen and northern anchovy) [Torok 1994].

2.3.3 Representation of Spatial Distribution of PCBs in San Francisco Bay

PCBs enter San Francisco Bay via numerous routes including urban runoff, atmospheric deposition, ground water, and inputs from the large watersheds of the Sacramento River and the San Joaquin River, as well as many smaller tributaries surrounding the Bay. Because of the large number of inputs into the Bay, the total PCB concentrations in sediments in San Francisco Bay vary considerably. ΣPCB concentrations range from virtually non-detectable levels to concentration as high as 9 mg/kg (dry sediment) [Davis 2004]. Water concentrations are much lower but also vary considerably. They range from approximately 77 pg/L to approximately 3,700 pg/L [SFEI, 1999]. The spatial variability in the total PCB concentrations can be expected to cause significant variation in the PCB concentrations in biota of the Bay. Organisms that do not move large distances (e.g. certain invertebrates such as mussels and polychaetes) are likely to reflect the PCB concentrations in their immediate environment. Hence, if they reside in a “hot spot”, PCB concentrations are likely to be greater than concentrations in organisms that inhabit less PCB polluted sections of the Bay. However, harbor seals, cormorants and terns and also several of the fish species investigated in this study have foraging areas that include large sections of the Bay and are therefore exposed to a wider range of PCB concentrations in the sediments. The PCB concentrations that are achieved in these organisms are expected

to reflect the “average” concentration to which they are exposed. Also, species that are widely distributed in the Bay will exhibit different spatially-averaged concentrations depending on the areas within the Bay where they reside and forage. If there would be information about the spatial distribution of wildlife and associated PCB concentrations in sediments in the Bay, it might be possible to calculate PCB concentrations in wildlife based on their foraging behavior. However, this information is not currently available. To calculate the PCB concentrations in wildlife species that are widely distributed in the Bay, we made the assumption that the available PCB sediment concentration data collected by monitoring programs in the Bay are able to represent the distribution of PCB concentrations to which the wildlife populations in the Bay are exposed. This assumption is reasonable for several reasons. First, PCB sediment concentration monitoring programs have included a large number of stations throughout the Bay (Figure 2.1). A large number of independent PCB concentration measurements (approximately 1,284) have been collected from these stations. This large data set is able to provide a reasonable representation of the spatial distribution of the PCB concentrations in the Bay. Secondly, the wildlife species included in the model are distributed over most of the Bay area and are year-round residents of the Bay.

It is possible to apply the model on a more site-specific basis (e.g. on a segment scale). In that case, the Bay wide spatial distributions used in this study can be replaced by more site-specific spatial concentration distributions. However, this requires better data on geographical distribution patterns of individual species and corresponding spatial distributions of PCB concentrations. However, given the wide spatial distribution of the key wildlife species in the model, it is important to caution against the application of the model on a small spatial or site-specific basis.

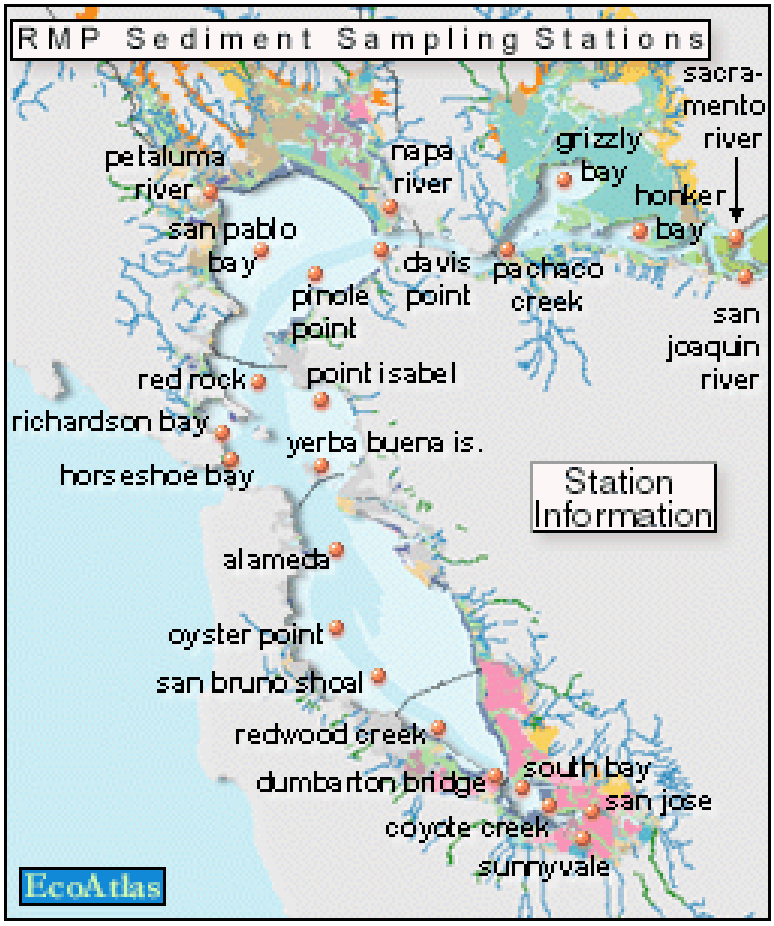

Figure 2.1: Locations of RMP sediment sampling stations in San Francisco Bay

2.3.4 Representation of Temporal Changes in PCB Concentrations

The San Francisco Bay food web bioaccumulation model applies a steady-state approach to estimate the PCB concentrations in biota from PCB concentrations in the sediments. The steady-state approach is based on the assumption that under the conditions of interest PCB concentrations have had sufficient time to exchange between water, sediments and the organisms of the food web to achieve a dynamic "equilibrium", where PCB concentrations no longer change over time. The steady-state approach does not preclude the possibility to represent the effect of seasonal changes in key environmental variables or to represent the effect of age on PCB concentration. The latter can be achieved by parameterizing the model for particular seasonal or age-specific conditions. However, the steady-state assumption does imply that, throughout the period of time that the seasonal

or age specific conditions apply, the PCB concentrations achieve a dynamic equilibrium. This assumption is in many cases appropriate for PCBs in smaller organisms (i.e. plankton, benthic invertebrates and juvenile fish), which exchange PCBs relatively quickly, causing a dynamic equilibrium to be established quickly. In the case of larger organisms (e.g. seals, large fish, birds) and more heavily chlorinated PCB congeners, the exchange of PCBs with the environment can become too slow to keep pace with the changing environmental conditions. In these instances, the PCB concentration is not at the dynamic equilibrium that the model predicts. To overcome this problem, non-steady-state or time-dependent calculations can be completed. However, these calculations are much more complicated, time-consuming than the steady-state calculations and further require extra time dependent input data that are largely unavailable. To keep the model simple, we have chosen to apply the steady-state approach. However, to capture the effect of seasonal variations on PCB concentrations we have applied a sensitivity analysis using Monte Carlo Simulation (MCS). As part of this method, PCB concentrations in biota are calculated as a function of a range of internal and external model variables. This produces a range of PCB concentrations that can be expected in the organism as a result of the variation in seasonal conditions. This range of concentrations can be considered a realistic estimate of the actual range in concentrations expected in the Bay for those PCBs and organisms that reach steady-state relatively quickly. For those PCB congeners and organisms that achieve steady-state slowly, we expect the predicted range of concentration to be an overestimate of the actual range as upper and lower values are unlikely to be reached throughout the period that the conditions apply. To capture the effect of changes in the PCB concentration with the age of the animal, we have introduced different age classes for some of the species in the model.

An important implication of the selection of the steady-state approach is that PCB concentrations in biota are directly proportional to the PCB concentrations in the Bay sediment. This means that temporal changes in the PCB concentrations in the biota of the Bay will match those in the sediments. We believe that this assumption is justified as the time response of the PCB concentrations in the sediment to changes in loadings and

external conditions is quite slow compared to the time response of PCB concentrations in biota. Davis [2004] estimated that the half-life time of PCBs in San Francisco Bay is approximately 20 years. A comparable half-life time of PCBs calculated in adult white croaker is approximately 100 d. This implies that the temporal response of the PCB concentration in larger fish is controlled by the time response of the sediments, which acts as the "slowest" compartment and the "rate controlling" step of PCB concentration changes over time. For modeling purposes, the concentration in the biota used in this model can therefore be determined as a constant multiplication factor of the concentration in the sediment. A time dependent approach was not considered necessary for the goals of this study.

In response to management actions, such as remediation, the model is able to provide realistic projections of the concentrations that will be achieved as a result of the remediation. The model is designed to predict the new equilibrium condition of SFB that will be achieved after remediation. The model is less capable of predicting how quickly the new equilibrium will be achieved after remediation if the remediation has an immediate effect on the Bay wide PCB concentration in the sediment. The latter is an unlikely scenario and therefore of secondary importance at this stage. In addition, models of the time response to remediation require information about the extent and the methods of remediation, which is currently not available. Developing a much more complex time dependent model is premature at this stage.

2.4 MODEL DESCRIPTION

2.4.1 General Model Description

The PCB food web bioaccumulation model for San Francisco Bay consists of two modules (i.e. the *science* module and the *management* module). The science module includes all the information (i.e. the model's internal and external variables, functional relationships and model performance evaluation data) to calculate the Biota Sediment

Accumulation Factor (BSAF) for individual PCB congeners and also for ΣPCBs. The BSAF is the main output of the model and represents the relationship between the PCB concentrations in biota (C_B) and that in the sediment (C_S) that is predicted by the model:

$$BSAF = C_B/C_S \quad (2.2)$$

Where C_B has units of g PCB/kg wet weight organism, C_S has units of g PCB/kg dry sediment and the BSAF has units of kg dry sediment/kg wet weight organism. A BSAF is calculated for each PCB congener in every species included in the model, including the seal and bird species. The BSAF is a quick and simple way to relate sediment and biota concentrations. The BSAF is further represented as a statistical distribution of values rather than a single point estimate to capture seasonal variations in the conditions of the Bay.

In the management module, the BSAF is used for two purposes. In a "forwards" calculation, the BSAF is used to assess the PCB concentration in fish and wildlife in the Bay (C_B) based on measured or anticipated PCB concentrations in the sediment (C_S):

$$C_B = BSAF \cdot C_S \quad (2.3)$$

In a "backwards" calculation, the PCB concentration in the sediment (C_S) is calculated based on a PCB concentration in a fish or wildlife species (C_B). This calculation is designed to determine target PCB concentrations in sediments that meet ecological and/or human health criteria that are expressed in terms of a PCB concentration C_B. This calculation is:

$$C_S = C_B / BSAF \quad (2.4)$$

To derive the BSAF, the model uses a number of chemical, biological and environmental parameters (e.g. the octanol-water partition coefficient, lipid content, weight,

temperature), which are referred to as model state variables. The model does not use PCB concentrations themselves. However, in the application of the model in the management module PCB concentration data are used. For example, in the forward calculation, actual PCB concentrations can be used to make predictions of the PCB concentration in fish and wildlife in the Bay that are expected to occur as a result of the PCB concentrations in the sediments. In this model application, the PCB concentration in the sediment is referred to as an "external variable" (an external variable is also sometimes referred to as a forcing function). In the backward calculation, the PCB concentration in fish or wildlife species is the external variable.

The food web bioaccumulation model consists of a number of mathematical expressions describing the uptake and elimination of PCBs in biota of the Bay. The expressions for air-breathing (seals, cormorants, terns) and water-breathing organisms (fish, benthic invertebrates, plankton) are fundamentally different. For this reason we describe the architecture of the model in three sections. The first section is for water breathing organisms and includes phytoplankton, zooplankton, aquatic invertebrates and fish. The second section describes the model for marine mammals that is used to derive the BSAF for harbor seals. The third section lays out the model for birds, which is used to assess the BSAF in cormorants and terns.

2.4.2 Detailed Bioaccumulation Model Description: Phytoplankton, Zooplankton, Aquatic Invertebrates, Fish

Figure 2.2 provides a conceptual overview of major routes of chemical uptake and elimination in aquatic organisms that rely on gas exchange with the water for respiration. Our model is based on the presumption that the exchange of PCB congeners between the organism and its ambient environment can be described by a single equation for a large number of aquatic organisms:

$$dM_B/dt=\{W_B\cdot(k_1\cdot[m_O\cdot\phi\cdot C_{WT,O} + m_P\cdot C_{WD,S}] + k_D\cdot\Sigma(P_i\cdot C_{D,i}))\} - (k_2 + k_E + k_M)\cdot M_B \quad (2.5)$$

where M_B is the mass (g) of the PCB congener in the organism, dM_B/dt is the net flux of PCB congener being absorbed or depurated by the organism at any point in time t (d), W_B is the weight of the organism (kg) at time t, k_1 is the clearance rate constant (L/kg · d) for uptake via the respiratory area (i.e. gills and skin), m_O is the fraction of the respiratory ventilation that involves overlying water, m_P is the fraction of the respiratory ventilation that involves sediment associated pore water, ϕ (unitless) is the fraction of the total chemical concentration in the overlying water that is freely dissolved and can be absorbed via membrane diffusion, $C_{WT,O}$ is the total concentration of the PCB congener in the water column above the sediments (g/L), $C_{WD,S}$ is the freely dissolved PCB congener concentration in the sediment associated pore (or interstitial) water (g/L), k_D is the clearance rate constant (kg/kg · d) for chemical uptake via ingestion of food and water, P_i is the fraction of the diet consisting of prey item i, $C_{D,i}$ is the concentration of PCB congener (g/kg) in prey item i, k_2 is the rate constant (d^{-1}) for elimination of PCBs via the respiratory area (i.e. gills and skin), k_E is the rate constant (d^{-1}) for the elimination of the PCB congener via excretion into egested feces and k_M is the rate constant (d^{-1}) for metabolic transformation of the PCB congener.

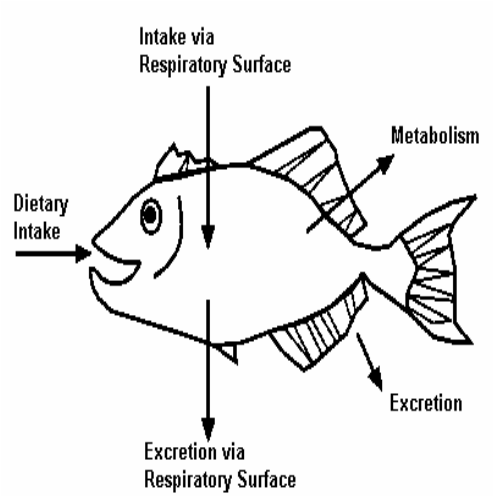

Figure 2.2: Conceptual diagram of the major uptake and elimination processes of PCBs in fish

For phytoplankton, algae and macrophytes, $k_{D,i}$ is zero and k_E is considered to be insignificant.

This model is based on several key assumptions. First, it is assumed that the PCB congener is homogeneously distributed within the organism as long as differences in tissue composition and phase partitioning are taken into account. There is considerable evidence that supports this assumption [e.g. Ernst and Goerke 1976]. Concentrations in specific fish tissues can therefore be calculated based on the composition of the fish tissues of interest. The latter is important for characterizing the risk experienced by fishermen who eat fish caught from the Bay. Secondly, it is assumed that the organism can be described as a single compartment in its exchange with its surrounding environment. Many studies can be quoted to support this [e.g. Branson et al. 1975]. The one-compartment model for an organism is best applied in situations such as the situation that exists in San Francisco Bay where variations in PCB concentrations in water and sediment are relatively slow over time. A third assumption of the model concerns the PCB congener elimination via egg deposition or sperm ejection. Studies in fish have shown that lipid-normalized concentrations of many persistent organic PCB congeners in eggs and adult female fish are approximately equal [e.g. Russell et al. 1999]. This implies that while egg deposition transfers a significant fraction of the PCB congener body burden from the adult female fish into the eggs, the lipid equivalent concentration within the organism remains the same. The mechanism in the model by which egg deposition lowers the internal concentration in the organism compared to fish that do not produce eggs (e.g. male fish), is through growth dilution associated with the formation of eggs in the fish. Growing eggs produces extra tissue in which PCB congeners reside, hence reducing the PCB concentration. However, equation 2.5 illustrates that this growth dilution effect is counteracted by uptake of PCB congener from water and the diet and that the balance of these processes controls the ultimate concentration in the organism.

As explained in section 2.3.4, equation 2.5 can be simplified by applying a steady-state assumption ($dM_B/dt = 0$), resulting in:

$$C_B = \{k_1 \cdot (m_O \cdot \phi \cdot C_{WT,O} + m_P \cdot C_{WD,S}) + k_D \cdot \sum P_i \cdot C_{D,i}\} / (k_2 + k_E + k_G + k_M) \quad (2.6)$$

where C_B is the PCB congener concentration in the organism (g/kg wet weight) (i.e. M_B/W_B). The steady-state assumption is reasonable for organisms in the Bay which have been exposed to the PCB congener over a long period of time and throughout their entire life. One of the implications of applying a steady-state assumption is that the growth of the organism needs to be expressed as a growth rate constant k_G, which is $dW_B/(W_B \cdot dt)$. The growth rate constant assumes that over the period of time the model applies, the growth of the organism can be represented by a constant fraction of the organism's body weight.

The bioaccumulation factor (BAF) is $C_B/C_{WT,O}$ and the wet weight based biota-sediment accumulation factor (BSAF) is C_B/C_S, where C_S is the concentration (g/kg dry sediment) in the bottom sediment:

$$BSAF = C_B/C_S \quad (2.7)$$

The BSAF is the key outcome of the San Francisco Bay food web bioaccumulation model as it provides the means to predict the concentrations of PCBs in biota from the PCB concentration in the sediments of the Bay. The various submodels for k_1, k_2, k_E, k_M, k_G and ϕ, used to estimate the BSAF are described below.

ϕ: PCBs have a high affinity for organic matter, such as particulate organic carbon (POC) and dissolved organic carbon (DOC) in the water column [McCarthy 1983, McCarthy and Jimenez 1985]. If associated with particulate or dissolved organic matter, the PCB congener is believed to be unavailable for uptake via diffusion into organisms. ϕ is the ratio of the freely dissolved water concentration C_{WD} (g/L) to the total water concentration C_{WT} (g/L). ϕ was estimated for non-ionizing PCBs as:

$$\phi = C_{WD} / C_{WT} = 1 / (1 + \chi_{POC} \cdot D_{POC} \cdot \alpha_{POC} \cdot K_{OW} + \chi_{DOC} \cdot D_{DOC} \cdot \alpha_{DOC} \cdot K_{OW}) \quad (2.8)$$

where χ_{POC} and χ_{DOC} are the concentrations of POC and DOC in the water (kg/L), respectively. D_{POC} and D_{DOC} are the disequilibrium factors for POC and DOC partitioning. They represent the degree to which POC-water and DOC-water distribution coefficients vary from POC-water and DOC-water equilibrium partition coefficients. D_{POC} or D_{DOC} values greater than 1.0 indicate distribution coefficients in excess of equilibrium partition coefficients, while values less than 1.0 represent conditions where equilibrium has not been reached. D_{POC} and D_{DOC} values equal to 1.0 represent equilibrium partitioning. Disequilibria between OC and water have been observed for a range of organic chemicals, including PCBs, in several ecosystems [e.g. Gobas and Maclean 2003] but their values remain difficult to predict at this point. In this study, we have used empirical water and sediment concentration data from the Bay to characterize D_{POC} and D_{DOC} in the model. In equation 2.8, α_{POC} and α_{DOC} are proportionality constants describing the similarity in phase partitioning of POC and DOC in relation to that of octanol. These proportionality constants can vary substantially among different types of organic carbon. Based on a study by Seth et al. [1999], we have assumed that α_{POC} can be estimated as 0.35 with error bars equivalent to a factor of 2.5. Following Burkhard et al. [2000] we have estimated α_{DOC} to be 0.08 with error bars equivalent to a factor of 2.5.

k_1 and k_2: The rate at which chemicals are absorbed from the water via the respiratory surface (e.g. gills and skin) is expressed by the aqueous uptake clearance rate constant k_1 (L/kg · d). In fish, invertebrates and zooplankton, it is viewed as a function of the ventilation rate G_V (L/d) and the diffusion rate of the chemical across the respiratory surface area [Walker 1987, Gobas 1993]:

$$k_1 = E_W \cdot G_V / W_B \quad (2.9)$$

where E_W is the gill chemical uptake efficiency and W_B is the wet weight of the organism (kg). E_W is a function of the K_{OW} of the PCB congener and is approximated based on observations in fish [Gobas and Mackay 1987]:

$$E_W = (A_{EW} + (B_{EW} / K_{OW}))^{-1} \quad (2.10)$$

where constant A_{EW} is 1.85 [± 0.13] and constant B_{EW} is 155 [± 0.50].

G_V was calculated based on an allometric relationship between wet weight and oxygen consumption for 200 different fish species [Thurston and Gehrke 1990] ranging in weight between $2.0 \cdot 10^{-5}$ and 60 kg under routine metabolic test conditions as well as G_V data for zooplankton and aquatic invertebrate species:

$$G_V = 1400 \cdot W_B^{0.65} / DO \quad (2.11)$$

where DO is the dissolved oxygen concentration in the water (mg O_2/L) and were available from empirical measurements of dissolved oxygen concentration made at RMP stations seasonally throughout the Bay between 1999-2001.

For algae, phytoplankton and aquatic macrophytes, we used a biphasic relationship for k_1 and k_2 based on a water-organic carbon two-phase resistance model:

$$k_1 = (A_P + ((B_P / K_{OW}))^{-1} \quad (2.12)$$

where A_P and B_P are constants (with units of time) describing the resistance to PCB uptake through respectively the aqueous and organic phases of the algae, phytoplankton or macrophyte. To obtain reasonable values for A_P and B_P for phytoplankton, we evaluated several data sets. Constant B_P (default value = 5.5 [± 3.7]) is derived by calibration to empirical k_2 values from various phytoplankton, algae and cyanobacteria

species over a range of K_{OW} using data in described in Koelmans et al. [1993, 1995, 1999]. Constant A_P (default value = 6.0 [± 2.0] · 10^{-5}) is derived from calibration to phytoplankton field BCF data from the Great Lakes [Swackhamer and Skoglund 1993 and Oliver and Niimi 1988]. A mean annual k_G value of 0.125 d^{-1} was selected based on studies by Alpine and Cloern [1988 and 1992].

The elimination rate constant k_2 (d^{-1}) is closely related to k_1 as both k_1 and k_2 involve the same processes of water ventilation and membrane permeation:

$$k_2 = k_1/K_{BW} \tag{2.13}$$

where K_{BW} (L/kg wet weight) is the biota-water partition coefficient. The partitioning of PCBs between biota in the Bay and water is believed to occur into the lipids, non-lipid organic matter (e.g. proteins and carbohydrates) and water. Each of these media has their own capacity to sorb and "store" PCB congeners. Hence, for every PCB congener in each organism of the Bay we define an organism-water partition coefficient K_{BW} on a wet weight basis (ww) as:

$$K_{BW} = k_1 / k_2 = v_{LB} \cdot K_{OW} + v_{NB} \cdot \beta \cdot K_{OW} + v_{WB} \tag{2.14}$$

where v_{LB} is the lipid fraction (kg lipid/kg organism ww), v_{NB} is the non-lipid organic matter (NLOM) fraction (kg NLOM/kg organism ww) and v_{WB} is the water content (kg water/kg organism ww) of the organism. β is a proportionality constant expressing the sorption capacity of NLOM to that of octanol. Based on previous work [Gobas et al. 1999], a value of approximately 0.035 ± 0.004 was chosen. This implies that the sorption affinity of NLOM for PCBs is approximately 3.5% that of octanol. While the sorption affinity of NLOM is low compared to that of lipid, it can play an important role in controlling the partitioning of organic chemicals in organisms that have low lipid contents (e.g. phytoplankton, algae, certain invertebrates). Good databases exist [e.g.

Payne et al. 1999] to parameterize the three phase partitioning model, especially for fish, crustaceans and shellfish consumed by humans.

For the calculation of the phytoplankton-water partition coefficient (K_{PW}) NLOM in equation 2.14 is replaced by non-lipid organic carbon (kg NLOC/kg organism ww) [Skoglund and Swackhamer 1999] with a proportionality constant of 0.35 as:

$$K_{PW} = v_{LP} \cdot K_{OW} + v_{NP} \cdot 0.35 \cdot K_{OW} + v_{WP} \qquad (2.15)$$

Since the BAF is a function of the ratio of k_1 and k_2, errors in the exact determination of G_V and E_W typically have a minor effect on the BAF as errors in k_1 will cancel out similar errors in k_2. This makes the model relatively insensitive to parameterization error in G_V and E_W and allows a single equation to represent ventilation rates and uptake efficiencies in a range of species. The partitioning properties of the chemical, represented by K_{BW} play a more important role. This is reasonable as the main roles of k_1 and k_2 are to describe how quickly or slowly equilibrium partitioning in the organism will be achieved. The model is most sensitive to k_1 and k_2 for substances that (i) are absorbed from water and food in comparable amounts and/or (ii) eliminated by gill ventilation at rates that are comparable to the combined elimination rate of feces egestion, metabolic transformation and growth dilution.

m_O, m_P: Organisms that are in close contact with the bottom sediments, such as benthic fish and invertebrates, can exchange PCB with sediment pore water. Freely dissolved chemical concentrations in pore water can exceed the overlying water concentrations as a result of sediment-water disequilibria, which can be very large under certain conditions [Gobas and Maclean 2003]. In many cases, benthic fish and invertebrates do not ventilate a large amount of pore water because of poor oxygen concentrations and low food content. Although pore water ventilation is likely small, it can have a significant effect on the BAF for PCBs that are at large sediment-water column disequilibria. For organisms that have no direct contact with the pore water, m_P is 0. In all cases m_O equals 1 - m_P.

$C_{WD,P}$: Freely dissolved concentrations of PCBs in pore water are estimated from the chemical concentration in the bottom sediment as [Kraaij et al. 2002]:

$$C_{WD,P} = C_{S,OC} \cdot \delta_S / K_{OC} \quad (2.16)$$

where $C_{WD,P}$ is the freely dissolved concentration of the PCBs in the pore water (g/L), $C_{S,OC}$ is the PCB concentration in the sediment normalized for organic carbon content (g/kg OC), δ_{OCS} is the density of the organic carbon in sediment (kg/L) and K_{OC} is the organic carbon-water partition coefficient.

***k_D and k_E*:** The rate at which PCBs are absorbed from the diet via the GIT is expressed by the dietary uptake clearance rate constant k_D (kg-food/kg-organism · d) and is a function of the dietary chemical transfer efficiency E_D, the feeding rate G_D (kg/d) and the weight of the organism W_B (kg) [Gobas 1993]:

$$k_D = E_D \cdot G_D / W_B \quad (2.17)$$

Empirical E_D observations are highly variable in aquatic invertebrates, ranging between 0 and 100% in amphipods, molluscs, oligochaetes, snails, clams and bivalves [Landrum and Poore 1988, Morrison et al. 1996, Lydy and Landrum 1993, Parkerton 1993, Bruner et al. 1994, Kukkonen and Landrum 1995, Wang and Fisher 1999, Mayer et al. 2001] and between 0 and 90% in fish [Gobas et al. 1993a, Parkerton 1993, Gobas et al. 1988, Gobas et al. 1993b, Fisk et al. 1988]. Explanations have been proposed for the variations in E_D, including differences among the sorption coefficient of chemicals in dietary matrices, the composition of dietary matrices (e.g. organic carbon and soot carbon content), the digestibility of the dietary matrix, metabolic transformation, steric hindrance in gut membrane permeation, experimental artifacts, differences in gut morphology and variability in food digestion between different species. Because of the large variability in the empirical data it is difficult to develop accurate models for the dietary uptake rate.

However, there are some notable trends in the E_D data that can provide guidance in model development. First, several authors have observed a reduction in dietary uptake efficiency with increasing K_{OW} for high K_{OW} chemicals in invertebrates [Parkerton 1993, Bruner et al. 1994] and fish [Parkerton 1993, Gobas et al. 1988]. Secondly, the average dietary chemical transfer efficiency (E_D) for chemicals with a log K_{OW} 4 – 6 is approximately 50% in aquatic invertebrates and fish that were fed continuously. These trends are consistent with a two-phase resistance model for gut-organism exchange which is further documented in [Gobas et al. 1988]. The following equation based on the lipid-water two-phase resistance model was selected to calculate the dietary absorption efficiencies of the PCB congeners:

$$E_D = (A_{ED} \cdot K_{OW} + B_{ED})^{-1} \qquad (2.18)$$

where constant A_{ED} is 8.5 [± 1.4]$\cdot 10^{-8}$ and constant B_{ED} is 2.0 [±0.6] for zooplankton, invertebrates and fish. We applied a general bioenergetic relationship, based on studies in trout [Weininger 1978], for estimating feeding rates in San Francisco Bay fish species and aquatic invertebrate species:

$$G_D = 0.022 \cdot W_B^{0.85} \cdot e^{(0.06 \cdot Tw)} \qquad (2.19)$$

where T_W is the mean water temperature in degrees Celsius. Filter feeding species have a distinct mechanism of dietary uptake that was represented as:

$$G_D = G_V \cdot C_{ss} \cdot \sigma \qquad (2.20)$$

where the feeding rate is a product of gill ventilation rate G_V (L/d), the concentration of suspended solids C_{ss} (kg/L) and the scavenging efficiency of particles σ (%) absorbed from the water.

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}) [Gobas et al. 1993] and was estimates as:

$$k_E = G_F \cdot E_D \cdot K_{GB} / W_B \qquad (2.21)$$

where G_F (kg-feces/kg-organism · d) is the fecal egestion rate and K_{GB} is the partition coefficient of the chemical between the GIT and the organism. G_F is a function of the feeding rate and the digestibility of the diet, which in turn is a function of the composition of the diet according to:

$$G_F = \{(1-\varepsilon_L) \cdot v_{LD}) + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \cdot G_D \qquad (2.22)$$

where ε_L, ε_N and ε_W are the dietary absorption efficiencies of lipid, NLOM and water, respectively. v_{LD}, v_{ND}, and v_{WD} are the overall lipid, NLOM and water contents of the diet, respectively. In fish, the absorption efficiencies of lipid and NLOM are approximately 90% and 50%, respectively [Gobas et al. 1999, Nichols et al. 2001].

Absorption and assimilation efficiencies for invertebrates range from 15 to 96% [Parkerton 1993, Gordon 1996, Berg et al. 1996, Roditi and Fisher 1999]. In general, these efficiencies are a reflection of the dietary matrix (e.g. organic matter quantity and quality) and the digestive physiology of the organism (e.g. feeding rates and gut retention time). Species with low absorption efficiencies (e.g. worms) typically feed on poor quality substrate (e.g. sediment or detritus) but maintain high feeding rates to obtain required nutrients for energy budgets and survival. A value of 75% is used for lipid and non-lipid organic matter absorption efficiencies in aquatic invertebrates.

In zooplankton, assimilation efficiencies for organic matter range from 55 to 85% [Connover, 1966], while carbon and phosphorus assimilation are measured at approximately 85% [Lehman 1993]. A value of 72% is assumed for lipid and non-lipid

organic matter absorption efficiencies in zooplankton. Water absorption varies between freshwater and marine organisms as a result of their distinct requirements for osmoregulatory balance. Since water is not a significant contributor to the storage capacity of PCBs its value has a negligible impact on the mechanism of biomagnification for these chemicals. The water absorption efficiency for all zooplankton, invertebrate and fish species was assumed to be 55%.

K_{GB}: The partition coefficient of the PCBs between the contents of the GIT and the organism, expresses the change in phase partitioning properties that occur as a result of the digestion of the diet after ingestion. It is estimated as:

$$K_{GB} = (v_{LG} \cdot K_{OW} + v_{NG} \cdot \beta \cdot K_{OW} + v_{WG}) / (v_{LB} \cdot K_{OW} + v_{NB} \cdot \beta \cdot K_{OW} + v_{WB}) \quad (2.23)$$

where v_{LG}, $v_{NG,}$, and v_{WG} are the lipid (kg lipid/kg digesta ww), NLOM (kg NLOM/kg digesta ww) and water (kg water/kg digesta ww) contents in the gut, respectively. The sum of these fractions (i.e. total digesta) approach 1 and are dependent on the absorption efficiency for each component of the diet as:

$$v_{LG} = (1-\varepsilon_L) \cdot v_{LD} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.24)$$

$$v_{NG} = (1-\varepsilon_N) \cdot v_{ND} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.25)$$

$$v_{WG} = (1-\varepsilon_W) \cdot v_{WD} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.26)$$

Because the bioaccumulation model (equation 2.6) is based on the ratio of k_D and k_E, which is $G_D/(G_F \cdot K_{GB})$, the model parameterization errors for the feeding rate G_D (and hence G_F, eq. 2.22) and the dietary uptake efficiency E_D tend to cancel out to a significant extent. Hence, the model can be expected to provide reasonable estimates of the BAF and

BSAF of PCBs in Bay organisms even if G_D and E_D are poorly characterized. This is an attractive feature of the model since the variability and error in G_D and E_D are often large.

k_G: In many cases, reliable data for the growth rate of organisms are available. Growth rates vary considerably among species and even within species as a function of size, temperature, prey availability and quality and other factors. For the majority of species included in the San Francisco Bay model, reliable growth rate data are not available. We therefore used the following generalized growth equations, based on [Thomann et al. 1989], to provide a reasonable approximation for the growth rate constant k_G (d^{-1}) of the aquatic species in the Bay. For zooplankton and invertebrates, we used:

$$k_G = I_{GR} \cdot W_B^{-0.2} \tag{2.27}$$

representative for temperatures around 10°C, while for fish species we used:

$$k_G = F_{GR} \cdot W_B^{-0.2} \tag{2.28}$$

Based on an average water temperature of approximately 15°C, I_{GR} and F_{GR} are the invertebrate (0.00035) and fish (0.0007) growth rate coefficients, respectively.

k_M: The rate at which a parent compound can be eliminated via metabolic transformation is represented by the metabolic transformation rate constant k_M (d^{-1}). This process is dependent on the PCB congener and the species in question. Aquatic micro- and macrophytes, invertebrates and fish very poorly metabolize the majority of PCB congeners. In this study, we have therefore assumed that for the PCB congeners considered in this model, k_M is negligible in these species.

Table 2.1 provides a summary for abiotic model state variables. Tables 2.2 and 2.3 provide a summary of model state variables for phytoplankton and all other aquatic biota (i.e. zooplankton, invertebrates and fish), respectively.

Table 21: A summary of abiotic model state variables, that require parameterization in the SFB food web model.

Definition	Parameter	Units
Mean air temperature	T_A	^oC
Mean water temperature	T_W	^oC
Dissolved oxygen concentration	DO	mg O_2/L
Practical salinity units	PSU	g/kg
Dissolved organic carbon content – water	OC_{WATER}	kg/L
Particulate organic carbon content – water	POC	kg/L
Concentration of suspended solids – water	C_{SS}	kg/L
Organic carbon content – sediment	$OC_{SEDIMENT}$	%
Chemical concentration – water	C_{WT}	ng/L
Octanol-water partition coefficient	K_{OW}	unitless
Octanol-air partition coefficient	K_{OA}	unitless
Non-lipid organic matter – octanol proportionality constant	β	unitless

Table 22: A summary of biotic state variables that require parameterization in the bioaccumulation model for phytoplankton.

