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AN EVALUATION OF METHODS FOR CALCULATING MEAN SEDIMENT QUALITY GUIDELINE QUOTIENTS AS INDICATORS OF CONTAMINATION AND ACUTE TOXICITY TO AMPHIPODS BY CHEMICAL MIXTURES

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Abstract—Mean sediment quality guideline quotients (mean SQGQs) were developed to represent the presence of chemical mixtures in sediments and are derived by normalizing a suite of chemicals to their respective numerical sediment quality guidelines (SQGs). Mean SQGQs incorporate the number of SQGs exceeded and the degree to which they are exceeded and are used for comparison with observed biological effects in the laboratory or field. The current research makes it clear, however, that the number and type of SQGs used in the derivation of these mean quotients can influence the ability of mean SQGQ values to correctly predict acute toxicity to marine amphipods in laboratory toxicity tests. To determine the optimal predictive ability of mean SQGQs, a total of 18 different chemical combinations were developed and compared. The ability of each set of mean SQGQs to correctly predict the presence and absence of acute toxicity to amphipods was determined using three independent databases (n = 605, 2753, 226). Calculated mean SQGQ values for all chemical combinations ranged from 0.002 to 100. The mean SQGQ that was most predictive of acute toxicity to amphipods is calculated as SQGQ1 = ((Σ ([cadmium]/4.21)([copper]/270)([lead]/112.18)([silver]/1.77)([zinc]/410)([total chlordane]/6)([dieldrin]/8)([total PAH_{oc}]/1,800)([total PCB]/400))/9). Both the incidence and magnitude of acute toxicity to amphipods increased with increasing SQGQ1 values. To provide better comparability between regions and national surveys, SQGQ1 is recommended to serve as the standard method for combination of chemicals and respective SQGs when calculating mean SQGQs.

Keywords—Sediment quality guideline quotients Amphipod Toxicity Chemical mixtures

INTRODUCTION

Although the use of empirically derived sediment quality guidelines (SQGs) in sediment monitoring and assessment has been the subject of debate, recent reports suggest SQGs continue to be widely used to predict when chemical concentrations are likely to be associated with a measurable biological response [1–5]. Use of SQGs has been encouraged by recent research that indicates reasonable predictive ability of SQGs [6], in combination with limited application or regional specificity of chemical guidelines derived through other methods [7–11]. The increasing use of SQGs results from a practical need for protective management tools when identifying areas where anthropogenic chemicals may present a risk to benthic biota. Unfortunately, the inappropriate application of SQGs has resulted in criticism of their use in sediment management. There is a need to continually reexamine the appropriate use of SQGs as management tools and to refine uses of SQGs to better predict toxicity and/or biological community impairment.

Empirically derived SQGs have been generated from large sets of synoptically collected chemical and biological data [6]. Sediment quality guidelines were developed primarily from field-collected sediments using statistical approaches that associate chemical concentration and biological response. They were established to demonstrate the individual chemical concentrations at which biological effects were expected to be present or absent [12]. Chemical mixtures can also be represented using SQGs and are generally calculated by normalizing each chemical found in the sediment to its respective SQG value and then averaging the resulting normalized values for a given suite of chemicals. These normalized chemical summaries (hereafter referred to as mean sediment quality guideline quotients, or mean SQGQs) represent complex chemical mixtures within each unique sediment sample as a quantitative numeric value that incorporates both the magnitude and number of SQGs exceeded. Mean SQGQs can be used to predict the probability of biological effects in the laboratory or field as previously demonstrated [12–14]. In this article, we report and compare a variety of methods for calculating mean SQGQs with the objective of proposing a standardized method for SQGQ calculation that improves the ability of SQGQs to predict whole sediment acute effects on amphipods.

METHODS

This research evaluated the type and number of analytes in the SQGQ calculation to find chemical combinations that best predicted biological effects, as indicated by marine amphipod mortality in sediment toxicity tests. Mean SQGQS were calculated using effects range-median (ERM) [15,16] and probable effects level (PEL) [17] SQG values for normalizing sediment chemical concentrations. The ERM and PEL sediment quality guidelines have been published for 10 individual trace metals, three individual pesticides, 13 individual polycyclic aromatic hydrocarbons (PAHs), three groupings of individual PAHs.

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Table 1. Mean sediment quality guideline quotients (SQGQ) chemical combinations using effects range median (ERM) sediment quality guideline (SQG) values

