Tier II Method for Evaluation of the Indirect Effects SQO

February 27, 2011

I. Introduction

This document describes the Tier II assessment approach developed for the indirect effects component of the Sediment Quality Objectives (SQO) program. It has been modified from the previous version[a] in response to constructive review comments provided by the SSC and Advisory Committee[b].

The document is organized into three sections. The introduction provides background on the assessment framework and key aspects of the approach. Section II describes the Tier II assessment approach in greater detail, including the key assumptions, equations, and steps of the approach. Section III provides an example illustrating the calculations and possible interpretation of the results.

Overview of indirect effects assessment framework

The purpose of the indirect effects assessment framework is to determine whether sediments meet California's narrative SQO for human health: *Pollutants shall not be present in sediments at levels that will bioaccumulate in aquatic life to levels that are harmful to human health.* The SQO for indirect effects applies only to bays and estuaries; the framework is not intended to be applied to open marine waters or freshwater systems.

This assessment determines whether sediment contamination at a site results in an unacceptable health risk to humans because of the consumption of contaminated fish and shellfish (i.e., seafood). Data for two types of information, referred to as indicators, are analyzed to make the assessment: risk from consuming seafood and the relative contribution of the site contamination to seafood contamination. The unit of assessment is the site, which is as an area of interest within a water body. The size and boundaries of a site are a function of the assessment's purpose and study design, which are identified by developing a conceptual site model. For some applications, a site may be equivalent to an entire bay or estuary, while other programs may require assessment within a portion of the water body.

This assessment framework is intended to provide a consistent method for interpreting monitoring data from several statewide programs. The results of the assessment are expected to be used for multiple purposes where the SQO applies, such as identifying impaired water bodies, assessing compliance with permit conditions, and prioritizing sites for management action. If a need for management action has been determined, a more comprehensive and specific risk assessment may be needed to delineate the spatial extent of the impact, identify sources, select management actions, and determine clean up goals. This evaluation would be based on a variety of considerations, including feasibility, likelihood or extent of environmental benefit, economic

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[a] "Proposed Stochastic Method for Evaluation of the Indirect Effects SQO" released May 6, 2010
[b] Scientific Steering Committee comments were documented in "Comments and Recommendations from SQO Scientific Steering Committee July 14, 2010."

impact, and other site-specific considerations, and is beyond the scope of the Tier II indirect effects assessment framework.

The framework's conceptual design is applicable to a variety of contaminants, while the specific tools described in this phase of the program are intended for assessing chlorinated hydrocarbon pollutants: DDTs, PCBs, chlordane, and dieldrin.

Treatment of uncertainty in the tiered assessment framework

The indirect effects assessment framework is tiered, with increasing complexity and site specificity in higher tiers. The human health risk calculation method is similar among the tiers, but the approach for incorporating uncertainty and variability varies. Uncertainty refers to lack of knowledge about specific factors, parameters, or models, while variability refers to observed differences attributable to true heterogeneity or diversity in a population or exposure parameter. A deterministic (i.e., based upon calculations that do not include a random element) approach is employed for Tier I to provide simplicity and ease of application. The Tier I approach addresses uncertainty and variability by employing conservative point estimates of key input parameter values. A stochastic approach (i.e., incorporating a random element into model calculations) is employed in Tier II and Tier III analyses to characterize the effects of uncertainty and variability of key parameters. The Tier II stochastic analysis is standardized and limited in scope to focus on the uncertainty and variability of a subset of general parameters that will be locally available and are expected to influence the assessment outcome (Table 1). If a Tier III analysis is employed, the specific modifications to the approach will be determined by the management and information needs for the site in question.

The Tier II assessment uses a stochastic simulation model to incorporate aspects of uncertainty and variability into the assessment. Instead of selecting a single point estimate for key parameters, the stochastic approach incorporates the entire probability distribution into the exposure model. Monte Carlo simulation is then employed to repeatedly and randomly select points across the probability distribution for each key parameter. The results of multiple simulations are recorded, and then combined into a probability distribution of results for each type of indicator.

The Tier II stochastic approach generates a distribution of results, which are evaluated at various points to estimate exposure risk and sediment contribution. The use and presentation of probability-based information provides additional information to aid in interpreting the results. For example, probability distributions of cancer risk to human consumers of seafood indicate how the risk varies for different portions of the population. Stochastic approaches have been used to evaluate human health risk in diverse regions, including the Palos Verdes Shelf (Wilson et al., 2001), the Housatonic River in New England (Weston Solutions, 2005), San Francisco Bay (Gobas and Arnot, 2005, 2010), and the New York-New Jersey Bight (Linkov et al., 2002).

Table 1. Proposed treatment of stochastic parameters in a Tier II application. Statewide estimates for some parameters will be provided in technical guidance documents and will be based on analysis of California data or best available information. Local estimates are based on data for the site being assessed.

Parameter	Data source for value	Data source for dispersion*	Focus of dispersion measurement	Primary causes of dispersion*	Notes
(CR) Seafood consumption rate	Statewide estimate or local site data (when available)	Statewide estimate or local estimate (when available)	Entire statistical population (i.e., standard deviation)	Variability	Need to assess potential impact to full population that consumes local seafood.
(Ct) Tissue chemistry concentration	Local data from site	Local estimate	Average (i.e., standard error)	Uncertainty	Site specific data needed on contaminant exposure. Exposure of human consumers will tend to average across sediment and tissue population over time.
(Cs) Sediment chemistry concentration	Local data from site	Local estimate	Average (i.e., standard error)	Uncertainty	Same as for tissue chemistry
(BAF) Bioaccumulation factor	Calculate using bioaccumulation model with combination of local and general parameters	Statewide estimate	Entire statistical population (i.e., standard deviation)	Variability plus uncertainty	Bioaccumulation model incorporates key site specific parameters. Uncertainty and variability in bioaccumulation within and across sites has been successfully measured and can be easily applied using a standard parameter (Burkhard et al., 2010; Gobas and Arnot, 2010)
(HR) Seafood home range	Statewide estimate	Statewide estimate	Entire statistical population (i.e., standard deviation)	Variability plus uncertainty	Local data will generally be unavailable. Movement range relatively uncertain.

*The term “dispersion” is used to indicate variability across a statistical population. Examples of measurements of dispersion include standard deviation, standard error of the mean, or coefficient of variation.

Use of a guild approach

A guild approach is employed to evaluate health risk and model exposure from sediments, as described elsewhere (SQO Science Team, 2010a). For this approach, finfish species in California estuaries and marine embayments are categorized in one of eight dietary guilds, based on trophic position and consumption of benthic prey. The guild approach is intended to provide biological realism, while having reasonable data requirements. The guiding principle is that incorporating information about seafood diet into target species selection and bioaccumulation modeling will provide a more realistic depiction of contaminant exposure than using generic assumptions. In particular, species that consume similar prey types will have similar food web exposure to sediment-associated contaminants.