Definition	Parameter	Units
Whole body lipid fraction	L	kg/kg
Whole body non-lipid organic carbon fraction	NLOC	kg/kg
Whole body water fraction	WC	kg/kg
Phytoplankton growth rate constant	K_G	d^{-1}
Constant A_P (equation 2.12)	A_P	d^{-1}
Constant B_P (equation 2.12)	B_P	d^{-1}

Table 23: A summary of model state variables that require parameterization in the bioaccumulation model for zooplankton, invertebrates and fish.

Definition	Parameter	Units
Wet weight	W	kg
Whole body lipid fraction	L	kg/kg
Whole body non-lipid organic matter fraction	NLOM	kg/kg
Whole body water fraction	WC	kg/kg
Percentage of respired pore water	P_W	%
Invertebrate growth rate coefficient	I_{GR}	unitless
Fish growth rate coefficient	F_{GR}	unitless
Metabolic transformation rate constant	k_M	d^{-1}
Fraction of prey item in diet	P_i	unitless
Lipid absorption efficiency	ε_L	%
NLOM absorption efficiency	ε_N	%
Water absorption efficiency	ε_W	%
Constant A_{EW} (equation 2.10)	A_{EW}	unitless
Constant B_{EW} (equation 2.10)	B_{EW}	unitless
Constant A_{ED} (equation 2.18)	A_{ED}	unitless
Constant B_{ED} (equation 2.18)	B_{ED}	unitless

2.4.3 Detailed Bioaccumulation Model Description for harbor Seals

Figure 2.3 [illegible] of PCB uptake and elimination i[illegible] and inhalation of air. Dietary uptal[illegible]Bs in the harbor seal. Elimination [illegible]ey include elimination of PCBs in [illegible]mination in urine. In addition, ther[illegible]bolized in harbor seals [Boon and R[illegible]eals can transfer PCBs into their off[illegible]ng and growth periods can also affect PCB concentrations. Several of these uptake and elimination processes occur at particular times of the year and are non-continuous. Harbor seals are known to fast and molt at particular times of the year and female animals give birth and nurse their pups for a period of approximately 4 weeks. To represent these processes in a relatively simple model, it is important to consider some key characteristics of PCBs. First, PCBs are lipophilic chemicals that build up high concentrations in the lipids of organisms.

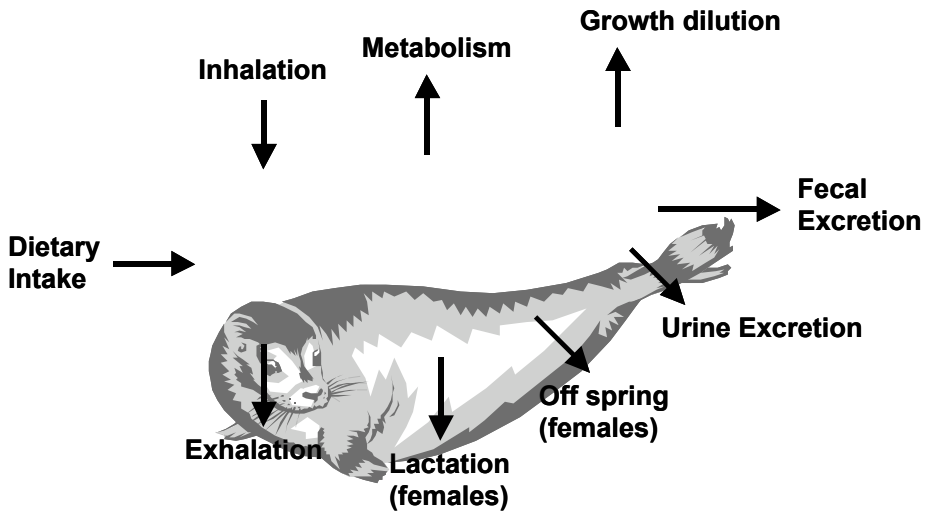

Figure 2.3: Conceptual diagram of the major uptake and elimination processes of PCBs in harbor seals

Seals contain large amounts of fat in their blubber (i.e. the lipid content of healthy harbor seals in the Bay varies between 36 to 50%), which means that the great majority of PCBs are found in the lipid tissues. Secondly, PCBs show a natural tendency to establish a chemical equilibrium. Within an organism like a seal this means that PCBs distribute themselves between various parts of the organism in a way that the concentrations in lipids of any part of the organism is approximately equal. In other words, the lipid-normalized concentration is approximately the same. This behavior of PCBs is of particular relevance to transfer of PCBs from female seals into their pups. If it can be assumed that PCBs in mother and pup achieve an internal equilibrium, then the lipid-normalized concentration in female seals will not change upon parturition. In essence, the reduction in the mass of PCBs in the mother upon parturition (due to transfer to the pup) is associated with a proportional drop in lipid mass, causing the lipid-normalized concentration to remain approximately the same. The same principle is at work during lactation. Assuming that PCB is equally distributed among fats in the nursing female, transfer of PCB in milk does not cause a change in concentration as proportional declines in PCB mass and lipid mass occur during lactation. The same philosophy applies to molting. While production of off-spring, lactation and molting are not expected to have an immediate effect on the lipid-normalized concentration in the seal, they do have a long-term concentration effect in seals because of the growth dilution effect that takes place during fetus development, milk production and skin formation. Seals have to grow body mass to accommodate these processes in addition to any net (year-to-year) increases in body weight. This process of growth takes place more gradually over the seal's life cycle and can be represented as a continuous process. Of course, the growth induced decline of the PCB concentration in seals is compensated by intake of PCB with the diet that makes growth possible. The balance between uptake and elimination is represented by the following mass balance equation:

$$dC_{HS,l}/dt = k_A C_{AG} + k_D.\Sigma(P_i \cdot C_{D,i}) - (k_O + k_E + k_U + k_G + k_P + k_L + k_M) \cdot C_{HS,l} \quad (2.29)$$

where $C_{HS,l}$ is the lipid-normalized concentration of the PCB congener in the seal and $dC_{HS,l}/dt$ is the net change in lipid-normalized concentration over time t (d). C_{AG} is the gaseous aerial concentration ($g \cdot L^{-1}$). k_A is the inhalation rate constant (L/kg lipid$\cdot d^{-1}$). k_D is the clearance rate constant (kg/kg lipid.d^{-1}) for PCB uptake via ingestion of food and water. P_i is the fraction of the diet consisting of prey item i and $C_{D,i}$ is the concentration of the PCB congener (g/kg) in prey item i. k_O is the rate constant (d^{-1}) for exhalation of PCB via the lungs. k_E is the rate constant (d^{-1}) for the elimination of the PCB congener via excretion into egested feces. k_U is the rate constant for urinary excretion of PCBs. k_G is the rate constant for growth dilution. This term accounts for year-to-year increases in the net growth of the animals. k_P is the rate constant for transfer of PCBs into the pups. It represents the increase in lipid mass (equivalent to the post-parturition lipid mass of the pup) over the duration of the gestation period. k_L is the rate constant for transfer of PCBs to the pups as a result of lactation. It portrays the growth of lipid mass of the female seals over the year that is transferred to the pup during lactation. k_G, k_P and k_L are expressed as fixed annual proportional increases in body lipid weight, i.e. $dW_{S,l}/(W_{S,l}.dt)$ where $W_{S,l}$ is the weight of the lipids in the seal, and has units of d^{-1}. k_M is the rate constant for metabolic transformation of the PCB congener. At steady-state, equation 2.29 can be simplified to:

$$C_{HS,l} = (k_A C_{AG} + k_D . \Sigma(P_i \cdot C_{D,i})) / (k_O + k_E + k_U + k_G + k_P + k_L + k_M) \qquad (2.30)$$

A whole organisms wet weight based concentration in the seal C_{HS} can be calculated from the lipid-normalized concentration as:

$$C_{HS} = L_{HS} \cdot C_{S,l} \qquad (2.31)$$

Because the whole organism lipid content undergoes significant changes throughout the year, the wet weight concentration in the seal can be expected to undergo changes of similar magnitude. These can be represented in the model by varying L_{HS}. Because the

lipid content in seals is high, the contribution of non-lipid organic matter as a storage compartment for PCBs is relatively insignificant.

The ratio of the PCB concentrations in the seal C_{HS} and the concentration in the sediment C_S is the biota-sediment accumulation factor (BSAF in units of kg dry sediment/kg wet weight):

$$BSAF = C_{HS}/C_S \tag{2.32}$$

The BSAF provides a simple means to anticipate the concentrations of PCBs in seals from the PCB concentration in the sediments of the Bay.

The various submodels for calculating k_D, k_A, k_O, k_E, k_U, k_G, k_P and k_L in the seal model are described below.

***k_D and k_E*:** The dietary uptake clearance rate constant k_D (kg-food/kg-lipid · d) for PCBs was estimated as a function of the dietary chemical transfer efficiency E_D, and reported measurements of the feeding rate G_D (kg/d) and the lipid mass of the organism $W_{S,l}$ (kg):

$$k_D = E_D \cdot G_D / W_{S,l} \tag{2.33}$$

The following equation based on the lipid-water two-phase resistance model was used to calculate the dietary absorption efficiencies of the PCB congeners in male and female seals:

$$E_D = (A_{ED} \cdot K_{OW} + B_{ED})^{-1} \tag{2.34}$$

where constant A_{ED} is 1.0 [± 0.17]·10^{-9} and constant B_{ED} is 1.025 [±0.00125] for harbor seals.

The rate constant for fecal excretion of PCBs in seals k_E (d^{-1}) was estimated as:

$$k_E = G_F \cdot E_D \cdot K_{GS,l} / W_{S,l} \quad (2.35)$$

where G_F (kg-feces/kg-organism · d) is the fecal egestion rate and $K_{GS,l}$ is the partition coefficient of the chemical between the GIT and seal lipids. G_F is a function of the feeding rate and the digestibility of the diet, which in turn is a function of the composition of the diet according to:

$$G_F = \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \cdot G_D \quad (2.36)$$

where ε_L, ε_N and ε_W are the dietary absorption efficiencies of lipid, NLOM and water, respectively. v_{LD}, v_{ND}, and v_{WD} are the overall lipid, NLOM and water contents of the diet, respectively. In seals, the absorption efficiencies of lipid and NLOM are assumed to be approximately 98% and 75%, respectively [Rosen et al. 2000 and Rosen and Trites. 2000].

The partition coefficient $K_{GS,l}$ of the PCBs between the contents of the GIT and the seal's body lipids is estimated as:

$$K_{GB} = (v_{LG} \cdot K_{OW} + v_{NG} \cdot \beta \cdot K_{OW} + v_{WG}) / K_{OW} \quad (2.37)$$

where v_{LG}, $v_{NG,}$, and v_{WG} are the lipid (kg lipid/kg digesta ww), NLOM (kg NLOM/kg digesta ww) and water (kg water/kg digesta ww) contents in the gut of the seal respectively. The sum of these fractions (i.e. total digesta) approach 1 and are dependent on the absorption efficiency for each component of the diet as:

$$v_{LG} = (1-\varepsilon_L) \cdot v_{LD} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.38)$$

$$v_{NG} = (1-\varepsilon_N) \cdot v_{ND} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.39)$$

$$v_{WG} = (1-\varepsilon_W) \cdot v_{WD} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.40)$$

k_A and k_O: The absorption rate of PCBs from inhalation of air is expressed by the inhalation clearance rate constant k_A (L/kg lipid · d):

$$k_A = E_A \cdot G_A / W_{S,l} \quad (2.41)$$

The rate constant for PCB elimination via exhalation k_O (d^{-1}) is related to k_A as inhalation and exhalation involve the same processes of lung ventilation and pulmonary membrane permeation:

$$k_O = k_A / K_{S,lA} \quad (2.42)$$

where $K_{S,lA}$ (L/kg lipid) is the partition coefficient of the PCB congener between the lipid biomass of the seal and the air, which was estimated from the octanol-air partition coefficient K_{OA} and the density of lipids δ_L (kg/L) as:

$$K_{S,lA} = k_A / k_O = K_{OA} \cdot \delta_L^{-1} \quad (2.43)$$

The urinary excretion rate constant k_U (d^{-1}) is calculated as:

$$k_U = G_U / (W_{S,l} \cdot K_{OW} \cdot \delta_L^{-1}) \quad (2.44)$$

where G_U is the urinary excretion rate (L/d) and K_{OW} is the octanol-water partition coefficient.

k_G, k_P, k_L: In this model, the "quasi" elimination rate constants for growth dilution of the PCB concentration in male and female harbor seals and elimination of PCB in off-spring and milk in female harbor seals, represent the reduction in the PCB concentration in the lipid biomass of the seals that is achieved due to the increase in lipid biomass as a result of growth, off spring production and lactation. Each of these rate constants is represented by the proportional increase in the lipid biomass per unit of time according to:

$$dW_{HS,l} / (W_{HS,l} \cdot dt) \qquad (2.45)$$

When calculating k_G, $dW_{HS,l}$ represents the increase in lipid mass achieved over a year. When assessing k_P, $dW_{HS,l}$ describes the mass of lipid of the pup at the time of birth. This lipid biomass is generated over the duration of the gestation period. To estimate k_L, $dW_{HS,l}$ describes the mass of lipid transferred to the pup in the milk over the length of the lactation period, i.e. the product of the lactation rate G_L (L/d) and the length of the lactation period t_L. To make a relatively simple steady-state solution of the model possible, we calculated the increase in the lipid biomass of the female seals as the sum of the lipid masses generated for growth, off-spring production and lactation and expressed it as a fraction of the animal's lipid biomass generated per unit of time.

k_M: harbor seals have been shown to metabolize certain PCB congeners at significant rates. This can have a significant effect on the magnitude of PCB concentrations that will be attained in harbor seals. It has been observed that PCBs exhibit congener specific metabolic transformation patterns [Boon and Reijnders 1987 and Boon et al. 1994, 1997]. It is therefore possible to estimate the metabolic transformation of each PCB congener relative to a reference congener. In studies with harbor seals [Boon and Reijnders 1987 and Boon et al. 1994, 1997], PCB 153 was observed to be the dominant PCB congener. Empirical data show that PCB 153 is also the dominant PCB congener in the harbor seals of SFB. To estimate the metabolic transformation rate constant of each PCB congener, we fit the model (i.e. equation 2.30) by changing the metabolic transformation rate

constant k_M to obtain PCB congener specific concentration ratios (i.e. concentrations of PCB_i / concentration of PCB 153) that matches the observed concentration ratios concentrations of PCB_i / concentration of PCB 153. The metabolic transformation rate constant of PCB 153 was assumed to be 0 d^{-1}. This method produced a set of gender and congener specific metabolic transformation rate constants which are listed in Table 1 of Appendix B. These values were used in the model calculations.

Table 2.4 summarizes state variables for the San Francisco Bay harbor seals.

Table 2.4: A summary of model state variables that require parameterization in the bioaccumulation model for harbor seals, Double-crested Cormorants and Forster's Tern.

Definition	Parameter	Units
Wet weight	W	kg
Whole body lipid fraction	L	kg/kg
Whole body non-lipid organic matter fraction	NLOM	kg/kg
Whole body water fraction	WC	kg/kg
Mean homeotherm temperature	T_H	^oC
Growth rate constant	K_G	d^{-1}
Fraction of prey item in diet	P_i	unitless
Lipid absorption efficiency	ε_L	%
NLOM absorption efficiency	ε_N	%
Water absorption efficiency	ε_W	%
Constant A_{ED} (equation 2.34 for seals and 2.52 for birds)	A_{ED}	unitless
Constant B_{ED} (equation 2.34 for seals and 2.52 for birds)	B_{ED}	unitless
Urine excretion rate (for harbor seals)	G_U	L/d
Metabolic transformation rate constant	k_M	d^{-1}

2.4.4 Detailed Bioaccumulation Model Description: Cormorants and Terns

A conceptual overview of the major routes of PCB uptake and elimination in cormorants and terms is presented in Figure 2.4. PCB uptake is due to dietary uptake and inhalation of air. Dietary uptake is believed to be the most important process for uptake of PCBs in these bird species. The mechanisms by which these bird species eliminate PCBs include the elimination of PCBs in exhaled air, PCB excreted in fecal matter, elimination in urine and metabolic transformation. During periods of growth, PCB concentrations can be affected by growth dilution, which is not a real elimination process but has the potential effect of reducing the PCB body burden in the animals.

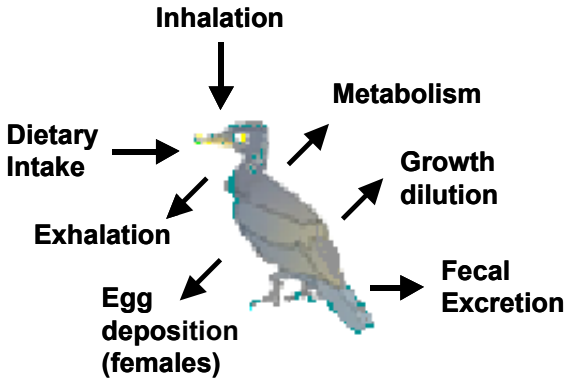

Figure 2.4: Conceptual diagram of the major uptake and elimination processes of PCBs in birds.

Female birds can also transfer PCBs into eggs. In the model, the effect of transferring PCBs to eggs on the maternal PCB body burden is assumed to be similar to that described above in the section on the bioaccumulation model for harbor seals. Again, we make the assumption that PCBs are well distributed among the lipid tissues in the bird. This assumption implies that the reduction in the mass of PCBs in the mother as a result of transfer of PCBs in the eggs is associated with a proportional drop in lipid mass, causing the lipid-normalized concentration to remain approximately the same. The wet weight based concentration in the female bird may undergo a change as a result of laying eggs,

due to the change in body composition (i.e. predominantly due to changes in lipid content). The main impact of producing eggs on the maternal PCB body burden is the result of the increase in body mass required to produce the eggs. Any growth induced decline of the PCB concentration in the female birds is compensated by intake of PCB with the diet that makes growth possible. The balance between uptake and elimination rates is represented by the following mass balance equation:

$$dC_{C,l}/dt = k_A C_{AG} + k_D.\Sigma(P_i \cdot C_{D,i}) - (k_O + k_E + k_G + k_C + k_M) \cdot C_{C,l} \qquad (2.47)$$

where $C_{C,l}$ is the lipid-normalized concentration of the PCB congener in either the cormorant or the tern; and $dC_{C,l}/dt$ is the net change in lipid-normalized concentration over time t (d). C_{AG} is the gaseous aerial concentration ($g \cdot L^{-1}$). k_A is the inhalation rate constant (L/kg lipid$\cdot d^{-1}$). k_D is the clearance rate constant (kg/kg lipid.d^{-1}) for PCB uptake via ingestion of food and water. P_i is the fraction of the diet consisting of prey item i and $C_{D,i}$ is the concentration of the PCB congener (g/kg) in prey item i. k_O is the rate constant (d^{-1}) for exhalation of PCB via the lungs of the birds. k_E is the rate constant (d^{-1}) for the elimination of the PCB congener via excretion into egested feces. k_G is the rate constant for growth dilution due to year-to-year increases in the net body mass of the birds. k_C is the rate constant for transfer of PCBs into eggs in female birds. It represents the increase in lipid mass due to egg production. k_M is the rate constant for metabolic transformation of the PCB congener in the bird.

At steady-state, equation 2.47 can be simplified to:

$$C_{C,l} = (k_A C_{AG} + k_D \cdot \Sigma(P_i \cdot C_{D,i})) / (k_O + k_E + k_G + k_C + k_M) \qquad (2.48)$$

The whole organisms wet weight based concentration can be calculated from the lipid-normalized concentration as;

$$C_C = L_C \cdot C_{C,l} \quad (2.49)$$

Where L_C is the lipid content of the cormorants or the terns. Since L_C can undergo significant changes throughout the year, the wet weight concentration in the seal can be expected to vary as well. This can be represented in the model by varying L_C.

The ratio of the PCB concentrations in the cormorants or the terms and the concentration in the sediment C_S is the biota-sediment accumulation factor ($BSAF_C$):

$$BSAF_C = C_C/C_S \quad (2.50)$$

The BSAF provides a simple means to anticipate the concentrations of PCBs in the cormorants or the terns from the PCB concentration in the sediments of the Bay.

The various submodels for calculating k_D, k_A, k_O, k_E, k_C and k_G in the models for the bird species are described below.

***k_D and k_E*:** The dietary uptake clearance rate constant k_D (kg-food/kg-lipid · d) for PCBs was estimated as a function of the dietary chemical transfer efficiency E_D, and reported measurements of the feeding rate G_D (kg/d) and the lipid mass of the organism $W_{C,l}$ (kg):

$$k_D = E_D \cdot G_D / W_{C,l} \quad (2.51)$$

The following equation based on the lipid-water two-phase resistance model was used to calculate the dietary absorption efficiencies of the PCB congeners in male and female birds:

$$E_D = (A_{ED} \cdot K_{OW} + B_{ED})^{-1} \quad (2.52)$$

where constant A_{ED} is 3.0 [± 0.49]·10^{-9} and constant B_{ED} is 1.04 [±0.002] for cormorants and terns.

The rate constant for fecal excretion of PCBs in cormorants and terns k_E (d^{-1}) was estimated as:

$$k_E = G_F \cdot E_D \cdot K_{GC,l} / W_{C,l} \quad (2.53)$$

where G_F (kg-feces/kg-organism · d) is the fecal egestion rate and $K_{GC,l}$ is the partition coefficient of the chemical between the GIT and the lipids of the birds. G_F is a function of the feeding rate and the digestibility of the diet, which in turn is a function of the composition of the diet according to:

$$G_F = \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \cdot G_D \quad (2.54)$$

where ε_L, ε_N and ε_W are the dietary absorption efficiencies of lipid, NLOM and water, respectively. v_{LD}, v_{ND}, and v_{WD} are the overall lipid, NLOM and water contents of the diet, respectively.

The partition coefficient $K_{GC,l}$ of the PCBs between the contents of the GIT and the body lipids of the birds is estimated as:

$$K_{GB} = (v_{LG} \cdot K_{OW} + v_{NG} \cdot \beta \cdot K_{OW} + v_{WG}) / K_{OW} \quad (2.55)$$

where v_{LG}, $v_{NG,}$, and v_{WG} are the lipid (kg lipid/kg digesta ww), NLOM (kg NLOM/kg digesta ww) and water (kg water/kg digesta ww) contents in the gut of the birds respectively. The sum of these fractions (i.e. total digesta) approach 1 and are dependent on the absorption efficiency for each component of the diet as:

$$v_{LG} = (1-\varepsilon_L) \cdot v_{LD} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.56)$$

$$v_{NG} = (1-\varepsilon_N) \cdot v_{ND} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.57)$$

$$v_{WG} = (1-\varepsilon_W) \cdot v_{WD} / \{(1-\varepsilon_L) \cdot v_{LD} + (1-\varepsilon_N) \cdot v_{ND} + (1-\varepsilon_W) \cdot v_{WD}\} \quad (2.58)$$

k_A and k_O: The absorption rate of PCBs from inhalation of air is expressed by the inhalation clearance rate constant k_A (L/kg lipid · d):

$$k_A = E_A \cdot G_A / W_{C,l} \quad (2.59)$$

The rate constant for PCB elimination via exhalation k_O (d^{-1}) is related to k_A as inhalation and exhalation involve the same processes of lung ventilation and membrane permeation:

$$k_O = k_A / K_{C,lA} \quad (2.60)$$

where $K_{C,lA}$ (L/kg lipid) is the partition coefficient of the PCB congener between the lipid biomass of the birds and the air, which was estimated from the octanol-air partition coefficient, i.e.:

$$K_{C,lA} = k_A / k_O = K_{OA} \cdot \delta_L^{-1} \quad (2.61)$$

K_U: The urinary excretion rate constant k_U (d^{-1}) is calculated as:

$$k_U = G_U / (W_{C,l} \cdot K_{OW} \cdot \delta_L^{-1}) \quad (2.62)$$

where G_U is the urinary excretion rate (L/d) and K_{OW} is the octanol-water partition coefficient.

k_G, k_C: The rate constants for growth dilution of the PCB concentration in male and female birds and deposition of PCB in eggs by female birds, are calculated from the reduction in the PCB concentration in the lipid biomass of the bird that can be expected to occur as the lipid biomass increases due to growth and egg production in the female bird. Each of these rate constants is represented by the proportional increase in the lipid biomass per unit of time according to:

$$dW_{HS,l} / (W_{C,l} \cdot dt) \qquad (2.63)$$

In equation 2.63, $dW_{C,l}$ represents the increase in lipid mass achieved over a year due to growth in the bird when calculating k_G. It represents the mass of lipid transferred into the egg when calculating k_C. This lipid biomass is generated over the duration of the gestation period. To keep the model simple, we calculated the increase in the lipid biomass of the female birds as the sum of the lipid masses generated for growth and egg production and expressed it as a fraction of the animal's lipid biomass generated per unit of time.

k_M Metabolic transformation rates of individual PCB congeners in Double-crested Cormorants were derived from empirical San Francisco Bay cormorant egg PCB concentration data using the same method described in section 2.4.3 for San Francisco harbor seals. These estimated metabolic rates were generally comparable to metabolic transformation rates derived from controlled laboratory studies in American kestrels (*Falco sparverius*) [Drouillard et al 2001]. The estimates of the metabolic transformation rate constants in cormorants were also used for the Forster's Tern. Appendix B illustrates the estimated metabolic transformation rate for each SFEI PCB congener.

Table 2.4 summarizes state variables for the bird species included in the model.

2.5 MODEL PARAMETERIZATION

2.5.1 General

The model parameterization is the phase in the model development where values for the model's state variables are selected to ensure that the model is representative of conditions in the Bay. This section lists the values for the various state variables that were chosen. These values are also documented in the Excel model that accompanies this report. In the parameterization we have attempted to make use of information reported in the scientific literature. For the great majority of the model input variables sufficient information is available to select appropriate values. However, we also encountered instances where required model input variables needed to be estimated because of a lack of appropriate data in the literature. In these cases we have documented the rationale of our selection.

2.5.2 Physical Chemical Properties of PCBs

The octanol-water (K_{OW}) and octanol-air (K_{OA}) partition coefficients of the PCB congeners that were used in the model calculations are summarized in Table 2.5 and also tabulated in the worksheet entitled "Input-1" in the San Francisco Bay Food Web Model. This Table lists the freshwater-based octanol-water partition coefficient at the mean ambient water temperature of the Bay of 14.9^{o}C. These were used to derive the saltwater-based octanol-water partition coefficient following Xie et al. [1997]. The saltwater-based K_{OW} values were used in the calculations of the distribution of the PCBs between fish and water of the Bay. The model also uses the freshwater-based octanol-water partition coefficient at 37.5^{o}C to represent partitioning between lipids and aqueous media (e.g. urine) in warm-blooded mammals and birds. Table 2.5 also includes the data used to represent the octanol-air partition coefficients at 13.7 and 37.5^{o}C. The latter values are used to represent the exchange of PCBs between the animal and the air via the lungs.

The uncertainty in log K_{OW}, as reported in Table 2.5, reflects uncertainty associated with observations of K_{OW} reported in the cited papers. We did not choose to measure the uncertainty in K_{OW} through a compilation of literature data. Compilations of this kind include data collected over many years and determined by different methods. Certain methods (e.g. shake-flask) provide unreliable values for the K_{OW} of PCBs. When these unreliable values are combined with better (and newer) quality data, large uncertainties are sometimes calculated. Uncertainty calculated in this fashion is not reflective of the actual (and currently accepted) uncertainty in the K_{OW} measurements.

2.5.3 Toxic Equivalency Factors for PCBs

The toxic equivalency factors for fish, bird and mammalian species were derived from Van den Berg et al. [1998] and are documented in Table 2.6. In the San Francisco Bay food web model, they can be found in the "management" worksheet. If new or better values become available, the existing values can be replaced by the new values.

Table 25: Molecular weight (MW) in g/mol, LeBas Molar volume (used to calculate the saltwater based K_{OW}) in cm^3/mol, the freshwater octanol-water partition coefficient (K_{OW}) at 14.9°C, the salt-water octanol-water partition coefficient (K_{OW}) at 14.9°C, the freshwater octanol-water partition coefficient (K_{OW}) at 37.5°C and the octanol-air partition coefficient (K_{OA}) at 13.7°C and 37.5°C. SD is one standard deviation expressed in logarithmic units.

PCB Congener	MW (g/mol)	LeBas Molar Volume (cm^3/mol)	*Ref.*	log K_{OW} 14.9 °C	Uncertainty (1 SD)	log K_{OW} [a] 14.9 °C	*Ref.*	log K_{OW} 37.5 °C	*Ref.*	log K_{OA} 13.7 °C	log K_{OA} 37.5 °C	*Ref.*
8	223.1	226.4	*1*	5.19	0.04	5.31	*2*	5.15	*2*	7.79	6.83	*2*
18	257.5	247.4	*1*	5.32	0.08	5.44	*3* [b]	5.28	*3* [d]	7.67	6.82	*4*
28	257.5	247.4	*1*	5.74	0.09	5.87	*2*	5.69	*2*	8.33	7.29	*2*
31	257.5	247.4	*1*	5.86	0.10	5.99	*2*	5.81	*2*	8.43	7.39	*2*
33	257.5	247.4	*1*	5.67	0.13	5.80	*3* [b]	5.63	*3* [d]	8.30	7.40	*4*
44	292.0	268.4	*1*	5.84	0.12	5.98	*3* [b]	5.80	*3* [d]	8.90	7.96	*4*
49	292.0	268.4	*1*	5.97	0.13	6.11	*3* [b]	5.93	*3* [d]	8.53	7.61	*4*
52	292.0	268.4	*1*	6.00	0.12	6.14	*2*	5.81	*2*	8.72	7.64	*2*
56	292.0	268.4	*1*	6.04	0.13	6.17	*3* [b]	6.00	*3* [d]	9.12	8.16	*4*
60	292.0	268.4	*1*	6.14	0.19	6.28	*3* [b]	6.10	*3* [d]	9.54	8.55	*4*
66	292.0	268.4	*1*	6.02	0.20	6.16	*3* [b]	5.98	*3* [d]	9.57	8.58	*4*
70	292.0	268.4	*1*	6.12	0.14	6.26	*3* [b]	6.08	*3* [d]	9.21	8.25	*4*
74	292.0	268.4	*1*	6.13	0.13	6.26	*3* [b]	6.09	*3* [d]	9.39	8.41	*4*
87	326.5	289.4	*1*	6.37	0.13	6.52	*3* [b]	6.33	*3* [d]	9.49	8.51	*4*
95	326.5	289.4	*1*	6.07	0.12	6.22	*3* [b]	6.03	*3* [d]	9.25	8.28	*4*
97	326.5	289.4	*1*	6.29	0.03	6.44	*3* [b]	6.25	*3* [d]	9.43	8.45	*4*
99	326.5	289.4	*1*	6.38	0.04	6.53	*3* [b]	6.34	*3* [d]	9.57	8.58	*4*
101	326.5	289.4	*1*	6.41	0.03	6.56	*2*	6.36	*2*	9.34	8.25	*2*
105	326.5	289.4	*1*	6.91	0.20	7.06	*2*	6.85	*2*	10.07	8.90	*2*
110	326.5	289.4	*1*	6.34	0.12	6.49	*3* [c]	6.28	*3* [e]	9.46	8.48	*4*

PCB Congener	MW (g/mol)	LeBas Molar Volume (cm^3/mol)	*Ref.*	log K_{OW} 14.9 °C	Uncertainty (1 SD)	log K_{OW} [a] 14.9 °C	*Ref.*	log K_{OW} 37.5 °C	*Ref.*	log K_{OA} 13.7 °C	log K_{OA} 37.5 °C	*Ref.*
118	326.5	289.4	*1*	6.78	0.14	6.93	*2*	6.72	*2*	9.91	8.74	*2*
128	361.0	310.4	*1*	6.82	0.19	6.98	*3* [c]	6.76	*3* [e]	10.19	9.16	*4*
132	361.0	310.4	*1*	6.57	0.06	6.73	*3* [c]	6.51	*3* [e]	9.96	8.94	*4*
138	361.0	310.4	*1*	7.30	0.24	7.46	*2*	7.25	*2*	10.19	9.05	*2*
141	361.0	310.4	*1*	6.80	0.08	6.96	*3* [c]	6.74	*3* [e]	10.26	9.22	*4*
149	361.0	310.4	*1*	6.65	0.07	6.81	*3* [c]	6.59	*3* [e]	9.96	8.94	*4*
151	361.0	310.4	*1*	6.63	0.06	6.79	*3* [c]	6.57	*3* [e]	10.01	8.99	*4*
153	360.9	310.4	*1*	6.97	0.06	7.13	*2*	6.91	*2*	10.02	8.78	*2*
156	361.0	310.4	*1*	7.04	0.24	7.20	*3* [c]	6.98	*3* [e]	10.82	9.74	*4*
158	361.0	310.4	*1*	6.90	0.21	7.06	*3* [c]	6.84	*3* [e]	10.48	9.43	*4*
170	395.5	331.4	*1*	7.21	0.13	7.38	*3* [c]	7.15	*3* [e]	10.97	9.89	*4*
174	395.5	331.4	*1*	7.06	0.11	7.23	*3* [c]	7.00	*3* [e]	10.69	9.62	*4*
177	395.5	331.4	*1*	7.04	0.11	7.21	*3* [c]	6.98	*3* [e]	10.80	9.73	*4*
180	395.5	331.4	*1*	7.25	0.09	7.42	*2*	7.19	*2*	10.73	9.51	*2*
183	395.5	331.4	*1*	7.15	0.12	7.32	*3* [c]	7.09	*3* [e]	10.97	9.88	*4*
187	395.5	331.4	*1*	7.12	0.11	7.29	*3* [c]	7.06	*3* [e]	10.79	9.71	*4*
194	429.8	352.4	*1*	7.85	0.19	8.03	*2*	7.79	*2*	11.70	10.46	*2*
195	430.0	352.4	*1*	7.48	0.16	7.66	*3* [c]	7.42	*3* [e]	11.58	10.45	*4*
201	430.0	352.4	*1*	7.54	0.16	7.72	*3* [c]	7.48	*3* [e]	11.38	10.26	*4*
203	430.0	352.4	*1*	7.56	0.17	7.74	*3* [c]	7.50	*3* [e]	11.55	10.43	*4*

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[a] Salinity correction Xie, WH, Shiu, WY, Mackay, D. 1997.

[b] +0.02 log units for temperature correction – estimated from ref 2 and ref 3

[c] +0.03 log units for temperature correction – estimated from ref 2 and ref 3

[d] -0.02 log units for temperature correction – estimated from ref 2 and ref 3

[e] -0.03 log units for temperature correction – estimated from ref 2 and ref 3

Table 2.6: Toxic Equivalency Factors (TEF) of PCB congeners in humans and wildlife.