Mean SQGQs using ERM guidelines[a]					
ERMQ1	ERMQ2	ERMQ3	ERMQ4	ERMQ5	ERMQ6
Antimony	Arsenic	Cadmium	Antimony	Arsenic	Arsenic
Arsenic	Cadmium	Chromium	Arsenic	Cadmium	Cadmium
Cadmium	Chromium	Copper	Cadmium	Chromium	Chromium
Chromium	Copper	Mercury	Chromium	Copper	Copper
Copper	Lead	Zinc	Copper	Lead	Lead
Lead	Mercury	Total DDT	Lead	Mercury	Mercury
Mercury	Silver	Dieldrin	Silver	Silver	Silver
Silver	Zinc	Total PCBs	Zinc	Zinc	Zinc
Zinc	2-Methylnaphthalene	Low mol wt PAHs	Total DDT	Total chlordane	Total chlordane
Total DDT (OC)	Dibenz[*a*,*h*]anthracene	High mol wt PAHs	Total chlordane	Dieldrin	Dieldrin
Total chlordane	Acenaphthene		Dieldrin	Total PCBs	Total PCBs
Dieldrin	Acenaphthylene		Total PCBs	Low mol wt PAHs	Low mol wt PAHs
Endrin	Anthracene		Low mol wt PAHs	High mol wt PAHs	Total PAHs
Total PCBs	Benz[*a*]anthracene		Total PAHs		
Low mol wt PAHs	Benzo[*a*]pyrene				
High mol wt PAHs	Chrysene				
	Fluorene				
	Fluoranthene				
	Naphthalene				
	Phenanthrene				
	Pyrene				
	p′*p*′-DDE				
	Total DDT				
	Total PCBs				

[a] ERMQ chemical combinations used effects range median SQGs [15,16] as critical values for mean quotient calculation except ERMQ1, which used an organic carbon normalized SQG [33] value for total DDT. OC = organic carbon; PCBs = polychlorinated biphenyls; PAHs = polycyclic aromatic hydrocarbons; mol wt = molecular weight.

two summed organochlorine pesticides, and the sum of 18 polychlorinated biphenyl congeners (PCBs) [15–17]. Guideline values for these 32 chemicals were selected because of published studies demonstrating the reliability and predictive ability of the individual guideline values [6,16]. Two different chemical combinations that were used in previous studies were compared initially and evaluated for their ability to correctly classify sediments as toxic or nontoxic. Based on the results of this comparison, 10 additional chemical combinations were sequentially tested using various combinations of the same chemicals and their respective SQGs. Each successive combination was an attempt by the investigators to improve mean SQGQ predictive ability based on the results of the previous combination. Six of the 12 calculation methods were based on various combinations of chemicals that were divided by their respective ERM guidelines (Table 1). Six PELQ calculation methods were based on various combinations of chemicals that were divided by their respective PEL guidelines (Table 2).

In an attempt to evaluate mean SQGQs that incorporated additional types of SQGs, an assessment of the predictive ability of individual SQGs was performed. The assessment included individual SQGs developed using correlative approaches, consensus approaches, and theoretical approaches. Individual SQGs were selected for inclusion in mean SQGQ quotient calculation methods when the values best predicted acute toxicity to amphipods for that chemical or chemical class and were representative of chemical concentrations most commonly found in field samples from the database (italicized entries in Table 3). A total of 15 individual SQGs were selected for use in additional chemical combinations. These SQGs were incorporated into six SQGQ calculation methods that were based on combinations of chemicals divided by a mixture of respective ERM, PEL, or other selected individual SQGs (Table 4).

Each mean quotient calculation method included chemicals and their respective SQGs for each of four major chemical groups (metals, pesticides, PAHs, PCBs). A total of 18 chemical combinations were evaluated.

All mean quotient calculations attempted to use the same summation methods for chemical classes (total chlordane, total DDT, total PCBs, low molecular weight PAHs, high molecular weight PAHs, total PAHs). This step was necessary for valid comparison of mean quotient calculations but presented limitations with large multistudy data sets because of differences in analyte lists among studies. The methods for summation of chemical classes used in this study are given in the Appendix [15,18–20]. Individual chemical quotients are calculated by dividing the measured concentration or class summation concentration in the sediment sample by the respective published sediment quality guideline value for each chemical for which individual SQGs were derived. A value greater than one indicates the chemical concentration in that sample exceeded its respective SQG. The mean SQGQ is obtained by calculating the mean of the resulting individual quotients for a given combination of chemicals. A generalized example of the calculation is

$$\text{mean sediment quality guideline quotient} = \left(\sum_{n} \left([\text{arsenic/SQG}][\text{chromium/SQG}][\text{copper/SQG}] \ldots \times [\text{total chlordane/SQG}][\text{total PCB/SQG}]\right)\right) \Big/ n$$

where n = total number of analytes.

Samples that were found to have chemical concentrations

Table 2. Mean sediment quality guideline quotient (SQGQ) chemical combinations using probable effects level (PEL) SQG values

Mean SQGQs using PEL guidelines[a]					
PELQ1	PELQ2	PELQ3	PELQ4	PELQ5	PELQ6
Arsenic	Cadmium	Cadmium	Arsenic	Arsenic	Arsenic
Cadmium	Chromium	Chromium	Cadmium	Cadmium	Cadmium
Chromium	Copper	Copper	Chromium	Chromium	Chromium
Copper	Lead	Mercury	Copper	Copper	Copper
Lead	Mercury	Zinc	Lead	Lead	Lead
Mercury	Nickel	Total DDT	Silver	Mercury	Mercury
Silver	Silver	Dieldrin	Zinc	Silver	Silver
Zinc	Zinc	Total PCBs	Total DDT	Zinc	Zinc
Total DDT (OC)	2-Methylnaphthalene	Low mol wt PAHs	Total chlordane	Total chlordane	Total chlordane
Total chlordane	Dibenz[*a*,*h*]anthracene	High mol wt PAHs	Dieldrin	Dieldrin	Dieldrin
Dieldrin	Acenaphthene		Total PCBs	Lindane	Lindane
Lindane	Acenaphthylene		Low mol wt PAHs	Total PCBs	Total PCBs
Total PCBs	Anthracene		Total PAHs	Low mol wt PAHs	Low mol wt PAHs
Low mol wt PAHs	Benz[*a*]anthracene			High mol wt PAHs	Total PAHs
High mol wt PAHs	Benzo[*a*]pyrene				
	Chrysene				
	Fluorene				
	Fluoranthene				
	Naphthalene				
	Phenanthrene				
	Pyrene				
	p'p'-DDE				
	Total DDT				
	Total PCBs				