The guild approach informs the assessment in two aspects. Information regarding guild membership aids in selecting local seafood species for monitoring to assess risk to seafood consumers. Additionally, guild-based diet attributes for selected species are incorporated into the bioaccumulation model to estimate the contribution of site sediments to local seafood exposure.

II. Tier II approach

In Tier II, the seafood chemistry and sediment chemistry data are both used to answer two key questions regarding sediment contamination at a site:

1. **Consumption risk:** To what extent are human consumers of seafood at risk from sediment-associated contaminants?
2. **Sediment contribution:** To what degree are sediments at the site under consideration contributing to that risk?

The first question is evaluated using the concentration of contaminants in seafood tissue samples from the site. A stochastic model of exposure to the consumer population is used to generate cumulative distribution functions of cancer risk and noncancer hazard. Percentiles along this distribution are then compared to risk thresholds, to categorize the site in terms of potential risk to consumers (i.e., the consumption risk).

The second question is evaluated by using the sediment chemistry data and site-specific bioaccumulation factors in a stochastic model to estimate tissue contaminant concentrations that would be expected due to site sediment contamination. This distribution of expected tissue contaminant concentrations is then compared to the average measured seafood tissue contaminant concentration at the site, and a distribution of percentages is calculated. The percentage of the observed seafood tissue chemistry that is due to site sediment chemical contamination (i.e., the sediment contribution) is the measurement outcome.

All calculations for consumption risk and sediment contribution are performed in a spreadsheet model. The model is set up by defining the monitored species, which fall into one of the dietary guilds, and their relative importance in the human diet. Other site-specific attributes, such as sediment and tissue chemistry are also entered. The calculations are then performed with stochastic simulations, generating distributions of three types of results: cancer risk and non cancer hazard due to the overall seafood diet of the human consumers (Figure 1), and sediment contribution to the seafood contamination (Figure 2).

Calculation of consumption risk

Consumption risk is based on calculations of cancer risk and noncancer hazard, that are in turn based on measured tissue contaminant concentrations from multiple species monitored at the site (Figure 1). Appropriate species are selected based on development of a conceptual site model, including consideration of the different dietary guilds present on the site. Background information to define guild membership is provided elsewhere (SQO Science Team, 2010a).

The calculations used to calculate risk are the same as those used by California's Office of Environmental Health Hazard Assessment (OEHHA) to develop seafood consumption guidelines and advisories (Klasing and Brodberg, 2008).

Carcinogens

(Eq. 1) RL = **TC** x **CR** x CSF x (ED/AT) x CRF / BW

Non-carcinogens

(Eq. 2) HQ = **TC** x **CR** x CRF / (RfD x BW)

Where
TC = tissue concentration for appropriate seafood species monitored at site (mg/kg)
AT = Averaging Time (yr)
BW = Body Weight (kg)
CR = Consumption Rate (kg/d)
CRF = Cooking Reduction Factor (unitless)
CSF = Cancer Slope Factor $(mg/kg/d)^{-1}$
ED = Exposure Duration (yr)
HQ =Hazard quotient for noncarcinogens (unitless)
RfD = Reference Dose (mg/kg/d)
RL = Cancer Risk Level (unitless)

In equations 1 and 2, the underlined and boldface parameters (tissue concentration and consumption rate) are varied stochastically in the Tier II Monte Carlo simulation. The tissue concentration (TC) is based on measurements of appropriate seafood species measured at the site. The stochastic assessment framework generates a distribution of exposure concentrations based on the combined results of all seafood species measured. Specifically:

(Eq. 3) $$\underline{TC} = \sum_{i=1}^{n} \underline{TC_i} \cdot p_i$$

Where i (1, 2, … n) are the individual species monitored, $\underline{TC}_i$ is the average tissue concentration for species i, and p_i is the proportion of the fish consumer diet represented by species i.

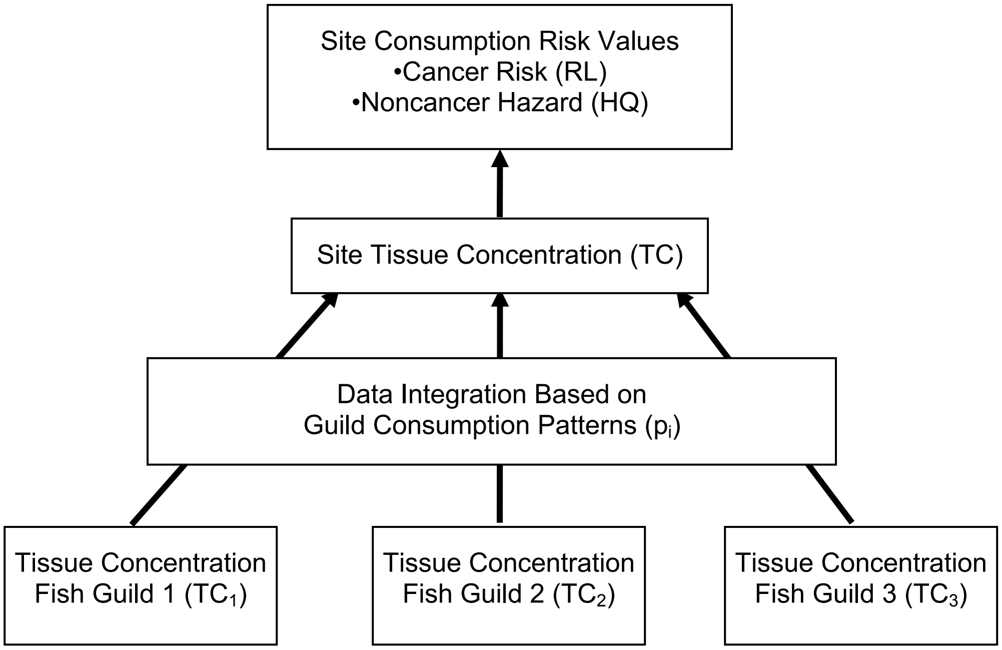

Figure 1. Strategy for determining the consumption risk to seafood consumers. The number of guilds included in the analysis depends of the conceptual site model.

Estimates of average and standard error of tissue contamination are calculated from multiple measurements for each species monitored. The relative proportion of each guild in the diet is determined as part of the site conceptual model. In general, these proportions are based on local catch or consumption data for each fish species.

Calculation of sediment contribution

Sediment contribution is calculated by comparing estimated vs. observed tissue contaminant concentration. Estimated tissue contaminant concentration is calculated for each species monitored (TE_i), where i (1, 2, … n) are the individual species monitored. TE_i is calculated based on measured sediment chemistry concentrations from the site, combined with a bioaccumulation model.

