Calculation and Uses of Mean Sediment Quality Guideline Quotients: A Critical Review

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Fine-grained sediments contaminated with complex mixtures of organic and inorganic chemical contaminants can be toxic in laboratory tests and/or cause adverse impacts to resident benthic communities. Effects-based, sediment quality guidelines (SQGs) have been developed over the past 20 years to aid in the interpretation of the relationships between chemical contamination and measures of adverse biological effects. Mean sediment quality guideline quotients (mSQGQ) can be calculated by dividing the concentrations of chemicals in sediments by their respective SQGs and calculating the mean of the quotients for the individual chemicals. The resulting index provides a method of accounting for both the presence and the concentrations of multiple chemicals in sediments relative to their effects-based guidelines. Analyses of considerable amounts of data demonstrated that both the incidence and magnitude of toxicity in laboratory tests and the incidence of impairment to benthic communities increases incrementally with increasing mSQGQs. Such concentration/response relationships provide a basis for estimating toxicological risks to sediment-dwelling organisms associated with exposure to contaminated sediments with a known degree of accuracy. This sediment quality assessment tool has been used in numerous surveys and studies since 1994. Nevertheless, mean SQGQs have some important limitations and underlying assumptions that should be understood by sediment quality assessors. This paper provides an overview of the derivation methods and some of the principal advantages, assumptions, and limitations in the use of this sediment assessment tool. Ideally, mean SQGQs should be included with other measures including results of toxicity tests and benthic community surveys to provide a weight of evidence when assessing the relative quality of contaminated sediments.

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1.0 Introduction

Numerical sediment quality guidelines (SQGs)have been demonstrated to be useful tools for assessing the quality of freshwater, estuarine, and marine sediments (*1*–*6*). Various agencies, regions, and programs in North America using a variety of approaches have developed these numerical values. The approaches have been selected to address the receptors that were considered (i.e., sediment-dwelling organisms, wildlife, or humans), the degree of protection to be afforded, the geographic area to which the values were to be applied (i.e., site-specific, regional, or national), and their intended uses (e.g., as informal screening tools, enforceable standards, or remediation objectives). SQGs have been derived with a variety of both theoretical methods that rely upon equilibrium partitioning models and empirical methods that rely upon analyses of matching, field-collected chemistry and biological effects data (*6*). For example, effects-range median (ERM; (*7*)), probable effects levels (PEL; (*8*)), probable effects concentrations (PECs; (*4*)), and sediment quality standards (SQS; (*5*)) have been derived in North America using empirical methods. As other examples, equilibrium partitioning sediment guidelines (ESG) were derived for mixtures of trace metals (*9*), and equilibrium partitioning sediment benchmarks (ESB) were derived for mixtures of polynuclear aromatic hydrocarbons (*10*).

Numerical sediment quality guidelines provide a basis for interpreting whole-sediment chemistry data by identifying the concentrations of chemicals of potential concern (COPCs) that can cause or substantially contribute to adverse effects on sediment-dwelling organisms (*4*). While such SQGs may provide valuable tools for determining if the concentrations of individual COPCs exceed acute or chronic toxicity thresholds, sediments are frequently contaminated with complex mixtures of chemicals and only rarely by a single substance. Some of the challenges of evaluating the ecotoxicology of complex mixtures, especially involving chemicals with different modes of action, were summarized (*11*). Often, the composition of the chemical mixtures can vary considerably within a study area or site, adding to the challenge of identification of the area most in need of further attention. For these reasons, additional tools (i.e., matching toxicity or benthic data and chemistry data) are required to assess the overall risks to sediment-dwelling organisms associated with exposure to sediments that contain mixtures of COPCs.

In response to the need for such tools in the management of contaminated sediments, a robust, yet simple, assessment tool has been developed for assessing the potential effects of contaminant mixtures in sediments (*4*, *12*–*17*). In those studies, mean SQG quotients (mSQGQ) were determined by

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calculating the arithmetic mean of the quotients derived by dividing the concentrations of chemicals in sediments by their respective SQGs. The result is a single, unitless, effect-based index of the relative degree of contamination that can provide a basis for determining the likelihood that a sediment sample would be toxic to sediment-dwelling organisms. Accordingly, mSQGQs provide a number of advantages in the interpretation of the significance of complex mixtures of potentially toxic substances in sediments. However, because this represents a relatively new tool, users of this approach should be aware of a number of important assumptions and limitations with the use of mean SQGQs. The purpose of this paper is to review the methods used to derive the quotients, the history of their use, and some of their advantages, assumptions, and limitations.

2.0 Derivation of Mean SQGQs

Mean SQGQs are typically calculated in a three-step process. First, each chemical concentration in the sample is divided by its respective SQG, resulting in an individual ratio of the concentration of that chemical in the sample to its respective SQG (i.e., a SQG quotient, SQGQ). Then, all the resulting quotients either for all individual chemicals (*14*) or several classes of chemicals (*16–18*) are summed. The individual quotients can be summed for classes of chemicals, typically including three classes: trace metals, polynuclear aromatic hydrocarbons (PAHs), and chlorinated organic hydrocarbons (COHs). This second approach tended to reduce variability in concentration/response relationships where individual SQGs differed in predictive ability (*16, 18*). Finally, either the sum of the individual quotients is divided by the number of SQGs or the sums of the three classes are divided by three to derive the mSQGQ value for each sample.

Any set of effects-based SQGs developed with the same or similar narrative intent can be used to derive the quotients. Mean SQGQs can be calculated with SQGs that were derived with empirical or theoretical (equilibrium-partitioning) methods. However, mean SQGQs have been calculated with guidelines derived with empirical methods more frequently than with those developed with theoretical methods (*6*). In addition, empirically derived guidelines are primarily intended for use in risk assessments, whereas those based on theoretical models are primarily intended to determine the cause of toxicity (*6*). We recommend that mean SQGQs should be calculated with guidelines from one approach or the other, not a combination of the two approaches. Because primarily SQGs derived with empirical methods have been used to calculate mean SQGQs, the focus of this paper is directed toward the empirical approach.