[a] PELQ chemical combinations used probable effects level (PEL) SQGs [17] as critical values for mean quotient calculations except for PELQ1, which used an organic carbon normalized SQG [33] value for total DDT. OC = organic carbon; PCBs = polychlorinated biphenyls; PAHs = polycyclic aromatic hydrocarbons; mol wt = molecular weight.

of the summation, to a value of one half of the given method detection limits. When one or more required chemicals were not analyzed for a particular sample, that sample was removed from the base data set and not included in evaluations of mean quotient calculation methods requiring that chemical. This step was necessary for valid comparison of the summation methods and the data sets to which they could be applied.

This study used chemical and biological data from three readily available sources as the basis for comparisons of predictive ability. The sources were the State of California's Bay Protection and Toxic Cleanup Program database (BPTCP), the National Oceanic and Atmospheric Administration's (NOAA's) national sediment toxicity (SEDTOX) database, and NOAA's Biscayne Bay survey in Florida. The BPTCP database included 605 coastal sediment samples for which synoptic chemical analyses and toxicity tests (*Eohaustorius estuarius* and *Rhepoxynius abronius*) were performed [21–27]. These data were used for initial comparisons between calculation methods developed by Fairey et al. [21] and Long et al. [6] and 10 additional chemical mixture combinations using ERM and PEL guidelines for mean quotient calculation. These data also were used to evaluate the predictive ability of a variety of individual SQGs with the objective of evaluating the predictive ability of six additional chemical mixture combinations that combined SQGs from different studies. The SEDTOX database included 2,753 sediment samples from studies throughout the coastal United States for which synoptic chemical analyses and whole sediment acute toxicity tests (*Ampelisca abdita, R. abronius*) were paired [28]. The SEDTOX data was used to confirm predictive accuracy of mean quotient calculation methods using BPTCP data and to further evaluate mean quotient calculation methods that included SQGs from mixed sources. The Biscayne Bay database [29] included 226 samples analyzed for sediment chemistry and toxicity (*A. abdita*) and was used as a third independent database for testing predictive accuracy.

Chemical data were combined in dBase IV database files and manipulated using dBase command programs. Mean SQGQ values derived from the various unique chemical combinations in each sample then were compared with synoptically measured toxicity test responses to assess how well each chemical combination predicted acute toxicity. Samples were classified as toxic for the BPTCP study when sample survival was significantly different from controls and less than a critical value determined using the minimum significant difference 90th percentile that was generated from BPTCP data (*Eohaustorius estuarius* survival in sample was less than 75% of survival in negative controls. *R. abronius* survival in sample was less than 77% of survival in negative controls) [21–27,30]. Samples were classified as toxic for the remaining studies when samples were significantly different from controls and less than 80% of negative controls [31].

MacDonald et al. [32] compared mean quotient values at five critical levels to assess associations with measured biological effects (<0.1, <0.5, >0.5, >1.0, and >1.5). Long and MacDonald [12] used similar levels but also included an additional level (>2.3) to better evaluate greater mean SQGQ values. Seven critical levels (Tables 5 & 6) were used in the current study, with one additional critical level (<0.2) included to better evaluate mean SQGQ values in the lower ranges, where the majority of samples fell.

In these analyses, we compared both the incidence (percentages) of acute toxicity and average amphipod survival above and below mean SQGQ critical values. The criteria for identification of optimal predictive ability were that the incidence of toxicity increased steadily and average survival decreased steadily as mean SQGQs increased; incidence of toxicity was low (<5%) and average survival high (>80%) when

Table 3. Sample counts and the incidence of acute toxicity to amphipods when effects range medians (ERMs), probable effects levels (PELs), or other individual sediment quality guidelines (SQGs) were exceeded using the Bay Protection and Toxic Cleanup Program (BPTCP) data (n = 605)