(Eq. 4) $TE_i = \underline{\mathbf{Cs}} * \underline{\mathbf{BAF_i}} * SA / \underline{\mathbf{HR_i}}$.

TE_i = estimated tissue contaminant concentration in species i contributed from site sediments
Cs = Measured contaminant concentration in sediment from the site
BAF_i = bioaccumulation factor for species i
SA = site area (km^2) or length across the site (km)
HR_i = seafood home range (km^2) or linear movement distance (km) for species i

Three parameters in Equation 4 were chosen for stochastic variation: sediment contaminant concentration (Cs), home range (HR_i), and bioaccumulation factor (BAF_i). These parameters were selected based on a combination of sensitivity of the outcome to their variation and ability to obtain local or statewide estimates of uncertainty or variability. Other parameters in Equation

4 are used as point estimates to achieve consistency with other State agencies (e.g., OEHHA), and to reduce the complexity of the analysis. These issues are discussed in greater detail in the sensitivity analysis document, distributed previously (SQO Science Team, 2010b).

Equation 4 employs a site use factor (i.e., SA/HR_i) to account for the movement of fish beyond the site boundaries. The site use factor is calculated differently for different guilds. Some species guilds have home range calculations on an area basis, while others only have linear movement distance information available. For guilds with established home range areas, Equation 4 compares home range area vs. site area to develop site use factor. For guilds that do not maintain specific home ranges, or have appropriate home range area data, Equation 4 estimates HR as the linear movement distance by individuals in the species. For these guilds, HR is compared to the site length (i.e., maximum linear distance across the site). In either case, the site use factor is set to equal to one when the home range is smaller than the site (i.e., SA > HR).

For each species i, sediment contribution (SC_i) is calculated as the percentage of observed tissue contaminant concentration (TC_i) due to estimated exposure to site sediment contaminants (TE_i):

(Eq. 5) $$SC_i\ (\%) = 100 * (TE_i / TC_i)$$

Equations 4 and 5 are calculated to estimate sediment contribution for each seafood species monitored at the site, and these results are combined to determine the site sediment contribution (Figure 2). The site sediment contribution (SC) is the weighted average estimated sediment contribution for all species:

(Eq. 6) $$SC = \sum_{i=1}^{n} SC_i \cdot p_i$$

where SC_i is the average estimated tissue concentration for species i, and p_i is the proportion of the fish consumer diet represented by species i.

<u>Site assessment steps</u>

Analyzing data and interpreting the results includes seven steps, which are illustrated in the detailed example (Section III):

- Step 1: Develop conceptual site model.
- Step 2: Input data for site-specific parameters.
- Step 3: Run the bioaccumulation model to calculate bioaccumulation factors for use in sediment contribution calculations.
- Step 4: Perform simulations to generate cumulative probability distributions of consumption risk and sediment contribution results.
- Step 5: Plot and evaluate results of the simulations.
- Step 6: Categorize results for the consumption risk and sediment contribution.
- Step 7: Compare the results for the two indicators to make a site assessment.

This process is conducted for each contaminant group separately. The final site assessment is based on the highest level of risk from site contamination obtained for any compound.

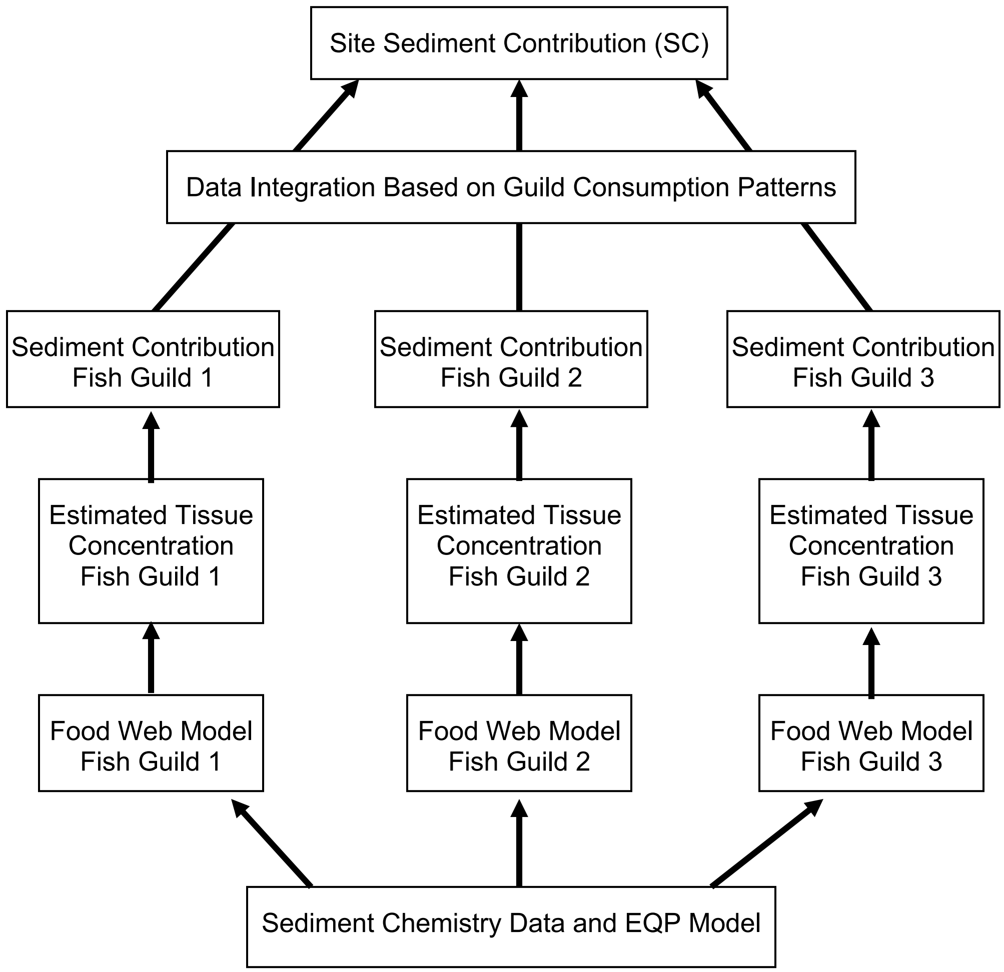

Figure 2. Strategy for determining the site sediment contribution to fish bioaccumulation. The number of guilds included in the analysis depends of the conceptual site model.