Sediment quality guidelines can be calculated on either a dry weight basis or after normalization to total organic carbon (TOC) or as ratios of simultaneously extracted metals to acid volatile sulfides. The use of SQGs derived with the same methods and the same narrative intent provides the most accurate representation of the degree of contamination. Both the sums and means can be used together to form a weight of evidence. However, the sums of quotients, but not the means, are subject to variability if different numbers of chemicals were measured in different samples. The summed approach is not advised if there are different numbers of chemicals analyzed among different samples. Typically, if a chemical concentration is less than the method detection limit (MDL), either one-half of the MDL is used or that chemical is deleted from the calculation and the denominator is adjusted accordingly. The latter procedure is typically used when the reported detection limit for a substance is greater than its respective SQG. The concentrations of individual chemicals and summed classes of those chemicals (for example, the PAHs) should not be double counted; either the concentrations of individual substances (e.g., naphthalene) or the summed concentrations of the classes should be used (e.g., total PAHs). Individual quotients are included in the calculations of the means if they are fractions of 1.0 or greater than 1.0.

Our collective experience has shown that the relationships between mean SQGQs and measures of biological effects often improved when only the most reliable SQGs are used in the formula (*4, 18–20*). The relative reliability of a particular set of SQGs may differ among study areas due to site-specific differences in the composition of the chemical mixtures. Statistical analyses, such as correlation analyses, of site-specific matching chemistry and measures of effects may be necessary to establish which set of SQGs is most reliable.

3.0 Advantages of Mean SQGQs

Mean SQGQs can provide a single, easily understood, effects-based numerical index of the relative degree of chemical contamination of sediment samples. The numbers of chemicals in a sample that exceed their respective SQGs can be summed as an indication of the presence of these substances at levels of concern. It is logical to rank a sample as more contaminated if it has numerous chemicals exceeding the SQGs than a sample with few or no chemical concentrations greater than the SQGs. However, by only calculating the number of SQGs exceeded, a chemical concentration that exceeds a SQG by a small amount and one that exceeds it by manyfold are treated the same. The mean SQGQ approach allows the analyst to account for not just the presence of the chemical at a concentration greater than the SQG, but also, the magnitude by which the SQG is exceeded in the sample.

The analyst can estimate the probability of observing sediment toxicity by comparing the mean SQGQ in a sample to previously published probability tables (*15, 17, 19*) or, preferably, by establishing site-specific exposure/response relationships. Alternatively, the analyst can apply the regression equations that have been developed to characterize concentration/response relationships (*12–14*). Two examples of concentration/response relationships are illustrated in Figure 1. Both studies compiled data from multiple data sets into one database and compared the incidence of toxicity over ranges in mean SQGQs. In freshwater, the incidence of significant 10- to 14-day mortality in the amphipod *Hyalella azteca* tests increased from 18% to 73% as mean PEC quotients increased over five ranges in values (*17*). In saltwater, the incidence of significant mortality in 10-day tests with *Ampelisca abdita* and *Rhepoxynius abronius* increased from 6% to 91% as mean SQGQs increased over 10 ranges in values (*19*). As indicated with the information summarized in Figure 1 and Tables 1–7, the mean SQGs can be used to establish the concentration/response relationships in large, combined databases as well as site-specific data. In the absence of local site-specific data, analysts can use this information to identify the levels of risk of toxicity that are acceptable and/or unacceptable.

Site maps that show gradients or other patterns in concentrations for numerous individual chemicals can be important elements of a sediment quality assessment. But, such maps can be confusing, especially when there are multiple gradients for multiple chemicals in a complex study area. By condensing the chemical data into a single index, such as mean SQGQs, or a set of three maps for chemical classes, the analyst can display, describe, and monitor just one variable (or three variables) over time and space.

Because mean SQGQs have been demonstrated to provide a reliable basis for classifying whole sediment samples as toxic and not toxic, these tools can form an important component in the remedial action planning process at contaminated sediment sites. That is, preliminary remediation goals (PRGs; i.e., target cleanup levels) can be established by setting remedial action objectives (RAOs) that specify the