PCB Congener	TEF – WHO Fish	TEF – WHO Birds	TEF – WHO Mammals
8	0.000000	0.000000	0.000000
18	0.000000	0.000000	0.000000
28	0.000000	0.000000	0.000000
31	0.000000	0.000000	0.000000
33	0.000000	0.000000	0.000000
44	0.000000	0.000000	0.000000
49	0.000000	0.000000	0.000000
52	0.000000	0.000000	0.000000
56	0.000000	0.000000	0.000000
60	0.000000	0.000000	0.000000
66	0.000000	0.000000	0.000000
70	0.000000	0.000000	0.000000
74	0.000000	0.000000	0.000000
87	0.000000	0.000000	0.000000
95	0.000000	0.000000	0.000000
97	0.000000	0.000000	0.000000
99	0.000000	0.000000	0.000000
101	0.000000	0.000000	0.000000
105	0.000005	0.000100	0.000100
110	0.000000	0.000000	0.000000
118	0.000005	0.000100	0.000100
128	0.000000	0.000000	0.000000
132	0.000000	0.000000	0.000000
138	0.000000	0.000000	0.000000
141	0.000000	0.000000	0.000000
149	0.000000	0.000000	0.000000
151	0.000000	0.000000	0.000000
153	0.000000	0.000000	0.000000
156	0.000005	0.000100	0.000500
158	0.000000	0.000000	0.000000
170	0.000000	0.000000	0.000000
174	0.000000	0.000000	0.000000
177	0.000000	0.000000	0.000000
180	0.000000	0.000000	0.000000
183	0.000000	0.000000	0.000000
187	0.000000	0.000000	0.000000
194	0.000000	0.000000	0.000000
195	0.000000	0.000000	0.000000
201	0.000000	0.000000	0.000000
203	0.000000	0.000000	0.000000

2.5.4 Environmental Conditions of the Bay

The input variables used to characterize the environmental conditions in the Bay are included in Table 2.7. These values can be found in worksheet "Input-1" in the San Francisco Bay Model.

Table 27: Model state variables selected to represent environmental conditions in San Francisco Bay. N/A – not applied.

Parameter	Input	Variability (+/-)	Units	Reference
Mean Water Temperature	14.9	1.3	^{O}C	*RMP SFB water data*
Mean Air Temperature	13.7	6.0	^{O}C	*Estimated*
Practical Salinity Units (PSU)	20.2	1.6	g/kg	*RMP SFB water data*
Dissolved Oxygen Concentration (DO)	8.09	1.1	mg O_2/L	*RMP SFB water data*
Dissolved Organic Carbon Content – Water (OC_{WATER})	2.10E-06	2.00E-07	kg/L	*RMP SFB water data*
Particulate Organic Carbon Content – Water (POC)	1.85E-06	1.50E-07	kg/L	*RMP Roberts 2002*
Concentration of Suspended Solids (C_{SS})	2.46E-05	2.50E-06	kg/L	*RMP SFB water data*
Organic Carbon Content- Sediment ($OC_{SEDIMENT}$)	1.02	0.50	%	*RMP SFB sediment data*
Density of Organic Carbon - Sediment (Docsed)	0.9	N/A	kg/L	*Mackay, D. 1991.*
Setschenow Proportionality Constant (SPC)	0.0018	N/A	L/cm^3	*Xie, WH, Shiu, WY, Mackay, D. 1997.*
Molar Concentration of Seawater @ 35 ppt (MCS)	0.5	N/A	mol/L	*Xie, WH, Shiu, WY, Mackay, D. 1997.*

2.5.5 Biological Variables

The species that are represented in the San Francisco Bay Food Web Model along with their body weight and lipid content are listed in Table 2.8. They include a total of 23 species, several age classes, male and female animals as well as their off-spring and eggs. A detailed account of the values chosen for each of the model state variables that require parameterization are presented in Appendix A. Appendix B includes the metabolic transformation rate constants used in the model. Tables 2.9 and 2.10 list the feeding preferences of the various species represented in the model. Figure 2.5 provides a schematic overview of organisms included in the San Francisco Bay food web and the representative trophic interactions considered in the model.

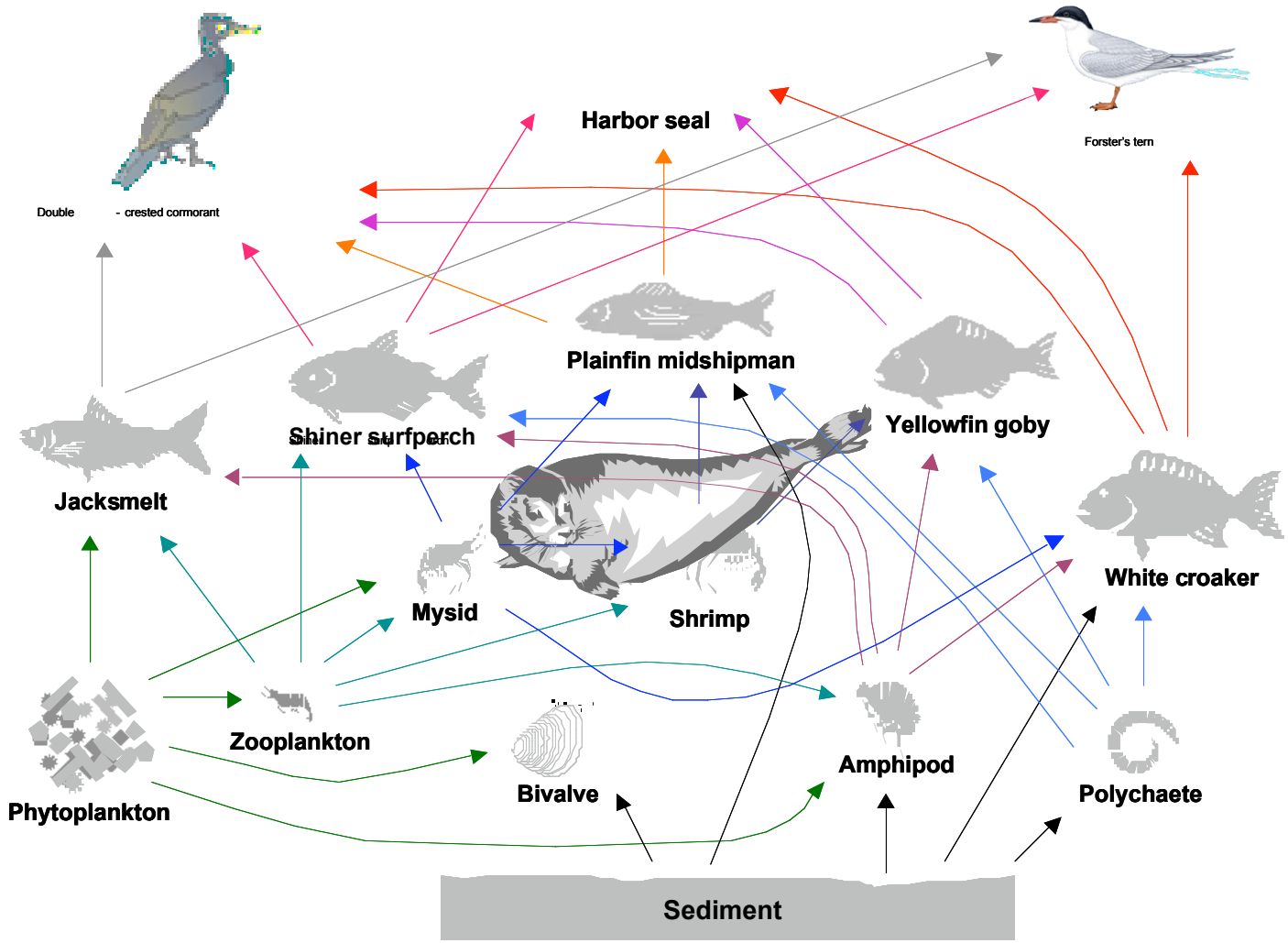

Figure 2.5: Conceptual diagram illustrating organisms included in the model and their trophic interactions.

Table 2.8: Species name, age class and sex of the species represented in the San Francisco Bay food web model.

Species #	Age Class	Species	Length (cm)	Weight (kg)	Reference	% Lipid content (1 SD)	Reference
Phytoplankton	N/A	phytoplankton (various sp, diatoms, algae sp.)	N/A	N/A	*N/A*	0.12 (0.02)	*Estimated from Mackintosh et al 2004*
Zooplankton	N/A	zooplankton (various sp. e.g., *Copepoda calanoid* or sp.)	N/A	7.10E-08	*Gobas and Wilcockson 2003*	0.75 (0.20)	*Estimated*
Benthic - 1	N/A	generic polychaete (e.g., *Neanthes succinea*)	N/A	1.10E-04	*Gobas and Wilcockson 2003*	0.75 (0.20)	*Estimated from Roberts et al 2002*
Benthic - 2	N/A	generic amphipod (e.g., *Ampelisca abdita* or sp.)	N/A	3.13E-06	Estimated	0.75 (0.20)	*Estimated from Roberts et al 2002*
Benthic - 3	N/A	generic cumacea (e.g., *Nippoleucon hinumensis*)	N/A	5.00E-06	*Estimated*	0.75 (0.20)	*Estimated from Roberts et al 2002*
Benthic - 4	N/A	*Mysis sp.*	N/A	1.50E-05	*Estimated*	1.0 (0.25)	*Estimated from Roberts et al 2002*
Benthic - 5	N/A	generic bivalve (e.g., *Mytilus californianus*) - included for model evaluation only	N/A	1.52E-03	*RMP sampling data 2000-2001*	6.99 (1.6)	*RMP sampling data 2000-2001*
Benthic - 6	N/A	generic bivalve (e.g., C*rassostrea gigas)* - included for model evaluation only	N/A	9.79E-04	*RMP sampling data 2000-2001*	9.37 (1.5)	*RMP sampling data 2000-2001*
Benthic - 7	N/A	generic polychaete (e.g., *Harmothoe imbricata*)	N/A	1.00E-07	*Gobas and Wilcockson 2003*	0.75 (0.20)	*Estimated from Roberts et al 2002*
Benthic - 8	N/A	generic shrimp (e.g., *Crangon sp.*)	N/A	3.72E-04	*Gobas and Wilcockson 2003*	1.5 (0.35)	*Estimated from Roberts et al 2002*
Fish - 1	0	*Cymatogaster aggregata* (shiner surfperch)	4.0	*1.31E-03*	*Estimated from Harvey et al 2000*	2.0 (0.5)	*Estimated from RMP sampling data 2000*
Fish - 2	0	*Atherinopsis californiensis* (jacksmelt)	8.0	4.00E-03	*Estimated from Harvey et al 2000*	1.2 (0.25)	*Estimated from RMP sampling data 2000*
Fish - 3	0	*Engraulis mordax* (Northern anchovy)	6.0	3.70E-03	*Estimated from Harvey et al 2000*	2.0 (0.5)	*Estimated from RMP sampling data 2000*

Species #	Age Class	Species	Length (cm)	Weight (kg)	Reference	% Lipid content (1 SD)	Reference
Fish - 4	0	*Genyonemus lineatus* (white croaker)	8.0	1.50E-02	*Estimated from Harvey et al 2000*	1.8 (0.4)	*Estimated from RMP sampling data 2000*
Fish - 5	>0	*Engraulis mordax* (Northern anchovy)	12.5	2.15E-02	*Estimated from Harvey et al 2000*	2.5 (0.6)	*Estimated from RMP sampling data 2000*
Fish - 6	>0	*Cymatogaster aggregata* (shiner surfperch)	11.2	5.13E-02	*RMP sampling data 2000*	2.62 (0.94)	*RMP sampling data 2000*
Fish - 7	>0	*Atherinopsis californiensis* (jacksmelt)	27.0	2.06E-01	*RMP sampling data 2000*	1.57 (0.73)	*RMP sampling data 2000*
Fish - 8	>0	*Acanthogobius flavimanus* (yellowfin goby)	15.0	3.00E-02	*Estimated from Andy Jahn Fish Gutz Survey*	3.0 (0.75)	*Estimated from RMP sampling data 2000*
Fish - 9	>0	*Porichthys notatus* (plainfin midshipman)	20.0	1.30E-01	*Estimated from Harvey et al 2000*	3.0 (0.75)	*Estimated from RMP sampling data 2000*
Fish - 10	>0	*Genyonemus lineatus* (white croaker)	26.1	3.71E-01	*Estimated from RMP sampling data 2000*	3.5 (0.75)	*Estimated from RMP sampling data 2000*
Avian - 1	Adult - male	*Phalacrocorax auritus* (Double-crested Cormorant)	N/A	2.50E+00	*1*	7.5 (1.5)	*6*
Avian - 2	Adult - female	*Phalacrocorax auritus* (Double-crested Cormorant)	N/A	2.40E+00	*1*	7.5 (1.5)	*6*
Avian egg - 1	Egg	*Phalacrocorax auritus* (Double-crested Cormorant)	N/A	4.49E-02	*1*	5.5 (0.53)	*7*
Avian - 3	Adult - male	*Sterna forsterii* (Forster's Tern)	N/A	1.90E-01	*2*	7.0 (1.5)	*7*
Avian - 4	Adult - female	*Sterna forsterii* (Forster's Tern)	N/A	1.75E-01	*2*	7.0 (1.5)	*7*
Avian egg - 2	Egg	*Sterna forsterii* (Forster's Tern)	N/A	2.13E-02	*2*	5.0 (0.5)	*7*
Mammal - 1	Adult - male	*Phoca vitulina richardsi* (harbor seal)	N/A	9.00E+01	*3,4*	43 (4.3)	*8*

Species #	Age Class	Species	Length (cm)	Weight (kg)	Reference	% Lipid content (1 SD)	Reference
Mammal - 2	Adult - female	*Phoca vitulina richardsi* (harbor seal)	N/A	8.00E+01	*3,4*	43 (4.3)	*8*
Mammal - 3	Juvenile	*Phoca vitulina richardsi* (harbor seal)	N/A	4.16E+01	*3,4*	40 (5)	*8*
Mammal - 4	Pup - 14 days	*Phoca vitulina richardsi* (harbor seal)	N/A	1.60E+01	*5*	25 (2)	*5,9*

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Table 2.9: Diet composition of fish and invertebrate species represented in the model. Diet items are presented in columns.

Species #	Age Class	Species	A	B	C	D	E	F	G	H	I	J	K	L	M	N	Ref.
Phytoplankton	N/A	Phytoplankton (various - diatoms, *algae sp.*)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	
Zooplankton	N/A	Zooplankton (e.g., *Copepoda calanoid*)	0	1	0	0	0	0	0	0	0	0	0	0	0	0	*1*
Benthos - 1	N/A	Generic polychaete (e.g., *Neanthes succinea*)	0.90	0.05	0.05	0	0	0	0	0	0	0	0	0	0	0	*2*
Benthos - 2	N/A	Generic amphipod (e.g., *Ampelisca abdita*)	0.3	0.35	0.35	0	0	0	0	0	0	0	0	0	0	0	*2*
Benthos - 3	N/A	Generic cumacea (e.g., *Nippoleucon hinumensis*)	0.15	0.65	0.2	0	0	0	0	0	0	0	0	0	0	0	*2*
Benthos - 4	N/A	*Mysis sp.*	0.1	0.45	0.45	0	0	0	0	0	0	0	0	0	0	0	*2*
Benthos - 5	N/A	Generic bivalve (e.g., *Mytilus californianus*) - included for model evaluation only	0.60	0.20	0.20	0	0	0	0	0	0	0	0	0	0	0	*2*
Benthos - 6	N/A	Generic bivalve (e.g., C*rassostrea gigas)* - included for model evaluation only	0.60	0.20	0.20	0	0	0	0	0	0	0	0	0	0	0	*2*
Benthos - 7	N/A	Generic polychaete (e.g., *Harmothoe imbricata*)	0.90	0.05	0.05	0	0	0	0	0	0	0	0	0	0	0	*2*
Benthos - 8	N/A	Generic shrimp (e.g., *Crangon sp.*)	0	0.3	0.3	0	0	0	0.4	0	0	0	0	0	0	0	*3*
Fish - 1	0	*Cymatogaster aggregata* (shiner surfperch)	0.05	0.05	0.25	0.05	0.25	0.25	0.05	0	0	0.05	0	0	0	0	*4*
Fish - 2	0	*Atherinopsis californiensis* (jacksmelt)	0	0.8	0.2	0	0	0	0	0	0	0	0	0	0	0	*4*
Fish - 3	0	*Engraulis mordax* (Northern anchovy)	0	0.2	0.35	0	0.2	0.15	0.1	0	0	0	0	0	0	0	*4*
Fish - 4	0	*Genyonemus lineatus* (white croaker)	0.05	0.05	0.2	0.15	0.1	0.1	0.1	0	0	0.15	0.1	0	0	0	*4*

Species #	Age Class	Species	A	B	C	D	E	F	G	H	I	J	K	L	M	N	Ref.
Fish - 5	>0	*Engraulis mordax* (Northern anchovy)	0	0.2	0.2	0	0.15	0.2	0.25	0	0	0	0	0	0	0	*4*
Fish - 6	>0	*Cymatogaster aggregata* (shiner surfperch)	0.05	0.05	0.1	0.1	0.2	0.2	0.15	0	0	0.1	0	0.05	0	0	*4*
Fish - 7	>0	*Atherinopsis californiensis* (jacksmelt)	0	0.65	0.20	0.05	0.05	0.05	0	0	0	0	0	0	0	0	*4*
Fish - 8	>0	*Acanthogobius flavimanus* (yellowfin goby)	0	0	0	0.2	0.15	0.15	0	0	0	0.2	0.25	0.05	0	0	*4*
Fish - 9	>0	*Porichthys notatus* (plainfin midshipman)	0.05	0	0	0.1	0.15	0.15	0.2	0	0	0.05	0.2	0.05	0	0.05	*4*
Fish - 10	>0	*Genyonemus lineatus* (white croaker)	0.05	0	0	0.20	0.15	0.15	0.15	0	0	0.20	0.05	0	0	0.05	*4*

A	Sediment	H	Benthic - 5
B	Phytoplankton	I	Benthic - 6
C	Zooplankton	J	Benthic - 7
D	Benthic - 1	K	Benthic - 8
E	Benthic - 2	L	shiner surfperch (0)
F	Benthic - 3	M	jacksmelt (0)
G	Benthic - 4	N	Northern Anchovy (0)

1 Estimated
2 Estimated from Roberts et al 2002
3 Estimated from Roberts et al 2002; Andy Jahn Personal Communication
4 Estimated from Andy Jahn Personal Communication; Fishbase (http://www.fishbase.org/search.cfm); California Department of Fish and Game (http://www.delta.dfg.ca.gov/baydelta/monitoring/); Cailliet, G. M., R. J. Larson, et al. 2000. Biological Characteristics of Nearshore Fishes of California: A Review of Existing Knowledge and Proposed Additional Studies. Moss Landing, CA, Moss Landing Marine Laboratories; Roberts et al 2002; SFEI 1999

Table 210: Diet composition of Double-crested Cormorants, Forster's Terns and harbor seals in the model. Diet items are presented in columns.

Species #	Age Class	Species	A	B	C	D	E	F	G	H	I	J	K	L	Ref.
Avian - 1	Adult - male	*Phalacrocorax auritus* (Double-crested Cormorant)	0	0	0	0	0.05	0.05	0.05	0.05	0.30	0.30	0.20	0	*1,2*
Avian - 2	Adult - female	*Phalacrocorax auritus* (Double-crested Cormorant)	0	0	0	0	0.05	0.05	0.05	0.05	0.30	0.30	0.20	0	*1,2*
Avian egg - 1	Egg	*Phalacrocorax auritus* (Double-crested Cormorant)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	*N/A*
Avian - 3	Adult - male	*Sterna Forsteri* (Forster's Tern)	0	0.15	0.15	0.15	0.15	0.1	0.1	0.05	0.05	0.05	0.05	0	*3*
Avian - 4	Adult - female	*Sterna Forsteri* (Forster's Tern)	0	0.15	0.15	0.15	0.15	0.1	0.1	0.05	0.05	0.05	0.05	0	*3*
Avian egg - 2	Egg	*Sterna Forsteri* (Forster's Tern)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	*N/A*
Mammal - 1	Adult - male	*Phoca vitulina* (harbor seal)	0	0	0	0	0	0.05	0.05	0.05	0.5	0.15	0.2	0	*4,5,6*
Mammal - 2	Adult - female	*Phoca vitulina* (harbor seal)	0	0	0	0	0	0.05	0.05	0.05	0.5	0.15	0.2	0	*4,5,6*
Mammal - 3	Juvenile	*Phoca vitulina* (harbor seal)	0.1	0	0	0	0	0.1	0.1	0.1	0.4	0.1	0.1	0	*4,5,6*
Mammal - 4	Pup – 14 days	*Phoca vitulina* (harbor seal)	0	0	0	0	0	0	0	0	0	0	0	1	*4,5,6*

Dietary preferences

A Generic shrimp (e.g., *Crangon sp*.)
B *Cymatogaster aggregata* (shiner surfperch) (0)
C *Atherinopsis californiensis* (jacksmelt) (0)
D *Engraulis mordax* (Northern anchovy) (0)
E *Genyonemus lineatus* (white croaker) (0)
F *Engraulis mordax* (Northern anchovy) (>0)
G *Cymatogaster aggregata* (shiner surfperch) (>0)
H *Atherinopsis californiensis* (jacksmelt) (>0)
I *Acanthogobius flavimanus* (yellowfin goby) (>0)
J *Porichthys notatus* (plainfin midshipman) (>0)
K *Genyonemus lineatus* (white croaker) (>0)
L Mother's milk

1 Hatch, J. J. and D. V. Weseloh, Eds. (1999). Double-crested Cormorant (*Phalacrocorax auritus*). The Birds of North America No. 441. Philadelphia, PA, The Birds of North America, Inc.

2 Stenzel, L. E., R. P. Henderson, et al. (1991). Breeding Population Size and Fledgling Success of Double-crested Cormorants on the Richmond-San Rafael Bridge and Farallon Islands, CA, 1988-1990.

3 McNicholl, M. K., P. E. Lowther, et al., Eds. (2001). Forster's Tern (*Sterna Forsteri*). The Birds of North America No. 595. Philadelphia, PA, The Birds of North America, Inc.

4 Kopec, D. A. and J. T. Harvey (1995). Toxic Pollutants, Health Indices and Population Dynamics of harbor Seals in San Francisco Bay, 1989-1992. Moss Landing, CA, Moss Landing Marine Laboratories: 89 p.

5 Grigg, E. K. (2003). Pacific harbor Seals (*Phoca vitulina richardsi*) in San Francisco Bay, California: A Review of the Literature. Oakland, CA, San Francisco Estuary Institute: 109 p.

6 Torok, M. L. (1994). Movements, Daily Activity Patterns, Dive Behavior, and Food Habits of harbor Seals (*Phoca vitulina richardsi*) in San Francisco Bay, California. M.S. Thesis, Calif. State Univ., Stanislaus, 87 p

2.6 MODEL IMPLEMENTATION IN EXCEL SPREADSHEET

The model is constructed in Microsoft Excel 2000 ® and uses the add-in program Crystal Ball ® [Decisioneering 2000] to conduct Monte Carlo Simulations. The model contains 22 worksheets. Users of the model only need to use one worksheet, i.e. the worksheet entitled "Management". Using this *management* module does not require the Crystal Ball add-in program or the skills required to use this particular program. We highly recommend that users of the model only use the management worksheet.

The other worksheets contain the submodels, data compilations used in the model and model calculations and results used for sensitivity analyses and model performance evaluations. These sheets contain the actual model calculations of the BSAFs for the various species and the data that are used to accomplish this. An overview of the contents of the various spreadsheets is presented in the worksheet "overview" in the attached Excel spreadsheet model. We do not recommend that users of the model make changes in these worksheets as they have an impact on the output of the model. The 21 worksheets that make up the *science* module of the model are included in the model to enable independent review of the model by expert reviewers.

The *management* module of the model includes two types of model calculations, i.e. the "forwards" and "backwards" calculations.

2.6.1 Forwards Calculation: Estimation of Total PCB Concentrations in Fish and Wildlife

In the "forwards" calculation, the PCB concentration in fish and wildlife in the Bay (C_B) is calculated based on a measured or anticipated PCB concentrations in the sediment (C_S). This means that the PCB concentrations in the sediments have to be entered and the model calculates the corresponding PCB concentrations in organisms of the San Francisco Bay food web. The concentration in the sediments is presented in a logarithmic

format as log C_S, such that the lognormal distribution of the sediment concentration can be presented as a normal distribution of log C_S. The model outcome, i.e. the BSAF is also presented in a logarithmic format as log BSAF, which provides the advantage that the lognormal distribution of the BSAF can be presented as a normal distribution of log BSAF. The model calculation that is conducted is:

$$\log C_B = \log C_S + \log BSAF \tag{2.64}$$

And C_B then follows as:

$$C_B = 10^{\log(C_B)} \tag{2.65}$$

This calculation is mathematically equivalent to:

$$C_B = BSAF \cdot C_S \tag{2.66}$$

Variability and error in the model input parameters (i.e. log C_S) and error in the model calculations (i.e. log BSAF) are propagated in the estimate of log C_B. The uncertainty in the biota concentrations is expressed by the standard deviation of the geometric mean concentration. It is expressed as the standard deviation (SD_{CB}) of log C_B. It is calculated from the standard deviations (SD_{BSAF}) of log BSAF estimates and the standard deviation (SD_{CS}) of the sediment concentrations are according to

$$SD_{CB} = \sqrt{(SD_{CS}^2 + SD_{BSAF}^2)} \tag{2.67}$$

In the forward calculation C_B is calculated for each congener and total-PCBs. Uncertainty in C_B is based on uncertainty in the concentration of total PCBs in the sediments and uncertainty in the BSAF. Variability and uncertainty in the BSAF is characterized by two methods, which are described in section 3.4. The first method applies Monte Carlo Simulation to estimate the uncertainty in the BSAF due to uncertainty in the model state

variables. This uncertainty in the BSAF (which includes variability and error in the model's state variables but not in C_S) is then applied to the observed (or anticipated) uncertainty in the sediment concentrations to calculate a distribution of PCB concentrations in biota. The second method of determining uncertainty is derived through a model performance analysis that involves a comparison of observed and model predicted BSAFs of total-PCBs.

In the *management* module, the model predictions of C_B are carried out for Shiner surfperch, jacksmelt, white croaker, Double-crested Cormorants, Forster's Terns and harbor seals. In the *science* module, BSAFs are derived for all species in the model. It is possible to include any of the species in the science module into the management module. However, to keep the management module relatively simple, we have limited the number of species in the display of the model results to those species that are most relevant for management purposes.

The predicted distributions in the PCB concentrations for various species in the Bay can be used to assess the frequency with which PCB concentrations exceed certain target threshold concentrations. This is illustrated in Figure 2.6 and involves representing the log-normal distributions of PCB concentration in biota as cumulative distributions. The y-axis then illustrates the fraction of PCB concentrations in the various species of the Bay that are expected to be larger or smaller than the target value of interest.

First, the effect of remediation on Bay wide PCB concentrations can be explored using the current model by entering the anticipated (i.e. after remediation) spatial concentration distribution after remediation. To do this, it is important to know the contribution of the hotspots to the Bay wide concentration distribution. The anticipated PCB sediment concentration distribution can be entered in the model, which will determine the effect of the change in Bay wide concentration distribution (due to remediation) on the Bay wide PCB concentrations in biota and associated human health and ecological risks. If more detailed information is available about the foraging behavior of a particular species or

sub-population, a foraging/migration specific PCB concentration distribution can be entered in the model to assess the distribution of PCB concentrations in those organisms. If the species foraging area includes a "hotspot", then the effect of remediation of the hotspot can be anticipated by entering the anticipated statistical sediment concentration distributions after remediation. It is important to emphasize that higher trophic levels organisms that migrate over wide areas of the Bay or are widely distributed over the Bay have a limited exposure to hotspots and declines in PCB sediment concentrations at these hotspots will only have proportional effect on the body burdens of these organisms.

The model architecture can be applied on a site-specific basis (e.g. a "hotspot") by entering the PCB concentration in sediments along with some other site-specific data at the hotspot. The resulting biota concentrations can then be compared to concentrations anticipated at the hotspot after remediation. This application is useful when assessing the impacts of remediation on local populations of relatively sedentary species (e.g. mussels, clams). This particular application of the model cannot be extended to higher trophic level organisms like harbor seals or bird species which have larger foraging areas.

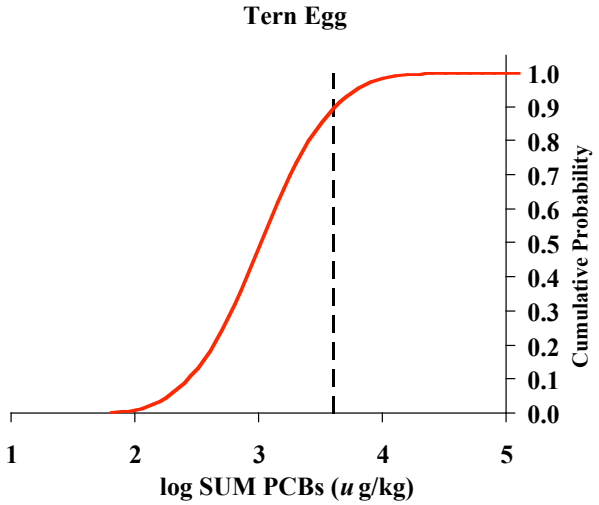

Figure 2.6 Illustrative example of a cumulative probability distribution of the ΣPCB concentration in Forster's Tern eggs in relation to a target concentration (dashed line). The cumulative probability distribution illustrates the probability of exceeding the PCB target threshold concentration.

2.6.2 Forwards Calculation: Estimation of the TEQ in Fish and Wildlife

The forward calculations also include estimates of the TEQ and its statistical distribution. The TEQ is based on 3 PCB congeners, i.e. PCBs 105, 118, 156. Like the total PCB concentrations, the TEQ is presented in logarithmic format as log TEQ. The uncertainty in the estimates of the TEQ are based on uncertainties in the PCB congeners concentrations in the sediments and their BSAF for those congeners for which TEF values were available. Because only 3 out of the 40 PCB congeners detected in the sediments exhibit a significant "dioxin" like toxicity, the predictions of TEQ values are based on a small number PCB congeners. The most potent PCB congeners (i.e. the PCB congeners with the highest TEFs) are not included in the calculated TEQs because concentration data in the sediments are not available for these congeners. We therefore expect that the predicted TEQs in this model values are underestimates of the actual TEQs in fish and wildlife in the Bay and should not be used for risk assessments at this point. To make more accurate predictions of the TEQ in fish and wildlife, it is important to include data on the sediment concentrations of those PCBs that are known to have a high "dioxin-like" toxicity and hence have a high TEF. These concentration data are not available at this time. To make better estimates of the toxicological significance of PCBs in the Bay, it is important to expand the chemical analysis of Bay sediments and biota in future monitoring programs to include PCB congeners which have high TEFs.

2.6.3 Forwards Calculation: Estimation of Upper-Bound Excess Cancer Risks in Bay Residents Consuming Local Fish

The forward calculations further include several methods to estimate the human health and ecological risks associated with the entered PCB concentrations for the Bay sediments. Two types of human health risk assessments are presented. The first risk assessment determines the upper-bound lifetime excess cancer risk, R, due to consumption of those fish species for which the model calculations are conducted. It follows the methodology used by the US EPA and is documented in US EPA [1996]. The assessment is based on the assumption that only Bay residents consume the fish species

for which the concentration C_B is derived by the model. The calculation for R (unitless) is:

$$R = F \times E \times DE \times CL \times Q \times C_B / (BW \times LT) \quad (2.68)$$

The rate of local Bay fish consumption F by a person (in kg fish per day) is set at 0.021 kg/d [SFEI 2003]. The dietary absorption efficiency of PCBs in human is set at 100% or 1. C_B is the concentration (in units of mg PCB/kg wet weight fish) of the PCB congener or total PCB in the fish that is consumed by members of the target population for which the risk assessment is conducted. The model calculates C_B. DE is the exposure duration to PCB contaminated fish from the Bay and set at 30 years. CL represents the loss of PCBs due to cooking of fish. It is set at a value of 0.75, which is a loss equivalent to 25% of the original PCB concentration. Q is the slope factor for PCBs and following the US-EPA IRIS database, is set at 2 $(mg/kg/d)^{-1}$. The body weight BW (in kg) is set at 70 kg, representing an adult human being. The lifetime LT of an adult person is set at 70 years. Alternative calculations of the excess cancer risk can be added in the spreadsheet.

2.6.4 Forwards Calculation: Estimation of Hazard to Human Health due to Consumption of San Francisco Bay Fish

The second type of human health risk assessment that is included in the model assumes that PCBs are not carcinogens. It is based on the derivation of a reference dose or an acceptable daily intake for PCBs. In the model, the hazard H is derived by first estimating the dose D (mg/kg/d) of PCBs for Bay residents consuming local fish:

$$D = F \times E \times CB \times CL / BW \quad (2.69)$$

And then dividing the dose D by the acceptable daily intake ADI (or reference dose) in mg/kg/d according to:

$$H = D/ADI \quad (2.70)$$

Where F is the rate of local Bay fish consumption F by a person (in kg fish per day) and set at 0.021 kg/d [SFEI 2003]. E is the dietary absorption efficiency of PCBs in human and set at 100% or 1. C_B is the concentration (in units of mg PCB/kg wet weight fish) of the PCB congener or total PCB in the fish that is consumed by members of the target population for which the risk assessment is conducted. The model calculates C_B and the hazard estimation is only based on the assumption that only the fish species for which the model calculations are conducted are being consumed. CL represents the loss of PCBs due to cooking of fish. It is set at 0.75 which is equivalent to 25% of the original PCB concentration. BW is the body weight BW (in kg) of an adult human being and is set at 70 kg. The ADI is set at 2.10^{-5} mg/kg/d following the US EPA IRIS database for Aroclor 1254. A value for H equal or greater than 1 indicates there is a potential that, under the scenario described above, PCBs in fish are hazardous to people consuming Bay fish. A value of H less than 1 indicates that there is no hazard.

2.6.5 Forwards Calculation: Characterization of the Potential for Ecological Effects to Fish and Wildlife

The model has the ability to make estimates of the frequency of occurrence of certain toxicological effects in those species that were included in the model. This is accomplished by comparing the cumulative frequency distribution of the total PCB concentrations in a species of San Francisco Bay to accepted body residue concentrations that have been observed to be associated with toxicological syndromes. Body residue concentrations are internal concentrations in a particular species that cause a certain effect. The cumulative frequency distribution represents the range of PCB concentrations that can be expected in that species of the Bay as a result of the PCB concentration in the sediments that is entered in the model. The cumulative frequency distribution can show what fraction of the population in the Bay is expected to contain PCB concentrations that exceed the threshold concentration associated with the toxic effect and hence can be expected to be adversely affected by PCBs.

The model can make similar estimates of effects based on the TEQ. However, since a good record of the presence of congeners with high TEF values in the sediments of the Bay does currently not exist, we do not recommend that the TEQ is used at this point to make estimates of ecological effects. Current calculations of the TEQ are expected to underestimate the actual TEQ in Bay fish and wildlife. The management sheet contains the calculations to conduct estimates of effects based on TEQs and can be activated when appropriate data become available.