Developing a conceptual site model

Step 1, development of a conceptual site model, is key to planning the assessment and formulating management decisions. Background on conceptual model development may be found in Cura et al. (1999) and Bridges et al. (2005); Davis et al. (2006) and Connor et al. (2004) provide two detailed examples. The conceptual site model should be based on local information and expertise. The conceptual site model should contain information needed to determine the following parameters:

- Site boundaries and site size
- Seafood consumer population characteristics (e.g., consumption rate)
- Seafood species to be monitored
- Site-specific modification to other parameters, as needed, such as seafood movement range or diet

A definition of the site boundaries and site size is needed to aid in data collection and data reduction, in addition to being a key input for the sediment contribution indicator. Site boundaries may be defined based on geomorphic and hydrologic boundaries, areas of management concern, previous boundary definitions (e.g., water body segments), and other local considerations. Another consideration is the spatial distribution of sediment contamination within a site. Some sites may contain specific areas of elevated contamination ("hotspots"), and it may be worthwhile to perform the assessment at multiple scales, including the hotspots, as well as less contaminated areas, to determine whether the assessment outcome would be different.

The seafood consumer population is chosen based on what is known about fishing practices and consumption rates at the site. Selection of an appropriate consumer population will aid in identifying available information on local consumption rates. Surveys from other California water bodies may be employed to determine consumption rates if local data are not available. Selection of seafood species of interest will be based on the fishing and consumption practices of local consumers, as well as species known to reside in the site, and representing predominant dietary guilds.

Categorization thresholds and integration of the results

Table 2 contains a set of provisional categorization thresholds for the approach, to be used in Step 6. The Water Board will ultimately decide the threshold values for SQO assessment. Evaluation of the consumption risk indicator employs a single threshold for cancer risk and noncancer hazard (Table 2a). This threshold is evaluated at three points on the consumption risk cumulative distribution: 95%, 75%, and 50%. The outcome category is determined based on the percent of seafood consumers that is below that threshold.

For sediment contribution, a distribution of likely sediment contributions is calculated to account for uncertainty and variability in model parameters (Equations 4 and 5). Similar to the consumption risk evaluation, the sediment contribution evaluation (Table 2b) employs a single threshold of percent contribution to seafood tissue concentration. The outcome category is determined based on the portion of modeled sediment results that is below that threshold. The evaluation is performed at three points on the sediment contribution distribution: 75%, 50%, and 25%.

Table 3 describes the proposed approach for integrating consumption risk and sediment contribution into an assessment decision for each contaminant (Step 7). The third column of Table 3 describes in narrative form the interpretation of each possible combination of the two indicators. The integrated results are summarized in categorical form as one of five numbered categories, with a higher level of potential health fish from the site indicated by a higher category number.

Table 2. Potential categories for a stochastic simulation approach to evaluate consumption risk (a); and sediment contribution (b). Note that all numeric values are provisional and included for illustration purposes only – final values would ultimately be selected by the Water Board.

2a. Consumption Risk

Consumer Group	Cumulative % of risk or hazard distribution	Cancer Risk			Noncancer Hazard	
		Threshold	Outcome		Threshold	Outcome
Virtually All	95%	$<10^{-5}$	1. Very Low		<1	1. Very Low
Most Consumers	75%	$<10^{-5}$	2. Low		<1	2. Low
Upper End Consumer	50%	$<10^{-5}$	3. Moderate		<1	3. Moderate
Average Consumer	50%	$\geq 10^{-5}$	4. High		≥1	4. High

2b. Potential categories for sediment contribution. Column 2 refers to the cumulative percent of modeled sediment results, and Column 3 refers to the calculated percent sediment contribution threshold.

Estimate of sediment contribution	Cumulative % of sediment contribution distribution	% Contribution Threshold	Outcome
Third quartile	75%	<50%	1. Very Low
Second quartile (median)	50%	<50%	2. Low
First quartile	25%	<50%	3. Moderate
First quartile	25%	≥50%	4. High

Table 3. Provisional site assessment for indirect effects SQO, combining consumption risk and sediment contribution. Five numbered categories of result are obtained. Final categories, relationships, and outcomes will be determined by the Water Board.

Consumption Risk	Sediment Contribution	Narrative description	Final category
1. Very Low	1. Very Low	Virtually all of the seafood consuming population is at an acceptable risk from seafood contamination. Very little of the seafood tissue burden is due to site sediments.	1
1. Very Low	2. Low	Virtually all of the seafood consuming population is at an acceptable risk from seafood contamination. A limited amount of the seafood tissue burden is due to site sediments.	1
1. Very Low	3. Moderate	Virtually all of the seafood consuming population is at an acceptable risk from seafood contamination. A substantial portion of the seafood tissue burden is due to site sediments.	1
1. Very Low	4. High	Virtually all of the seafood consuming population is at an acceptable risk from seafood contamination. Most of the seafood tissue burden is due to site sediments.	1
2. Low	1. Very Low	Most seafood consumers are at an acceptable risk from seafood contamination. Very little of the seafood tissue burden is due to site sediments.	1
2. Low	2. Low	Most seafood consumers are at an acceptable risk from seafood contamination. A limited amount of the seafood tissue burden is due to site sediments.	1
2. Low	3. Moderate	Most seafood consumers are at an acceptable risk from seafood contamination. A substantial portion of the seafood tissue burden is due to site sediments.	2
2. Low	4. High	Most seafood consumers are at an acceptable risk from seafood contamination. Most of the seafood tissue burden is due to site sediments.	2
3. Moderate	1. Very Low	Average seafood consumers are at an acceptable risk from seafood contamination. Very little of the seafood tissue burden is due to site sediments.	2
3. Moderate	2. Low	Average seafood consumers are at an acceptable risk from seafood contamination. A limited amount of the seafood tissue burden is due to site sediments.	3
3. Moderate	3. Moderate	Average seafood consumers are at an acceptable risk from seafood contamination. A substantial portion of the seafood tissue burden is due to site sediments.	4
3. Moderate	4. High	Average seafood consumers are at an acceptable risk from seafood contamination. Most of the seafood tissue burden is due to site sediments.	5
4. High	1. Very Low	Average seafood consumers are at an unacceptable risk from seafood contamination. Very little of the seafood tissue burden is due to site sediments.	2
4. High	2. Low	Average seafood consumers are at an unacceptable risk from seafood contamination. A limited amount of the seafood tissue burden is due to site sediments.	3
4. High	3. Moderate	Average seafood consumers are at an unacceptable risk from seafood contamination. A substantial portion of the seafood tissue burden is due to site sediments.	4
4. High	4. High	Average seafood consumers are at an unacceptable risk from seafood contamination. Most of the seafood tissue burden is due to site sediments.	5

III. A Tier II case study example

A case study is presented using monitoring data to illustrate the Tier II stochastic approach, and graphical depictions of output. The example focuses on a water-body scale assessment, which is expected to be the typical application. In this example, assessment example, DDT concentrations in sport fish and sediment sampled in San Francisco Bay are evaluated and integrated to make a site assessment.