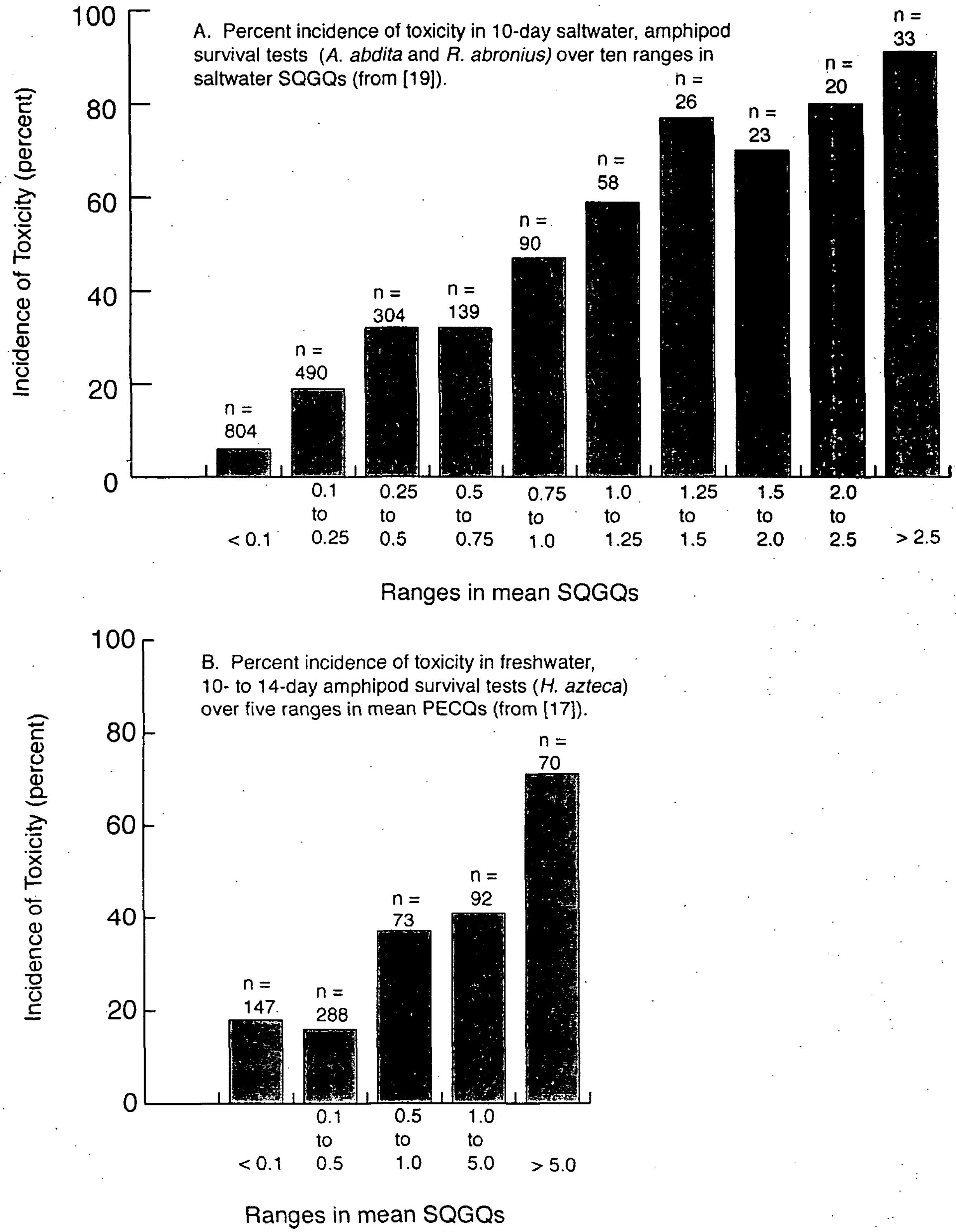

FIGURE 1. Percent incidence of toxicity in amphipod survival tests over ranges in mean sediment quality guideline quotients (SQGQs) in databases compiled nationwide for saltwater and freshwater sediments.

maximum incidence or magnitude of toxicity that is considered to be acceptable, post-remediation. Then, either the published concentration/response relationships or, preferably, site-specific relationships can be used to calculate the mean SQGQ that corresponds to the RAO (*14, 22, 23*). Either national, or, preferably, site-specific, concentration/response relationships can be used to derive such PRGs. It is recommended that site-specific sediment chemistry and toxicity

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data should be obtained to confirm that the selected toxicity thresholds provide the desired level of protection for ecological receptors at the site (*24*). Such PRGs for chemical mixtures (i.e., those based on mean SQGQs) tend to be easier to apply and more accurate than PRGs for numerous individual chemicals. Importantly, such PRGs accompanied by direct measures of toxicity are most relevant when removal or capping represent the preferred remedial alternatives. Different tools are required if source control represents the preferred alternative or total maximum daily loads (TMDLs) need to be developed. These tools may include sediment spiking experiments, toxicity identification studies, and bioaccumulation modeling.

It has been our collective experience that concentration/response relationships in large-scale sediment quality assessments (e.g., those that encompass entire lakes, estuaries, bays) often improve as the data set is focused down to smaller areas that involve only a single pollution gradient with a specific chemical mixture. Accordingly, SQGs and mean SQGQs derived with site-specific information often are more accurate predictors of the presence and absence of toxic effects than guidelines prepared with data from nationwide or other larger-scale databases. In addition, confidence in the use of a set of SQGs in management decisions can increase within smaller areas with site-specific studies of their predictive ability (*24*).

4.0 Assumptions Related to the Application of Mean SQGQs

Mean SQGQs have been calculated most frequently with SQGs derived with empirical approaches, such as the ERM, PEL, and PEC values, in which measures of adverse effects were associated with, but not necessarily caused by, specific chemicals. In contrast to SQGs derived with mechanistic or theoretical approaches in which an exposure/response relationship is determined with single chemicals, most SQGs derived with empirical approaches rely upon field-collected samples in which mixtures of chemicals occur. Although the derivation and use of mean SQGQs with empirically derived guidelines is intuitively appealing, there are a number of important assumptions that are associated with the use of this approach. These assumptions should be considered when using mean SQGQs, especially because causality cannot always be inferred when using empirically derived SQGs (*25*). Some assumptions and limitations may not be obvious to analysts, while others will seem intuitive. None of them should preclude the use of this assessment tool.

Additivity. By normalizing the concentrations of different kinds of chemicals to their respective SQGs and then summing and averaging the individual quotients, the assumption is made that the contributions of each chemical to toxicity are additive. That is, the assumption is made that the chemicals in the sample are not acting antagonistically or synergistically. There is no conclusive empirical evidence of this additivity in nature for all chemicals for which there are SQGs. Because sets of commonly used SQGs include a wide variety of chemicals, it is possible that the assumption of additivity is not correct (*25*). Antagonism between different chemicals has been reported in limited laboratory experiments (*26*). However, there is evidence of additivity in bioassays of clean sediments spiked with individual chemicals and combinations of these chemicals (*27–31*). These studies indicated that responses in bioassays generally were additive when chemicals were first tested separately, then tested in combinations or mixtures. Field confirmation of additivity has been reported in numerous studies in which either the incidence or the severity of toxicity and/or benthic impairment increased incrementally as mean SQGs increased (Figure 1; (*24*); Section 6 below).

Mode of Toxicity. By using the mean SQGQ approach, the assumption is made that all of the chemicals accounted for with the SQGs have the same mode (mechanism) of toxicity. Specifically, the assumption is made that all of them are acting as acute and/or chronic toxins. Such nonionic organic compounds have been referred to as narcotics (*32*). Most of the commonly used SQGs were derived with data from acute toxicity tests or benthic community indices. Thus, by calculating mean SQGQs for multiple chemicals, it is assumed that these chemicals act the same way in test samples as they did in the studies performed to derive the SQGs. That is, the assumption is that these chemicals are not acting primarily, for example, as teratogens, pro-mutagens, mutagens, or carcinogens. If chemicals such as benzo[*a*]-pyrene, polychlorinated biphenyls, or mercury have multiple modes of action, it is assumed that, in this situation, they are acting as direct toxicants that would reduce survival and/or growth of test organisms. It follows, then, that although they represent an integrated tool with which to predict a measurable biological response, mean SQGQs cannot be used to reliably predict effects other than acute or chronic toxicity. Also, it is assumed that the mean SQGQs are not being used to predict bioaccumulative effects in fish, wildlife, or humans.