To illustrate the application of the model to make assessments of the toxicological significance of PCB concentrations in harbor seals, we used the threshold effect concentration for total PCBs of 11 μg/g lipid proposed by Kannan et al. [2000]. This threshold concentration is based on studies by Boon et al. [1987] and Brouwer et al. [1989], who reported respectively a NOAEL of 5.2 μg/g lipid and a LOAEL of 25 μg/g lipid. Kannan et al. [2000] provide a discussion on uncertainties associated with the reported NOAEL and LOAEL and propose a threshold effects concentration for PCBs in harbor seals. The threshold concentration was calculated as the geometric mean of the NOAEL and LOAEL by Kannan et al. [2000].

To illustrate the application of the model to estimate the toxicity of total PCBs in Double-crested Cormorants we used wet weight based concentrations of 3.6 to 6.8 ppm, reported and reviewed by Hoffman et al. [1996]. These concentrations were associated with embryonic mortality, beak deformities and club foot in the field. To simplify the characterization of possible effects on Double-crested Cormorants we used a threshold effect concentration of 4 μg/g wet weight body mass.

To estimate the potential for PCB to cause toxic effects in Forster's Terns, we used wet weight based concentrations of 6 to 26 ppm in eggs, reported and reviewed by Hoffman et al. [1996] based on data by Kubiak et al. [1989], Hoffman et al. [1987] and Tillit et al [1993]. These concentrations in eggs were associated with embryonic mortality, impaired reproductive success, subcutaneous edema of head and neck, AHH induction and beak

deformities [Hoffman 1996]. For the characterization of the toxic effects in Forster's Terns we used a threshold effect concentration of 6 μg/g wet weight in eggs in the model.

Based on each effect concentration in each species, an ecological risk index (ERI) is calculated as:

$$ERI = C_B / C_{THRESHOLD} \quad (2.71)$$

Threshold effect concentrations may change as new information becomes available. Also, toxicological endpoints are also subject to debate and different authors are likely to propose different values associated with effects. For these reasons, we have presented the management sheet in a form that allows the user to vary the threshold effect concentrations by simply adding the preferred value in the appropriate cell in the spreadsheet.

2.6.6 Backwards Calculation: Estimation of Total PCB Concentrations in Sediments from PCB Concentration in Fish and Wildlife

In the "backwards" calculation, the PCB concentration in the sediment (C_S) is calculated based on a PCB concentration in a fish or wildlife species (C_B). This calculation is designed to determine target PCB concentrations in sediments that meet ecological and/or human health criteria that are expressed in terms of a PCB concentration C_B. The calculation that is conducted is:

$$\log C_S = \log C_B - \log BSAF \quad (2.72)$$

Which is equivalent to:

$$C_S = C_B / BSAF \quad (2.73)$$

Where C_B is now the external variable that needs to be entered and the BSAF is calculated by the model. The backwards calculations are presented for total PCBs. The calculations can also be conducted for TEQs. However, considering the lack of knowledge of the composition of PCBs that is needed to make meaningful TEQ calculations, the backwards TEQ calculations are not included in the current version of the model.

Uncertainty in the model error is included in the backwards calculation in terms of the uncertainty in the BSAF, which is calculated by the model as described above. In addition, it is possible, when entering the PCB concentrations in the biota, to include an accepted variability in the target biota concentration C_B in the Bay. In that case, the uncertainty in the BSAF and C_B is combined in the model to determine a distribution of PCB concentrations in the sediments that are expected to produce the entered distribution of PCB concentrations in fish or wildlife species.

3. METHODOLOGY

3.1 GENERAL

To test and evaluate the PCB food web bioaccumulation model for San Francisco Bay, we conducted a *sensitivity analysis,* a *model performance analysis* and an *uncertainty analysis*.

The *sensitivity analysis* assesses the impact of variability and/or error in the model's state variables (e.g. organism weight, lipid content, temperature etc.) on the model outcome (i.e. the BSAF of total PCBs in Bay fish and wildlife). The sensitivity analysis is useful in determining the effect that errors in model state variables might have on the model outcome. Sensitive variables are variables that have a relatively large impact on the model outcome, i.e. a small change in the value of the variable produces a relatively large change in the model outcome. A less sensitive variable is a variable that causes a relatively small change in model outcome given the same change in the value of the variable. The sensitivity analysis can therefore provide valuable insights into the selection of the parameters that need to be included in the uncertainty analysis. It is important to include sensitive parameters in the uncertainty analysis. The sensitivity analysis is described in section 3.2.

The role of the model *performance analysis* is to evaluate the accuracy of the model predictions. It is based on a comparison of the model predicted BSAFs to independent, observed BSAFs of PCB congeners in fish and wildlife in the Bay. It is important to recognize that this San Francisco Bay food web model does not make use of measured

concentrations of PCBs in sediment and biota. The measured concentration data in sediments and biota data are therefore not used in the model development and can therefore be viewed as independent. The only exception is in the estimation of metabolic transformation rate constants of PCB congeners in harbor seals and bird species where observed concentrations ratios of PCB congeners and PCB153 in these organisms were used to estimate congener specific metabolic transformation rates. The measured concentration data are used to test and evaluate the model's performance. The performance analysis is described in section 3.3.

The role of the *uncertainty analysis* is to assess the error in the model calculations. The uncertainty analysis is important because the magnitude of the model needs to be considered when interpreting the results of the model calculations for management purposes. We present two types of model uncertainty analyses in this report. The first method is based on a comparison of model predicted and observed PCB concentrations. It uses calculated differences between observed and predicted BSAFs of total PCBs to assess the uncertainty of the model calculations. The second method applies a stochastic technique (Monte Carlo Simulation (MCS)) to assess the effect of inherent variability and error associated with the model's state variables on the model predictions. Both methods of uncertainty analysis have their strengths and limitations. The uncertainty calculated by comparing observed and predicted concentrations has the advantage that the estimate of the model uncertainty is grounded in empirical observations. However, it is subject to the limitations of the sampling programs used to obtain the PCB concentrations in sediments and biota of the Bay. The uncertainty calculated through Monte Carlo Simulation has a strong theoretical foundation. However, it is subject to difficulties associated with the characterization of errors in model parameters and it cannot include errors in model architecture. When applying model results for management purposes, it is prudent to consider uncertainty calculated by both methods. The uncertainty analysis is described in section 3.4.

3.2 SENSITIVITY ANALYSIS

Each state variable in the model displays a certain natural variability. For example, the model relies on the water temperature, which varies spatially and temporally throughout the Bay. In addition, the measurement of each state variable includes a certain amount of error. For example, reading the temperature off a thermometer can be associated with an error of 0.5 or 0.1 degree. The range of values due to variability and error reflect a certain degree of uncertainty in the actual value of the model variable (e.g. water temperature) selected for use in the model. This uncertainty carries through the model and is reflected in the model outcome. If the state variable is a sensitive variable, then the variability and error in the state variable produce a relatively large range of model outcomes. A relatively insensitive state variable produces a smaller range of model outcomes given the same variability or error.

The objective of the sensitivity analysis is to provide insight into the relative importance of the various state variables of the model. This is useful in the analysis of the internal mechanics of the model. It can be used to characterize potential errors in the model and to develop a better understanding of the relationship between the processes that control the behavior of PCBs in the San Francisco Bay food web.

The sensitivity analysis was conducted for each of the model state variables (I) that require parameterization. The model state variables that were included in the sensitivity analysis are listed in Tables 2.1 to 2.4. The sensitivity analysis then involved changing each model variable (I) at a time by a fixed amount (ΔI). The change (ΔO) that occurred in model outcome (O) was then calculated and the model state variable's sensitivity S was determined as:

$$S = \left(\frac{(\Delta O / O)}{(\Delta I / I)} \right) \tag{3.1}$$

The quantity S describes the sensitivity of O to changes in I. To calculate the sensitivity of the model input variable's sensitivity, a 10% reduction of the "mean" value used in the model was used, i.e. ($\Delta I / I = -0.1$). The resulting change in model outcome O (i.e., BSAF for SFEI ΣPCBs) was reported for phytoplankton, a filter feeding benthic invertebrate (i.e. Pacific oyster), a fish species (i.e. white croaker), an adult male cormorant and an adult male seal. This provides an illustrative and representative assessment of sensitivity in the San Francisco food web model.

The sensitivity analysis included all model state variables that require parameterization. The model variables included in the sensitivity analysis fall into two general categories. Abiotic variables describe attributes of San Francisco Bay watershed and biotic parameters describe characteristics of specific organisms. The abiotic parameters included in the sensitivity analysis were air temperature, water temperature, dissolved oxygen concentration, salinity (which affects K_{OW}), dissolved organic carbon in the water column, particulate organic carbon in the water column, concentration of suspended solids, organic carbon content of bottom sediments and the non-lipid organic matter-to-octanol proportionality constant (Table 2.1). The biotic variables included in the sensitivity analysis were organism wet weight, lipid content, non-lipid organic matter content, water content, the fraction of pore water ventilated by fish and invertebrates, particle scavenging efficiency of filter feeders, phytoplankton growth rate, invertebrate and fish growth rate coefficients (i.e., constants in equations 2.27 and 2.28, respectively), seal growth rate, lipid absorption efficiency, non-lipid organic matter absorption efficiency, water absorption efficiency and body temperatures of homeotherms. Also included in the sensitivity analysis were constants in equations 2.10, 2.12, 2.18, 2.34 and 2.52. The biotic state variables included in the model parameters are summarized in Tables 2.2, 2.3 and 2.4.

3.3 MODEL PERFORMANCE ANALYSIS

The model performance analysis involved the comparison of the model predicted sediment-receptor concentration relationship for each PCB congener i, $BSAF_{P,i}$, to the observed sediment-receptor concentration relationship, $BSAF_{O,i}$, for all PCB congeners i for which relevant observed concentration data were available. To do this, we used measured PCB congener concentrations in sediment and water as input parameters for the calculation of the PCB concentrations in the various biological organisms considered in the model. We then calculated the $BSAF_{P,i}$ by dividing the calculated concentration in the organisms by the concentration in the sediment. The $BSAF_{O,i}$ was derived by dividing measured PCB concentration in biota by the measured concentration in the sediment. Empirical PCB concentration data were available for harbor seals, Forster's Terns, Double-crested Cormorants, jacksmelt, shiner surfperch, white croaker, Pacific oysters and California mussels. To quantitatively express this measure of model performance, we use the model bias MB, which is derived on a species-specific basis:

$$MB_j = 10^{\left(\sum_{i=1}^{n} \frac{\left[\log\left(BSAF_{P,i} / BSAF_{O,i} \right) \right]}{n} \right)} \qquad (3.2)$$

In essence, MB_j is the geometric mean (assuming a log-normal distribution of the ratio $BSAF_{P,i}$ / $BSAF_{O,i}$) of the ratio of predicted and observed BSAFs for all PCB congeners i in a particular species j included in the analysis. MB is a measure of the systematic over- (MB>1) or under-prediction (MB<1) of the model. For example, MB = 2 indicates that the model over-predicts the empirical PCB congener concentrations in the species of interest on average by a factor of 2. Conversely, a model bias of 0.5 indicates that the model under-predicts PCB congener concentrations on average by a factor of 2. It should be stressed that in the calculation of MB, over- and under-estimations of the observed BSAF values for individual PCB congeners have a tendency to cancel out. Hence, MB tracks the central tendency of the ability of the model to predict PCB congener

concentrations. It is a useful measure of model performance if total PCBs (_PCB) are of primary interest.

The variability of over- and under-estimation of measured values is represented by the 95% confidence interval of MB (i.e. 95% CI = antilog(geometric mean ± ($t_{v,\ 0.05}$ × standard deviation)). The 95% confidence interval represents the range of BSAFs that includes 95% of the observed BSAFs. It is a measure of the variability and uncertainty of the model predictions. Due to the log-normal distribution of the ratio of predicted and observed BSAFs, this variability can be expressed as a factor (rather than a term) of the geometric mean. For example, if the 95% confidence interval of the MB is 3, it means that 95% of the predicted/observed BSAF ratios of the PCB congeners are found between MB/3 and MB x 3. In other words, 95% of the observed congener-specific BSAFs are found between the

Predicted BSAF x MB/3 (3.3)

and

Predicted BSAF x MB x 3 (3.4)

In addition to the analysis of model performance on a congener-specific basis, we also investigated the model performance for the estimation of the BSAF of ΣPCBs. To do this, we used the measured congener-specific PCB concentrations in sediment and water as input parameters for the calculation of the PCB concentrations in the various biological organisms considered in the model. Congener-specific concentrations in biological organisms were then summed to determine a ΣPCB concentration observed in sediments ($C_{S,\ \Sigma PCB}$) and model calculated for biota ($C_{B,\ \Sigma PCB}$). We then calculated the $BSAF_{P,\ \Sigma PCB}$ by dividing the calculated concentration in the organisms by the concentration in the sediment, i.e. ($C_{B,\ \Sigma PCB}$ / $C_{S,\ \Sigma PCB}$). The $BSAF_{O,\ \Sigma PCB}$ was derived by dividing measured PCB concentration in biota by the measured concentration in the sediment. To

quantitatively express model performance on for ΣPCB, we used the model bias MB*, which is derived on a species-specific basis:

$$MB_j{}^* = 10^{\left(\sum_{i=1}^{m} \frac{\left[\log\left(BSAF_{P,\Sigma PCB} \,/\, BSAF_{O,\Sigma PCB} \right) \right]}{m} \right)} \qquad (3.5)$$

MB_j^* is the geometric mean (assuming a log-normal distribution of the ratio $BSAF_{P,\,\Sigma PCB}$ / $BSAF_{O,\,\Sigma PCB}$) of the ratio of predicted and observed BSAFs for ΣPCB in species j. MB^* is a measure of the systematic over- ($MB^*>1$) or under-prediction ($MB^*<1$) of the BSAF for ΣPCB by the model. The 5th and 95th percentiles of MB* represent the variability of over- and under-estimation of measured values. The 95% confidence interval represents the range of BSAFs for ΣPCB in species j that includes 95% of the observed BSAFs for ΣPCB in species j. It is a measure of the variability and uncertainty of the model predictions. As a result of the log-normal distribution of the ratio of predicted and observed BSAFs, the error of MB^* can be expressed as a factor (rather than a term) of the geometric mean. For example, if the 95% confidence interval of the MB* is 3, it means that 95% of the predicted/observed BSAF ratios of the PCB congeners are found between MB*/3 and MB* x 3. In other words, 95% of the observed BSAFs for ΣPCBs are found between the

Predicted BSAF x MB*/3 (3.6)

and

Predicted BSAF x MB* x 3 (3.7)

The model's predictability of the BSAF for PCB congeners and ΣPCB improve when MB and MB^* approach 1.0 and their 95% confidence interval becomes smaller.

One of the key characteristics of MB and MB^* and their 95% confidence interval is that it represents many sources of error including model parameterization errors and errors in model structure and philosophy as well as analytical and sampling 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. Because of these characteristics MB and its 95% confidence interval are useful measures when forecasting actual PCB concentrations in biota on a larger spatial (e.g. Bay wide) scale.

Most of the measured concentration data used in the model performance evaluation were collected as part of RMP in 1999, 2000 and 2001. The time period in which the sediment concentrations were collected by the RMP coincided with the period in which biota samples were collected. The only exception was for harbor seals. Harbor seal samples were collected between 1989 and 1993. The RMP monitors PCB concentrations in the filter feeders *Mytilus californianus* (California mussels) and *Crassostrea gigas* (Pacific oyster); three fish species, i.e. jacksmelt (*Atherinopsis californiensis)*, white croaker (*Genyonemus lineatus)* and shiner surfperch (*Cymatogaster aggregate)*, and eggs from a resident bird species (i.e. the Double-crested Cormorant, *Phalacrocorax auritus*). The eggs were collected from year-round colony residents that eat fish from SFB [Davis et al 2004]. Empirical data from these studies collected at the Richmond Bridge Station in May (1999-2001) were used to assess model performance.

An extensive PCB monitoring program does not currently exist for SFB harbor seals and PCB congener specific data are rarely reported. Risebrough et al. [1980] reported ΣPCB levels in blubber collected in the mid-1970s using Aroclor standards that ranged from a low of 16 ppm, for a pup, to 500 ppm (lipid weight) for an adult male. Kopec and Harvey [1995] reported ΣPCB residues ranging between 2.5 and 267 ppm lipid weight and a mean concentration of 51 ppb (wet weight) in plasma and whole blood samples collected in 1991-1992 for 14 seals (males and females). Because the whole blood lipid content varied from 0.06% to 0.50% depending on the extraction method, the authors expressed

concern about this uncertainty. Lydersen et al. [2002] concluded that monitoring PCB levels in seals from blood samples can lead to variable results due to feeding events and changes in the physiological condition of the animals. Blubber samples are less sensitive to fluctuating lipid contents than blood samples and concentrations of PCBs in blubber samples are expected to be more reflective of equilibrium conditions in the whole organism. PCB data from blubber samples of adult SFB harbor seals (1989-1993) prepared for the San Francisco Regional Board by the California Department of Toxic Substances Control Hazardous Materials Laboratory were used to evaluate model performance. This data set included congener specific concentrations, lipid content of the blubber samples, as well as seal gender and approximate age, which are important for model parameterization and evaluation. The PCB concentration data span a 4-year period and the data selected for the model performance analysis was collected in the same season (early spring). Samples from decomposing animals and tissues were excluded from the evaluation. The average age of the females and males are 15 and 9.5 years, respectively. The measured _PCB concentrations ranged from 10 to 277 ppm (lipid weight). The geometric mean _PCB concentrations (based on the 40 SFEI PCB congeners) were approximately 21 and 22 mg/kg lipid from the female and male seals, respectively.

3.4 UNCERTAINTY ANALYSIS

The uncertainty in the BSAF of ΣPCB in fish and wildlife of San Francisco Bay was determined by two methods. The first method was based on a comparison of observed and predicted BSAFs, discussed in section 3.3. This method uses the model bias MB^* and its 95% confidence intervals, defined in section 3.3, to represent the uncertainty in the model predicted BSAFs of ΣPCB.

The application of field monitoring data to characterize the uncertainty in the model calculations enhances the credibility of the model as model calculations are directly

compared to available empirical data. However, it should be stressed that any shortcomings of the monitoring data sets are reflected in the uncertainty estimate of the model. The empirical concentration data that are used in the estimation of the model uncertainty have several limitations. One important limitation is that the PCB monitoring programs in San Francisco Bay have limited spatial coverage. For example, biota sample collections (e.g. harbor seals, cormorants, white croaker) have only been conducted in certain areas of the Bay. Hence, PCB concentrations in these organisms may not provide an accurate representation of the distribution of the concentrations throughout the Bay. Also, the available PCB concentration data have a limited temporal coverage. As a result, the measured PCB concentrations are unlikely to provide an adequate representation of the temporal variations in concentrations. For that reason, it is useful to assess the model uncertainty by a second method which attempts to incorporate the geographical and temporal variations in PCB concentrations in the estimate of model uncertainty.

The second method of uncertainty analysis that was performed applies a stochastic technique (Monte Carlo Simulation (MCS)) to assess the effect of inherent variability and error associated with the model state variables on the model predictions. This methodology is based on the representation of the model state variables by statistical distributions rather than point estimates. The distribution represents the uncertainty in the value of the model variable selected for use in the model. The distribution expresses how the state variables may vary due to geographical location, time of the year, differences in behavior among individuals of a species and other factors. In MCS, these distributions are repeatedly sampled and the sampled values are used in the model to produce a distribution of model outcomes (i.e. BSAFs). This distribution of model results represents the variability in the model outcome due to variability and error in the model's state variables (e.g., temperature, organic carbon content, lipid contents, etc). The uncertainty in all state variables contributes to the magnitude of the range of model outcomes; however, they are not necessarily additive.

MCS were conducted within the Excel spreadsheets using Crystal Ball [Decisioneering 2000]. Each MCS involved 10,000 trials. Some simplifying assumptions were made to improve the transparency of the computationally complex simulation calculations. First, only model parameters that were found to be sensitive (in the sensitivity analysis) were included in the MCS. Hence, relatively insensitive model parameters were excluded. The uncertainties in these model variables were assumed to have an insignificant effect on the uncertainty in the model outcome (i.e. BSAF). For example, mean air temperature is not used in the bioaccumulation calculation of many species in the food web model and is not a sensitive variable in the calculation of bioaccumulation air breathing organisms where the variable is used. Likewise, biotic parameters such as the organism's water content and water absorption efficiency are also insensitive model variables. This is because water does not contribute significantly to the storage capacity of hydrophobic chemicals like PCBs in biota. Secondly, model variables that exhibit a strong co-dependence with other variables in the model were excluded from the analysis. For example, lipid contents generally co-vary with organism weights. While organism weight may have a small impact on model output (largely through allometric relationships controlling feeding and growth), lipid content is a much more sensitive variable since it is a key parameter controlling the partitioning processes for PCBs. Thus, lipid contents for SFB food web organisms were included in the MCS while the organism's wet weight was excluded from the simulations. Other examples of co-dependence are the regression coefficients in the regression equations. In this case, the coefficient with the greatest sensitivity was included in MCS whereas the other regression coefficient was excluded. Thirdly, uncertainty in the feeding preferences were excluded from the MCS because (i) there is insufficient information to characterize the uncertainties in these state variables, (ii) feeding preferences are highly interdependent and therefore unsuitable for MCS, and (iii) the feeding preferences are not sensitive variables as long as changes in feeding preferences do not include large changes in trophic status of the organism's diet items. The model state variables that were included in the MCS, their values and distributions are summarized in Tables 3.1 – 3.4.

The MCS include distributions for the concentrations of PCB congeners in the water. The model internalizes PCB water concentrations in the calculation of the BSAF. Estimates of the variability of the PCB concentration in the water were based on measured PCB concentration in water from a number of sampling stations for the period between 1999 and 2001. Log-normal PCB water concentration distributions were used for MCS.

Primary production is highly variable spatially and seasonally in San Francisco Bay. Primary producers (e.g. phytoplankton) are also subject to periods of rapid growth (i.e. blooms). Thus for MCS a log-normal distribution was selected to characterize "phytoplankton" growth rate with the standard deviation equal to the mean input (i.e. 0.125 day^{-1}).

Table 3.1: A summary of abiotic model state variables used for the MCS in the SFB food web model.

Parameter	Mean	Variability (1 SD)	Distribution
T_W	14.9	1.3	Normal
DO	8.09	1.1	Log-normal
PSU	20.2	1.6	Log-normal
OC_{WATER}	$2.1 \bullet 10^{-6}$	$2.0 \bullet 10^{-7}$	Log-normal
POC	$1.85 \bullet 10^{-6}$	$1.5 \bullet 10^{-7}$	Log-normal
C_{SS}	$2.46 \bullet 10^{-5}$	$2.5 \bullet 10^{-6}$	Log-normal
$OC_{SEDIMENT}$	1.02	0.50	Log-normal
C_{WT}	Appendix C	Appendix C	Log-normal
β	$3.5 \bullet 10^{-2}$	$3.5 \bullet 10^{-3}$	Normal

Table 3.2: A summary of phytoplankton state variables used for the MCS in the SFB food web model.

Parameter	Mean	Variability (1 SD)	Distribution
L	0.0012	0.0002	Normal
NLOC	0.06	0.002	Normal
K_G	0.125	0.125	Log-normal
A_P	$6.0 \bullet 10^{-5}$	$2.0 \bullet 10^{-5}$	Normal

Table 3.3: A summary of zooplankton, invertebrate and fish state variables used for the MCS in the SFB food web model.

Species	Parameter	Mean	Variability (1 SD)	Distribution
All zooplankton, invertebrates and fish	L	Table 2.8	Table 2.8	Normal
All zooplankton, invertebrates and fish	NLOM	0.20	0.01	Normal
All zooplankton, invertebrates and fish	A_{ED}	$8.5 \cdot 10^{-8}$	$1.4 \cdot 10^{-8}$	Normal
All zooplankton, invertebrates and fish	A_{EW}	1.85	0.13	Normal
All zooplankton and invertebrates	I_{GR}	$3.5 \cdot 10^{-4}$	$3.5 \cdot 10^{-5}$	Normal
All fish	F_{GR}	$7.0 \cdot 10^{-4}$	$7.0 \cdot 10^{-5}$	Normal
Zooplankton	ε_L	0.72	0.02	Normal
Zooplankton	ε_N	0.72	0.02	Normal
Invertebrates	ε_L	0.75	0.02	Normal
Invertebrates	ε_N	0.75	0.02	Normal
Fish	ε_L	0.90	0.02	Normal
Fish	ε_N	0.50	0.02	Normal
Invertebrates (benthic filter feeders)	P_W	0.20	0.02	Normal
Invertebrates (benthic detritovores)	P_W	0.10	0.01	Normal
Invertebrates (shrimp, mysids)	P_W	0.05	0.01	Normal
Fish (benthic)	P_W	0.05	0.005	Normal

Table 3.4: A summary of harbor seal, Double-crested Cormorant and Forster's Tern state variables used for the MCS in the SFB food web model.

Species	Parameter	Mean	Variability (1 SD)	Distribution
All birds and seals	L	Table 2.8	Table 2.8	Normal
All birds and seals	NLOM	0.20	0.01	Normal
All birds	A_{ED}	$3.0 \bullet 10^{-9}$	$4.9 \bullet 10^{-10}$	Normal
All birds	ε_L	0.95	0.02	Normal*
All birds	ε_N	0.75	0.02	Normal
All seals	A_{ED}	$1.0 \bullet 10^{-9}$	$1.7 \bullet 10^{-10}$	Normal
All seals	ε_L	0.98	0.02	Normal*
All seals	ε_N	0.75	0.02	Normal
Adult male seals	K_G	$7.5 \bullet 10^{-5}$	$7.5 \bullet 10^{-6}$	Normal
Adult female seals	K_G	$1.0 \bullet 10^{-5}$	$1.0 \bullet 10^{-6}$	Normal
Juvenile seals	K_G	$1.0 \bullet 10^{-3}$	$1.0 \bullet 10^{-4}$	Normal

*upper boundary set to 99.8%

3.5 MODEL APPLICATION

As part of this report, we will illustrate the application of the model to make estimates of the concentrations of total PCBs (_PCB) and PCB congeners in organisms of the San Francisco Bay food web based on current PCB concentrations in the sediments of the Bay. To do this we will first make "forwards" calculations. These calculations are carried out in the management sheet of the model. Secondly, we will apply the model in an illustrative fashion to make estimates of the concentrations of total PCBs in the Bay sediments that can be expected to meet a set of criteria that are of ecological and human health relevance. This is done using the "backwards" calculations. They are also carried out in the management sheet of the model.

3.5.1 Forwards Calculations

To illustrate the application of the model to make estimates of the concentrations of total PCBs and PCB congeners in organisms of the San Francisco Bay food web based on current PCB concentrations in the sediments of the Bay, we calculated concentrations of PCB congeners in three fish species, cormorant eggs, tern eggs and male and female seals from current PCB congener concentrations in the sediments.

To accomplish this, we first compiled sediment concentration data from all RMP monitoring stations in the Bay for the period between 1999 and 2001. In total 1,284 samples were available [RMP 1999, 2000, 2001]. Congener concentrations reported as "non-detected" were replaced by half (50%) of the method detection limit (MDL) but only if detectable values were reported for 25% or more of the measurements for that period of time. Otherwise, non-detectable concentrations were not included in the analysis. This method provides a reasonable balance between skewing the data towards lower values in cases where the frequency of non-detects was high and skewing the data towards higher values by excluding the non-detects from the statistical analysis. For each congener, a statistical analysis of the concentration data was then conducted to determine

the statistical distribution of the PCB concentrations in the sediments. In all cases, PCB congener concentrations were represented by log-normal distributions. A similar procedure was used for _PCB, where the total PCB concentration was determined as the sum of the concentrations of 40 PCB congeners as described in section 2.3.1. We derived statistical distributions of the PCB concentrations in the Northern, Central and Southern sections of the Bay. To determine section wide distributions of the PCB congener concentrations in the Northern section of the Bay, we combined data from RMP sampling stations in Petaluma River, San Pablo Bay, Pinole Point and Davis Point. PCB concentration distribution for the Central section of the Bay were derived from the RMP stations in Alameda, Red Rock, Point Isabel, Richardson Bay, Horseshoe Bay, Oakland Inner harbor, San Leandro Bay and Yerba Buena Island. PCB concentration distribution data for the Southern section of the Bay were based on data from stations in Oyster Point, San Bruno Shoal, Redwood Creek, Dumbarton Bridge, Coyote Creek, Sunnyvale, San Jose and South Bay. We also developed distribution for the entire Bay based on mean reported concentrations from each monitoring station. The PCB concentration distributions for the Northern, Central and Southern sections of the Bay can be used to represent the exposure conditions for those species that predominantly reside in specific areas of the Bay. The Bay wide distributions are used to assess the exposure of species that have large foraging areas or for species that are distributed over the entire Bay. In our approach we have assumed that the RMP network of monitoring stations provides an appropriate spatial representation of the PCB concentrations to which these organisms are exposed. We think the latter is a reasonable assumption as monitoring stations are located throughout the Bay and distributed reasonably homogenously among the various sections of the Bay. Future monitoring programs that include sampling along a Bay wide intersect is likely to provide additional insight in the spatial distribution of PCB concentrations throughout the Bay. Information from this program is likely to be useful in characterizing the extent to which Bay organisms are exposed to PCBs. PCB congener concentrations in sediments and water that were used in the model to represent current (i.e. 1999-2001) conditions are listed in Appendix C.

In the next step we calculated the PCB congener concentration in San Francisco Bay biota from the BSAF and the PCB congener concentrations in the sediments according to

$$\log C_B = \log BSAF + \log C_S \qquad (3.8)$$

In this calculation, the spatial distribution of PCB congener concentrations in the Bay sediments was represented by the standard deviation (SD_{CS}) of the mean log C_S (i.e. of the geometric mean of the concentration in the sediments collected as part of the RMP sediment sampling program). Variability in log BSAF was represented by the standard deviation (SD_{BSAF}) of log BSAF (i.e. the geometric mean of the BSAF). The effect of variability and error in the PCB congener concentrations in the sediments and uncertainty the BSAF estimates on the PCB congener concentrations in biota was expressed by the standard deviation (SD_{CB}) of log C_B (i.e. the geometric mean of the _PCB concentration in the biota) and calculated as:

$$SD_{CB} = \sqrt{(SD_{CS}^2 + SD_{BSAF}^2)} \qquad (3.9)$$

The _PCB concentration was then calculated as the sum of the congener concentrations.

Based on the geometric mean of the _PCB concentrations in biota, we calculated an upper bound excess lifetime human cancer risk and a human health hazard index for San Francisco Bay fishermen who consume local fish according to equations 2.68 to 2.70. We also calculated an ecological risk index for fish, cormorant and tern eggs and harbor seals based on the geometric mean of the PCB concentrations in these organisms according to equation 2.71. Finally, to provide better insights into the significance of the spatial and temporal distribution of the PCB concentrations, we compared distributions of _PCB concentrations in San Francisco Bay biota to _PCB concentrations associated with human health risk and ecological risk targets. The target concentrations in fish and wildlife are listed in the management worksheet of the model and in Table 3.5.

Table 3.5: Internal concentrations in San Francisco Bay sport fish and wildlife associated with a 1:100,000 upper-bound excess human cancer risk, a human health hazard index in excess of 1 and excess of the NOAEL, LOAEL, the threshold effect concentration and the concentration required to cause a 5% exceedence of the threshold effect concentration.

Endpoint	Organism	Concentration (µg/kg wet weight)
Human Excess Lifetime Cancer Risk (1:100,000)	shiner surfperch	52
Human Health Hazard (H = 1)	shiner surfperch	207
Ecological Risk - ΣArochlor	shiner surfperch	20
Human Excess Lifetime Cancer Risk (1:100,000)	jacksmelt	52
Human Health Hazard (H = 1)	jacksmelt	207
Ecological Risk - ΣArochlor	jacksmelt	20
Human Excess Lifetime Cancer Risk (1:100,000)	white croaker	52
Human Health Hazard (H = 1)	white croaker	207
Ecological Risk - ΣArochlor	white croaker	20
Ecological Risk – LOAEL	Cormorant Egg	5000
Ecological Risk – LOAEL	Tern Egg	4000
Ecological Risk - Threshold Effect (11,000 µg/kg lipid)	Male harbor Seal	4730
Ecological Risk - LOAEL (25,000 µg/kg lipid)	Male harbor Seal	10750
Ecological Risk - NOAEL (5,000 µg/kg lipid)	Male harbor Seal	2150
Ecological Risk - 5% exceedence of Threshold Effect	Male harbor Seal	1500
Ecological Risk - Threshold Effect (11,000 µg/kg lipid)	Female harbor Seal	4730
Ecological Risk - LOAEL (25,000 µg/kg lipid)	Female harbor Seal	10750
Ecological Risk - NOAEL (5,000 µg/kg lipid)	Female harbor Seal	2150
Ecological Risk - 5% exceedence of Threshold Effect	Female harbor Seal	1000

3.5.2 Backwards Calculations

In the backwards calculation, the ΣPCB concentration in the sediment expected to meet ΣPCB concentrations in fish and wildlife associated with various human health and ecological risks was calculated as:

$$\log C_S = \log C_B - \log BSAF \qquad (3.10)$$

The BSAF of ΣPCB is calculated in the forwards calculations based on the current composition of PCB congeners in sediments of the Bay. The current composition of PCBs was determined based on sediment samples collected from the RMP stations between 1999 and 2001 as described in section 3.5.1. The BSAF for ΣPCB is therefore specific for the PCB composition in the Bay. The concentration of ΣPCB in the sediment (C_S) that is calculated also presumes that the composition of the PCB concentration in the Bay is the same as that is entered in the forward calculations to represent the current conditions. Hence, congener specific concentrations can be calculated from the ΣPCB concentration under the assumption that the PCB congener profile is similar to that in current sediments (or PCB congener profiles entered in the forwards calculations of the management sheet).

To derive target concentrations for _PCB in sediments of San Francisco Bay, human health and ecological risk targets (in this report, the values summarized in Table 3.1) were entered as log C_B in equation 3.10. log BSAF of _PCB was then subtracted to calculate log C_S which was used to determine the target _PCB concentration in the sediments as $10^{\log C_S}$. This target _PCB concentration in the sediment represent the geometric mean concentration of _PCB in sediments of San Francisco that needs to be achieved to meet the human health and ecological risk targets. The uncertainty in the BSAF that is introduced in the derivation of the target sediment concentrations represents the uncertainty in the model's calculation of the geometric mean concentration of _PCB

in sediments of San Francisco that meet the human health and ecological risk targets. It is important to stress that the model calculates a geometric mean target sediment concentration for _PCB. Theoretically, there are many statistical distributions of the sediment concentrations that exhibit the same geometric mean. This means that there are many different Bay-wide _PCB sediment concentration distributions that are consistent with the human health and ecological risk targets used in the model calculations. From a management perspective this is important information because it implies that a wide range of management options may be available to achieve human health and ecological risk objectives.

4. RESULTS AND DISCUSSION

This section summarizes the results of the sensitivity analysis, the model performance analysis the uncertainty analysis and the application of the model. The model itself is attached in Appendix D. The file name of the model is SFB Food Web Bioaccumulation Model for PCBs.xls.