Note: The purpose of this example is to illustrate how the Tier II stochastic approach would be performed. The parameter values used are provisional values. Future analyses and discussion will be used to refine selection of the parameter values. Also note that the data used in the example have been compiled from multiple studies whose study designs may not be optimal for SQO assessment.

Step 1: Develop conceptual site model.

This example was developed by the Science Team to illustrate the indirect effects assessment framework and approach. As such, the conceptual site model described here draws from conceptual models developed elsewhere. This example will illustrate some of the considerations and decisions that inform conceptual site model development for SQO assessment. The conceptual site model will begin with a general description of the water body and pollutant of concern. As described in the previous section, the conceptual site model will include treatment of site boundaries, site size, the fish consumer population, and seafood species of interest.

Background: A detailed conceptual site model for DDTs and other legacy pesticides in San Francisco Bay was developed in Connor et al. (2004). San Francisco Bay is the largest estuary on the Pacific coast of the Americas, extending from the confluence of the Sacramento and San Joaquin Rivers to the Golden Gate, where the Bay meets the Pacific Ocean. The pesticides DDTs, chlordanes, and dieldrin remain in the San Francisco Estuary as a result of agricultural and residential applications from the early to late 20th century (Connor et al., 2007). The Bay is listed as impaired by legacy pesticides on California’s 303(d) list (State Water Resources Control Board, 2009) because of an interim fish consumption advisory developed by OEHHA (OEHHA, 1997). The advisory was based on a 1994 fish tissue study (SFBRWQCB, 1995), which indicated that legacy pesticides, PCBs, mercury, and dioxins were present at levels of potential concern. Sources of pesticides entering the Bay include runoff from the Central Valley, runoff from local watersheds, municipal and industrial discharges, atmospheric deposition, erosion of sediments buried beneath the active sediment layer, and dredging and disposal of deep sediments (Connor et al., 2007). The Regional Monitoring Program for Water Quality (RMP), a comprehensive contaminant and water quality monitoring program, has collected annual data on legacy pesticide concentrations in San Francisco Bay water, sediments, and bivalves since 1993 (SFEI, 2005). The RMP also monitors concentrations of legacy pesticides in sport fish every three years (Greenfield et al., 2003; Greenfield et al., 2005; Hunt et al., 2008), with the most recent sampling event in 2009. A conceptual model for the San Francisco Bay food web has also been developed (Gobas and Arnot, 2005; Davis et al., 2006). This model indicates that one of the pathways for contaminant exposure to anglers is the pathway evaluated by the indirect effects SQO assessment: consumption of seafood exposed to sediment contaminants via food web biomagnification (Figure 3).

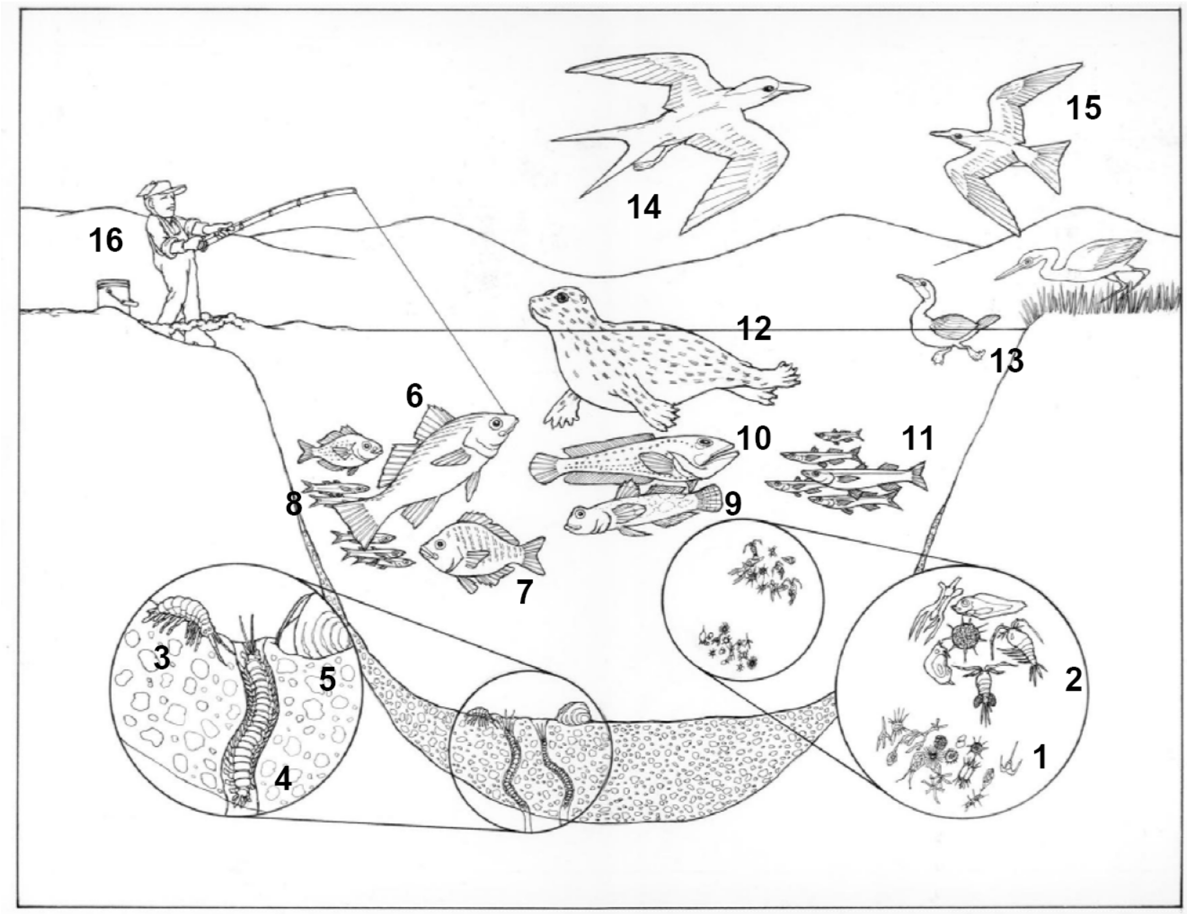

Figure 3. Conceptual model for the San Francisco Bay food web. Legacy pollutants enter the food web via accumulation by phytoplankton (1) at the base of the food web. Concentrations then increase with each step up the food web, reaching maximum concentrations and posing the greatest health risks in species that consume Bay fish. Phytoplankton (1) are consumed by small animals including zooplankton (2) and invertebrates such as amphipods (3), worms (4), or clams (5). Invertebrates in the sediment also accumulate contaminants directly from sediment through ingestion of particles and from contact with sediment porewater. Fish consume the zooplankton and invertebrates and receive a higher dose of bioaccumulative compounds. Humans (16) and wildlife species consume the fish and receive higher doses. Wildlife consume smaller fish species such as yellowfin goby (9), plainfin midshipmen (10), and anchovy (11). Humans consume larger species such as white croaker (6), shiner surfperch (7), and jacksmelt (8). Wildlife species of concern for bioaccumulation and effects include harbor seals (12), cormorants (13), Forster's terns (14), and the endangered least tern (15). Figure and caption reprinted from Davis *et al.* (2006).