Causality. The chemicals that are accounted for in the calculations of mean SQGQs may differ in their contribution to the observed toxic effects, but nevertheless chemicals in sediments typically act together as a mixture to elicit a toxic effect. One chemical or class of chemicals at a site may be the major drivers of risks of toxicity, but these chemicals likely do not act alone. Some chemicals in the mixture in a sediment sample may have a relatively minor contribution to a measure of toxicity as compared to other substances in the sample. Nevertheless, the assumption is made that the causes of toxicity are attributable to the mixtures of chemicals in the sediments, including those not measured or not accounted for with the SQGs, not some natural variable. A corollary to these assumptions is that sediments would not be expected to contain unmeasured toxicants or chemicals not accounted for with the SQGs when they do not indicate toxic effects and have low mean SQGQs. Also, these mixtures of chemicals often co-vary in concentration with each other, occurring at low concentrations in the least contaminated samples and occurring in high concentrations in the most contaminated samples. If these assumptions are true, then it follows that site-specific SQGs derived from analyses of matching chemistry and biological data acquired in a small-scale study may not be directly applicable to other sites where other mixtures of chemicals exist. Consistent with this observation, sediment standards developed specifically for Puget Sound (state of Washington) were not recommended for application in other regions (*33*). For example, site-specific guidelines developed by analysis of data from a site contaminated with PCBs and mercury may not accurately predict toxicity in another site in which the chemicals of concern are, say, primarily divalent trace metals or PAHs. Therefore, it has been recommended that site-specific data should be generated to evaluate the predictive ability of SQGs at individual study sites (*12, 13, 24*). Methods and guidance on site-specific studies of predictive ability have been provided previously (*24*).

Relative Risk of Toxicity. Use of the mean SQGQ approach assumes that samples from a study site with the same or similar mean SQGQs, but with different chemical characteristics, would have the same or similar probabilities of being toxic if they were subjected to toxicity testing. That is, the assumption is made that the relative risk of toxicity posed by two samples with the same mean SQGQs, but with different mixtures or proportions of chemicals, would be the same. Otherwise, the chemical index scores generated by calculating mean SQGQs would be meaningless as estimates of relative risk. This assumption could mean that samples with extremely different chemical characteristics but the same mean SQGQs would be classified the same. For example, a sample with only one chemical elevated in concentration above the SQG and none others at detectable concentrations and a second sample with multiple chemicals only slightly elevated in concentrations could have similar mean SQGQs and, therefore, ostensibly the same probability of causing toxicity. There is evidence that this is a safe assumption because both the degree of mortality and the incidence of toxicity tend to increase in a predictable pattern as mean SQGQs increase in large data sets composed of samples with differing chemical mixtures (*17, 19, 21*). Such concentration/response relationships have been reported in multiple saltwater and freshwater studies and all of these studies demonstrate incremental increases in adverse effects over ranges of increasing mean SQGQs, regardless of the composition of the chemical mixtures (*20, 24*). However, the degree of variability in toxicity among samples within the same range in mean SQGQs at a site may reflect, at least in part, the degree of variability in the composition of the chemical mixtures among the samples.

5.0 Limitations in the Use of Mean SQGQs

Potential users of this tool should be aware of several important limitations in the approach. None of these limitations should preclude use of the mean SQGQ assessment tool.

First, it can be difficult to reach agreement regarding the level of mean SQGQs to be used as unacceptable and acceptable for classification of samples at a site. It is rarely possible to identify chemical concentrations that cause toxic effects in 100% of samples. Intuitively, a mean quotient of 1.0 could be viewed as mean SQG unity and indicative of an important point in a scale of contamination, much like a hazard quotient. However, it can be more meaningful at a site to identify an inflection point in the data to distinguish between nontoxic (i.e., reference or background) sites and adversely affected sites. Such inflection point(s) along the chemical contamination scale can be important to determine where primarily safe conditions end and where primarily toxic conditions begin. These inflection points can differ considerably among sites. The inflection point can differ as functions of the nature of the chemical mixtures at the site, the SQGs that were used, and the sensitivity of the test of toxicity used at the site. The most accurate and objective way to establish the inflection point from primarily safe levels to primarily toxic levels using this tool is to calibrate the mean SQGQs to the matching results of toxicity tests and/or benthic community composition analyses. Such calibration is optimal when done with site- or location-specific data. However, barring the availability of site-specific data, calibrations can be made with large data sets previously reported (*15, 17, 19, 21, 24, 34–37*).

Second, it is important to recognize that the mean SQGQ tool is not a panacea. As is the case with any multi-parameter index, by condensing data from multiple chemicals into one index, information on individual chemicals will be masked. Although mean SQGQs can be used as stand-alone assessment tools for classifying sediment contamination, they are best used with other information, such as the data from toxicity tests. Use of this tool should not preclude examination of the individual chemical data, including those for ammonia, total organic carbon (TOC), and other water quality variables. Other chemicals for which there are no SQGs may be important at the site (e.g., chlorpyrifos and other pesticides), especially for measures of effects other than toxicity (i.e., for bioaccumulative substances). It is important to understand that mean SQGQs cannot be used to accurately predict the uptake and bioaccumulation of sediment-bound chemicals by fish, wildlife, and humans.

Third, mean SQGQs can be used only to account for the presence and concentrations of chemicals for which the mean SQG quotients were calculated. That is, the mean quotients cannot be assumed to be surrogates for other unmeasured substances or measured substances for which there were no SQGs. They may, in fact, be accurate surrogates of the presence of other substances, but such co-variance must be determined empirically with site-specific data. In addition, mean SQGQs calculated with guidelines derived with empirical methods may not be accurate indicators of which chemicals in the sediments were the cause of toxicity or benthic impairment. Additional analyses, such as toxicity identification evaluations and laboratory bioassays of clean sediments spiked with known chemicals, may be needed to accurately determine causality (*6*).

Fourth, because the mean SQGQs were not initially derived as regulatory standards or criteria, their usage is not widely addressed in regulatory or risk assessment methods manuals. Some regulatory and regulated entities may object to their use in enforcement and remediation activities because mean SQGQs were not initially derived for those purposes. However, the derivation and interpretation of mean PEC quotients is included in guidance manuals issued for sediment quality assessments by the Great Lakes National Program Office of U.S. EPA (*38–40*). In addition, numerical sediment quality criteria have been established in British Columbia (Canada) based on mean PELQs (*41*).