Chemical name	ERM[b]	No. samples > ERM	% Toxic	PEL[c]	No. samples > PEL	% Toxic	Other SQGs	No. samples > SQG	% Toxic
Antimony	*25 µg/g*	3	67	NA	NA	NA	200 µg/g [11]	0	NA
Arsenic	*70 µg/g*	2	100	41.6 µg/g	6	67	700 µg/g [11]	1	100
Cadmium	9.6 µg/g	3	100	*4.21 µg/g*	11	100	NA	NA	NA
Chromium	*370 µg/g*	7	71	160.4 µg/g	87	36	270 µg/g [11]	22	50
Copper	*270 µg/g*	69	70	108.2 µg/g	206	56	1,300 µg/g [11]	3	100
Lead	218 µg/g	15	93	*112.18 µg/g*	64	75	660 µg/g [11]	3	100
Mercury	0.7 µg/g	110	55	0.696 µg/g	110	55	*2.1 µg/g* [11]	19	68
Nickel	51.6 µg/g	76	(41)	42.8 µg/g	108	(44)	NA	NA	NA
Silver	3.7 µg/g	6	100	*1.77µg/g*	44	75	6.1 µg/g [11]	1	100
Zinc	*410 µg/g*	76	78	271 µg/g	141	65	1,600 µg/g [11]	5	100
Total chlordane	*6 ng/g* [15]	185	54	4.79 ng/g	210	52	NA	NA	NA
Total DDT	46.1 ng/g	214	49	51.7 ng/g	203	(50)	100 µg/g OC [33]	9	33
Dieldrin	*8 ng/g*	30	90	4.3 ng/g	53	79	20 µg/g OC [9]	0	NA
Endrin	45 ng/g	0	NA	NA	NA	NA	*0.76 µg/g OC* [9]	2	100
Lindane	NA	NA	NA	0.99 ng/g	9	67	*0.37 µg/g OC* [9]	2	100
Total PCB	180 ng/g	164	53	188.79 ng/g	157	54	*400 ng/g* [35]	80	65
Acenaphthene	500 ng/g	3	33	88.9 ng/g	42	53	230 µg/g OC [9]	0	NA
Acenaphthylene	640 ng/g	0	NA	127.89 ng/g	31	58	NA	NA	NA
Anthracene	1,100 ng/g	27	41	245 ng/g	107	51	NA	NA	NA
Fluorene	540 ng/g	10	(50)	144.35 ng/g	48	(48)	NA	NA	NA
2-Methylnaphthalene	670 ng/g	3	67	201.28 ng/g	19	63	NA	NA	NA
Naphthalene	2,100 ng/g	1	100	390.64 ng/g	9	(44)	NA	NA	NA
Phenanthrene	1,500 ng/g	27	55	543.53 ng/g	86	57	240 µg/g OC [9]	8	50
Low mol wt PAHs	3,160 ng/g	25	(44)	1,442 ng/g	72	51	24,000 ng/g [11]	1	0
Benz[*a*]anthracene	1,600 ng/g	32	43	692.53 ng/g	100	52	NA	NA	NA
Benzo[*a*]pyrene	1,600 ng/g	59	53	763.22 ng/g	115	54	NA	NA	NA
Chrysene	2,800 ng/g	31	(45)	845.98 ng/g	103	52	NA	NA	NA
Dibenz[*a,h*]anthracene	260 ng/g	73	62	134.61 ng/g	115	54	NA	NA	NA
Fluoranthene	5,100 ng/g	18	(50)	1,493.54 ng/g	84	(48)	300 µg/g OC [9]	13	38
Pyrene	2,600 ng/g	44	48	1,397.6 ng/g	111	(54)	NA	NA	NA
High mol wt PAHs	9,600 ng/g	71	51	6,676.14 ng/g	100	51	69,000 ng/g [11]	1	100
Total PAHs	44,792 ng/g	5	60	16,770.54 ng/g	45	(47)	*1,800 µg/g OC* [20]	10	60

[a] The number of samples exceeding individual SQGs and the percentage of those samples determined to be toxic were used in selecting which SQGs were reasonably predictive of toxicity to amphipods and were representative of concentrations commonly found in BPTCP samples. Selected SQGs (italics) were used in mean calculation methods that incorporated individual SQGs from a variety of sources. PCB = polychlorinated biphenyl; PAH = polycyclic aromatic hydrocarbon; OC = organic carbon; NA = not applicable; mol wt = molecular weight.
[b] [16].
[c] [17].

Table 4. Mean sediment quality guideline quotient (SQGQ) chemical combinations using effects range median (ERM) probable effects level (PEL) and other individual SQGs values

Mean SQGQs using combinations of individual SQGs[a]					
SQGQ1	SQGQ2	SQGQ3	SQGQ4	SQGQ5	SQGQ6
Cadmium	Cadmium	Cadmium	Cadmium	Arsenic	Antimony
Copper	Chromium	Chromium	Chromium	Cadmium	Arsenic
Lead	Copper	Copper	Copper	Copper	Cadmium
Silver	Lead	Lead	Lead	Lead	Chromium
Zinc	Silver	Silver	Silver	Silver	Copper
Total chlordane	Zinc	Zinc	Zinc	Zinc	Lead
Dieldrin	Total chlordane	Lindane	Total chlordane	Total chlordane	Mercury
Total PCBs	Dieldrin	Dieldrin	Dieldrin	Dieldrin	Silver
Total PAHs	Endrin	Endrin	Total PCBs	Lindane	Zinc
	Total PCBs	Total PCBs	Total PAHs	Total PCBs	Total chlordane
	Total PAHs	Total PAHs		Total PAHs	Dieldrin
					Endrin
					Lindane
					Total PCBs
					Total PAHs

[a] SQGQ chemical combinations used ERM, PEL, and other individual SQGs as critical values.
biphenyl; PAHs = polycyclic aromatic hydr...