4.1 MODEL SENSITIVITY

The model sensitivity analysis illustrates the extent to which variability in each of the model state variables contributes to variability in the BSAF. The sensitivity analysis involved varying individual model state variables by 10% of the selected values for the model calculations and reporting the resulting variability in the BSAF as described in Section 3.1. Table 4.1 and Tables 4.2 to 4.4 report the sensitivity in the BSAF for ΣPCB for abiotic and biotic state variables, respectively.

Table 4.1 indicates that all abiotic parameters included in the sensitivity analysis exhibited an impact on the model outcome. The lowest sensitivity was observed for the air temperature, which is only used in the calculations for the harbor seal and the two bird species. The particulate organic carbon content in the water column is a sensitive parameter in the model. This is not surprising since this parameter contributes to the quantity of chemical that is available in the water column for uptake by phytoplankton, invertebrates and fish. A reduction in the particulate organic carbon content in the water column results in a higher concentration of freely dissolved chemical in the water that can be absorbed by organisms via water respiration and passed on to predators when

organisms are consumed. Water temperature is another relatively sensitive abiotic variable as it affects several key processes such as the feeding rate of organisms, the gill ventilation rate in fish and the partitioning properties of the chemical between water, air and lipids.

Table 4.1: Sensitivity of abiotic state variables on the BSAF of PCBs in selected species represented in the San Francisco Bay food web bioaccumulation model. N/A – parameter is not applicable to the species.

Parameter (symbol)	Phytoplankton	Invertebrate	Fish	Male Cormorant	Male Seal
Mean air temperature (T_A)	N/A	N/A	N/A	0.00	0.00
Mean water temperature (T_W)	0.00	0.00	-0.65	-0.63	-0.63
Dissolved oxygen concentration (DO)	0.00	0.46	-0.37	-0.27	-0.24
Practical salinity units (PSU)	0.06	-0.04	-0.19	-0.17	-0.16
Dissolved organic carbon content – water (OC_{WATER})	0.07	0.03	0.05	0.06	0.06
Particulate organic carbon content – water (POC)	0.69	0.30	0.46	0.57	0.60
Concentration of suspended solids – water (C_{SS})	0.00	-0.54	-0.22	-0.36	-0.37
Organic carbon content – sediment ($OC_{SEDIMENT}$)	0.00	0.32	0.15	0.10	0.09
NLOM proportionality constant (β)	N/A	-0.07	0.02	0.49	0.57

Tables 4.2 to 4.4 illustrate the sensitivity of the biotic state variables of the SFB model. Certain parameters such as organism water content and water absorption efficiency do not have significant impacts on model outputs. On the other hand, parameters such as lipid content (and organic carbon content in phytoplankton), lipid absorption efficiency and non-lipid organic matter absorption efficiency are more sensitive variables and have

a greater effect on the model outcome. Lipids and organic carbon (in phytoplankton) are the main site within organisms where bioaccumulation of PCBs occurs. The lipid digestion efficiency and the non-lipid organic carbon (i.e. protein and carbohydrate) digestion efficiency are the most sensitive parameters in the model. These parameters control the lipid and organic matter content in the gastrointestinal tract of an organism following a feeding event and are largely responsible for the dietary biomagnification of PCBs. The growth rate (e.g. phytoplankton and seals) and the coefficients used to calculate the growth rate (in invertebrates and fish) are also sensitive model state variables. This is due to the fact that the growth rate is one of the most important depuration mechanisms in the model for higher K_{OW} PCBs.

The sensitivity analysis indicates that properties controlling the partitioning of the PCBs and dietary magnification play key roles in the San Francisco Bay food web bioaccumulation model. This is consistent with the fundamental architecture of the model, which is to a large degree based on (i) the chemical partitioning of PCBs between the organism and water or air, (ii) the dietary magnification of PCB, and (iii) growth dilution.

Table4.2: Sensitivity of biotic model state variables on the BSAF of PCBs in phytoplankton species represented in the San Francisco Bay food web bioaccumulation model.

Parameter (symbol)	Phytoplankton Sensitivity
Whole body lipid fraction (L)	-0.03
Whole body non-lipid organic carbon fraction (NLOC)	-0.55
Whole body water fraction (WC)	0.00
Phytoplankton growth rate constant (K_G)	0.47
Constant A_P (equation 2.12)	0.46
Constant B_P (equation 2.12)	0.01

Table 4.3: Sensitivity of biotic state variables on the BSAF of PCBs in representative invertebrate (Pacific oyster) and fish (white croaker) species in the San Francisco Bay food web bioaccumulation model. N/A – parameter is not applicable to the species.

Parameter (symbol)	Invertebrate Sensitivity	Fish Sensitivity
Wet weight (W)	0.07	-0.03
Whole body lipid fraction (L)	-0.55	-0.64
Whole body non-lipid organic matter fraction (NLOM)	-0.07	-0.13
Whole body water fraction (WC)	0.00	0.00
Percentage of respired pore water (Pw)	-0.23	-0.01
Invertebrate growth rate coefficient (I_{GR})	0.46	N/A
Fish growth rate coefficient (F_{GR})	N/A	0.26
Particle scavenging efficiency (σ)	0.05	N/A
Lipid absorption efficiency (ε_L)	-0.07	-1.03
NLOM absorption efficiency (ε_N)	-0.08	-0.48
Water absorption efficiency (ε_W)	0.00	0.00
Constant A_{EW} (equation 2.10)	-0.05	-0.10
Constant B_{EW} (equation 2.10)	0.00	0.00
Constant A_{ED} (equation 2.18)	0.00	0.00
Constant B_{ED} (equation 2.18)	0.00	0.00

Table 4.4: Sensitivity of biotic model state variables on representative mammal (i.e. adult male seal) and bird (i.e. adult male cormorant) species in the San Francisco Bay food web bioaccumulation model. N/A – parameter is not applicable to the species.

Parameter (symbol)	Avian Sensitivity	Mammal Sensitivity
Wet weight (W)	0.00	0.00
Whole body lipid fraction (L)	-0.87	-0.71
Whole body non-lipid organic matter fraction (NLOM)	-0.08	-0.01
Whole body water fraction (WC)	0.00	0.00
Mean homeotherm temperature (T_H)	0.00	0.00
Seal growth rate constant (k_G)	N/A	0.15
Lipid absorption efficiency (ε_L)	-4.45	-4.50
NLOM absorption efficiency (ε_N)	-1.34	-1.34
Water absorption efficiency (ε_W)	0.00	0.00
Constant A_{ED} (equation 2.34 for seals and 2.52 for birds)	0.00	0.00
Constant B_{ED} (equation 2.34 for seals and 2.52 for birds)	0.00	0.00

Table 4.5: Model calculated log BSAFs and their uncertainty (expressed as the standard deviation of log BSAF and calculated by Monte Carlo simulations) of various PCB congeners in white croaker, Double-crested Cormorant eggs and adult female harbor seals.

PCB	white croaker		Cormorant (Egg)		Adult Seal (Female)	
	log BSAF	SD	log BSAF	SD	log BSAF	SD
8	0.15	0.25	0.18	0.28	0.77	0.24
18	0.16	0.20	0.05	0.22	0.76	0.25
28	0.47	0.20	1.64	0.21	1.09	0.23
31	0.74	0.27	0.51	0.29	1.38	0.28
33	0.35	0.18	0.08	0.20	0.95	0.24
44	0.61	0.21	0.37	0.22	1.36	0.24
49	0.93	0.22	0.71	0.24	2.36	0.23
52	0.89	0.25	0.61	0.28	2.69	0.25
56	0.72	0.20	0.77	0.22	1.87	0.25
60	0.77	0.22	0.83	0.24	1.81	0.26
66	0.97	0.29	2.19	0.32	2.02	0.28
70	1.00	0.29	0.87	0.32	2.33	0.29
74	0.65	0.23	1.83	0.25	2.20	0.29
87	0.82	0.20	1.03	0.23	1.30	0.22
95	0.91	0.30	0.63	0.33	2.02	0.26
97	1.10	0.30	0.68	0.33	0.92	0.28
99	1.13	0.25	2.37	0.27	2.93	0.25
101	1.26	0.24	1.01	0.26	2.88	0.23
105	1.15	0.23	2.39	0.28	1.94	0.24
110	1.16	0.27	0.84	0.29	2.23	0.25
118	1.32	0.28	2.58	0.31	2.36	0.27
128	1.34	0.34	2.60	0.37	3.19	0.34
132	1.26	0.29	1.53	0.31	2.74	0.28
138	1.37	0.28	2.63	0.32	3.22	0.27
141	1.30	0.29	1.19	0.33	2.44	0.28
149	1.34	0.29	1.24	0.32	2.49	0.26
151	1.04	0.20	0.61	0.24	1.12	0.21
153	1.58	0.33	2.87	0.36	3.45	0.30
156	1.08	0.20	2.01	0.23	2.42	0.23
158	1.07	0.20	2.00	0.24	2.51	0.23
170	1.55	0.36	2.83	0.39	3.42	0.32
174	1.47	0.33	1.08	0.37	1.79	0.30
177	1.21	0.24	2.17	0.27	2.82	0.24
180	1.49	0.32	2.77	0.36	3.36	0.30
183	1.49	0.33	2.76	0.37	3.35	0.30
187	1.38	0.28	2.65	0.32	3.21	0.27
194	1.12	0.27	2.35	0.31	2.94	0.26
195	1.15	0.22	2.37	0.26	2.94	0.29
201	1.36	0.24	2.62	0.28	1.67	0.23
203	1.11	0.20	2.33	0.24	2.85	0.21

4.2 MODEL PERFORMANCE

To test the model's ability to estimate concentrations of PCB congeners in biota of San Francisco Bay, the model was applied to make predictions of the BSAF and concentrations of PCB congeners and _PCB concentrations in several organisms in San Francisco Bay based on measured concentrations of PCBs in the sediment. The model predicted BSAFs ($BSAF_{P,i}$) were then compared to the observed BSAFs ($BSAF_{O,i}$) for those species for which empirical values were available. This methodology is described in more detail in section 3.3.

Figures 4.1 to 4.8 illustrate model predicted and observed BSAFs for the approximately 40 PCB congeners included in the RMP monitoring program. These Figures present the results of performance analyses in organisms of different trophic levels and guilds and illustrate that the observed BSAFs exhibit a considerable range of values. This variability in the observed BSAF includes spatial variability as the observed BSAFs are based on measured PCB concentrations in biota and sediments of the Bay, which vary among locations in the Bay.

Figures 4.1 to 4.8 also illustrate the predicted log BSAFs and their 95% confidence intervals. The standard deviations are based on Monte Carlo Simulation incorporating the uncertainty in the model's state variables. They do not include variability due to spatial differences in PCB concentrations in the sediments. The Figures show that the model predicted BSAFs are well within the range of the observed values. The geometric mean BSAFs model predictions are generally in close proximity to observations. Figures 4.1 to 4.8 further illustrate that the "congener patterns" of PCBs in all of the organisms, which represent the composition of the PCB mixture, are reasonably well reproduced by the model. This indicates that the apparent agreement between observations and predictions for the BSAFs is similar among the congeners of the PCB mixtures.

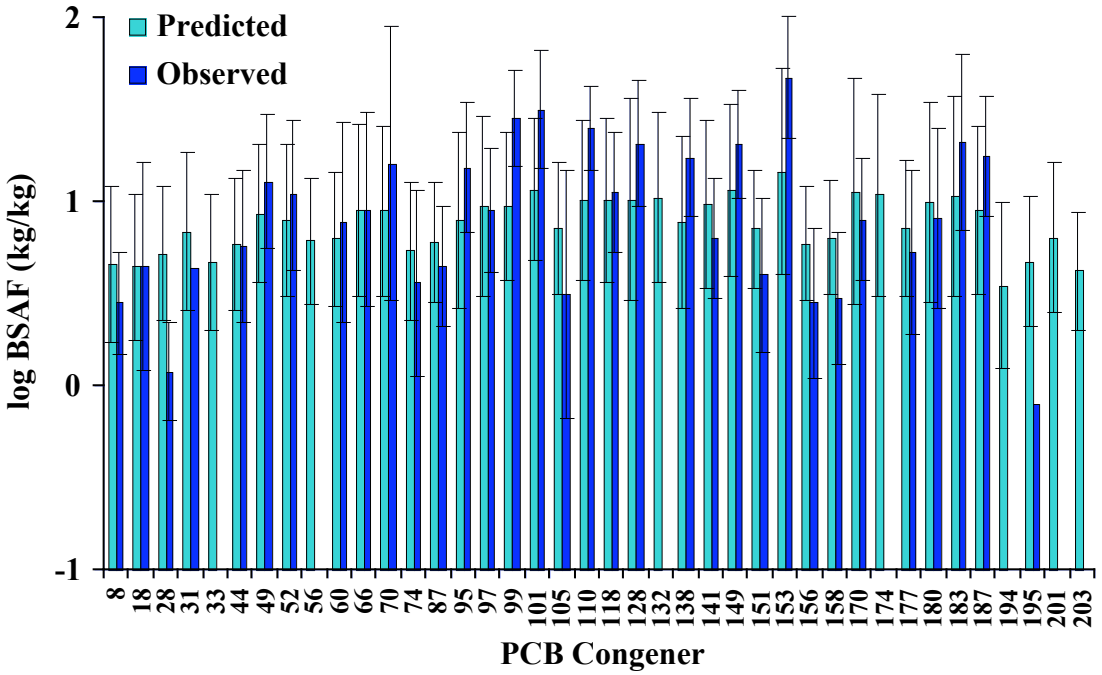

Figure 4.1: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in California mussels (*Mytilus californianus*) in San Francisco Bay.

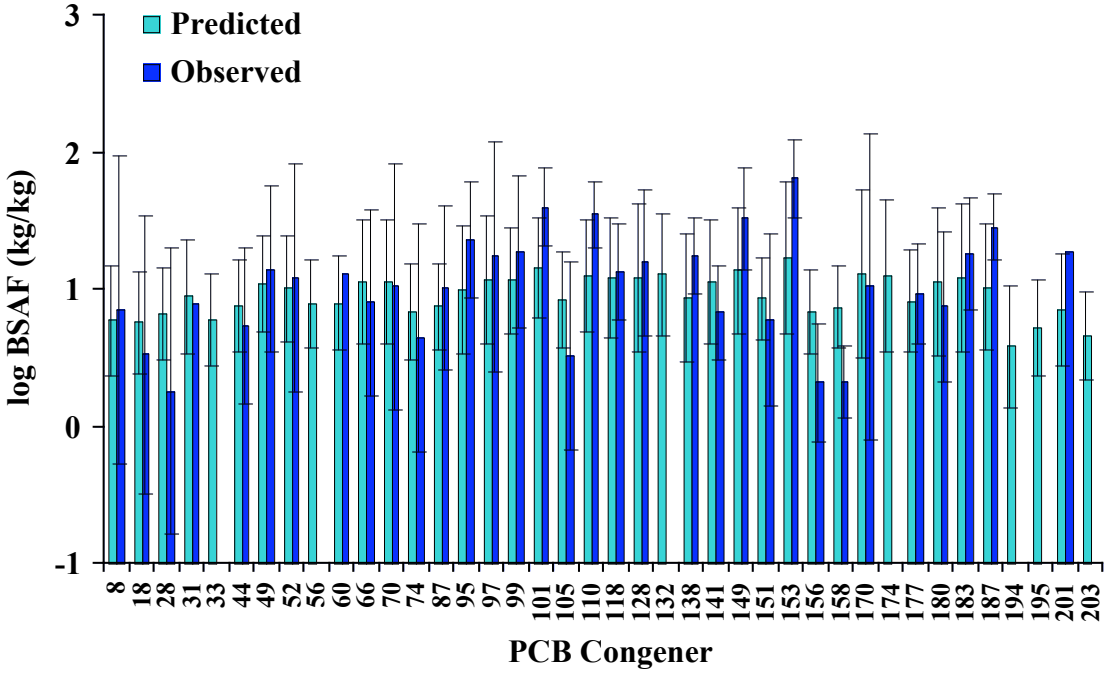

Figure 4.2: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in Pacific oysters (*Crassostrea gigas*) in San Francisco Bay.

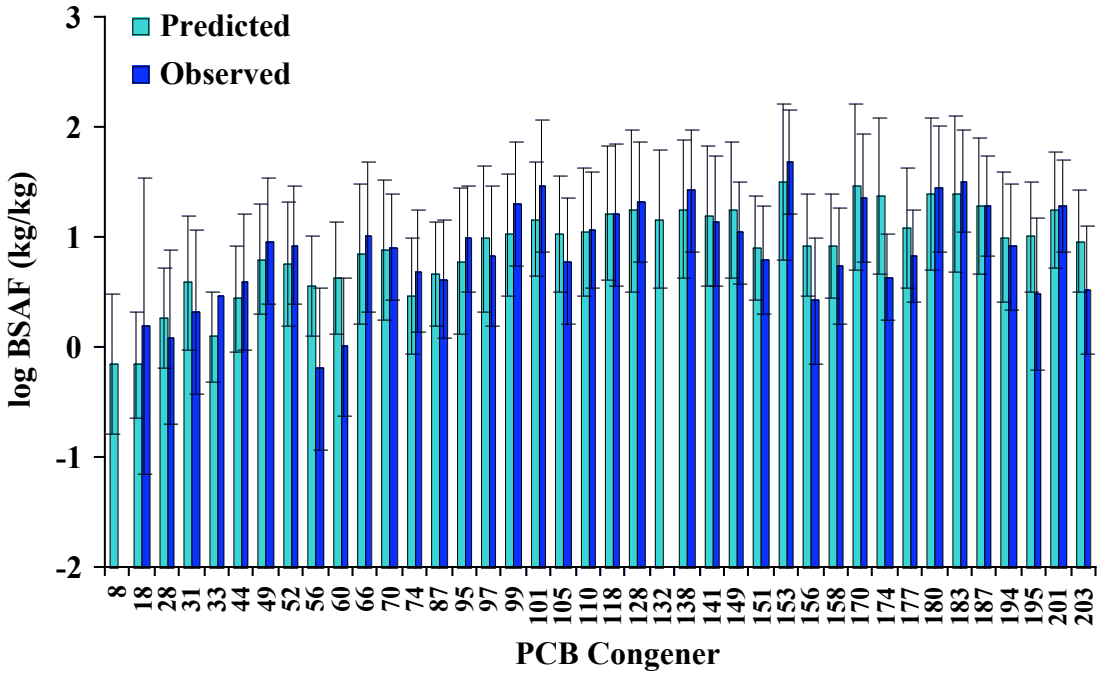

Figure 4.3: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in shiner surfperch (*Cymatogaster aggregate*) in San Francisco Bay.

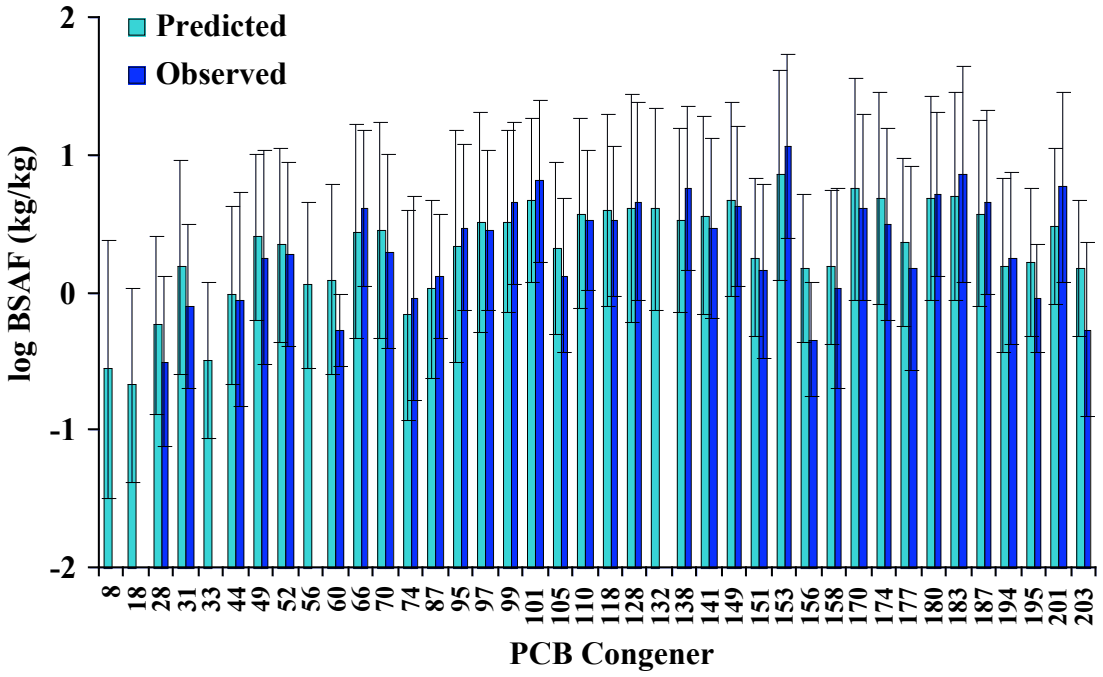

Figure 4.4: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in jacksmelt (*Atherinopsis californiensis*) in San Francisco Bay.

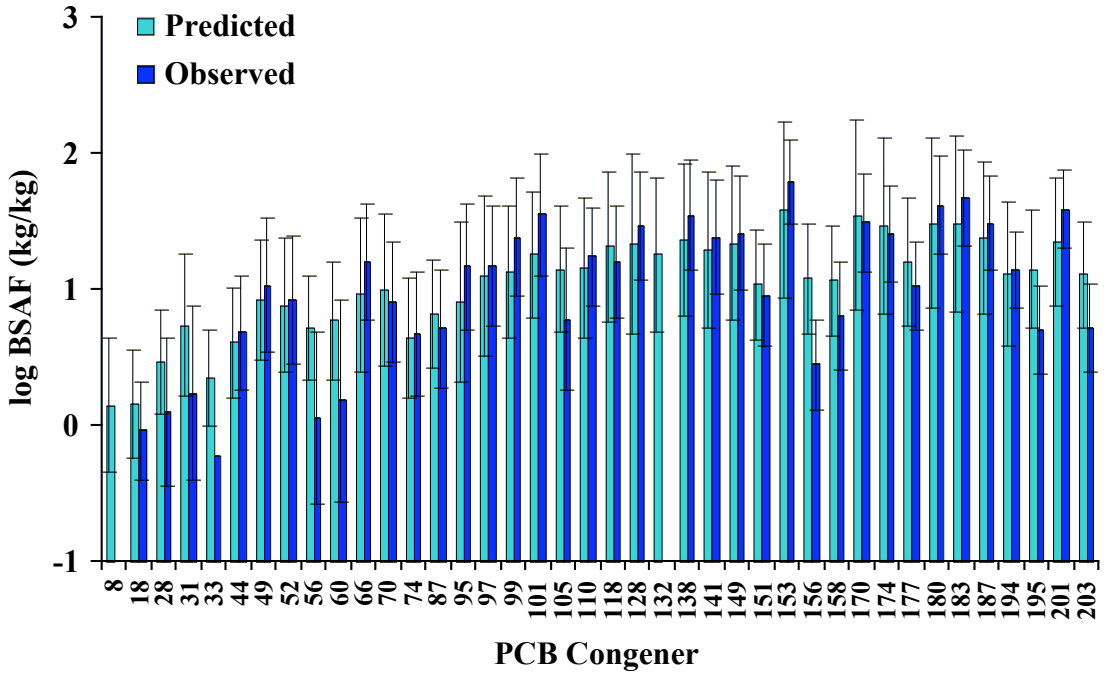

Figure 4.5: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in white croaker (*Genyonemus lineatus*) in San Francisco Bay.

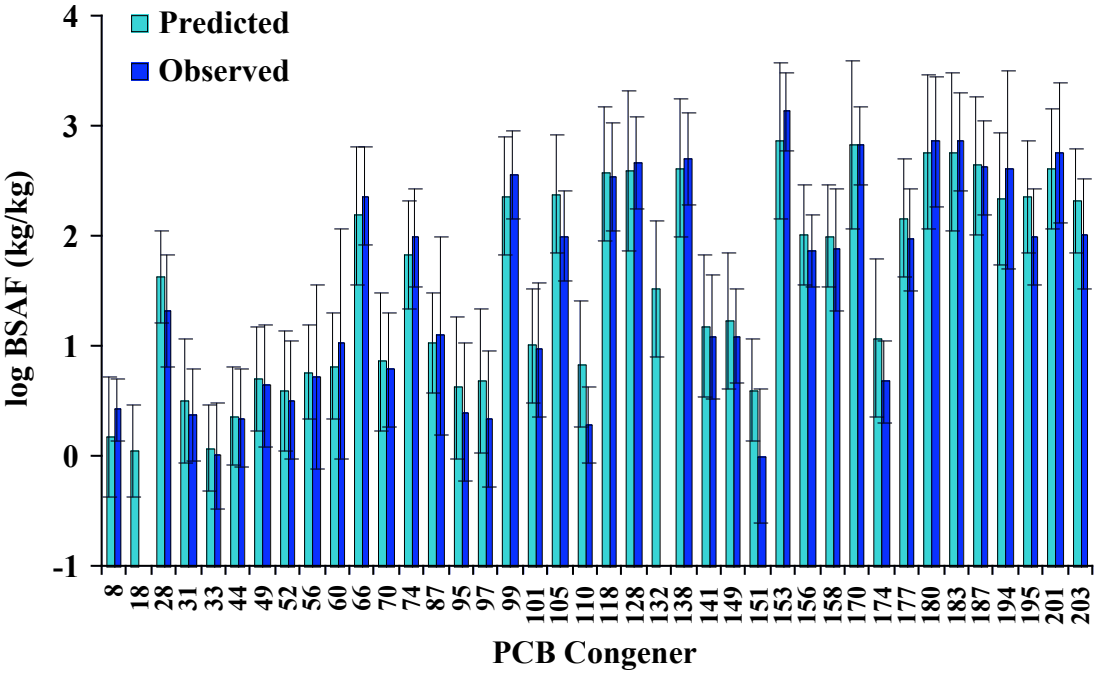

Figure 4.6: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in eggs of Double-crested Cormorants (*Phalacrocorax auritus*) in San Francisco Bay.

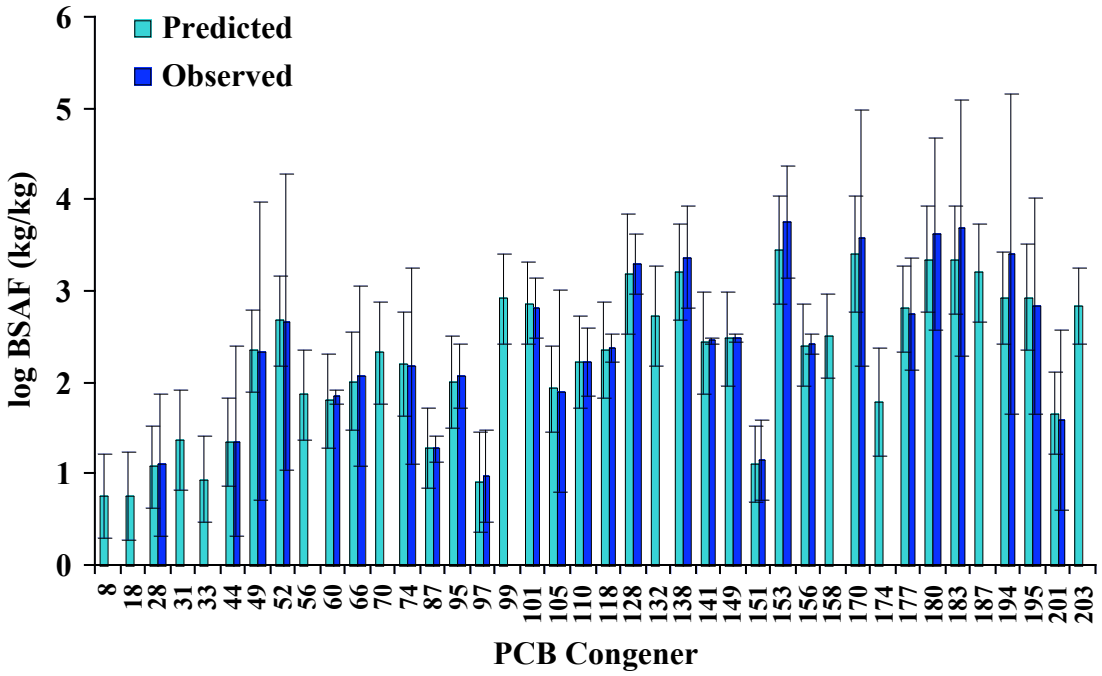

Figure 4.7: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in adult female harbor seals (*Phoca vitulina richardsi)* in San Francisco Bay.

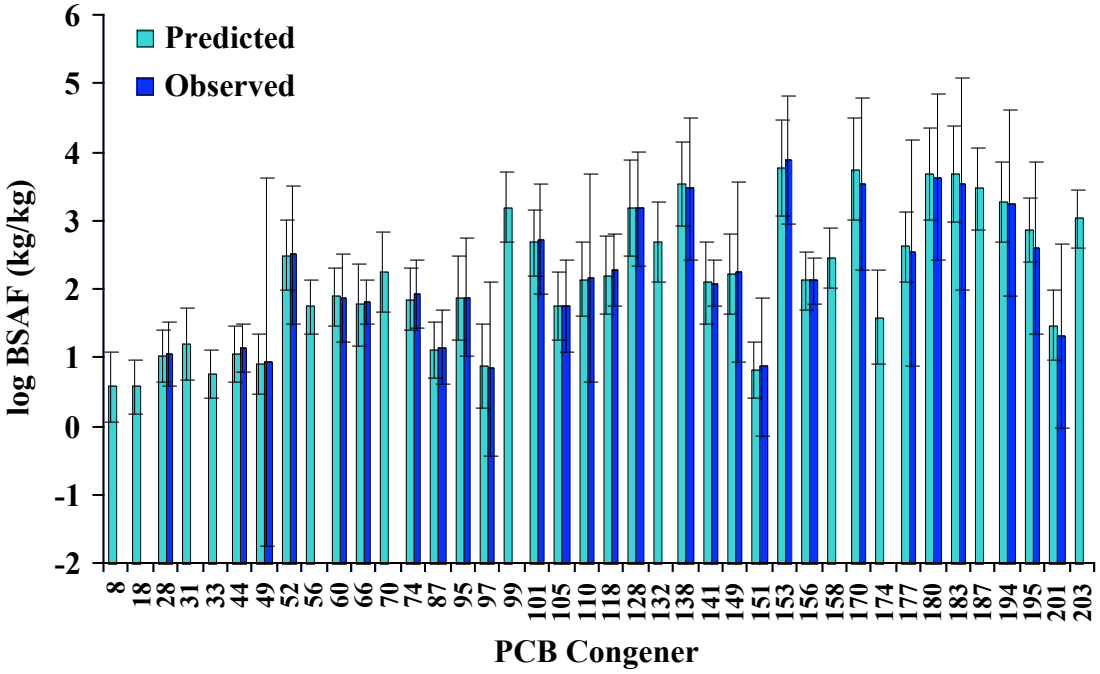

Figure 4.8: Model predicted and observed BSAFs (kg dry sediment/kg wet weight organism) of approximately 40 PCB congeners in adult male harbor seals (*Phoca vitulina richardsi)* in San Francisco Bay.

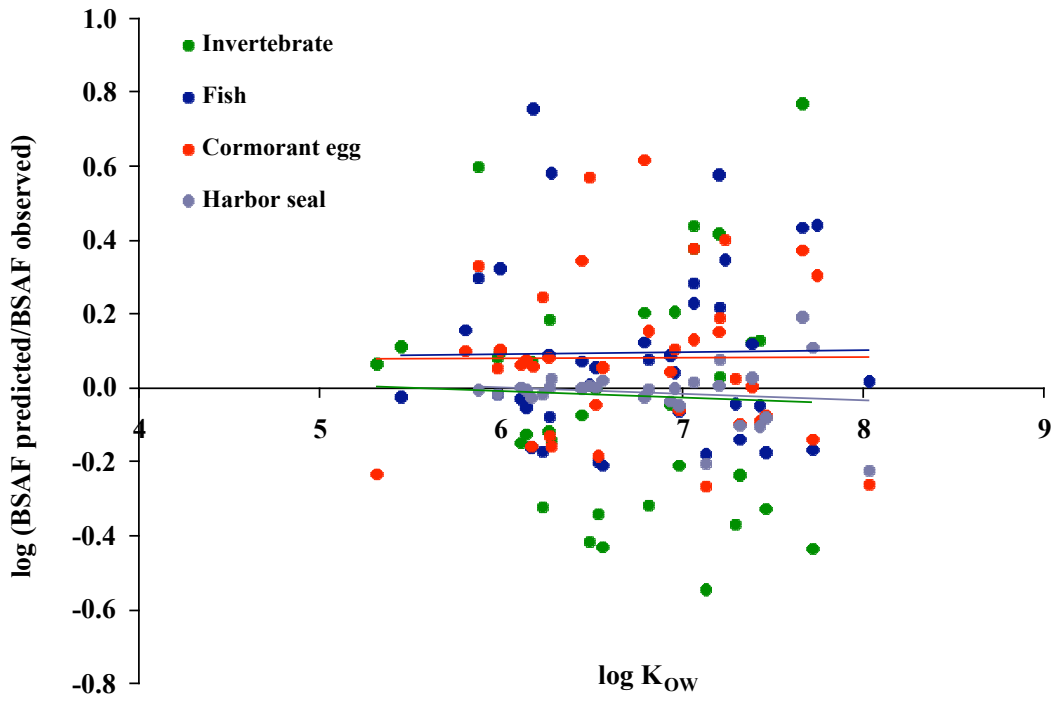

Figure 4.9: Comparison of the predicted and observed BSAFs in Bay organisms for PCB congeners of varying octanol-water partition coefficients. A log ($BSAF_{predicted}/BSAF_{observed}$) equal to 0 indicates perfect agreement between observed and predicted BSAFs.

Figure 4.9 further illustrates the ability of the model to estimate concentrations of PCBs in biota of the San Francisco Bay food web. It expresses and quantifies the level of agreement between observed and predicted means of the BSAFs in the various species as $BSAF_{predicted}/BSAF_{observed}$ for the PCB congeners and explores the relationship between the ratio of observed and predicted BSAFs and the octanol-water partition coefficient of the PCB congeners. It illustrates that among the different PCB congeners, the log ($BSAF_{predicted}/BSAF_{observed}$) ranges between approximately -0.6 and 0.8. For example, the log ($BSAF_{predicted}/BSAF_{observed}$) among individual PCB congeners in Double-crested Cormorant eggs ranges between approximately -0.27 and 0.61. This implies that among the PCB congeners in cormorant eggs, the worst agreement between observed and predicted BSAFs was equivalent to a factor $10^{0.61}$ or 4.0. This was for PCB congener 151.

Linear regression of log ($BSAF_{predicted}/BSAF_{observed}$) vs. log K_{OW} illustrates that over- and under-estimations of the BSAF by the model is not related to the hydrophobicity of the PCB congeners. It also illustrates the regression line is close to 0, indicating that the average ratio of $BSAF_{predicted}/BSAF_{observed}$ is close to 1.