6.0 Applications of Mean SQGQs

History of Use and Development. Mean SQGQs initially were calculated in evaluations of chemistry data generated in sediment quality surveys conducted in marine bays and estuaries by the National Oceanic and Atmospheric Administration (NOAA), as a part of its National Status and Trends Program. In partnerships with the states of Florida and California, surveys were conducted in Tampa Bay (FL) (*42, 43*) and San Pedro Bay (CA) (*44*), respectively. In the reports from both surveys, mean ERM quotients were calculated to compare and rank the degree of contamination among sampling sites, using the ERM values of ref *7*. Mean ERM quotients were calculated in subsequent surveys of Boston Harbor (MA), Savannah River (GA), Charleston Harbor (SC), Biscayne Bay (FL), western Florida panhandle (FL), Sabine Lake (TX), San Diego Bay (CA), San Pedro Bay (CA), and Puget Sound (WA) conducted by NOAA and state agency partners. Results of these surveys were published in a series of technical reports and journal articles (*45–52*). Using the PEL values derived by MacDonald et al. (*8*), mean PEL quotients also were calculated for the report on the Biscayne Bay survey (*47*).

The relationships between both the degree of response and percent incidence of toxicity in laboratory toxicity tests and ranges in both the mean ERM- and mean PEL quotients were evaluated with large data sets compiled from saltwater studies completed nationwide (*15, 21*). In their evaluations of regional monitoring data from San Francisco Bay (CA), Thompson et al. (*53*) reported significant correlation coefficients between mean ERM quotients and percent amphipod survival. The manner in which the quotients were calculated was revised by using a combination of ERMs, PELs, and other SQGs to establish the best statistical relationships between mean SQGQs and both percent incidence of toxicity and mean amphipod mortality (*19*). Results of toxicity tests were compared among ranges of increasing mean ERM quotients in Southern California (*54*). Using both the ERMs and the Washington State SQS values, Long et al. (*52*) described the degree of contamination in Puget Sound sediments.

The relationships between mean SQGQs and the incidence of impaired benthic communities were described in analyses conducted with estuarine data sets (*36, 37*). The predictive

TABLE 1. Incidence of Toxicity (IOT) and Magnitude of Toxicity (MOT) within Two Ranges in Mean Probable Effect Concentration Quotients (PECQs) in the Calcasieu Estuary, Louisiana (data from ref *12*)

species tested	duration of exposure (days)	endpoint measured	mean PECQ <0.31 n^a	mean PECQ <0.31 IOT (%)	mean PECQ <0.31 MOT (% survival)	mean PECQ >0.31 n	mean PECQ >0.31 IOT (%)	mean PECQ >0.31 MOT (% survival)
Hyalella azteca	10 d	survival	73	22	82	12	50	54
	28 d	survival	63	29	84	12	83	52
Ampelisca abdita	10 d	survival	97	58	56	29	90	23

[a] n = number of samples.

abilities of mean PEC quotients were evaluated in separate databases generated for the saltwater sediments of the Calcasieu estuary in Louisiana (*12*) and the Tampa Bay estuary (*22*). The relationships between indices of macrobenthic community composition and mean ERMQs were determined in San Francisco Bay (*55*). The responses of acute and chronic toxicity tests to a range in mean ERMQs were compared in upper Chesapeake Bay (MD) (*56*).

In freshwater, the first application of this approach was in a study of the contamination of sediments in the Great Lakes (*16*). Both maximum and summed quotients were used to classify the degree of chemical contamination. Using the PEC values prepared by MacDonald et al. (*4*) for freshwater, concentration/response relationships were determined in several studies (*16–18, 34, 35, 38–40*). In a study of the St. Louis River Area of Concern (*34, 35*), mean PEC quotients were compared to results of both amphipod and chironomid toxicity tests. The concentration/response relationships observed in the study site were compared to those in data compiled from other Great Lakes sites. Concentration/response relationships were described for both amphipod and chironomid toxicity tests with data from up to 670 samples (*13*). Similar analyses were performed with data from a survey of Barton Springs (TX) (*58*), the Grand Calumet River and Indiana Harbor (*23, 59*), the southeastern United States (*14*), and with data from the upper Columbia River Basin (*13*). For the Calcasieu Estuary (Louisiana), the relationships between mean PECQs and the survival and incidence of toxicity to the freshwater amphipod *Hyalella azteca* and the marine amphipod *Ampelisca abdita* were determined to support an assessment of risks to the benthic invertebrate community and to develop preliminary remediation goals (*12*). The size of the area and the volume of material to be dredged was established with mean PECQs in a remedial investigation/feasibility study for Onondaga Lake (NY), based on inflection points calibrated to the response in laboratory tests with chironomids and amphipods (*60*).

The predictive abilities of most currently available SQGs were summarized in large databases compiled for a Pellston Workshop on "Use of Sediment Quality Guidelines and Related Tools for the Assessment of Contaminated Sediments" convened by the Society of Environmental Toxicology and Chemistry (*6, 20, 24*). In this workshop, matching chemical and toxicological data from most major regions of the United States were compiled and evaluated. Many of the data sets that were evaluated and compared involved the derivation of mean SQG quotients. As a part of this workshop, the attendees compared the concentration/response relationships among data sets using various mean SQG quotients and results of either toxicity tests or benthic community analyses. Data from over 8000 samples were compiled by the contributors to represent the current state of the science. In all data sets tested thus far, the relative risks of observing either toxicity in laboratory tests or benthic community impairment increased incrementally with increasing mean SQGQs, regardless of which SQGs were used (*20, 24*).

Case Studies of Exposure/Response Relationships using Mean SQGQs. In all cases that involve the delineation and remediation of a contaminated sediment site, narrative goals must be established for sediment quality that represent acceptable and unacceptable conditions. For example, the site managers may chose to protect 95% of the benthic species, or to eliminate acute toxicity to 80% of test organisms, or eliminate liver neoplasms in 90% of resident demersal fish. Once a narrative goal or a set of goals is established, the sediment quality analysts can use the available data to determine the chemical conditions necessary to attain these goals. The following case studies are summarized as examples of the concentration/response relationships reported previously using mean SQGQs and measures of toxicity and/or benthic community effects. These examples were included because they represent a wide range in the kinds of biological effects endpoints and their differential sensitivities and they exemplify conditions in both freshwater and saltwater.