Site boundaries and size: DDT exposure to humans via fish consumption is a potential concern throughout San Francisco Bay, demonstrated by all Bay segments being 303d listed as impaired for DDTs (State Water Resources Control Board, 2009). This case study example will evaluate the entire Bay, with site boundaries including the entire estuarine and marine portion, up to the upper boundary of the Bay (Chipps Island, at the base of the Sacramento-San Joaquin River Delta). This upper boundary also includes the home range for most sport fish species targeted by fish consumers within the Bay. For probabilistic calculation of sediment contribution to seafood contamination (Equations 4 and 5, pp. 6 and 7), the area of the entire bay is 896 km^2 (Melwani et al., 2008), and the length of the Bay, measured as distance from the Bay-Delta boundary to the Golden Gate is 64 km. Assessment of subembayments or of specific more contaminated areas targeted for management of DDT contamination (e.g., Lauritzen Channel, Richmond Harbor, Lee et al., 1994; U. S. EPA, 1994) could result in different outcomes.

The fish consumer population: The San Francisco Bay human population includes consumers of fish at both sport and subsistence consumption rates (Chiang, 1998; SFEI, 2000). To indicate risk to both recreational and subsistence consumers, this case study will assume a target population that includes both subpopulations. Specifically, the consumption rate distribution will be based on a survey of all anglers who recently consumed local fish (SFEI, 2000). This survey targeted all fishers encountered at multiple popular fishing locations for sport and subsistence fishing. The daily consumption rate among recent consumers (based on 4 week recall, and adjusted for avidity bias) was used. The arithmetic mean consumption rate was 23.02 g/d and the standard deviation was 32.05 (Table K29, line 3, SFEI, 2000). This distribution chosen represents recent consumers (past 4 weeks only) rather than all sport fishers. This population includes both sport and subsistence fishers.

Seafood species of interest: The conceptual model of the San Francisco Bay food web (Figure 3) aids in identifying sport fish species of interest for local site managers. Shiner perch, white croaker, and jacksmelt are among the species of local interest (Figure 3). The Regional Monitoring Program for Water Quality in San Francisco Bay (RMP) has previously identified additional sport fish for monitoring, based on popularity among local consumers, posing high potential risk due to elevated contaminant concentrations, and representing different dietary guilds within the Bay food web. In addition to shiner perch, white croaker, and jacksmelt, the RMP also monitors four other species of interest: California halibut, leopard shark, white sturgeon, and striped bass. Among the seven species, appropriate species for SQO assessment are shiner perch, white croaker, California halibut, and leopard shark. However, California halibut generally only occur in deeper portions of Central Bay, and are not reflective of exposure throughout most of the Bay. Based on these constraints, the case study will include three species: shiner perch, white croaker, and leopard shark. Each of these species is routinely monitored by the RMP, and is appropriate for SQO assessment, based on sediment association, limited home range, and consumption by anglers.

Step 2: Input data for site-specific parameters.

In the second step of the analysis, data are summarized and entered into a Decision Support Tool, which performs calculations for Steps 3 and 4. The stochastic approach requires explicit local specification of estimates of dispersion for consumption rate, tissue contamination, and sediment contamination. For this case study, consumption rate parameters were defined in Step 1. In Tier II analysis, consumption rate would be based on a statewide guidance value or local consumption rate data if available (Table 1).

Seafood tissue and sediment chemistry concentrations would be collected locally for the site (Table 1). Consistent with the revised framework, in this example the tissue chemistry data are calculated and entered by species, to account for among-species differences in bioaccumulation (Equation 3, Figure 1). Based on the conceptual site model, sum DDT concentrations (mean and SE) were calculated for three finfish species: leopard shark, white croaker, and shiner perch. Data were collected and available from 2003, 2006, and 2009. Average and standard error tissue concentrations for sum DDTs, and average tissue lipid concentrations for these species (Table 4) were calculated and entered into the Decision Support Tool. Because insufficient data are available to establish the relative proportion of each species consumed by individual consumers, an equal relative proportion of consumption was assumed.

Table 4. Seafood input parameters used in the assessment example.

Species	Dietary guild	Sum DDTs Mean ± SE ($ng\ g^{-1}$)	Lipids (%)
Leopard shark	Benthic with piscivory	7.26 ± 1.62	0.37
White croaker	Benthic without piscivory	37.09 ± 4.90	5.33
Shiner perch	Benthic and pelagic without piscivory	21.82 ± 0.89	1.32

Sediment chemistry data were developed on a Bay-wide basis to correspond to the Bay-wide tissue data. These were based on 80 samples collected as part of a probabilistic survey design collected in 2002 and 2004 (Lowe et al., 2004)[c]. The average sum DDTs concentration was 1.86 ng/g and the standard error of the mean was 0.23. Average concentrations for each individual DDT compound, and sediment TOC were also determined, to enable calculation of the bioaccumulation factor. Site area and length were determined to enable site use factor calculation (Table 5).

Table 5. Additional site specific parameters entered into the spreadsheet model tool for the assessment example.

Parameter	Value Employed	Data Source
Seafood Consumption Rate	23.02 ± 32.05 g/d	SFEI (2000)
Sediment TOC	1.30 %	RMP Data Query*
Site area	896 km^2	Melwani et al (2008)
Length of site	64 km	Google Earth Query
Sediment sum DDT concentrations	1.86 ± 0.23 ng/g	RMP Data Query*
Sediment DDT congener profile (ng/g)	op-DDD = 0.20 op-DDE = 0.05 op-DDT = 0.03 pp-DDD = 0.91 pp-DDE = 0.92 pp-DDT = 0.18	RMP Data Query*

* http://www.sfei.org/RMP/report

[c] 4 of the 80 data points were below detection limits. To account for these censored observations, summary statistics were generated using methods for censored environmental data. Specifically, the package NADA (developed for R 2.10.1 by Dennis Helsel) was used to calculate average and standard deviation using the Regression on Order Statistics Method (Helsel 2005).

Step 3: Run the bioaccumulation model to calculate bioaccumulation factor for the sediment contribution calculation.