Table 5. Comparison of mean sediment quality guideline quotient chemical combinations using the Bay Protection and Toxic Cleanup Program (BPTCP) data (n = 605[a]); ERM = effects range median; PEL = probable effects level

SQGQ range[c]	ERMQ1 (n = 528)[b]	ERMQ2 (n = 395)	ERMQ3 (n = 569)	ERMQ4 (n = 533)	ERMQ5 (n = 533)	ERMQ6 (n = 531)
>2.3	n = 6, 100%	n = 9, 33%	n = 24, 50%	n = 19, 58%	n = 9, 100%	n = 8, 100%
>1.5	n = 17, 88%	n = 13, 46%	n = 46, 61%	n = 34, 65%	n = 23, 83%	n = 20, 85%
>1.0	n = 50, 78%	n = 31, 42%	n = 92, 62%	n = 52, 63%	n = 63, 78%	n = 55, 78%
>0.5	n = 122, 62%	n = 94, 50%	n = 205, 51%	n = 161, 53%	n = 147, 57%	n = 136, 60%
<0.5	n = 406, 37%	n = 301, 37%	n = 364, 38%	n = 372, 38%	n = 386, 37%	n = 395, 36%
<0.2	n = 227, 36%	n = 175, 36%	n = 149, 38%	n = 182, 37%	n = 202, 36%	n = 212, 35%
<0.1	n = 65, 31%	n = 65, 39%	n = 38, 29%	n = 38, 29%	n = 53, 23%	n = 53, 23%
SQGQ range[c]	PELQ1 (n = 528)	PELQ2 (n = 394)	PELQ3 (n = 569)	PELQ4 (n = 528)	PELQ5 (n = 533)	PELQ6 (n = 531)
>2.3	n = 14, 100%	n = 20, 35%	n = 39, 59%	n = 29, 66%	n = 16, 94%	n = 13, 100%
>1.5	n = 50, 76%	n = 45, 44%	n = 85, 64%	n = 61, 66%	n = 55, 76%	n = 48, 75%
>1.0	n = 91, 70%	n = 36, 50%	n = 142, 58%	n = 113, 63%	n = 95, 69%	n = 87, 74%
>0.5	n = 197, 53%	n = 127, 48%	n = 274, 51%	n = 241, 49%	n = 202, 53%	n = 199, 54%
<0.5	n = 331, 36%	n = 267, 36%	n = 295, 35%	n = 287, 37%	n = 331, 35%	n = 332, 35%
<0.2	n = 88, 29%	n = 118, 37%	n = 66, 35%	n = 63, 33%	n = 81, 30%	n = 82, 29%
<0.1	n = 29, 21%	n = 33, 24%	n = 7, 14%	n = 2, 0%	n = 5, 0%	n = 5, 0%
SQGQ range[c]	SQGQ1 (n = 561)	SQGQ2 (n = 561)	SQGQ3 (n = 563)	SQGQ4 (n = 561)	SQGQ5 (n = 528)	SQGQ6 (n = 528)
>2.3	n = 16, 94%	n = 14, 93%	n = 3, 100%	n = 16, 94%	n = 11, 100%	n = 5, 100%
>1.5	n = 42, 76%	n = 32, 81%	n = 7, 100%	n = 39, 82%	n = 20, 82%	n = 14, 100%
>1.0	n = 81, 70%	n = 58, 72%	n = 18, 72%	n = 71, 69%	n = 39, 77%	n = 30, 77%
>0.5	n = 160, 60%	n = 149, 62%	n = 98, 73%	n = 163, 59%	n = 123, 64%	n = 108, 71%
<0.5	n = 400, 36%	n = 411, 36%	n = 465, 36%	n = 398, 36%	n = 405, 36%	n = 420, 35%
<0.2	n = 187, 30%	n = 132, 28%	n = 178, 31%	n = 126, 28%	n = 207, 32%	n = 203, 36%
<0.1	n = 50, 32%	n = 3, 66%	n = 10, 30%	n = 17, 18%	n = 57, 30%	n = 27, 30%

[a] In the BPTCP database, 250 sediment samples were acutely toxic to amphipods (41%) while 355 were not toxic.
[b] The count reflects the number of BPTCP samples for which the particular chemical combination could be calculated.
[c] For each SQGQ range, the number of samples with mean quotient values exceeding the respective critical value are given as well as the percentage of those samples exceeding the critical value that were acutely toxic to amphipods.

mean SQGQs were low (<0.1); incidence of toxicity was high (>90%) and average survival was low (<50%) when mean SQGQs were high (>2.3); and when predictive ability was similar across SQGQ ranges for different calculation methods, sample counts were compared to find methods that correctly predicted toxicity for the largest number of samples in each data set.