Estuarine sediments from the Calcasieu Estuary (Louisiana) were tested with both the freshwater amphipod *Hyalella azteca* (10- and 28-day exposures) and the marine amphipod *Ampelisca abdita* (10-day tests) (*12*). The percent incidence of toxicity and average percent survival were compared between a group of samples with mean PECQs ≤0.31 and a group of samples with mean PECQs >0.31 (Table 1). A mean PECQ of 0.31 was determined as the critical value (inflection point) in this study by examining the distribution of both the mean PECQs and the toxicity test results. The incidence of toxicity was considerably higher and the average percent survival was lower in the samples with mean PECQ >0.31 relative to the less contaminated samples. The 10-day tests with *A. abdita* appeared to be more sensitive than the 10-day tests with *H. azteca*; however, a considerable gain in sensitivity in the latter tests occurred with 28-day exposures.

In a study of the freshwater sediments of the lower Columbia River (state of Washington,), results were obtained for three toxicity tests (*H. azteca, Chironomus dilutus, Ceriodaphnia dubia*) and compared over four ranges in mean PEC quotients (*13*). In all three tests, the percentages of samples classified as toxic were lowest in sediments with the lowest mean PEC quotients (<0.1) and the incidence of toxicity increased incrementally as the quotients increased, peaking in the most contaminated samples (quotients >5.0) (Table 2). The concentration/response relationships differed among the three different tests in the first three ranges in mean PECQs, but the percentages of samples that were toxic were remarkably similar in the most contaminated sediments (75 to 81%).

In a study of the sediments of Indiana Harbor (Indiana), the mean PEC quotients that corresponded with 20% and 50% probabilities of toxicity in tests with *H. azteca* were determined with a logistic regression model (*61*). Then, the actual incidence of toxicity within the three ranges in mean PECQs defined with these two values were determined (Table 3). Mean PECQs were calculated for the trace metals alone, the PAHs alone, and the sums of the quotients for metals,

TABLE 2. Incidence of Toxicity (IOT) within Four Ranges in Mean Probable Effect Concentration Quotients (PECQs) in the Columbia River, Washington (data from ref *13*)

			Mean PECQ							
			<0.1		0.1–1.0		>1.0		>5.0	
species tested	duration of exposure (days)	endpoint measured	*n*[a]	IOT (%)	*n*	IOT (%)	*n*	IOT (%)	*n*	IOT (%)
Hyalella azteca	7–14 d	survival	19	11	58	26	47	51	21	81
Chironomus dilutus	≥20 d	survival	5	0	20	15	12	58	5	80
Ceriodaphnia dubia	7–10 d	survival or reproduction	7	14	7	29	12	33	4	75

[a] *n* = number of samples.

TABLE 3. Incidence of Toxicity (IOT) within Three Ranges in Mean Probable Effect Concentration Quotients (PECQs) in the Indiana Harbor Area of Concern, Indiana (data from ref *23*)

			incidence of toxicity[a] (pct)					
mixture model	P_{20}[b]	P_{50}	*n*[c]	$<P_{20}$	*n*	$P_{20}-P_{50}$	*n*	$>P_{50}$
mean PECQ for metals	0.84	2.5	69	13	25	52	22	73
mean PECQ for PAHs[d]	1.9	5.8	81	11	8	50	27	93
mean PECQ for metals, PAHs, PCBs	2.9	5.5	81	14	11	45	24	92

[a] Based on the results of 28-day survival tests with the amphipod, *Hyalella azteca*. [b] P_{20}; P_{50} = sediment quality guideline quotient that corresponds with a 20% or 50% probability of observing toxicity. [c] *n* = number of samples. [d] PAHs = polycyclic aromatic hydrocarbons; PCBs = polychlorinated biphenyls.

PAHs, and polychlorinated biphenyls (PCBs). In all three cases, the incidence of toxicity (11–14%) was lowest in the least contaminated sediments and increased to approximately 50% in the intermediate category. The highest incidence of toxicity (73–93%) occurred in samples with mean PECQs for metals, PAHs, and for metals/PAHs/PCBs greater than 2.5, 5.8 and 5.5, respectively. Also, the lack of an increase in toxicity when the data for metals and PCBs were added to the quotients for PAHs alone suggests that these groups were less important contributors to toxicity than the PAHs.

In the St. Louis River (Wisconsin and Minnesota), toxicity tests were performed with *H. azteca* and *C. dilutus* and results were compared over four ranges in mean PECQs (*34*) (Table 4). In both tests, the lowest incidence of toxicity (7%) occurred in the least contaminated sediments, toxicity increased incrementally as the quotients increased, and peaked (75–100%) in the most contaminated samples. The numbers of samples (4 or 5) in the most contaminated category were relatively small.

Both the composition of benthic assemblages and results of two toxicity tests were compared to mean PEL quotients in the marine sediments of Tampa Bay (Florida) (*22*). Three ranges in mean PEL quotients were identified in this study that distinguished the results of the biological tests (Table 5). Average sea urchin fertilization success in tests of pore waters differed by a factor of approximately 6 between the most and least contaminated sediments, whereas average amphipod survival decreased by only 14%. Five indices of benthic community composition decreased incrementally with increasing mPELQs with up to a 25-fold difference in averages between the most and least contaminated samples. These results are typical of the relatively greater sensitivity of indices of benthic community composition and of sea urchin fertilization tests than the 10-day amphipod survival test (*36, 37*). In addition, some of the variability among stations in benthic community composition may have been attributable to the effects of co-varying natural factors such as sediment texture, TOC, depth, salinity, etc.