Once data entry is complete, the next step is to calculate the bioaccumulation factor (BAF) for each fish species included in the assessment. The Decision Support Tool contains a macro that calculates the estimated tissue concentrations (TE) for each compound entered (in this case, each of the six DDT congeners) and sums these results to obtain a single TE (i.e., for sum DDTs). The BAF is then calculated as the quotient of estimated tissue concentration divided by observed sediment concentration for sum DDTs (i.e., BAF = TE/Cs). The BAF calculations are performed separately for each dietary guild, with the results applied to the selected finfish species in Step 4.

Step 4: Perform simulations to generate cumulative probability distributions of results.

A Monte Carlo simulation methodology (McKone and Bogen, 1991) is employed to obtain cumulative probability distributions for consumption risk and sediment contribution. This simulation uses the YASAIw add-in Monte Carlo simulation macro[d] for Excel (Eckstein and Riedmueller, 2002; Pelletier, 2009), which the user installs prior to using the Decision Support Tool. In the typical application, 10,000 simulations are performed. The following simulation outputs are automatically recorded for further evaluation:

1. **Consumption risk:** carcinogenic risk and noncancer hazard predicted from the tissue chemistry data.
2. **Sediment contribution:** the estimated tissue contaminant concentration predicted from the sediment chemistry data.

Step 5: Plot and evaluate results of the simulations.

The stochastic approach lends itself to graphical depiction and interpretation. There are a number of methods to describe the results, and in a typical application the user will generate some exploratory graphics to illustrate the findings. The Monte Carlo simulation macro contains tools for calculating cumulative distribution functions (Figures 4, 5, and 7), and histograms. Monte Carlo simulation output data can also be used to generate box and whiskers plots (Figures 6 and 8) and simple tabulations (Table 6).

Figures 4 and 5 illustrate the cumulative distribution functions for cancer risk and noncancer hazard resulting from the stochastic simulations. Figures 4 and 5 and the underlying data can be used to make inferences regarding the cancer risk and noncancer hazard to various components of the modeled consumer population. Figure 4 illustrates that about 80% of the modeled consumer population is exposed to less than a 10^{-6} increased risk of cancer and all of the population less than a 10^{-5} increased risk of cancer. Figure 5 illustrates that 70% of the population has a noncancer hazard less than 0.01 and all of the population has a noncancer hazard less than 0.1.

Figure 6 illustrates the results of the cancer risk results in box and whiskers plot format. This graphical depiction may be more easily interpreted by individuals unfamiliar with cumulative distribution plots. The results indicate that the 5th percentile, 25th percentile,

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[d] Developed by Greg Pelletier, Washington Department of Ecology, available for download at http://www.ecy.wa.gov/programs/eap/models.html

median, and 75th percentile consumer would all have a cancer risk less than 10^{-6}. The 95th percentile consumer would have a cancer risk of approximately 2.5 x 10^{-6} (i.e., between 10^{-6} and 10^{-5}).

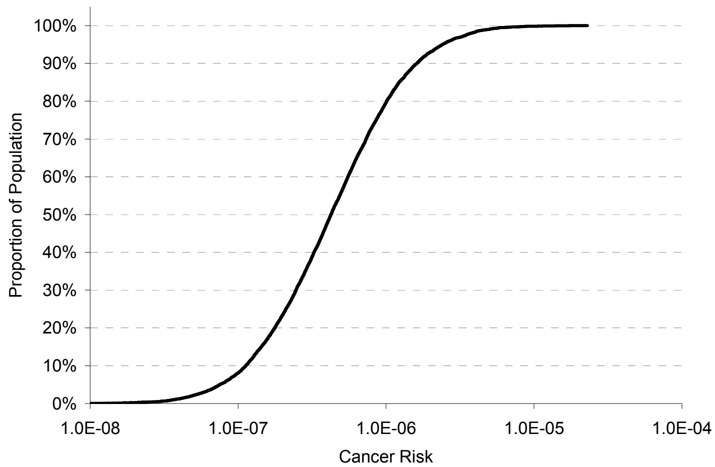

Figure 4. Cumulative distribution function of cancer risk for the consumption risk simulation results. Note log scale x-axis.

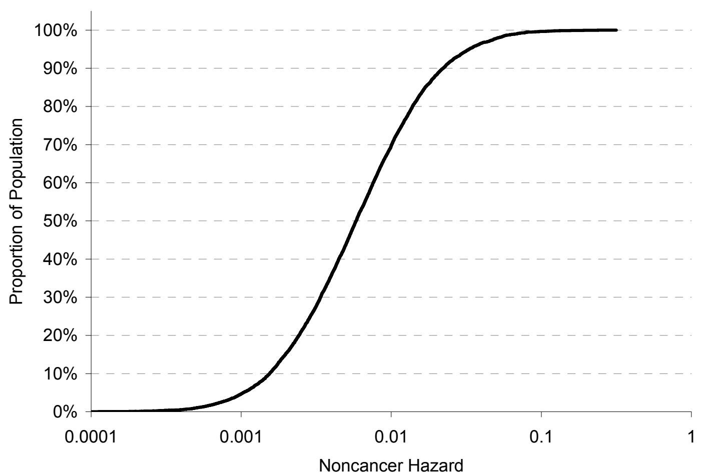

Figure 5. Cumulative distribution function of noncancer hazard for the consumption risk simulation results. Note log scale of x-axis.

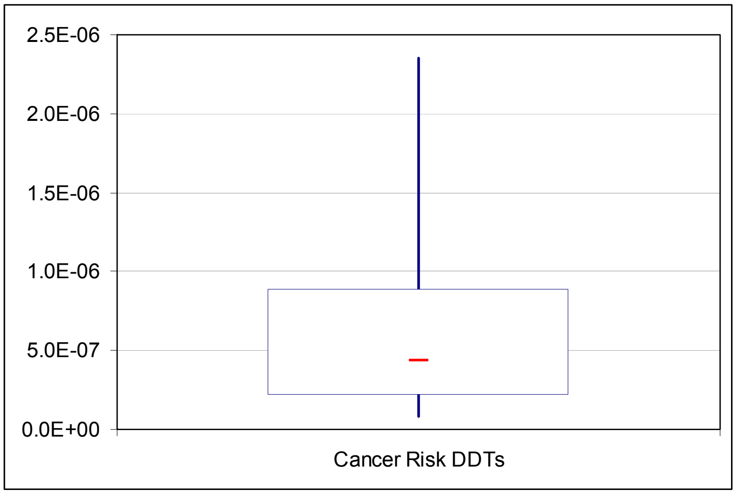

Figure 6. Box and whiskers plot depiction of cancer risk for the consumption risk simulation results. Top whisker = 95%, bottom whisker = 5%, red line = median (50%), and box = quartiles (25%, 75%). Note: y-axis uses scientific notation but is on a linear scale.