Table 4.6 illustrates that the mean Model Bias (MB) among the 40 PCB congeners ranges between 0.86 for female harbor seals to 1.32 for the white croaker and is close to 1 for all organisms. This illustrates that the model produces little systematic over- or under-estimation of PCB congener concentrations. The 95% confidence intervals of the mean model bias ranges between a factor of 1.55 for male harbor seals to 4.65 for white croaker. This illustrates that over- and under-estimations of the BSAF for individual PCB congeners can be considerable. However, over-estimation of the BSAF for certain congeners are cancelled out by under-estimation of the BSAF for other congeners, producing a mean BSAF for PCB congeners among the various species of the Bay that is within 2 to 32% (depending on the species) of the observed mean values. This indicates that the apparent systematic error in the model is relatively small. It further implies that while the model may produce estimates of the BSAF for some congeners that can be substantially over- or under-estimated, it can be expected to produce estimates of the BSAF of total PCB concentrations that are in good agreement with the observed concentrations. This is an encouraging sign and suggests that the model may be able to make realistic predictions of the BSAF of _PCBs, i.e. the relationship between _PCB concentrations in sediments and biota in San Francisco Bay.

Figures 4.10 and 4.11 illustrate model predicted and observed BSAFs for _PCB. The observed log BSAF of _PCB, contain 95% confidence intervals ranging between approximately 0.4 (for cormorants) and 1.0 (for male harbor seals) and reflecting considerable variability among the observed BSAFs in the Bay. Figures 4.10 and 4.11 also illustrate the predicted log BSAFs and their standard deviations calculated through Model Bias (MB*) and Monte Carlo Simulation (MCS), respectively. The figures illustrate that the model predicted BSAFs of _PCB are well within the range of the observed values. Table 4.6 illustrates that the mean Model Bias (MB^*) of the BSAF of

_PCB (Equation 3.5) ranges between 0.71 for Pacific oysters to 1.22 for the male harbor seals and is close to 1 for all organisms. This illustrates that the model predicted BSAFs of _PCB are in good agreement with the observed BSAFs and fall well within the range of BSAFs that have been observed in the Bay. The model calculations of the BSAF of _PCB do not appear to contain a significant degree of bias in terms of either an over- or under-estimation of the observed BSAFs. The 95% confidence intervals of the mean model bias MB^* range between a factor of 2.0 for California mussels to 10 for male harbor seals (Table 4.6). The confidence intervals of the MB^* illustrate the range of predicted BSAFs of _PCB that include 95% of the BSAF observations in the Bay. The 95% confidence intervals of MB^* are used as a measure of the expected variability around the mean BSAFs of _PCBs predicted by the model for organisms of the Bay. The confidence intervals can be viewed as the uncertainty in the BSAF model estimates for _PCBs. They play an important role in assessing what the probability is that concentrations of _PCBs in organisms of the Bay exceed various ecological and human health criteria.

Table 4.6: The mean model bias for specific congeners (MB) and ΣPCBs (MB*), their 95% confidence intervals, sample size (n) and logarithmic equivalents i.e. log MB and log MB* and their standard deviations (SD) for several species of San Francisco Bay.

Species	Name	MB (n)	Log MB (SD)	MB* (n)[a]	Log MB* (SD)
California mussel	*Mytilus californianus*	0.98 (33) 0.24 – 4.00	-0.01 (0.31)	0.73 (13) 0.36 – 1.48	-0.13 (0.14)
Pacific oyster	*Crassostrea gigas*	0.92 (33) 0.23 – 3.60	-0.04 (0.30)	0.71 (9) 0.30 – 1.76	-0.15 (0.17)
shiner surfperch	*Cymatogaster aggregate*	1.16 (38) 0.31 – 4.30	0.06 (0.29)	0.96 (18) 0.30 – 3.11	-0.02 (0.24)
jacksmelt	*Atherinopsis californiensis*	1.14 (35) 0.47 – 2.72	0.06 (0.19)	0.95 (15) 0.24 – 3.67	-0.02 (0.28)
white croaker	*Genyonemus lineatus*	1.32 (38) 0.37 – 4.65	0.12 (0.28)	1.00 (24) 0.37 – 2.67	0.00 (0.21)
Double-crested Cormorant	*Phalacrocorax auritus*	1.18 (38) 0.43 – 3.19	0.07 (0.22)	0.84 (8) 0.33 – 2.16	-0.08 (0.18)
Male harbor seal	*Phoca vitulina*	1.04 (28) 0.70 – 1.55	0.02 (0.09)	1.22 (4) 0.12 – 12.4	0.09 (0.36)
Female harbor seal	*Phoca vitulina*	0.86 (28) 0.46 – 1.59	-0.06 (0.14)	0.78 (2) 0.12 – 4.87	-0.11 (0.19)

a. 95% confidence interval (CI) = antilog (geometric mean ± ($t_{\nu, 0.05}$ × standard deviation))

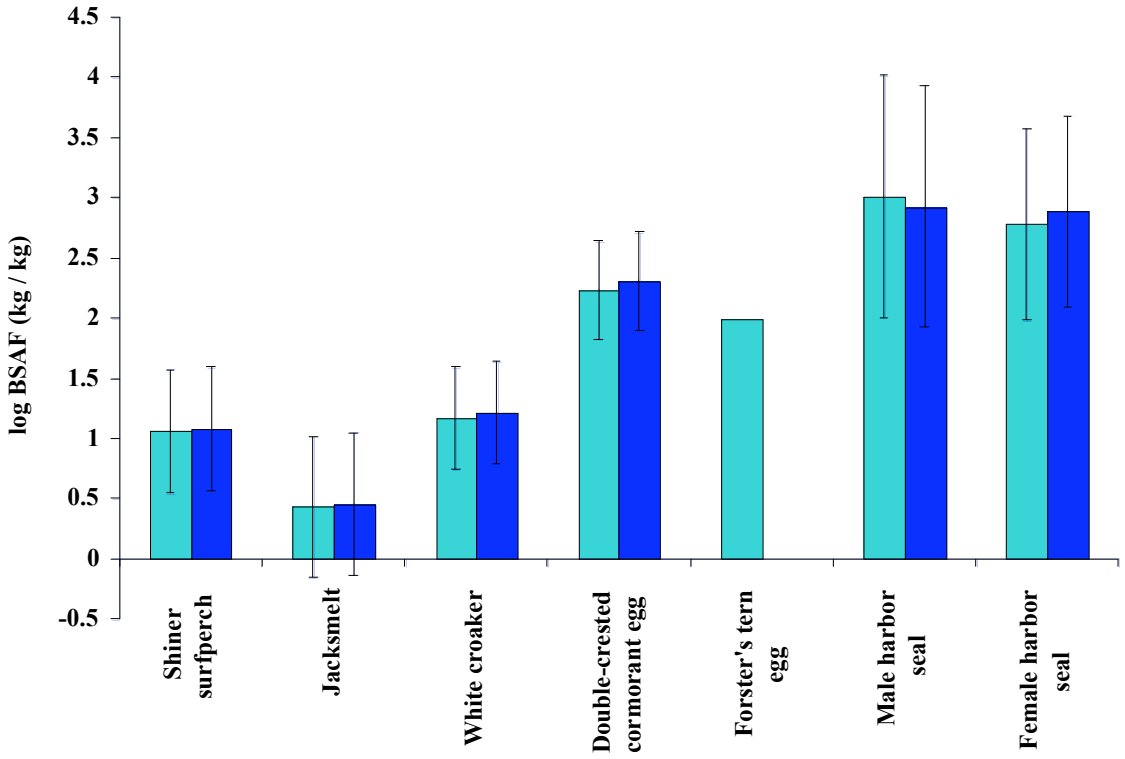

Figure 4.10: Model predicted (green) and observed (blue) mean BSAFs (kg dry sediment/kg wet weight organism) of _PCBs in several species in San Francisco Bay. Error bars represent 95% confidence intervals. Confidence intervals of the model predicted log BSAF reflect the 95% confidence intervals of the mean MB*.

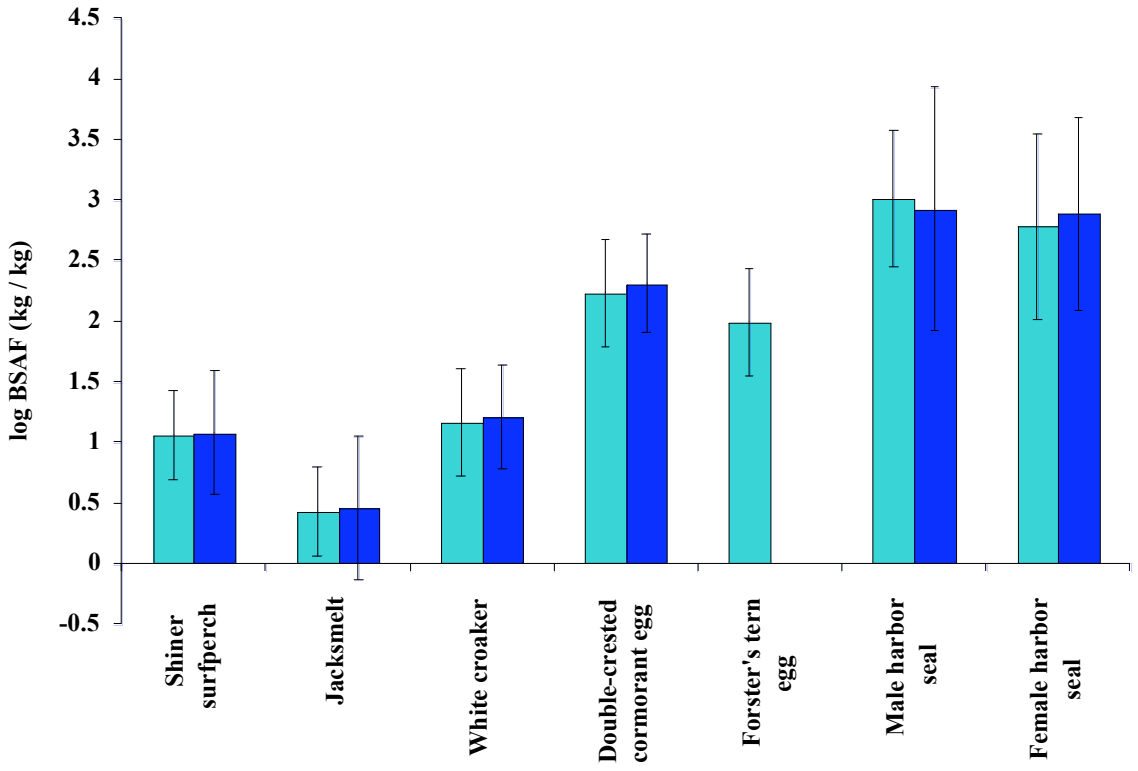

Figure 4.11: Model predicted (green) and observed (blue) mean BSAFs (kg dry sediment/kg wet weight organism) of _PCBs in several species in San Francisco Bay. Error bars represent 95% confidence intervals. Confidence intervals of the model predicted log BSAF are calculated through Monte Carlo Simulation.

4.3 UNCERTAINTY ANALYSIS

The uncertainty in the calculations of the BSAF of ΣPCB in fish and wildlife of San Francisco Bay was assessed by applying two methods, which are discussed in section 3.4. One method uses the 95% confidence intervals of the model bias (MB^*) for _PCBs, defined in section 3.3, to express the uncertainty in the model predicted BSAFs of ΣPCB. The 95% confidence intervals are presented in Table 4.6. They ranged between a factor of 2.0 for California mussels to 10 for male harbor seals. This illustrates that BSAFs of PCBs in the various species of San Francisco Bay exhibit considerable variability. This variability needs to be considered when applying the model to make calculations of PCB concentrations in biota. For this reason, the 95% confidence intervals of the MB* are used as estimates of the uncertainty of the model. The uncertainty of the model can be viewed as the range of predicted BSAFs that can be expected to include 95% of the actual BSAFs in the Bay.

The second method of uncertainty analysis that was performed involved the application of Monte Carlo Simulation to assess the effect of inherent variability and error in the model state variables on the model outcome. Table 4.5 illustrates the model uncertainty of the BSAF for individual PCB congeners in white croaker, cormorant eggs and adult female harbor seals calculated by Monte Carlo Simulation. Figures 4.1 to 4.8 illustrate the BSAFs of PCB congeners and their 95% confidence intervals calculated by Monte Carlo Simulation. Figure 4.11 illustrates the magnitude of the uncertainty in the BSAFs for _PCBs calculated by Monte Carlo Simulation. Figures 4.10 and 4.11 illustrates that both methods used to determine the magnitude of model uncertainty produce comparable results. This implies that the selection of methodology for estimating model uncertainty is of little consequence, i.e. both methods arrive at comparable estimates of the magnitude of model uncertainty.

4.4 MODEL APPLICATION

4.4.1 Forwards calculation

Figure 4.12 compiles ΣPCB concentrations from a total of 1,284 sediment samples collected from San Francisco Bay between 1999 and 2001 under the RMP sediment sampling program. It illustrates the distribution of PCB concentrations in the Bay and shows that there is a substantial variability in the ΣPCB concentrations in the sediments of the various sections of the Bay (i.e. North, Central and South). The ΣPCB concentration distributions range by approximately 2 orders of magnitude in the Northern and Southern sections of the Bay, and by 3 orders of magnitude in the Central section of

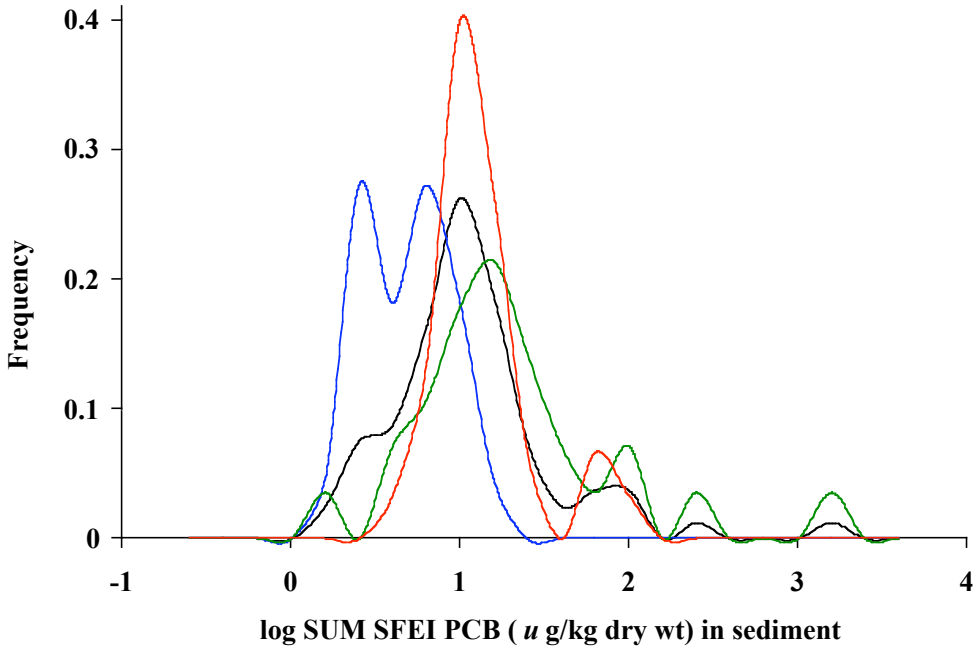

Figure 4.12: Distributions of ΣPCB concentrations in sediments in the Northern (blue line), Southern (red line) and Central (green line) sections of San Francisco Bay as well as the distribution for the entire Bay (black line) based on a total of 1,284 samples collected at RMP stations between 1999 and 2001.

the Bay. ΣPCB concentrations in the Northern section of the Bay are somewhat lower than those in the Central and Southern sections of the Bay. This suggests that the Northern section of the Bay is less contaminated with PCBs than the other sections of the Bay. To represent the concentrations of the PCB congeners in the sediments of the Bay, we have chosen to compile all the data and express the Bay wide concentration by a single log-normal distribution. As discussed earlier, we think that this is appropriate as the species included in the model are either distributed over large sections of the Bay and have a large foraging area encompassing many areas in the Bay. Figure 4.12 (black line) illustrates that the Bay wide distribution of the ΣPCB concentrations in the sediments conforms well to the distributions in the Southern and Central sections of the Bay. However, the geometric mean of the Bay wide distribution is larger than that for the Northern section of the Bay.

Figure 4.13 illustrates the Bay wide log-normal distribution of the ΣPCB concentrations used in the model (red line) in relation to the actual distribution of all 1,284 sediment concentrations in the Bay (black line). This Figure shows that the log-normal distribution that was used in the model to represent the current level of PCB contamination in the Bay is in reasonable agreement with the actual distribution of the 1,284 sediment concentration data from the Bay. The geometric mean of this distribution is approximately 11.6 μg/kg dry sediment. The 95% confidence interval of the geometric mean is equivalent to a factor of 7.4. This indicates that fish and wildlife in the Bay are exposed to PCB concentrations that vary substantially in the Bay. The model application is geared to assessing the Bay wide distribution of the PCB concentrations in fish and wildlife of the Bay that can be expected based on the observed distribution of PCB concentrations in the sediments.

Figures 4.14 to 4.20 illustrate the results of the model calculations of the ΣPCB concentration in some key species of the San Francisco Bay food web. In these figures, the red lines represent the ΣPCB concentration in each of the species based on the distribution of ΣPCB concentrations in the Bay sediment and the contribution to the

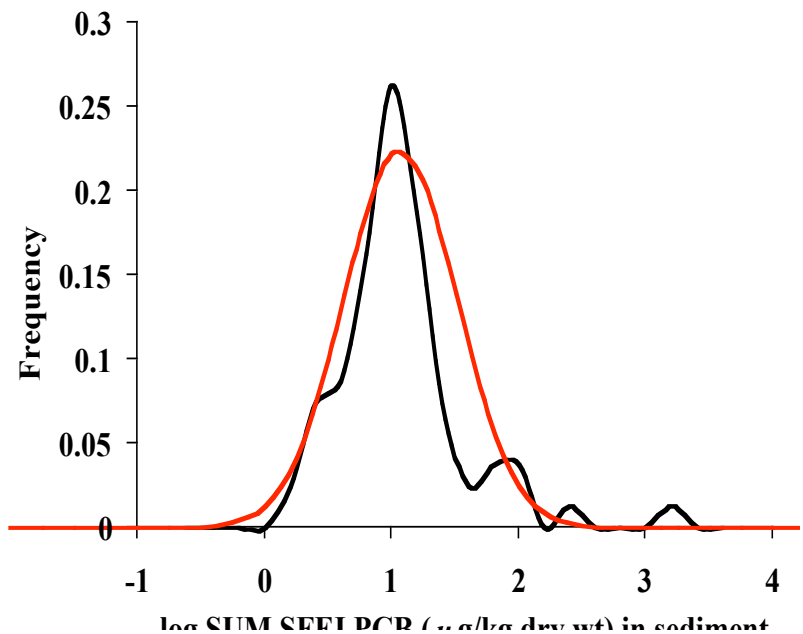

Figure 4.13: Distributions of ΣPCB concentrations in sediments of San Francisco Bay. The black line represents actual distribution based on 1,284 sediment concentration data collected at RMP stations between 1999 and 2001. The red line represents the distribution used in the model application.

variability in the PCB concentration in biota by the model calculated through Monte Carlo Simulation (MCS). The predicted ΣPCB concentration distributions include uncertainty in the BSAF as well as the variability in the _PCB concentrations in the sediments illustrated in Figure 4.13. These calculations therefore incorporate variability in both the external variable (the PCB concentration in the sediment) and uncertainty in the model calculations. It should be stressed that the distribution of the predicted PCB concentrations in biota is therefore not solely a reflection of model uncertainty, but also reflects the variability in PCB concentrations in the sediments of the Bay. In fact, the variability of the PCB concentrations in the Bay sediments is the largest contributor to 95% confidence intervals of the predicted geometric mean ΣPCB concentrations depicted in Figures 4.14 to 4.20.

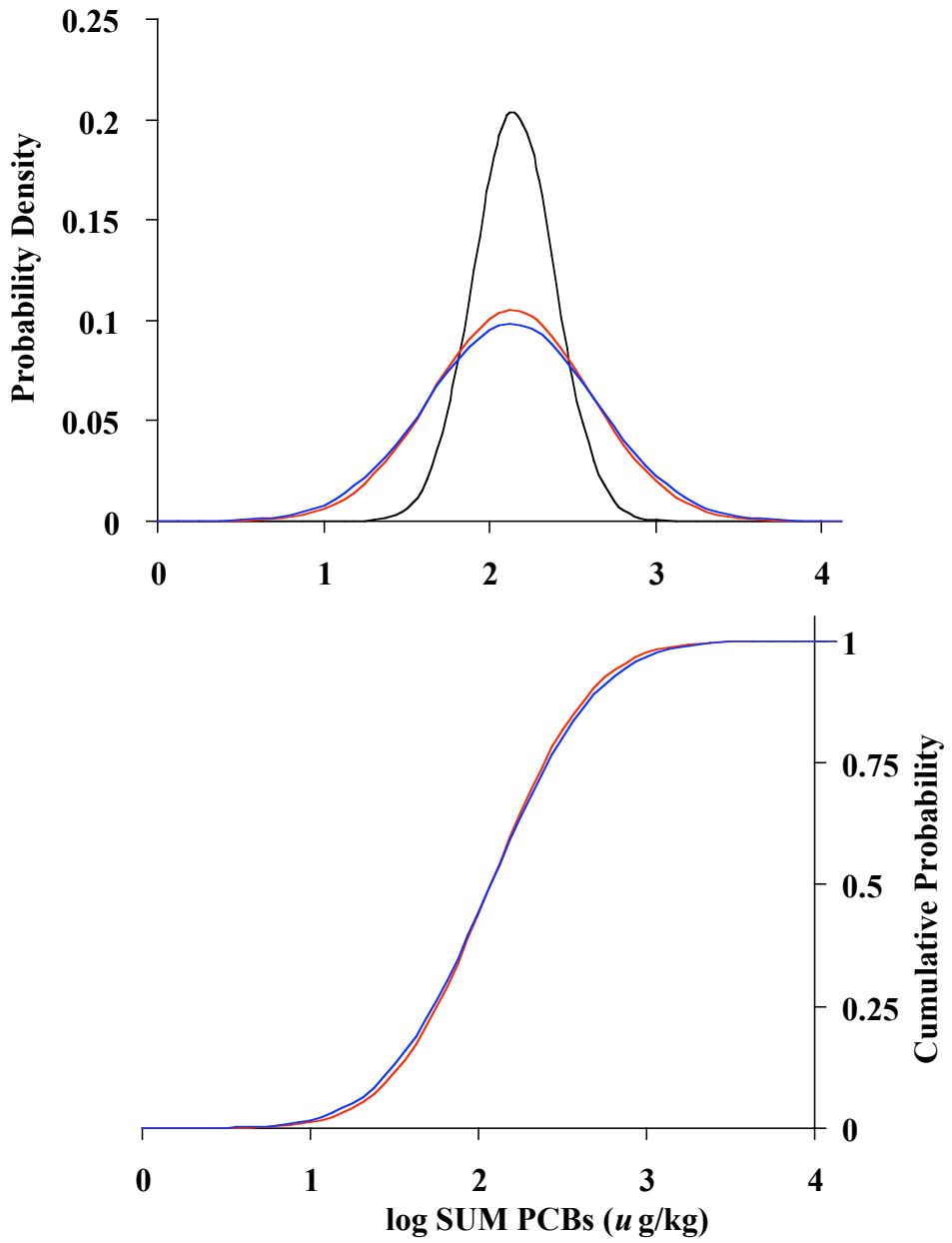

Figure 4.14: Normal (top) and cumulative (bottom) probability distributions for the ΣPCB concentrations in shiner surfperch in San Francisco Bay for the period between 1999 and 2001. The red line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MCS). The blue line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MB*). The black line represents the distribution of observed concentrations in the Bay from data collected in 2000.

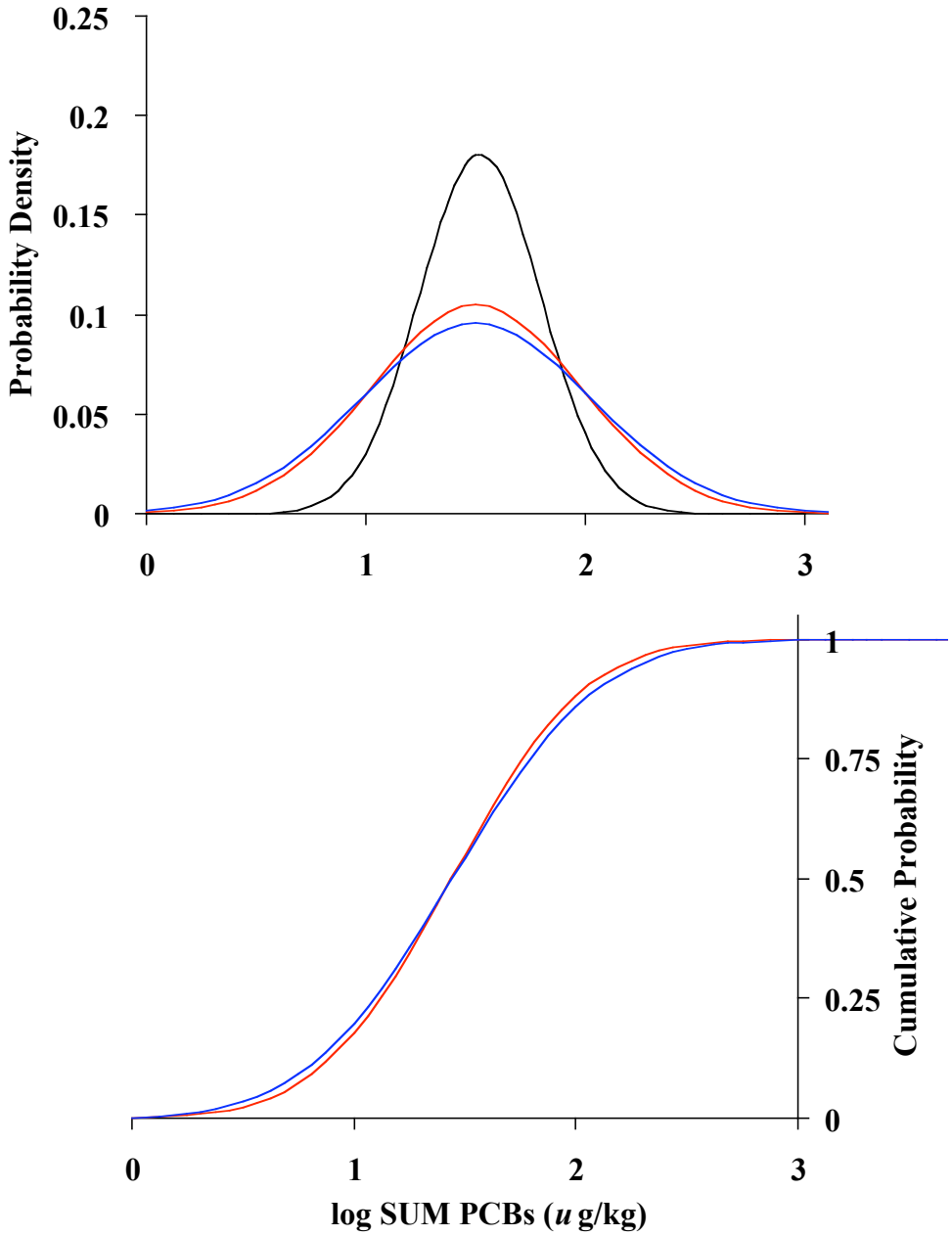

Figure 4.15: Normal (top) and cumulative (bottom) probability distributions for the ΣPCB concentrations in jacksmelt in San Francisco Bay for the period between 1999 and 2001. The red line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MCS). The blue line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MB*). The black line represents the distribution of observed concentrations in the Bay from data collected in 2000.

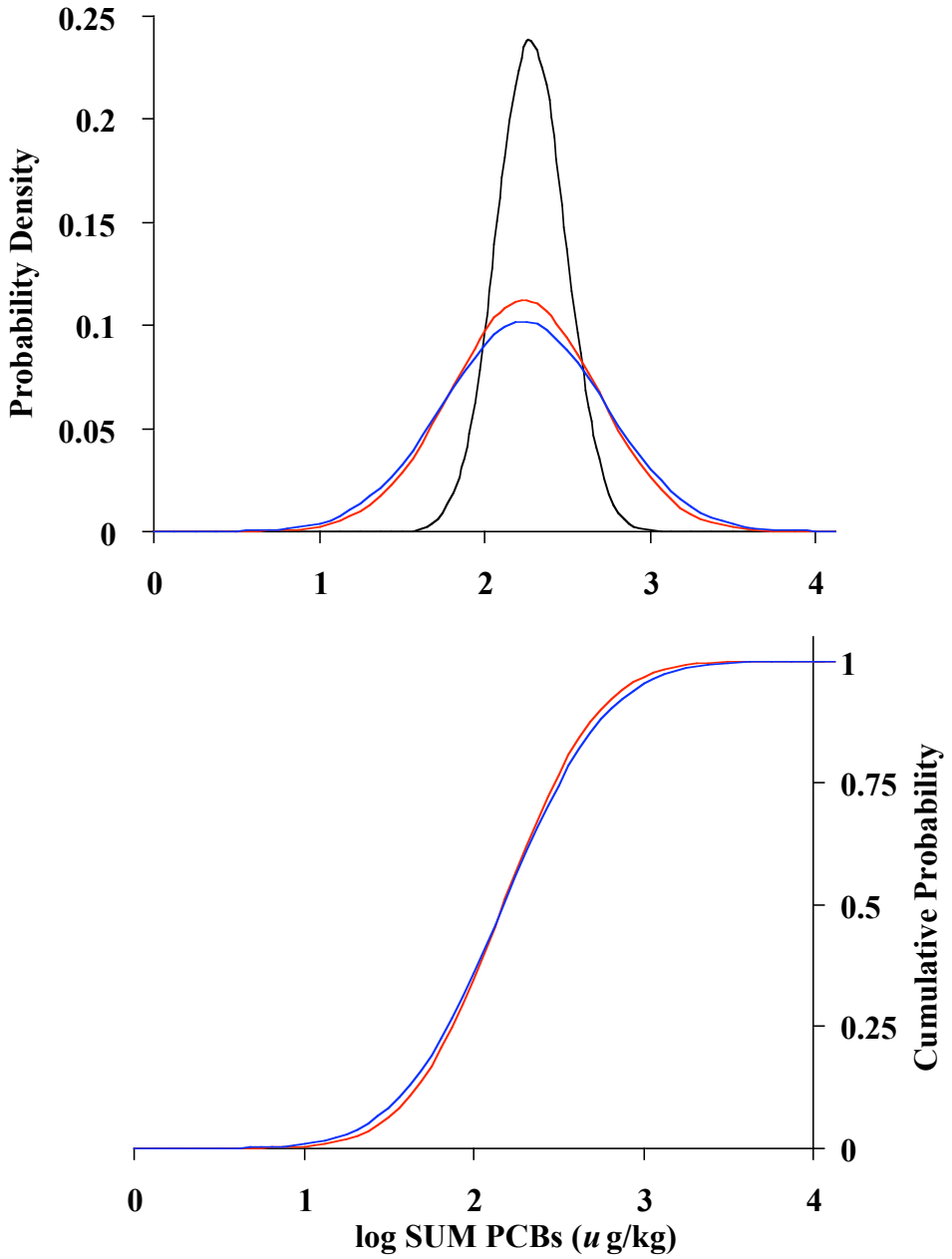

Figure 4.16: Normal (top) and cumulative (bottom) probability distributions for the ΣPCB concentrations in white croaker in San Francisco Bay for the period between 1999 and 2001. The red line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MCS). The blue line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MB*). The black line represents the distribution of observed concentrations in the Bay from data collected in 2000.

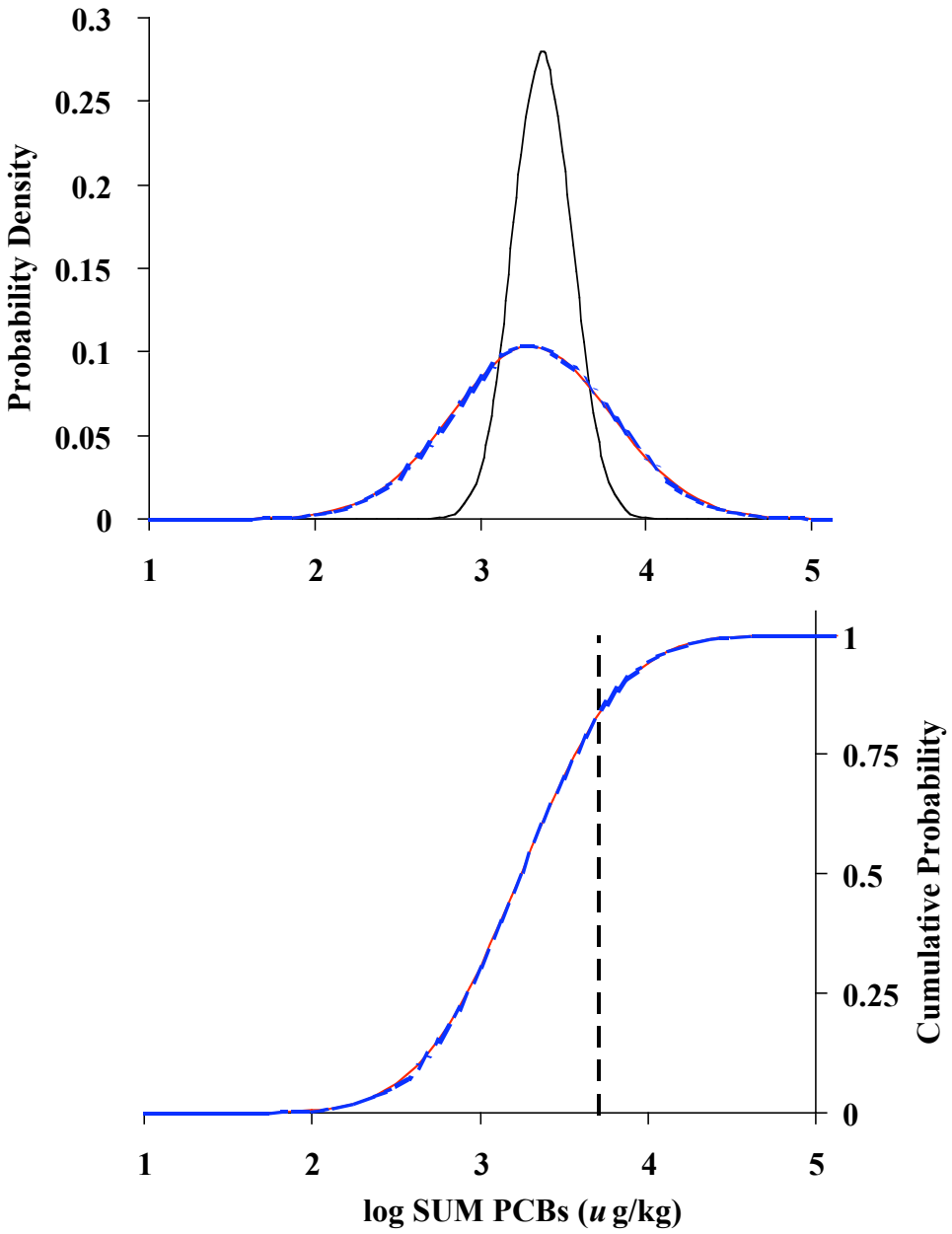

Figure 4.17: Normal (top) and cumulative (bottom) probability distributions for the ΣPCB concentrations in Double-crested Cormorant eggs in San Francisco Bay for the period between 1999 and 2001. The red line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MCS). The blue line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MB*). The black line represents the distribution of observed concentrations in the Bay from data collected in 2000.The dashed line represents a LOAEL of 5.0 mg/kg.