Measures of both acute toxicity and of benthic community composition were recorded in a survey of Biscayne Bay (Florida) (*47*). A portion of this survey included the maritime Port of Miami area and the adjoining saltwater reaches of the lower Miami River. Six benthic metrics and results of three toxicity tests are contrasted among three ranges in mean ERM quotients (Table 6). Average amphipod survival (*A. abdita*) and Microtox EC50 concentrations decreased slightly from the least contaminated to the intermediate category, then decreased greatly in the most contaminated sediments, whereas percent sea urchin fertilization in pore waters did not differ among the three categories. Whereas the abundance of all benthic species did not distinguish among categories, the numbers of species and the abundance of pollution-sensitive arthropods, amphipods, and ampeliscid amphipods diminished steadily and incrementally as chemical contamination increased. The average abundance of pollution-tolerant capitellid polychaetes increased along this contamination gradient. These data also agree with the observations made in previous estuarine studies of the relatively greater sensitivity of the benthos to low levels of contamination as compared to that of the 10-day amphipod survival test (*36, 37*). Also, as reported for other regions, many of the benthic metrics co-varied among stations with both the mean ERM quotients and measures of sediment texture, TOC, and salinity (*47*).

A large-scale survey of Puget Sound (state of Washington) involved analyses of chemistry, toxicity, and benthic community composition in 300 samples (*52*). The survey area

TABLE 4. Incidence of Toxicity (IOT) within Four Ranges in Mean Probable Effect Concentration Quotients (PECQs) in the St. Louis River Area of Concern (Wisconsin and Minnesota) (data from ref *34*)

			incidence of toxicity (pct)							
species tested	duration of exposure (days)	endpoint measured	*n*[a]	<0.1	*n*	0.1–1.0	*n*	>1.0	*n*	>5.0
Hyalella azteca	10 d	survival or growth	44	7	90	13	15	40	4	75
Chironomus dilutus	10 d	survival or growth	46	7	84	13	16	56	5	100

[a] *n* = number of samples.

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TABLE 5. Magnitude of Toxicity (MOT) and Benthic Invertebrate Indices within Three Ranges in Probable Effect Level Quotients (PELQs) in Tampa Bay, Florida (data from ref *22*)

		mean PEL quotient					
		<0.05		0.05–0.33		≥0.34	
benthic metric/ toxicity test	endpoint measured	n^a	mean (SD)^b	n	mean (SD)	n	mean (SD)
sea urchin fertilization (*Arbacia punctulata*)	pct.	33	48 (31)	66	41 (35)	42	8.3 (19)
amphipod survival (*Ampelisca abdita*)	pct.	29	91.5 (6)	42	86.7 (5)	25	78.0 (14)
Shannon–Wiener diversity index	index	342	3.46 (0.97)	157	2.01 (1.30)	36	1.09 (1.09)
total abundance	no./m$^{2\,c}$	342	9620 (13000)	157	7200 (11900)	36	3070 (4900)
amphipod abundance	no./m^2	340	1820 (5050)	157	1610 (5540)	36	72 (194)
gastropod abundance	no./m^2	342	953 (2040)	157	195 (412)	36	40 (130)
capitellid polychaete abundance	no./m^2	342	335 (763)	157	335 (1010)	36	18 (52)

^{a} n = number of samples. ^{b} SD = standard deviation. ^{c} no./m^2 = number per meter square.

TABLE 6. Magnitude of Toxicity (MOT) and Benthic Invertebrate Indices within Three Ranges in Mean Effects Range Median Quotients (ERMQs) in Biscayne Bay/Lower Miami River, Florida (data from ref *47*)

		mean ERM quotient					
		<0.03		0.03–0.2		≥0.2–2.0	
benthic metric/toxicity test	endpoint measured	n^a	mean (SD)^b	n	mean (SD)	n	mean (SD)
amphipod survival (*Ampelisca abdita*)	percent	28	96 (7)	37	93 (18)	20	41 (32)
sea urchin fertilization (*Arbacia punctulata*)	percent	28	84 (20)	37	76 (25)	20	85 (24)
microtox microbial bioluminescence	mean EC_{50}^{c}	28	144 (309)	37	105 (231)	20	23 (43)
total abundance	no./sample	10	613 (231)	12	427 (374)	7	471 (408)
number of species	no./sample	10	91 (16)	12	58 (35)	7	6 (2)
arthropod abundance	no./sample	10	179 (98)	12	96 (139)	7	10 (14)
amphipod abundance	no./sample	10	92 (71)	12	35 (77)	7	6 (12)
ampeliscid abundance	no./sample	10	3 (3)	12	2 (6)	7	0 (0)
capitellid polychaete abundance	no./sample	10	5 (3)	12	15 (13)	7	204 (279)

^{a} n = number of samples. ^{b} SD = standard deviation. ^{c} mean EC_{50} = mean effective concentration of sediment that caused a 50% reduction in light production.

TABLE 7. Magnitude of Toxicity (MOT) and Benthic Invertebrate Indices within Five Ranges in Mean Effects Range Median Quotients (ERMQs) in Puget Sound, Washington (data from ref *52*)

		mean ERM quotient									
		<0.1		0.1–0.2		≥0.2–0.4		≥0.4–1.0		>1.0–4.2	
benthic metric/ toxicity test	endpoint measured	n^a	mean (SD)^b	n	mean (SD)	n	mean (SD)	n	mean (SD)	n	mean (SD)
amphipod survival (*Ampelisca abdita*)	percent	89	97 (7)	122	98 (4)	43	99 (4)	30	97 (6)	16	96 (6)
sea urchin fertilization (*S. purpuratus*)^c	percent	89	105 (15)	122	102 (20)	43	97 (30)	30	75 (40)	16	84 (26)
microtox microbial bioluminescence	mean EC_{50}^{d}	89	16 (27)	122	7 (16)	43	9 (15)	30	17 (36)	16	18 (24)
cytochrome p450 induction	B[a]p equiv.^{f}	89	6 (5)	122	13 (13)	43	30 (34)	30	93 (106)	16	249 (469)
total abundance	no./sample^f	89	797 (1040)	122	569 (450)	43	1140 (1288)	30	927 (825)	16	881 (450)
number of species	no./sample	89	71 (26)	122	44 (18)	43	46 (23)	30	59 (28)	16	60 (22)
dominance index	no./sample	89	15 (9)	122	8 (5)	43	7 (5)	30	8.3 (5.6)	16	8 (8)
arthropod abundance	no./sample	89	188 (351)	122	112 (170)	43	285 (387)	30	107 (135)	16	55 (78)
echinoderm abundance	no./sample	89	20 (59)	122	24 (74)	43	82 (162)	30	6 (15)	16	0.4 (1)
phoxocephalidae abundance	no./sample	89	13 (24)	122	6 (12)	43	17 (31)	30	1 (2)	16	1 (1)
Aphelochaeta spp. abundance	no./sample	89	51 (284)	122	75 (228)	43	122 (311)	30	323 (581)	16	331 (358)