RESULTS

As shown by the sample count for the BPTCP database (Table 5), the number of samples that lend themselves to a particular calculation method differs dramatically among methods (n = 394–569 out of 605). This variability is due to periodic expansions of the analyte list for the BPTCP over the program's seven years. In general, the lower the number of analytes included in the calculation method, the more likely the derivation could be completed for the majority of samples. Results demonstrate an increased number of samples being available for SQGQ calculation and biological comparison when SQG chemicals were limited.

Using the BPTCP database, toxicity to marine amphipods (*E. estuarius* and *R. abronius*) in 605 sediment samples was compared with calculated mean quotient values. Based on BPTCP comparisons with controls and the minimum significant difference, 250 samples were classified as acutely toxic (41%) and 355 were classified as nontoxic (59%). Calculated mean quotient values from sediment samples for all derivation methods ranged from 0.031 (lowest multiple chemical indicator) to 10.9 (greatest multiple chemical indicator).

In the BPTCP data, there was a wide range in the patterns in toxicity among the different calculation methods (Table 5). Generally, SQGQ values above the greater critical values were associated with greater proportions of toxic samples while those below the lower critical values were associated with reduced proportions of toxic samples. In two cases (ERMQ2, PELQ2), the incidence of toxicity did not increase appreciably with increasing chemical concentration. In four cases (ERMQ3, ERMQ4, PELQ3, PELQ4), the increase in toxicity was minimal with increasing chemical concentration. One hybrid combination of several types of sediment quality guidelines for mean quotient calculation (SQGQ6) resulted in the greatest association with the incidence of toxicity to amphipods (100% for values >2.3 and 100 % for values >1.5). In general, predictive ability improved when mean quotient calculations utilized SQGs developed using a variety of comparative statistical approaches (e.g., ERM, PEL, consensus, equilibrium partitioning). Associations with the incidence of toxicity were lowest for all methods when mean quotient values dropped below 0.1.

Using SEDTOX data, 2,753 samples were examined for associations between toxicity to marine amphipods (*E. estuarius*, *A. abdita*, and *R. abronius*) and all 18 mean quotient calculation methods. Of these samples, 484 were classified as toxic (18%) and 2,269 were classified as nontoxic (82%). The lower incidence of toxicity reflects the primary program goal of identifying general spatial status and temporal trends along the coastal margins of the United States rather than investigation of contaminated sites as with BPTCP. Calculated mean

Table 6. Comparison of mean sediment quality guideline quotient (SQGQ) calculation methods using SEDTOX database, Biscayne Bay (FL, USA) and combined data; effects range median = (ERM); probable effects level = (PEL)