Figures 7 and 8 indicate the cumulative distribution function and box and whiskers plot for the percent sediment contribution to tissue chemistry. Note that in Figure 7, the x-axis indicates the percent sediment contribution to tissue burden, whereas the y-axis indicates the statistical proportion of the population. In Figure 8, the y-axis indicates the percent sediment contribution to tissue burden, with the box and whiskers indicating different points on the statistical percentile of the population. Both figures illustrate that the most probable result is a sediment contribution of approximately 65% to 90% of observed seafood tissue chemistry, with plausible results ranging from approximately 50% to 100%.

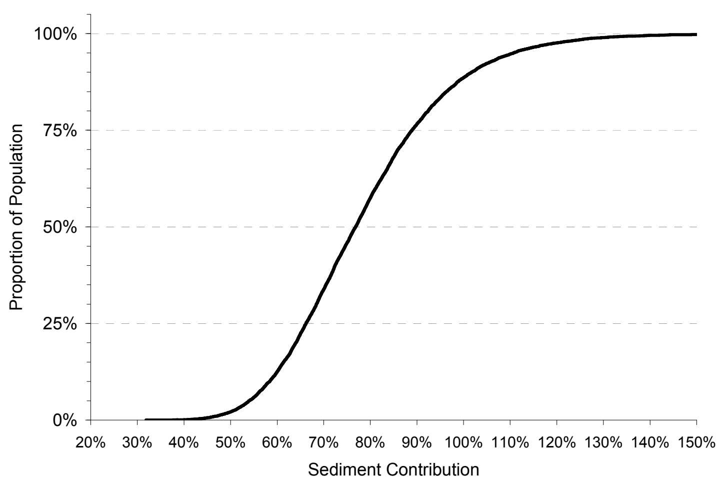

Figure 7. Cumulative distribution plot of sediment contribution to observed seafood contaminant concentrations. Note: linear scale.

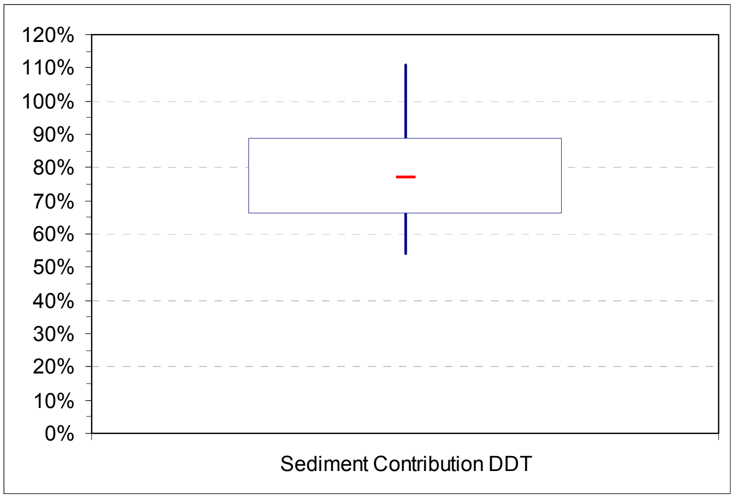

Figure 8. Box and whiskers plot depiction of sediment contribution to seafood tissue chemistry. Top whisker = 95%, bottom whisker = 5%, red line = median (50%), and box = quartiles (25%, 75%).

Step 6. Categorize results for the consumption risk and sediment contribution. The categorical results for each indicator are obtained by comparing simulation results at specific points on the distributions to threshold values (Table 2, Table 6). For consumption risk, the calculated cancer risk and noncancer hazard at points on the cumulative distribution are compared to the threshold for each outcome category (Table 7). The outcome for consumption risk is based on the highest point on the cumulative distribution for which the cancer risk and noncancer hazard results fall below the threshold (Table 2a). In this example, the consumption risk outcome is the same for cancer risk and noncancer hazard. The results for the highest percentile values (95%) are below both the cancer risk threshold (10^{-5}) and noncancer hazard (1.0) thresholds, resulting in a consumption risk category of Very Low (Tables 6 and 7).

Table 6. Summary stochastic simulation results for the Tier II example. Bold cells highlighted in grey are compared to provisional thresholds in this case study example.

	Noncancer hazard	Cancer risk	Sediment Contribution
Statistic	Tissue	Tissue	Sediment
5%	0.001	8.E-08	54%
25%	0.003	2.E-07	**66%**
Median (50%)	**0.006**	**4.E-07**	**77%**
75%	**0.01**	**9.E-07**	**89%**
95%	**0.03**	**2.E-06**	111%

Table 8 indicates the outcome for sediment contribution. In this example, the estimated sediment contribution for the first quartile value (25%) is 66%. In other words, the 25%ile estimate of the sediment population is predicted to contribute 66% to the total seafood tissue burden. This is greater than the 50% provisional threshold for sediment contribution, resulting in a category of High sediment contribution.

Table 7. Outcome of consumption risk stochastic simulation results for the Tier II example. The outcome for each type of risk is highlighted in color.

Cumulative % of distribution	Cancer Risk				Noncancer HQ		
	Result	Threshold	Outcome		Result	Threshold	Outcome
95%	2×10^{-6}	$<10^{-5}$	**Very low**		0.03	<1	**Very low**
75%	9×10^{-7}	$<10^{-5}$	Low		0.01	<1	Low
50%	4×10^{-7}	$<10^{-5}$	Moderate		0.006	<1	Moderate
50%	4×10^{-7}	$\geq 10^{-5}$	High		0.006	≥1	High

Table 8. Outcome of stochastic simulation for sediment contribution for the Tier II example.

Cumulative % of distribution	Sediment contribution	Threshold	Outcome
75%	89%	<50%	1. Very low
50%	77%	<50%	2. Low
25%	66%	<50%	3. Moderate
25%	66%	≥50%	**4. High**

Step 7. Integrate the consumption risk and sediment contribution results to make a site assessment.

The categorical scores for the consumption risk (Table 7) and sediment contribution (Table 8) categories are combined to obtain a site assessment for indirect effects, following Table 3. In this example, the site sediments have a high contribution to the seafood tissue burden. However, virtually all of the seafood consuming population is estimated to be at an acceptable risk from consuming local seafood. This results in a site classification of 1, the lowest category (Table 9).

Table 9. Outcome of integrating consumption risk and sediment contribution for the Tier II example. The integration follows Table 3.

Consumption Risk	Sediment Contribution	Narrative description	Final category
1. Very Low	4. High	Virtually all of the seafood consuming population is at an acceptable risk from seafood contamination. Most of the seafood tissue burden is due to site sediments.	1

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