^{a} n = number of samples. ^{b} SD = standard deviation. ^{c} *S. purpuratus* = *Strongylocentrotus purpuratus*. ^{d} mean EC_{50} = mean effective concentration of sediment that caused a 50% reduction in light production. ^{e} B[a]p equiv. = Benzo[a]pyrene equivalents, ug/g. ^{f} no./sample = number per 0.1m^2 sample.

included urban bays, deep channels, large basins, small rural bays, inlets, and fjords. Apparently because of their relatively low sensitivity, average amphipod survival in solid-phase sediments, percent fertilization of sea urchin eggs in pore waters, and Microtox EC50's in tests of organic extracts were similar over five ranges in mean ERMQs (from <0.1 to 1.0–4.2) (Table 7). However, cytochrome p450 induction in a Human Reporter Gene System assay of organic solvent extracts increased steadily with increases in the mean ERM quotients, resulting in a 42-fold difference between the average response in the most and least contaminated samples. Total abundance of the benthic invertebrates did not change substantially as contamination increased. However, total numbers of species and the numbers of dominant species decreased in the second range of mean SQGQs and remained low as contamination increased. The abundance of pollution-sensitive arthropods, echinoderms, and phoxocephalid amphipods generally diminished, whereas the abundance of pollution-tolerant polychaetes (*Aphelochaeta* spp.) increased as levels of contamination increased. Therefore, there was strong evidence of benthic disturbance at relatively low levels of contamination that did not cause an increase in toxicity in laboratory tests. However, the composition of the benthos in Puget Sound varied with both the mean ERM quotients and with co-varying measures of depth, near-bottom salinity, sediment texture, and TOC content (*52*).

The general exposure-response relationships for mean SQG quotients and laboratory toxicity tests were determined in evaluations of databases compiled from sediment quality surveys conducted nationwide in both saltwater and freshwater (Figure 1). Toxicity tests were performed with amphipods in both databases. The saltwater data were compiled from estuaries and marine bays along the Atlantic, Pacific, and Gulf of Mexico coasts of the United States (*19*). The freshwater data were compiled from the Great Lakes and other midwestern lakes and harbors (*17*). In both cases, the incidence of toxicity was relatively low in sediments with mean SQGQs of less than 0.1 and increased to approximately 50% as the quotients increased to 1.0 or greater. The incidence of toxicity peaked at 70–90% in both databases with quotients >5.0 in freshwater and >2.5 in saltwater. These data indicated that the concentration/response relationships observed in individual survey areas (Tables 1–7), also are apparent over larger spatial scales in data compiled from numerous locations. Therefore, these data corroborate the concentration/response relationships of increasing toxicity and benthic impairment with increases in either mean SQGQs or numbers of SQGs exceeded previously reported from analyses of many data sets (*6*).

In a recent experiment, the response of *H. azteca* exposed in laboratory toxicity tests was compared to the response of benthic invertebrates colonizing contaminated sediments in the field (*62*). Specifically, exposures were conducted with dilutions of field-collected sediments contaminated primarily with PAHs, PCBs, and metals. Measures of survival, growth, or reproduction in 42-d laboratory sediment toxicity tests with *H. azteca* were required to predict toxic effects observed on benthic communities exposed to similar sediments in the field. Importantly, effects on the benthic invertebrates colonizing the trays containing contaminated sediments occurred at lower chemical concentrations compared to concentrations that were toxic in 10-day laboratory mortality tests with *H. azteca*. The IC50 (50% inhibition concentration) for 42-day *H. azteca* reproduction was estimated to occur at a mean PECQ of about 0.6 and an IC50 for nematode colonization was estimated to occur at a mean PECQ of about 2.1. These mean PECQ effect concentrations were similar to mean PECQ effect concentrations observed in a database for 28- to 42-day *H. azteca* toxicity tests with field-collected sediment, reflecting the greater sensitivity of the longer term tests (*16, 17*). Results of this study indicate that use of chronic laboratory tests and manipulative field experiments may be needed to estimate impacts observed on benthic communities exposed to contaminated sediments in addition to estimating impacts using synoptic surveys of benthic communities.

7.0 Summary of Observations and Future Considerations

Since the mid-1990s, sediment quality analysts have used the basic concept of classifying the relative degree of chemical contamination of sediments with mean SQG quotients. Several federal agencies, multiple state and provincial agencies, many regional ambient monitoring programs, and environmental consulting firms have used the approach. It has been incorporated into risk assessments at contaminated sediment sites and accepted and published in the peer-reviewed scientific literature and in government publications. Analyses of large freshwater and saltwater data sets have shown that both the magnitude of response and the incidence of toxicity and/or benthic community impacts generally increase as mean SQGQs increase. However, these data also demonstrated that the inflection points of transition from primarily nontoxic conditions to impacted conditions often are site-specific. Nevertheless, there is considerable evidence that this assessment tool can be predictive of the presence or absence of toxic effects with a quantifiable degree of confidence.

Mean SQGQs provide the advantage of condensing complicated information from numerous chemicals into a single effects-based index that accounts for both the presence of chemicals and their concentrations relative to SQGs. Thus, this approach can be used to interpret complicated data with a single index for estimating relative risks of effects upon benthic macroinvertebrates. However, an understanding of several important assumptions and limitations to the use of this tool is critical to using it correctly. This tool is used best in sediment quality assessments as one of multiple lines of evidence with which to classify the relative quality of sediments. The weight of evidence necessary in a sediment quality assessment should be a function of the weight and cost of the decisions to be made with the data from the assessment (*6*).

We expect that further improvements in this assessment tool will arise in future years with additional research. Research is needed to increase our understanding of the effects of natural sedimentological factors (i.e., grain size, TOC, depth) versus anthropogenic chemicals in causing or contributing to the impairment of the resident benthos. More sensitive, whole sediment toxicity tests with both acute and chronic endpoints are needed to improve sensitivity without substantially increasing costs. Effects-based, SQGs are needed for more chemicals, especially relatively new toxicants in flame-retardants, personal care products, and pesticides.

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