	Comparison of SQGQ calculation methods to toxicity using SEDTOX data (n = 2,753[a])[b]								
QGQ nge[c]	SQGQ1 (n = 1,435)	SQGQ2 (n = 977)	SQGQ3 (n = 1,134)	SQGQ4 (n = 1,367)	SQGQ5 (n = 1,385)	SQGQ6 (n = 946)	PELQ1 (n = 1,286)	ERMQ2 (n = 1,668)	ERMQ6 (n = 1,399)
2.3	n = 19, 89%	n = 17, 53%	n = 12, 0%	n = 19, 79%	n = 15, 73%	n = 9, 11%	n = 28, 71%	n = 13, 54%	n = 19, 79%
1.5	n = 33, 88%	n = 29, 66%	n = 24, 30%	n = 32, 81%	n = 30, 77%	n = 25, 60%	n = 58, 69%	n = 25, 64%	n = 31, 84%
1.0	n = 70, 78%	n = 52, 70%	n = 49, 51%	n = 58, 76%	n = 58, 72%	n = 40, 60%	n = 116, 56%	n = 46, 72%	n = 61, 77%
0.5	n = 216, 48%	n = 184, 42%	n = 183, 40%	n = 205, 45%	n = 176, 46%	n = 136, 48%	n = 241, 40%	n = 127, 52%	n = 168, 47%
0.5	n = 1,218, 8%	n = 792, 6%	n = 949, 9%	n = 1,161, 6%	n = 1,206, 8%	n = 809, 7%	n = 1,045, 5%	n = 1,541, 8%	n = 1,231, 7%
0.2	n = 1,022, 5%	n = 636, 3%	n = 766, 5%	n = 955, 4%	n = 1,007, 4%	n = 666, 3%	n = 822, 3%	n = 1,378, 6%	n = 1,049, 4%
0.1	n = 768, 4%	n = 459, 2%	n = 515, 3%	n = 656, 3%	n = 746, 3%	n = 487, 2%	n = 537, 3%	n = 1,196, 5%	n = 806, 4%
	Comparison of SQGQ calculation methods to toxicity using Biscayne Bay data (n = 226[d])								
QGQ nge	SQGQ1 (n = 226)	SQGQ2 (n = 226)	SQGQ3 (n = 226)	SQGQ4 (n = 226)	SQGQ5 (n = 226)	SQGQ6 (n = 219)	PELQ1 (n = 226)	ERMQ2 (n = 226)	ERMQ6 (n = 226)
2.3	n = 6, 100%	n = 4, 100%	n = 0	n = 6, 100%	n = 4, 100%	n = 3, 100%	n = 5, 100%	n = 0	n = 4, 100%
1.5	n = 9, 100%	n = 7, 100%	n = 3, 100%	n = 7, 100%	n = 7, 100%	n = 6, 100%	n = 12, 83%	n = 3, 67%	n = 9, 89%
1.0	n = 18, 83%	n = 15, 87%	n = 6, 100%	n = 16, 81%	n = 14, 86%	n = 9, 100%	n = 20, 75%	n = 6, 67%	n = 14, 86%
0.5	n = 24, 71%	n = 23, 74%	n = 18, 78%	n = 23, 74%	n = 23, 74%	n = 19, 79%	n = 26, 65%	n = 17, 77%	n = 24, 71%
0.5	n = 202, 4%	n = 203, 4%	n = 208, 5%	n = 203, 4%	n = 203, 4%	n = 200, 5%	n = 200, 4%	n = 208, 6%	n = 202, 4%
0.2	n = 187, 4%	n = 188, 4%	n = 193, 4%	n = 187, 4%	n = 188, 4%	n = 188, 4%	n = 180, 4%	n = 198, 5%	n = 189, 4%
0.1	n = 156, 4%	n = 163, 4%	n = 167, 4%	n = 158, 4%	n = 162, 4%	n = 166, 4%	n = 131, 5%	n = 180, 4%	n = 162, 4%
	Comparison of SQGQ calculation methods to toxicity using minimized common data from 3,584 samples (n = 1,692[e])								
GQ ge[c]	SQGQ1 (n = 1,692)	SQGQ2 (n = 1,692)	SQGQ3 (n = 1,692)	SQGQ4 (n = 1,692)	SQGQ5 (n = 1,692)	SQGQ6 (n = 1,692)	PELQ1 (n = 1,692)	ERMQ2 (n = 1,692)	ERMQ6 (n = 1,692)
3	n = 32, 100%	n = 32, 75%	n = 15, 20%	n = 34, 94%	n = 26, 92%	n = 17, 53%	n = 45, 87%	n = 18, 56%	n = 28, 89%
5	n = 62, 87%	n = 58, 76%	n = 33, 48%	n = 59, 88%	n = 50, 84%	n = 45, 78%	n = 112, 76%	n = 37, 65%	n = 55, 85%
0	n = 127, 80%	n = 107, 76%	n = 65, 63%	n = 115, 78%	n = 98, 78%	n = 79, 71%	n = 214, 65%	n = 75, 65%	n = 118, 81%
5	n = 315, 56%	n = 316, 54%	n = 263, 56%	n = 321, 56%	n = 282, 57%	n = 263, 60%	n = 416, 50%	n = 210, 57%	n = 290, 57%
5	n = 1,377, 13%	n = 1,376, 13%	n = 1,429, 10%	n = 1,371, 13%	n = 1,410, 12%	n = 1,429, 11%	n = 1,276, 13%	n = 1,481, 17%	n = 1,402, 15%
2	n = 1,039, 8%	n = 946, 7%	n = 977, 8%	n = 960, 6%	n = 1,073, 9%	n = 1,057, 9%	n = 859, 5%	n = 1,245, 14%	n = 1,091, 10%
1	n = 724, 4%	n = 619, 3%	n = 604, 3%	n = 655, 3%	n = 740, 4%	n = 680, 4%	n = 540, 3%	n = 1,009, 11%	n = 766, 4%

the SEDTOX database, 484 sediment samples were acutely toxic to amphipods (18%) while 2,269 were not toxic.
e count (n values in the column heads) reflects the number of samples in each database for which the particular chemical combination could be calculated.
r each SQGQ range, the number of samples with mean quotient values exceeding the respective critical value are given as well as the percentage of those samples exceeding the critical value t were acutely toxic to amphipods.
the Biscayne Bay database, 25 sediment samples were acutely toxic to amphipods (11%) while 201 were not toxic.
the minimized common database, 371 sediment samples were acutely toxic to amphipods (22%) while 1,321 were not toxic.

quotient values for all 18 methods ranged from 0.01 to 100. The unique combination most predictive of toxicity to amphipods was SQGQ1. This combination of mixed sediment quality guidelines for mean quotient calculation resulted in the greatest association with the incidence of toxicity to amphipods (89% for values >2.3 and 88% for values >1.5; Table 6). Other derivation methods yielded reduced associations (30%–81%) with observed toxicity for values greater than 1.5 (Table 6). The incidence of toxicity invariably was less than 10% in samples with lesser mean quotient values (<0.5).

As with the BPTCP database, there was a significant difference in the total number of SEDTOX samples for which mean quotient values could be calculated using different chemical combinations. Totals ranged between 946 and 1,668 and represented 35 to 60% of the available data. The method that used the greatest number of chemicals (24 for ERMQ2) in the mean quotient calculations yielded the largest number of calculated SQGQ values (Table 6) but also demonstrated some of the lowest incidences of associated toxicity. Including the large number of individual PAHS in the ERMQ2 calculation was conducive to use of the data set but did not improve associations with acute amphipod toxicity. The SQGQ1, which incorporated only nine chemicals (no individual PAHs) and most accurately predicted toxicity, could be calculated for 1,435 samples, representing slightly more than one half of the available data.