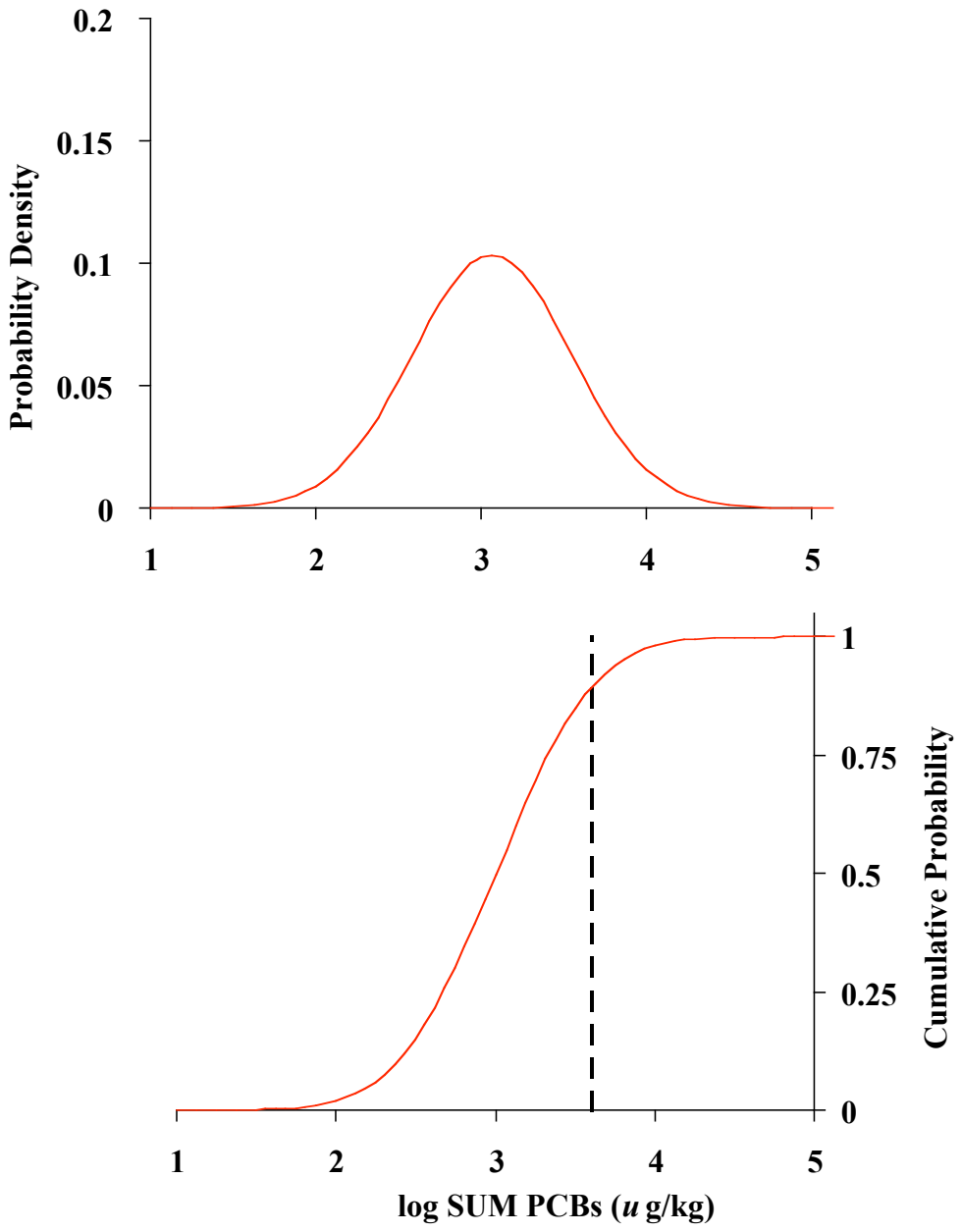

Figure 4.18: Normal (top) and cumulative (bottom) probability distributions for the ΣPCB concentrations in Forster's Tern eggs in San Francisco Bay for the period between 1999 and 2001. The red line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MCS). The dashed line represents a LOAEL of 4.0 mg/kg.

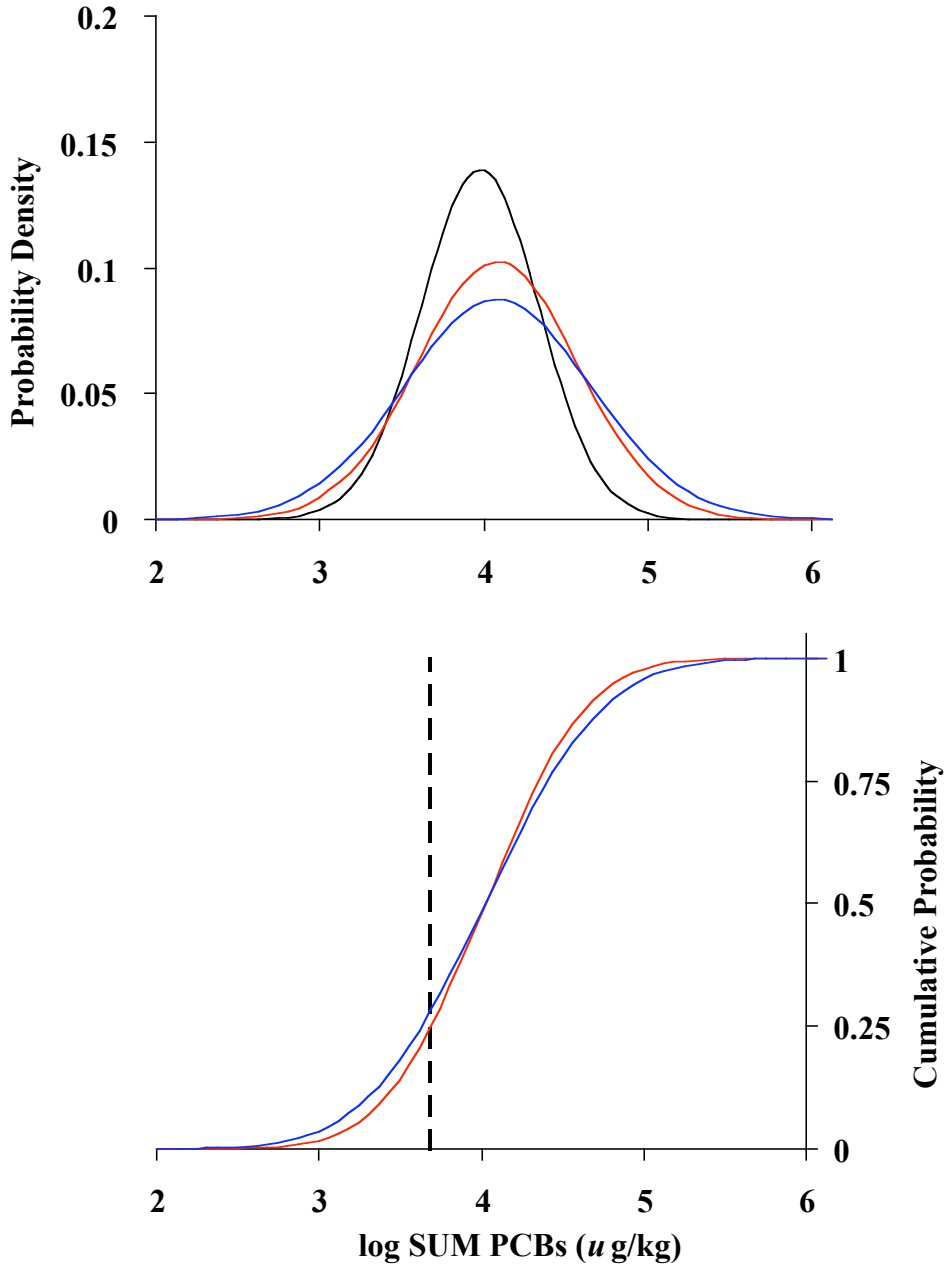

Figure 419: Normal (top) and cumulative (bottom) probability distributions for ΣPCB concentrations in adult male harbor seals in San Francisco Bay for the period between 1999 and 2001. The red line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MCS). The blue line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MB*). The black line represents the distribution of observed concentrations in the Bay from data collected 1992 - 1993. The dashed line represents an effect threshold concentration of 11.0 µg/kg lipid.

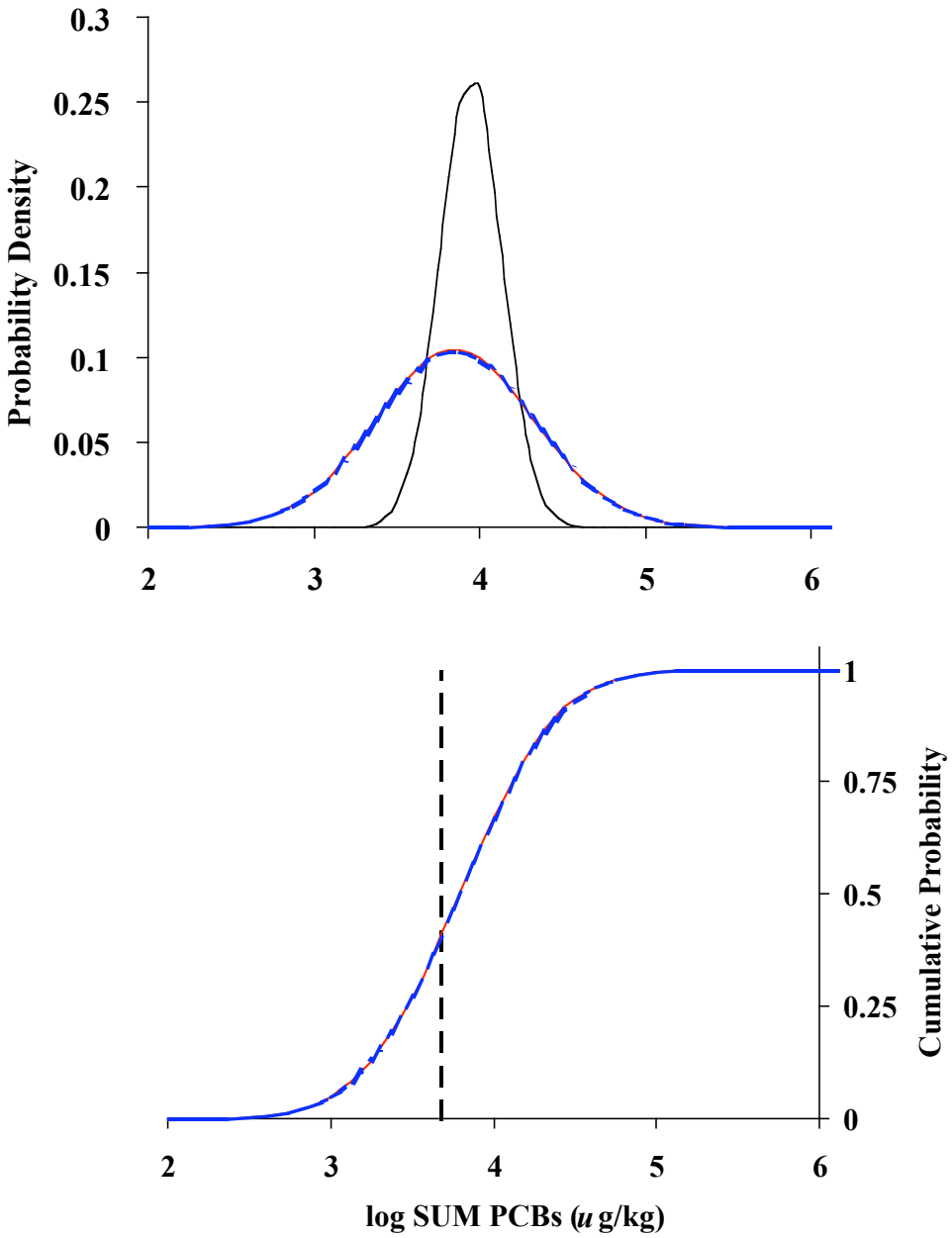

Figure 420: Normal (top) and cumulative (bottom) probability distributions for ΣPCB concentrations in adult female harbor seals in San Francisco Bay for the period between 1999 and 2001. The red line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MCS). The blue line represents concentration distribution predictions based on spatial variability in sediment concentrations and uncertainty in the model (MB*). The black line represents the distribution of observed concentrations in the Bay from data collected 1989 - 1993. The dashed line represents an effect threshold concentration of 11.0 µg/kg lipid.

The blue lines in Figures 4.14 to 4.20 represent the ΣPCB concentrations in each of the species based on the spatial variability in the ΣPCB concentrations in the sediments of the Bay as well as model uncertainty estimated by the model performance analysis for ΣPCB (i.e. MB*). The predicted PCB concentration distributions in biota therefore incorporate model uncertainty in the BSAF calculation (determined by comparison of observed and predicted BSAFs and expressed as the 95% confidence intervals of MB^*), and variability in the Bay wide _PCB concentration in the sediment. Figures 4.14 to 4.20 illustrate that the method of uncertainty analysis has little effect on the shape of the ΣPCB concentration distributions. This is due to the fact that (i) the variability in the Bay wide sediment concentrations (i.e. the model input) is large and greater than the contribution of uncertainty in the BSAF model and (ii) the methods for estimating model uncertainty, i.e. Monte Carlo Simulation and the comparison between observed and predicted BSAFs, produce comparable outcomes. The ΣPCB concentration distributions illustrate that large variations can be expected in the PCB concentrations within fish and wildlife in the Bay as a result of the spatial distribution of the PCB concentrations in the sediments of the Bay.

The black lines in Figures 4.14 to 4.20 represent the distributions of observed _PCB concentrations in the various species of the Bay. Figures 4.14 and 4.15 show that the geometric means of observed and model predicted _PCB concentrations in shiner surfperch, jacksmelt and white croaker are comparable. The distribution of observed PCB concentrations does not show the degree of spatial variations expected based on the spatial distribution of the PCB concentrations in the sediments. The latter may be due to the fact that the fish sampling programs were carried out in certain areas of the Bay. The observed concentrations in these fish species may therefore not fully represent the spatial distribution of PCB concentrations in these species within the Bay. The observed PCB concentration distribution can be expected to lie within the model predicted PCB concentration. This is because the PCB sediment concentration data (used to estimate the PCB concentration in biota) provides a good representation of the spatial variability in the PCB concentrations in the sediments of the Bay.

Figure 4.17 shows that model predicted and observed PCB concentration distributions for Double-crested Cormorants show similar features as those in the fish species. The geometric mean of the observed ΣPCB concentration distribution in the cormorants is slightly higher than that calculated by the model, but the distributions of observed PCB concentrations lies well within the distribution of predicted concentrations in the Bay.

Distributions of observed _PCB concentrations in male harbor seals are in good agreement with the distributions of model calculated distributions that include both spatial variability and variability in model state variables (Figure 4.19). Male harbor seals are the only species in the Bay that exhibit a variation in PCB concentrations that reflect the spatial distribution of the PCB concentrations in the sediments. The small sample size available to construct the distribution of observed PCB concentrations in male harbor seals (n=4) may be a significant factor contributing to this observation.

The observed geometric mean of the ΣPCB concentration in adult female harbor seals is somewhat larger than the model predicted geometric mean concentration. However, Figure 4.20 illustrates that the distributions of observed and predicted ΣPCB concentrations largely overlap. The fact that seals were collected between 1989 and 1993 while the PCB concentrations were collected between 1999 and 2001 may be a contributing factor to the apparent underestimation of the PCB concentrations in the seal. It is possible that PCB concentrations in sediments have fallen since 1993. This reduction in exposure concentrations may be reflected in lower internal concentrations in female seals which due to their off spring production and lactation can respond more quickly to reductions in exposure conditions than male seals. Similar to the results for fish and cormorants, the distribution of the observed PCB concentrations do not reflect the degree of spatial variability anticipated by the model based on the spatial distribution of PCB concentrations in the Bay. The latter may be due to the limited geographical range of the seal collections while sediment samples were collected over a large section of the Bay.
There are several general conclusions that can be reached from the comparison of the observed and model predicted distributions of _PCB concentrations. First, model

predictions of the concentrations of PCB congeners and ΣPCB based on the distributions of current PCB concentrations in the Bay showed a good agreement with the distributions of observed PCB concentrations. The geometric means of observed and predicted PCB concentrations were essentially identical (i.e. within 29% of the model predicted geometric mean) for all species investigated in the model. Secondly, the distributions of observed PCB concentrations fell within the distribution of predicted concentrations. The observation that the range of observed PCB concentrations in fish and wildlife species was in most cases smaller than the range of predicted PCB concentrations in the Bay are expected to be due to differences in the spatial coverage of the sample collection programs. Sediment samples were taken from many more areas of the Bay than fish, bird egg and harbor seal samples. As a result, the PCB concentrations in some of the fish and wildlife species of the Bay may not represent the full spatial variation in _PCB concentrations that is expected by the model. It is also possible that the PCB sediment concentration distribution for the Bay, which was derived from the RMP monitoring data, does not provide an accurate description of the actual distribution of the PCB concentrations in the sediments of the Bay or the PCB concentrations distribution experienced by the biota of the Bay. Perhaps, areas that are very contaminated with PCBs and areas that are devoid of PCB contamination are over presented in the sediment concentration database. To ascertain this possibility it is important to further explore the geostatistical distribution of PCB concentrations in the Bay.

Table 4.7 lists the outcome of the model calculations of the human health risks and hazards as well as ecological risks for various species based on the geometric mean of current (i.e. between 1999 and 2001) PCB concentrations in sediments of the Bay. It illustrates that, based on the model predicted geometric mean PCB concentrations in biota of the Bay, the human cancer risk criterion of 1.10^{-5} (for members of the public consuming fish from San Francisco Bay) can be expected to be exceeded in shiner surfperch and white croaker, but not in jacksmelt which due to its feeding characteristics generally contain lower PCB concentrations and hence lower associated excess cancer risk estimates. The human health hazard index for the consumption of shiner surfperch,

white croaker and jacksmelt ranges between 0.15 and 0.84 and hence are lower than the criterion of 1 used to identify a hazard to humans consuming these fish species at the rate presumed in this study. The ecological risk index calculated for Double-crested Cormorant and Forster's Tern eggs are 0.40 and 0.29 respectively, indicating that the model predicted geometric mean concentration of PCBs in the Bay is less than the LOAEL. In both male and female harbor seals, the geometric mean PCB concentration exceeds the threshold effect concentration substantially. In male harbor seal, the geometric mean PCB concentration also exceeds the LOAEL by a small amount (i.e. ERI is 1.1). When comparing the geometric mean concentration to the criteria values, it is important to stress that the geometric means apply to relatively wide distributions. Hence, even if the mean concentration falls below a criterion value, a substantial number of PCB concentrations in biota of the Bay can be expected to exceed the criteria.

Table 4.7: The geometric mean of the ΣPCB concentrations in various species of San Francisco Bay and associated measures of human health and ecological risk, including the upper bound estimate of the excess lifetime cancer risk in humans (Human Health Risk – Cancer), the human health hazard index (Human Health Risk – Threshold), and the Ecological Risk Index based on the LOAEL (Ecological Risk – ERI (LOAEL)).

Organism	Criterion	Tissue Concentration ΣPCBs (SFEI) (μg/kg wet weight)	Risk Measure
shiner surfperch	Human Health Risk - Cancer	135	$2.61 \cdot 10^{-5}$
shiner surfperch	Human Health Risk - Threshold	135	0.652
jacksmelt	Human Health Risk - Cancer	31.5	$0.61 \cdot 10^{-5}$
jacksmelt	Human Health Risk - Threshold	31.5	0.152
white croaker	Human Health Risk - Cancer	174	$3.36 \cdot 10^{-5}$
white croaker	Human Health Risk - Threshold	174	0.839
Cormorant Egg	Ecological Risk – ERI (LOAEL)	2010	0.402
Tern Egg	Ecological Risk – ERI (LOAEL)	1150	0.287
Male harbor Seal	Ecological Risk - Threshold Effect	11700	2.5
Female harbor Seal	Ecological Risk - Threshold Effect	7070	1.5

Figures 4.14 to 4.20 (bottom sections) show the model predicted PCB concentrations in terms of cumulative probability distributions. These distributions can be used to assess the probability that ΣPCB concentrations in the various biological receptors can be expected to exceed the criteria for human health and ecological risk. The distributions reflect the spatial variations in the PCB concentrations in the Bay. Examples of the exceedence for some criteria are included in the Figures. Table 4.8 lists the probability that ΣPCB concentrations exceed the criteria (listed in Table 3.5) investigated in this study. It shows that there is a substantial probability that the human health and ecological risk levels are exceeded in the Bay. For example, the probability that PCB concentrations exceed threshold effects concentration in harbor seals is approximately 70 to 73% for males and around 56% for females. The probability of exceeding the excess human

cancer risk of one in hundred thousand is 75 - 76% and 82 - 84% in shiner surfperch and white croaker respectively. The probabilities of exceeding the various human health and ecological risk measures are dependent on the shape of the distributions. As illustrated in Figures 4.14 to 4.20 the (narrower) distribution of the PCB concentrations based on variability in model state variables alone (i.e. not including spatial variability) predicts different probabilities of exceeding human health and ecological criteria. A narrower distribution produces smaller probabilities of exceedence in cases where the geometric mean is less than the criterion value. However, it produces greater probabilities of exceedence in cases where the geometric mean is greater than the criterion value. Hence, if the spatial variation in PCB concentration is overestimated by the sediment concentration data from the RMP monitoring program, then the probabilities of exceeding the human health hazard index of 1 for all 3 fish species will be less than that described in Table 4.8. Similarly, the probabilities of exceeding the ecological risk index (ERI) of 1 in eggs of Double-crested Cormorants and Forster's Terns will be smaller than the values depicted in Table 4.8. However, in that case, the probabilities of exceeding excess human cancer risk criteria of 1:100,000 as a result of consumption of shiner surfperch and white croaker can be expected to be greater than those presented in Table 4.8. Also, the probabilities of ΣPCB concentrations exceeding the threshold effect concentration for ΣPCBs in seals can be expected to be greater than the values presented in Table 4.8. The cumulative frequency distributions in the spreadsheet allow several of these scenarios to be investigated.

Table 4.8: Probabilities that the ΣPCB concentrations in various San Francisco Bay species can be expected to be equal or exceed internal tissue concentrations associated with various human health and ecological risk criteria. Probabilities are determined from the PCB concentration distributions derived from the Model Bias (MB*) and Monte Carlo Simulation (MCS) and depicted in Figures 4.12 to 4.18 as blue and red lines, respectively.

Organism	Criterion	Tissue Concentration ΣPCB (SFEI) (μg/kg wet weight)	MB*	MCS
shiner surfperch	Human Health Risk — Cancer	51.9	0.75	0.76
shiner surfperch	Human Health Risk — Threshold	207	0.30	0.29
jacksmelt	Human Health Risk — Cancer	51.9	0.29	0.27
jacksmelt	Human Health Risk — Threshold	207	0.05	0.03
white croaker	Human Health Risk — Cancer	51.9	0.82	0.84
white croaker	Human Health Risk — Threshold	207	0.37	0.36
Cormorant egg	Ecological Risk — LOAEL	5000	0.16	0.17
Tern egg	Ecological Risk — LOAEL	4000	N/A	0.11
Male harbor seal	Ecological Risk — Threshold Effect	4730	0.70	0.73
Female harbor seal	Ecological Risk — Threshold Effect	4730	0.56	0.56

4.4.2 Backwards calculation

The purpose of the backwards calculation is to recommend a PCB concentration in the sediment that meets human health and ecological risk criteria. The selection of human health and ecological risk criteria is typically subject to debate and judgment. Different criteria may emerge and also how the criteria are applied to empirical data or data from models may vary depending on the goals of remedial initiatives. We have constructed the model in such a fashion that new criteria can be easily entered in the model. As part of this study we have applied the model to calculate Bay wide geometric mean concentrations of ΣPCB in the sediments that are expected to result in Bay wide geometric mean concentrations that meet various human health and ecological criteria in San Francisco Bay. One of the consequences of this application of the model is that at the calculated sediment concentrations, it is expected that the PCB concentrations in approximately half the population of the Bay exceeds the criterion value while the PCB concentration in the other half of the population will be less than the criterion value. This is due to the considerable spatial and temporal variability in the PCB concentrations in the Bay. An alternative application of the model that was explored in this study is the calculation of the geometric mean PCB concentration in the Bay sediments that is expected to result in a 5% exceedence of criterion values. For male and female harbor seals, which appear to be the most sensitive ecological receptors explored in this study, we calculated the geometric mean PCB concentration in the Bay that is expected to result in a distribution of PCB concentrations in Bay harbor seals in which the PCB concentration in only 5% of the Bay harbor seals exceed the threshold effects concentrations.

Table 4.9 shows the Bay wide geometric mean concentrations of ΣPCB in the sediments that are expected to result in Bay wide geometric mean concentrations that meet human health and ecological criteria in San Francisco Bay. Table 4.9 also illustrates the uncertainty in the back calculation of the geometric mean PCB concentration in the sediment. The uncertainty is expressed in terms of the 95% confidence intervals of the

geometric mean PCB concentration in the sediment. Two 95% confidence intervals are provided, i.e. one determined from the comparison of observed and predicted BSAF (MB*) and the other determined through Monte Carlo Simulation (MCS). They express uncertainty in the BSAF used in the back calculation. They do not reflect the spatial variability in the PCB concentrations in the sediments of the bay. Figures 4.21 and 4.22 present the same data in graphical form. If it can be assumed that a concentration of 11.6 μg/kg dry weight is a reasonable estimate of the current geometric mean of the ΣPCB concentrations in sediments of the Bay, then Table 4.9 suggests that current sediment concentrations meet several human health and ecological risk criteria. Non-cancer risk hazard indices for the consumption of all three fish species of primary interest in the Bay are less than 1 based on the current geometric mean ΣPCB concentrations in sediments of the Bay. Also, the 1.10^{-5} excess human cancer risk criterion will not be exceeded for Bay residents consuming jacksmelt under current conditions in the Bay. Also, current ΣPCB concentrations in sediments of the Bay can be expected to cause geometric mean ΣPCB concentrations in female harbor seals that are below the LOAEL, but not the NOAEL. However, current ΣPCB concentrations in sediments of the Bay can be expected to produce geometric mean ΣPCB concentrations in fish and wildlife that do not meet all other criteria investigated in this study. Table 4.9 illustrates the levels that need to be achieved to meet the various human health and ecological risk criteria. For example, it shows that human excess lifetime cancer risk criterion of 1.10^{-5} for Bay fish consumption can be expected to be met in all three fish species investigated if the geometric mean ΣPCB concentrations in sediments is reduced to a value of 3.5 μg/kg dry weight (or a log C_S of 0.54 ± 0.12 (SD)). The threshold effects concentration can be met in male and female harbor seals if the geometric mean ΣPCB concentrations in sediments drop to values of 4.5 and 7.7 μg/kg dry weight, respectively. As explained earlier, a geometric mean ΣPCB concentration in sediments of the Bay of 4.5 μg/kg dry weight still implies that approximately half the population of male harbor seals can be expected to exceed the threshold effect concentration. The geometric mean ΣPCB concentrations in sediments that are required to produce only a 5% exceedence of the threshold effect concentration in male and female harbor seals are 1.4 and 1.6 μg/kg dry weight, respectively.

The model can help to explore other future scenarios for the PCB concentration in the Bay. We encourage this as we developed the model with this purpose in mind. Also, the calculation of target sediment concentrations based on risk assessment is included for illustrative purposes only. Risk estimates needed to determine target PCB concentrations in the sediments of the Bay may vary depending on ecological and human health objectives and the current state of science. The calculations for evaluating alternative scenarios based on the current model (i.e. the BSAF used in the calculations) are relatively simple when using the management worksheet.

Finally, it is important to recognize that the PCB concentrations derived through back calculation are geometric mean values. They are the Bay wide means of logarithmic distributions of PCB concentrations in the sediments. Theoretically, there can be many different distributions that have the same mean. This implies that different PCB sediment concentration distributions in San Francisco can meet the ecological and human health criteria illustrated in Table 4.9 (as long as they exhibit the same mean). This also means that there may be different management options that can be considered to meet the same ecological and human health goals.

Table 4.9: Bay wide geometric mean ΣPCB concentrations in the sediments and their 95% confidence intervals (CI) derived from the model bias (MB*) and Monte Carlo Simulation (MCS) that are expected to result in Bay wide geometric mean concentrations that meet various human health and ecological criteria in San Francisco Bay.

Criterion	Organism	Concentration in Organism (μg/kg wet weight)	Concentration in Sediment (μg/kg dry weight)	95% CI – MB* (μg/kg dry weight)	95% CI – MCS (μg/kg dry weight)
Human Excess Lifetime Cancer Risk (1:100,000)	shiner surfperch	52	4.4	1.4 - 14.5	1.9 - 10.3
Human Health Hazard (H = 1)	shiner surfperch	207	17.8	5.5 - 57.9	7.6 - 41.3
Human Excess Lifetime Cancer Risk (1:100,000)	jacksmelt	52	19.0	4.9 - 73.5	8.1 - 44.5
Human Health Hazard (H = 1)	jacksmelt	207	75.9	19.6 - 294.1	32.3 - 178.1
Human Excess Lifetime Cancer Risk (1:100,000)	white croaker	52	3.5	1.3 - 9.3	1.2 - 9.7
Human Health Hazard (H = 1)	white croaker	207	13.9	5.2 - 35.7	5.0 - 38.9
Ecological Risk - LOAEL	Cormorant egg	5000	28.7	11.2 - 73.9	10.3 - 80.0
Ecological Risk - LOAEL	Tern egg	4000	40.1	N/A	14.5 - 110.9
Ecological Risk - Threshold Effect (11,000 μg/kg lipid)	Male harbor seal	4730	4.5	0.4 - 45.9	1.2 - 16.4
Ecological Risk - LOAEL (25,000 μg/kg lipid)	Male harbor seal	10750	10.3	1.0 - 104.3	2.8 - 37.3
Ecological Risk - NOAEL (5,000 μg/kg lipid)	Male harbor seal	2150	2.1	0.2 - 20.9	0.6 - 7.5

Criterion	Organism	Concentration in Organism (μg/kg wet weight)	Concentration in Sediment (μg/kg dry weight)	95% CI – MB* (μg/kg dry weight)	95% CI – MCS (μg/kg dry weight)
Ecological Risk - 5% exceedence of Threshold Effect	Male harbor seal	1500	1.4	0.1 - 14.5	0.4 - 5.2
Ecological Risk - Threshold Effect (11,000 μg/kg lipid)	Female harbor seal	4730	7.7	1.2 - 48.3	1.3 - 45.1
Ecological Risk - LOAEL (25,000 μg/kg lipid)	Female harbor seal	10750	17.6	2.8 - 109.8	3.0 - 102.5
Ecological Risk - NOAEL (5,000 μg/kg lipid)	Female harbor seal	2150	3.5	0.6 - 22.0	0.6 - 20.5
Ecological Risk - 5% exceedence of Threshold Effect	Female harbor seal	1000	1.6	0.3 - 10.2	0.3 - 9.5

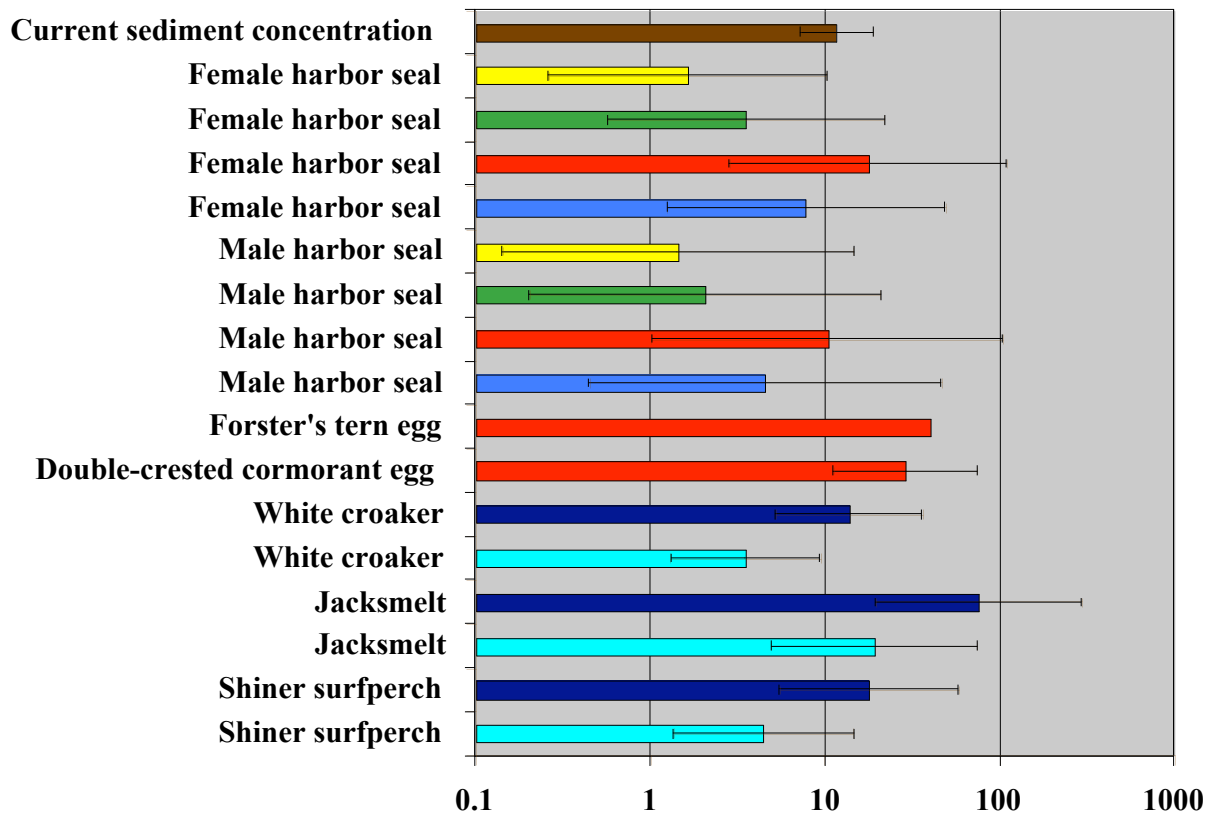

Figure 421: Target concentrations of ΣPCB in sediments (μg/kg dry weight) expected to meet various human health and ecological risk objectives. The brown bar reflects the current ΣPCB concentration in the sediment of SFB. Green and red bars reflect ΣPCB concentration expected to meet the NOAEL and LOAEL, respectively. Blue bars are ΣPCB concentrations in the sediment that meet the threshold effect concentration. Dark blue and light blue bars reflect ΣPCB concentrations that meet the human health risk criteria based on the calculation of respectively the human health hazard and the upperbound estimate of excess lifetime cancer risk in humans eating fish from San Francisco Bay. The yellow bars are the expected ΣPCB concentrations that will not exceed the threshold effect concentration in more than 5% of the population. The error bars reflect the 95% confidence intervals of the current measured sediment concentrations and the model predictions calculated using model bias (MB*).

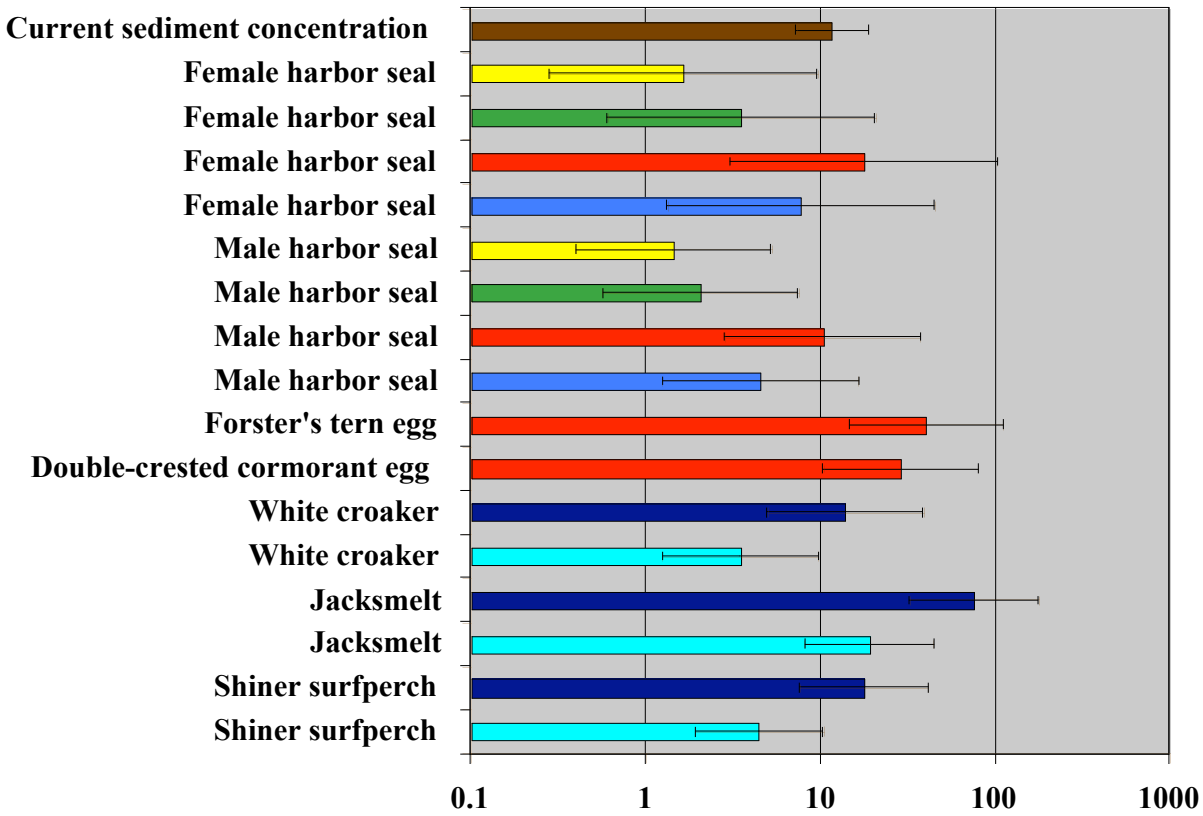

Figure 422: Target concentrations of ΣPCB in sediments (μg/kg dry weight) expected to meet various human health and ecological risk objectives. The brown bar reflects the current ΣPCB concentration in the sediment of SFB. Green and red bars reflect ΣPCB concentration expected to meet the NOAEL and LOAEL, respectively. Blue bars are ΣPCB concentrations in the sediment that meet the threshold effect concentration. Dark blue and light blue bars reflect ΣPCB concentrations that meet the human health risk criteria based on the calculation of respectively the human health hazard and the upperbound estimate of excess lifetime cancer risk in humans eating fish from San Francisco Bay. The yellow bars are the expected ΣPCB concentrations that will not exceed the threshold effect concentration in more than 5% of the population. The error bars reflect the 95% confidence intervals of the current measured sediment concentrations and the model predictions calculated using model bias (MCS).

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6. APPENDICES

Appendix A: Overview of species specific model state variables of the San Francisco Bay PCB food web model that require parameterization.

PARAMETER	VALUE / INPUT	REFERENCE
SPECIES	**PHYTOPLANKTON / ALGAE**	
Lipid Content (%)	0.12%	Mackintosh, CE et al ES&T 2004
NLOC Content (%)	6.00%	Mackintosh, CE et al ES&T 2004
Growth Rate Constant - k_G (1/day)	1.25E-01	Alpine, A. E. and J. E. Cloern (1988) and Alpine, A. E. and J. E. Cloern (1992)
Aqueous phase resistance constant (Ap) (1/day)	6.00E-05	Arnot and Gobas ET&C 2004
Organic phase resistance constant (Bp) (1/day)	5.50E+00	Arnot and Gobas ET&C 2004
SPECIES	**ZOOPLANKTON - 1**	
Species Name	*Copepoda & sp.*	
Weight (kg)	7.10E-08	Gobas and Wilcockson 2003
Lipid Content (%)	0.75%	Estimated from Roberts et al 2002
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	9.41E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	72.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	72.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004
SPECIES	**INVERT - 1**	
Species Name	*Neanthes succinea*	
Weight (kg)	1.10E-04	Gobas and Wilcockson 2003
Lipid Content (%)	0.75%	Estimated from Roberts et al 2002 and Gobas and Wilcockson 2003
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004

Fraction of Respired Pore Water (Pw)	15.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	2.17E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**INVERT - 2**	
Species Name	*Amphelisca sp*	
Weight (kg)	3.13E-06	Estimated
Lipid Content (%)	0.75%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	10.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	4.42E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**INVERT - 3**	
Species Name	*Nippoleucon hinumensis*	
Weight (kg)	5.00E-06	Estimated
Lipid Content (%)	0.75%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	10.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	4.02E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**INVERT - 4**	
Species Name	*Mysis sp.*	
Weight (kg)	1.50E-05	Arnot and Gobas ET&C 2004
Lipid Content (%)	1.00%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	5.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004

E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	3.23E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**INVERT - 5**	
Species Name	*Mytilus californianus*	
Weight (kg)	1.52E-03	Regional Monitoring Program (2000-2001)
Lipid Content (%)	6.99%	Regional Monitoring Program (2000-2001)
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	20.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.28E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**INVERT - 6**	
Species Name	*Crassostrea gigas*	
Weight (kg)	9.79E-04	Regional Monitoring Program (2000-2001)
Lipid Content (%)	9.37%	Regional Monitoring Program (2000-2001)
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	20.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.40E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**INVERT - 7**	
Species Name	*Harmothoe imbricata*	
Weight (kg)	1.00E-07	Gobas and Wilcockson 2003
Lipid Content (%)	0.75%	Estimated from Roberts et al 2002 and Gobas and Wilcockson 2003
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	15.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	8.79E-03	Arnot and Gobas ET&C 2004

Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**INVERT - 8**	
Species Name	*Crangon sp.*	
Weight (kg)	3.72E-04	Gobas and Wilcockson 2003
Lipid Content (%)	1.50%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	5.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.70E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	75.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	75.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 1**	
Species Name	*shiner surfperch*	
Weight (kg)	1.31E-03	Estimated from Harvey et al 2000
Lipid Content (%)	2.0%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	2.64E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 2**	
Species Name	*jacksmelt*	
Weight (kg)	4.00E-03	Estimated from Harvey et al 2000
Lipid Content (%)	1.2%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	2.11E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004

Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 3**	
Species Name	*Northern anchovy*	
Weight (kg)	3.70E-03	Estimated from Harvey et al 2000
Lipid Content (%)	2.0%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	2.15E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 4**	
Species Name	*white croaker*	
Weight (kg)	1.50E-02	Estimated from Harvey et al 2000
Lipid Content (%)	1.8%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.62E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 5**	
Species Name	*Northern anchovy (>juvenile)*	
Weight (kg)	2.15E-02	Estimated from Harvey et al 2000
Lipid Content (%)	2.5%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.51E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004

Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 6**	
Species Name	*shiner surfperch (>juvenile)*	
Weight (kg)	5.13E-02	Regional Monitoring Program (2000)
Lipid Content (%)	2.6%	Regional Monitoring Program (2000)
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.27E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 7**	
Species Name	*jacksmelt (>juvenile)*	
Weight (kg)	2.06E-01	Regional Monitoring Program (2000)
Lipid Content (%)	1.6%	Regional Monitoring Program (2000)
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	0.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	9.60E-04	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	**FISH - 8**	
Species Name	*yellowfin goby (>juvenile)*	
Weight (kg)	3.00E-02	Estimated from Andy Jahn Fish Gutz Survey
Lipid Content (%)	3.0%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	5.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.41E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	FISH - 9	
Species Name	*plainfin midshipman (>juvenile)*	
Weight (kg)	1.30E-01	Estimated from Harvey et al 2000
Lipid Content (%)	3.0%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	5.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	1.05E-03	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	FISH - 10	
Species Name	*white croaker (>juvenile)*	
Weight (kg)	3.71E-01	Regional Monitoring Program (2000)
Lipid Content (%)	3.5%	Estimated
NLOM Content (%)	20.0%	Arnot and Gobas ET&C 2004
Fraction of Respired Pore Water (Pw)	5.0%	Estimated
E_D - Constant A	8.50E-08	Derived from Arnot and Gobas ET&C 2004
E_D - Constant B	2.00E+00	Arnot and Gobas ET&C 2004
Growth Rate Constant - k_G (1/day)	8.54E-04	Arnot and Gobas ET&C 2004
Metabolic Transformation Rate Constant - k_M (1/day)	0.00E+00	Arnot and Gobas ET&C 2004
Lipid Digestion Efficiency (ε_L)	90.0%	Arnot and Gobas ET&C 2004
NLOM Digestion Efficiency (ε_N)	50.0%	Arnot and Gobas ET&C 2004
Water Digestion Efficiency (ε_W)	55.0%	Arnot and Gobas ET&C 2004

SPECIES	AVIAN - 1	
Species Name	*Cormorant (Male)*	
Weight (kg)	2.50E+00	Hatch, J. J. and D. V. Weseloh, Eds. (1999)
Lipid Content (%)	7.5%	Hatch and Weseloh 1999; Glaser and Connolly 2002
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	3.00E-09	Derived from Drouillard ET&C 2000
E_D - Constant B	1.04E+00	Derived from Drouillard ET&C 2000
Lung Respiration Rate (G_V) - (L/day)	2.48E+03	US EPA 1993
Food Ingestion Rate - (G_D) (kg-food/day)	7.50E-01	Hatch and Weseloh 1999
Growth Rate Constant - k_G (1/day)	0.00E+00	Hatch and Weseloh 1999; Glaser and Connolly 2002
Lipid Digestion Efficiency (ε_L)	95.0%	Derived from Drouillard ET&C 2000
NLOM Digestion Efficiency (ε_N)	75.0%	Estimated
Water Digestion Efficiency (ε_W)	85.0%	Derived from Kelly and Gobas ES&T 2003

SPECIES	**AVIAN - 2**	
Species Name	*Cormorant (Female)*	
Weight (kg)	2.40E+00	Hatch and Weseloh 1999; Glaser and Connolly 2002
Lipid Content (%)	7.5%	Hatch and Weseloh 1999; Glaser and Connolly 2002
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	3.00E-09	Derived from Drouillard ET&C 2000
E_D - Constant B	1.04E+00	Derived from Drouillard ET&C 2000
Lung Respiration Rate (G_V) - (L/day)	2.41E+03	US EPA 1993
Food Ingestion Rate - (G_D) (kg-food/day)	7.20E-01	Hatch and Weseloh 1999
Growth Rate Constant - k_G (1/day)	0.00E+00	Hatch and Weseloh 1999; Glaser and Connolly 2002
Clutch Size (CS) (kg/year)	1.80E-01	Based on 1 clutch/yr & mean of 4 eggs/clutch (Hatch and Weseloh 1999)
Lipid Digestion Efficiency (ε_L)	95.0%	Derived from Drouillard ET&C 2000
NLOM Digestion Efficiency (ε_N)	75.0%	Estimated
Water Digestion Efficiency (ε_W)	85.0%	Derived from Kelly and Gobas ES&T 2003

SPECIES	**AVIANEGG - 1**	
Species Name	*Cormorant (Egg)*	
Weight (kg)	4.49E-02	Hatch and Weseloh 1999
Lipid Content (%)	5.50%	Estimated from Glaser and Connolly 2002
NLOM Content (%)	15.00%	Estimated

SPECIES	**AVIAN - 3**	
Species Name	*Tern (Male)*	
Weight (kg)	1.90E-01	McNicholl, M. K., P. E. Lowther, et al., Eds. (2001)
Lipid Content (%)	7.0%	Estimated
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	3.00E-09	Derived from Drouillard ET&C 2000
E_D - Constant B	1.04E+00	Derived from Drouillard ET&C 2000
Lung Respiration Rate (G_V) - (L/day)	3.41E+02	US EPA 1993
Food Ingestion Rate - (G_D) (kg-food/day)	4.18E-02	McNicholl et al 2001
Growth Rate Constant - k_G (1/day)	0.00E+00	Hatch and Weseloh 1999; Glaser and Connolly 2002
Lipid Digestion Efficiency (ε_L)	95.0%	Derived from Drouillard ET&C 2000
NLOM Digestion Efficiency (ε_N)	75.0%	Estimated
Water Digestion Efficiency (ε_W)	85.0%	Derived from Kelly and Gobas ES&T 2003

SPECIES	**AVIAN - 4**	
Species Name	*Tern (Female)*	
Weight (kg)	1.75E-01	McNicholl et al 2001
Lipid Content (%)	7.0%	Estimated
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	3.00E-09	Derived from Drouillard ET&C 2000

E_D - Constant B	1.04E+00	Derived from Drouillard ET&C 2000
Lung Respiration Rate (G_V) - (L/day)	3.21E+02	US EPA 1993
Food Ingestion Rate - (G_D) (kg-food/day)	3.85E-02	McNicholl et al 2001
Growth Rate Constant - k_G (1/day)	0.00E+00	Hatch and Weseloh 1999; Glaser and Connolly 2002
Clutch Size (CS) (kg/year)	6.39E-02	based on 1 clutch/yr & mean of 3 eggs/clutch (McNicholl et al 2001)
Lipid Digestion Efficiency (ε_L)	95.0%	Derived from Drouillard ET&C 2000
NLOM Digestion Efficiency (ε_N)	75.0%	Estimated
Water Digestion Efficiency (ε_W)	85.0%	Derived from Kelly and Gobas ES&T 2003

SPECIES	**AVIANEGG - 2**	
Species Name	*Tern (Egg)*	
Weight (kg)	2.13E-02	McNicholl et al 2001
Lipid Content (%)	5.50%	Estimated from Glaser and Connolly 2002
NLOM Content (%)	15.00%	Estimated

SPECIES	**Mammal - 1**	
Species Name	*Adult Seal (Male)*	
Weight (kg)	9.00E+01	Derived from Kopec, D. A. and J. T. Harvey (1995) and Grigg, E. K. (2003).
Lipid Content (%)	43.0%	Derived from Lydersen, C., J. Wolkers, et al. (2002) and Bowen et al 1992
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	1.00E-09	Derived from Moser, G. A. and M. S. McLachlan (2002) and Moser, G. A. and M. S. McLachlan (2001).
E_D - Constant B	1.03E+00	Derived from Moser and McLachlan 2002 & 2001
Lung Respiration Rate (G_V) - (L/day)	3.51E+04	Derived from Hickie 1999
Food Ingestion Rate - (G_D) (kg-food/day)	6.30E+00	Grigg, E. K. (2003).
Growth Rate Constant - k_G (1/day)	7.50E-05	Estimated
Urinary Excretion Rate Constant - (G_U) (L/day)	3.45E-01	Estimated
Lipid Digestion Efficiency (ε_L)	98.0%	Based on Rosen and Trites Can. J. Zool. 2000, Moser and McLachlan 2002 & 2001 and Kelly and Gobas ES&T 2003
NLOM Digestion Efficiency (ε_N)	75.0%	Kelly and Gobas ES&T 2003
Water Digestion Efficiency (ε_W)	85.0%	Kelly and Gobas ES&T 2003

SPECIES	**Mammal - 2**	
Species Name	*Adult Seal (Female)*	
Weight (kg)	8.00E+01	Derived from Kopec, D. A. and J. T. Harvey (1995) and Grigg, E. K. (2003).
Lipid Content (%)	43.0%	Derived from Lydersen, C., J. Wolkers, et al. (2002) and Bowen et al 1992
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	1.00E-09	Derived from Moser and McLachlan 2002 & 2001
E_D - Constant B	1.03E+00	Derived from Moser and McLachlan 2002 & 2001
Lung Respiration Rate (G_V) - (L/day)	3.21E+04	Derived from Hickie 1999

Food Ingestion Rate - (G_D) (kg-food/day)	8.80E+00	Grigg, E. K. (2003).
Growth Rate Constant - k_G (1/day)	1.00E-05	Estimated
Urinary Excretion Rate Constant - (G_U) (L/day)	4.82E-01	Estimated
Lactation Rate Constant - (G_L) (L/day)	9.60E-01	Derived from Cottrell PE, Jeffries S, Beck B, Ross PS 2002, Bowen et al 2001, Bowen et al 1992
Lipid Content Fetus (LFetus) (%)	11.0%	Derived from Cottrell PE, Jeffries S, Beck B, Ross PS 2002, Bowen et al 2001, Bowen et al 1992
NLOM Content Fetus (NLOMFetus) (%)	20.0%	Arnot and Gobas ET&C 2004 and Kelly and Gobas ES&T 2003
WC Fetus (WCFetus) (%)	69.0%	Arnot and Gobas ET&C 2004 and Kelly and Gobas ES&T 2003
Weight - Fetus (Vfetus) (kg)	1.10E+01	Cottrell PE, Jeffries S, Beck B, Ross PS 2002
Lipid Digestion Efficiency (ε_L)	98.0%	Based on Rosen and Trites Can. J. Zool. 2000, Moser and McLachlan 2002 & 2001 and Kelly and Gobas ES&T 2003
NLOM Digestion Efficiency (ε_N)	75.0%	Kelly and Gobas ES&T 2003
Water Digestion Efficiency (ε_W)	85.0%	Kelly and Gobas ES&T 2003

SPECIES	**Mammal - 3**	
Species Name	*Juvenile Seal*	
Weight (kg)	4.16E+01	Derived from Kopec, D. A. and J. T. Harvey (1995) and Grigg, E. K. (2003).
Lipid Content (%)	40.0%	Derived from Lydersen, C., J. Wolkers, et al. (2002) and Bowen et al 1992
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	1.00E-09	Derived from Moser and McLachlan 2002 & 2001
E_D - Constant B	1.03E+00	Derived from Moser and McLachlan 2002 & 2001
Lung Respiration Rate (G_V) - (L/day)	1.97E+04	Derived from Hickie 1999
Food Ingestion Rate - (G_D) (kg-food/day)	3.33E+00	Grigg, E. K. (2003).
Growth Rate Constant - k_G (1/day)	1.00E-03	Estimated
Urinary Excretion Rate Constant - (G_U) (L/day)	1.83E-01	Estimated
Lipid Digestion Efficiency (ε_L)	98.0%	Based on Rosen and Trites Can. J. Zool. 2000, Moser and McLachlan 2002 & 2001 and Kelly and Gobas ES&T 2003
NLOM Digestion Efficiency (ε_N)	75.0%	Kelly and Gobas ES&T 2003
Water Digestion Efficiency (ε_W)	85.0%	Kelly and Gobas ES&T 2003

SPECIES	**Mammal - 4**	
Species Name	*Seal Pup*	
Weight (kg)	1.60E+01	Cottrell PE, Jeffries S, Beck B, Ross PS 2002
Lipid Content (%)	25.0%	Derived from Cottrell PE, Jeffries S, Beck B, Ross PS 2002, Bowen et al 2001 and Bowen et al 1992
NLOM Content (%)	20.0%	Estimated
E_D - Constant A	1.00E-09	Derived from Moser and McLachlan 2002 & 2001
E_D - Constant B	1.03E+00	Derived from Moser and McLachlan 2002 & 2001

Lung Respiration Rate (G_V) - (L/day)	5.76E+03	Derived from Hickie 1999
Food Ingestion Rate - (G_D) (kg-food/day)	9.60E-01	Grigg, E. K. (2003).
Growth Rate Constant - k_G (1/day)	2.50E-02	Derived from Cottrell PE, Jeffries S, Beck B, Ross PS 2002
Urinary Excretion Rate Constant - (G_U) (L/day)	3.22E-02	Estimated
Lipid Content Milk (Lmilk) (%)	45.0%	Bowen, W. D., O. T. Oftedal, et al. (1992)
NLOM Content Milk (NLOMmilk) (%)	10.0%	Bowen, W. D., O. T. Oftedal, et al. (1992)
WC Milk (WCmilk) (%)	45.0%	Bowen, W. D., O. T. Oftedal, et al. (1992)
Lipid Digestion Efficiency (ε_L)	98.0%	Based on Rosen and Trites Can. J. Zool. 2000, Moser and McLachlan 2002 & 2001 and Kelly and Gobas ES&T 2003
NLOM Digestion Efficiency (ε_N)	75.0%	Kelly and Gobas ES&T 2003
Water Digestion Efficiency (ε_W)	85.0%	Kelly and Gobas ES&T 2003

Appendix B: Metabolic transformation rates of PCB congeners in harbor seals and birds

Table B-1 Male harbor seals

PCB Congener	Estimated k_M	Male Seal Empirical Congener - X / 153	Male Seal Model Congener - X / 153
8	2.00E-02	N/A	2.45E-04
18	2.00E-02	N/A	4.26E-04
28	1.50E-02	1.61E-03	2.02E-03
31	2.00E-02	N/A	1.04E-03
33	2.00E-02	N/A	7.35E-04
44	2.00E-02	8.59E-04	9.67E-04
49	6.00E-02	3.72E-04	4.60E-04
52	1.00E-03	2.69E-02	3.27E-02
56	5.00E-03	N/A	5.66E-03
60	4.00E-03	4.55E-03	6.46E-03
66	9.00E-03	2.45E-03	2.99E-03
70	3.00E-03	N/A	1.03E-02
74	3.00E-03	5.47E-03	6.23E-03
87	3.00E-02	1.92E-03	2.30E-03
95	6.00E-03	6.06E-03	7.85E-03
97	1.00E-01	2.44E-04	3.54E-04
99	1.00E-04	N/A	1.53E-01
101	2.00E-03	4.75E-02	5.65E-02
105	1.50E-02	7.05E-03	9.13E-03
110	6.00E-03	1.66E-02	2.13E-02
118	8.00E-03	2.82E-02	3.14E-02
128	5.00E-04	3.80E-02	5.05E-02
132	2.00E-03	N/A	2.83E-02
138	1.00E-04	5.89E-01	7.35E-01
141	1.00E-02	3.32E-03	4.37E-03
149	8.00E-03	2.37E-02	2.96E-02
151	1.00E-01	1.20E-03	1.43E-03
153	0.00E+00	1.00E+00	1.00E+00
156	5.00E-03	1.46E-02	1.94E-02
158	2.00E-03	N/A	2.86E-02
170	0.00E+00	1.35E-01	2.82E-01
174	5.00E-02	N/A	1.78E-03
177	2.00E-03	4.11E-02	6.39E-02
180	0.00E+00	3.92E-01	5.71E-01
183	0.00E+00	9.54E-02	1.67E-01
187	1.00E-04	N/A	4.70E-01
194	0.00E+00	7.01E-02	9.45E-02
195	7.00E-04	1.51E-02	3.75E-02
201	5.00E-02	4.13E-04	7.36E-04
203	3.00E-04	N/A	1.07E-01

Table B-2 Female harbor seals

PCB Congener	Estimated k_M	Female Seal Empirical Congener - X / 153	Female Seal Model Congener - X / 153
8	2.00E-02	N/A	7.89E-04
18	2.00E-02	N/A	1.37E-03
28	2.00E-02	2.43E-03	4.91E-03
31	2.00E-02	N/A	3.34E-03
33	2.00E-02	N/A	2.37E-03
44	1.50E-02	1.91E-03	4.06E-03
49	2.00E-03	1.29E-02	2.69E-02
52	0.00E+00	5.18E-02	1.07E-01
56	5.00E-03	N/A	1.61E-02
60	7.00E-03	5.61E-03	1.15E-02
66	7.00E-03	5.99E-03	1.13E-02
70	3.00E-03	N/A	2.68E-02
74	1.00E-03	1.28E-02	2.91E-02
87	3.00E-02	3.44E-03	7.53E-03
95	6.00E-03	1.24E-02	2.29E-02
97	1.50E-01	4.49E-04	7.94E-04
99	1.00E-04	N/A	1.76E-01
101	1.00E-03	7.86E-02	1.87E-01
105	1.50E-02	1.35E-02	2.89E-02
110	7.00E-03	2.65E-02	5.49E-02
118	8.00E-03	4.84E-02	9.46E-02
128	0.00E+00	6.92E-02	1.08E-01
132	2.00E-03	N/A	6.70E-02
138	0.00E+00	6.33E-01	8.99E-01
141	6.00E-03	1.06E-02	2.06E-02
149	6.00E-03	5.55E-02	1.13E-01
151	8.00E-02	3.08E-03	5.95E-03
153	0.00E+00	1.00E+00	1.00E+00
156	3.00E-03	3.96E-02	7.96E-02
158	2.00E-03	N/A	6.78E-02
170	0.00E+00	2.01E-01	2.80E-01
174	5.00E-02	N/A	5.92E-03
177	1.00E-03	8.96E-02	2.12E-01
180	0.00E+00	5.21E-01	5.69E-01
183	0.00E+00	1.79E-01	1.66E-01
187	1.00E-04	N/A	5.39E-01
194	0.00E+00	1.35E-01	9.22E-02
195	1.00E-04	3.62E-02	9.10E-02
201	5.00E-02	1.01E-03	2.44E-03
203	3.00E-04	N/A	1.49E-01

Table B-3 Double-crested Cormorant, same estimates applied to Forster's Tern

PCB Congener	Estimated k_M	Cormorant Egg Empirical Congener - X / 153	Cormorant Egg Model Congener - X / 153
8	1.50E-01	7.23E-04	7.80E-04
18	2.00E-01	N/A	1.04E-03
28	0.00E+00	1.69E-02	6.68E-02
31	3.00E-01	7.44E-04	1.74E-03
33	3.00E-01	5.23E-04	1.22E-03
44	3.00E-01	7.77E-04	1.62E-03
49	3.00E-01	1.08E-03	2.30E-03
52	3.50E-01	1.55E-03	3.39E-03
56	1.50E-01	2.30E-03	4.87E-03
60	1.50E-01	3.53E-03	4.54E-03
66	0.00E+00	4.95E-02	6.38E-02
70	2.50E-01	1.57E-03	3.51E-03
74	0.00E+00	3.46E-02	4.73E-02
87	1.00E-01	9.49E-03	1.58E-02
95	3.50E-01	1.11E-03	3.60E-03
97	5.00E-01	4.39E-04	1.79E-03
99	0.00E+00	1.54E-01	1.87E-01
101	3.50E-01	4.70E-03	9.89E-03
105	0.00E+00	7.08E-02	3.11E-01
110	4.00E-01	1.26E-03	8.63E-03
118	0.00E+00	2.92E-01	5.97E-01
128	0.00E+00	6.63E-02	1.07E-01
132	1.00E-01	N/A	1.59E-02
138	0.00E+00	5.69E-01	8.87E-01
141	2.50E-01	1.88E-03	4.43E-03
149	2.50E-01	9.29E-03	2.46E-02
151	5.00E-01	9.19E-04	7.05E-03
153	0.00E+00	1.00E+00	1.00E+00
156	1.00E-02	4.62E-02	1.21E-01
158	1.00E-02	3.23E-02	8.09E-02
170	0.00E+00	1.49E-01	2.79E-01
174	5.00E-01	9.53E-04	4.43E-03
177	1.00E-02	6.34E-02	1.82E-01
180	0.00E+00	3.75E-01	5.65E-01
183	0.00E+00	1.11E-01	1.65E-01
187	0.00E+00	2.89E-01	5.68E-01
194	0.00E+00	9.07E-02	9.20E-02
195	0.00E+00	2.15E-02	9.38E-02
201	0.00E+00	6.26E-02	8.43E-02
203	0.00E+00	4.64E-02	1.74E-01

Appendix C: PCB congener concentrations in sediments and water that were used in the model to represent current (i.e. 1999-2001) conditions.

PCB Congener	Sediment Concentration (ng/kg dry weight) log transformed	Variability (+/- 1 SD) log transformed	Sediment Concentration (ng/g dry weight)	Variability (+/- 1 SD)
8	2.24E+00	4.41E-01	1.75E-01	1.72E+01
18	2.48E+00	6.93E-01	3.04E-01	2.99E+01
28	2.71E+00	6.25E-01	5.15E-01	5.06E+01
31	2.31E+00	5.48E-01	2.04E-01	2.00E+01
33	2.52E+00	6.25E-01	3.32E-01	3.26E+01
44	2.35E+00	3.90E-01	2.25E-01	2.21E+01
49	2.20E+00	5.53E-01	1.57E-01	1.55E+01
52	2.48E+00	4.80E-01	3.05E-01	2.99E+01
56	2.44E+00	4.70E-01	2.76E-01	2.71E+01
60	2.33E+00	3.95E-01	2.15E-01	2.11E+01
66	2.14E+00	5.86E-01	1.39E-01	1.36E+01
70	2.21E+00	5.35E-01	1.64E-01	1.61E+01
74	2.36E+00	5.04E-01	2.27E-01	2.23E+01
87	2.69E+00	4.84E-01	4.87E-01	4.78E+01
95	2.45E+00	5.80E-01	2.84E-01	2.79E+01
97	2.10E+00	5.13E-01	1.27E-01	1.25E+01
99	2.43E+00	4.14E-01	2.72E-01	2.67E+01
101	2.51E+00	6.02E-01	3.23E-01	3.18E+01
105	2.65E+00	4.04E-01	4.49E-01	4.42E+01
110	2.63E+00	5.60E-01	4.22E-01	4.15E+01
118	2.73E+00	4.72E-01	5.43E-01	5.34E+01
128	1.96E+00	5.30E-01	9.15E-02	8.99E+00
132	2.21E+00	2.63E-01	1.62E-01	1.60E+01
138	2.86E+00	5.81E-01	7.22E-01	7.10E+01
141	1.99E+00	5.01E-01	9.78E-02	9.61E+00
149	2.69E+00	5.02E-01	4.85E-01	4.76E+01
151	2.77E+00	4.89E-01	5.87E-01	5.76E+01
153	2.67E+00	5.14E-01	4.68E-01	4.60E+01
156	2.60E+00	4.80E-01	3.99E-01	3.92E+01
158	2.43E+00	3.29E-01	2.71E-01	2.66E+01
170	2.15E+00	5.00E-01	1.43E-01	1.40E+01
174	2.10E+00	5.18E-01	1.27E-01	1.25E+01
177	2.64E+00	4.01E-01	4.32E-01	4.24E+01
180	2.52E+00	5.45E-01	3.32E-01	3.26E+01
183	1.99E+00	5.51E-01	9.79E-02	9.62E+00
187	2.64E+00	4.23E-01	4.40E-01	4.32E+01
194	2.15E+00	4.73E-01	1.42E-01	1.40E+01
195	2.14E+00	4.61E-01	1.38E-01	1.35E+01
201	1.85E+00	5.53E-01	7.09E-02	6.96E+00
203	2.46E+00	4.62E-01	2.86E-01	2.81E+01

PCB Congener	Total Water Concentration (pg/L) log transformed	Variability (+/- 1 SD) log transformed	Total Water Concentration (ng/g)	Variability (+/- 1 SD)
8	9.86E-01	5.20E-01	9.68E-06	3.31E-06
18	9.50E-01	4.01E-01	8.91E-06	2.52E-06
28	1.20E+00	3.60E-01	1.60E-05	2.29E-06
31	1.15E+00	4.20E-01	1.40E-05	2.63E-06
33	7.85E-01	3.37E-01	6.09E-06	2.17E-06
44	9.80E-01	3.44E-01	9.54E-06	2.21E-06
49	1.17E+00	2.99E-01	1.48E-05	1.99E-06
52	1.36E+00	3.70E-01	2.31E-05	2.35E-06
56	9.73E-01	3.37E-01	9.39E-06	2.17E-06
60	8.17E-01	4.05E-01	6.56E-06	2.54E-06
66	1.11E+00	4.18E-01	1.28E-05	2.62E-06
70	1.11E+00	4.26E-01	1.29E-05	2.67E-06
74	5.31E-01	5.36E-01	3.39E-06	3.44E-06
87	8.85E-01	4.44E-01	7.68E-06	2.78E-06
95	1.26E+00	4.73E-01	1.80E-05	2.97E-06
97	9.42E-01	4.44E-01	8.76E-06	2.78E-06
99	1.23E+00	3.60E-01	1.69E-05	2.29E-06
101	1.47E+00	3.03E-01	2.92E-05	2.01E-06
105	9.98E-01	4.61E-01	9.95E-06	2.89E-06
110	1.50E+00	3.70E-01	3.20E-05	2.34E-06
118	1.48E+00	4.06E-01	3.00E-05	2.55E-06
128	7.08E-01	5.07E-01	5.10E-06	3.21E-06
132	1.02E+00	4.08E-01	1.05E-05	2.56E-06
138	1.57E+00	4.32E-01	3.71E-05	2.70E-06
141	6.81E-01	4.42E-01	4.80E-06	2.76E-06
149	1.54E+00	3.97E-01	3.47E-05	2.49E-06
151	1.11E+00	3.91E-01	1.29E-05	2.46E-06
153	1.70E+00	4.14E-01	5.07E-05	2.60E-06
156	5.88E-01	5.37E-01	3.87E-06	3.45E-06
158	5.17E-01	5.03E-01	3.29E-06	3.18E-06
170	1.13E+00	4.76E-01	1.34E-05	2.99E-06
174	9.54E-01	4.59E-01	8.99E-06	2.88E-06
177	1.02E+00	4.56E-01	1.04E-05	2.86E-06
180	1.42E+00	4.44E-01	2.64E-05	2.78E-06
183	8.69E-01	4.52E-01	7.39E-06	2.83E-06
187	1.36E+00	4.23E-01	2.26E-05	2.65E-06
194	9.08E-01	4.71E-01	8.08E-06	2.96E-06
195	4.02E-01	5.15E-01	2.53E-06	3.28E-06
201	6.77E-01	3.48E-01	4.75E-06	2.23E-06
203	6.82E-01	4.91E-01	4.81E-06	3.10E-06

Appendix D: Excel spreadsheet model including the food web bioaccumulation model for PCBs in San Francisco Bay.