Most mean quotient calculation methods provided good predictive ability in the Biscayne Bay data (Table 6). Both SQGQ6 and SQGQ1 predicted equally well based on the number and percentage of samples that were toxic (100%) when mean quotient values were greater than 1.0 and 1.5, respectively. The incidence of toxicity was greater than 70% for SQGQ6 and SQGQ1 when values were greater than 0.5, while values less than 0.5 were toxic less than 5% of the time.

To demonstrate general relationships between acute toxicity to amphipods and SQGQ values, data from all three sources were combined into a single data set. Reduction of the combined data set of 3,584 samples to only those samples that could be used in all 18 quotient calculation methods resulted in a common data set of 1,692 samples. Calculated mean quotient values for all 18 methods ranged from 0.002 to 100. The SQGQ1 resulted in the greatest association with the incidence of toxicity to amphipods (100% for values >2.3 and 87% for values >1.5). A low incidence of toxicity (4%) was observed when SQGQ1 values were less than 0.1 (Table 6). Table 7 identifies the percentages of samples that were acutely toxic for 12 ranges of SQGQ1 values. Also expressed is the magnitude of the toxic response (as mean % survival) over the same SQGQ1 ranges. The SQGQ1 values were highly correlated with the incidence ($r^2 = 0.901$, $p < 0.001$) and magnitude ($r^2 = 0.913$, $p < 0.001$) of acute toxicity (Fig. 1).

Table 7. Acute amphipod toxicity associated with SQGQ1 ranges for common samples from combined NOAA/BPTCP/Biscayne Bay database (n = 1,692)[a]

SQGQ1 range	Range average	No. of samples	% of Samples toxic	Average % survival	Average no. ERMs exceeded
0–0.1	0.04	724	4	95	0.03
0.1–0.25	0.16	389	19	83	0.3
0.25–0.5	0.35	262	33	76	1.6
0.5–0.75	0.62	113	32	76	3.3
0.75–1.0	0.87	77	52	70	5.4
1.0–1.25	1.1	44	68	53	6.3
1.25–1.5	1.36	21	81	56	6.7
1.5–2	1.62	21	67	45	7.6
2–2.5	2.2	11	91	36	9.5
2.5–3.0	2.72	10	100	35	9.4
3.0–3.5	3.23	10	100	20	10.2
>3.5	4.63	10	100	13	12.2

[a] NOAA = National Oceanic and Atmospheric Administration; BPTCP = Bay Protection and Toxic Cleanup Program; SQGQ = sediment quality guideline quotient; ERM = effects range medians

DISCUSSION

Mean SQGQs have been used previously to compare toxicity test response and observed benthic community response to concentrations of a mixture of 16 chemicals in coastal sediments from California, USA [21]. Similarly, Long et al. [6] used mean SQGQs to compare observed toxicity test response with a mixture of 24 chemicals in test sediments from a national database (n = 1,068). Both these studies found a pattern of increasing incidence of toxicity in sediments with increasing mean SQGQ values and identified critical levels above which biological effects could be predicted. Each of these studies used effects range median values to derive mean SQGQs, but chemicals used in the quotient calculation methods were not identical. Long et al. [6] used 13 individual SQGs to represent the individual polycyclic aromatic hydrocarbon compounds in the average, while Fairey et al. [21] represented the PAHs by using two individual SQGs, one each for low and high molecular weight PAH classes. Another difference is that Long et al. [6] represented the organochlorine pesticides using ERMs for p',p'-DDE and total DDT, while Fairey et al. [21] represented organochlorine pesticides using ERMs for total chlordane, dieldrin, endrin, and an organic carbon normalized value for DDT [33]. These seemingly minor differences had the potential of yielding dramatically different results. For example, there is poor correlation (Pearson's correlation, r^2 = 0.119) between mean SQGQ values calculated by these two mean SQGQ calculation methods in the present paper (ERMQ1 [21] and ERMQ2 [6]; Table 2) using chemical data from California's Bay Protection and Toxic Cleanup Program (BPTCP; n = 605). Investigation of outliers that grouped far from predicted values indicated that chemical mixtures were dominated by DDT or PAHs in those particular California samples. As demonstrated in Table 3, the predictive abilities of ERM SQGs for DDT and most individual PAHs were low using BPTCP data. Inclusion of these individual SQGs in the mean SQGQ calculation method reduced the overall predictive ability of the mean ERMQ2 values. Using ERMQ1, 88% of the most contaminated samples (ERMQ1 > 1.5) were observed to be toxic to amphipods (*R. abronius* and *E. estuarius*), while the incidence of associated toxicity drops to 46% for ERMQ2 values >1.5 (Table 5). Also of note is that the mean quotient calculation method requiring the greatest number of chemicals (ERMQ2) resulted in the fewest samples available for mean quotient calculation. Missing chemical analytes over multiple years of the program limited the utility of the ERMQ2 values as indicators of chemical mixture concentration in this data set. These results demonstrate how selection of individual SGQs to be included in the mean SQGQ, in this case particularly with DDT and PAHs, can influence the outcome of any subsequent analysis.

In the data analysis reported here, the ability of mean SQGQs to accurately predict the probability of observing an associated biological effect is dependent

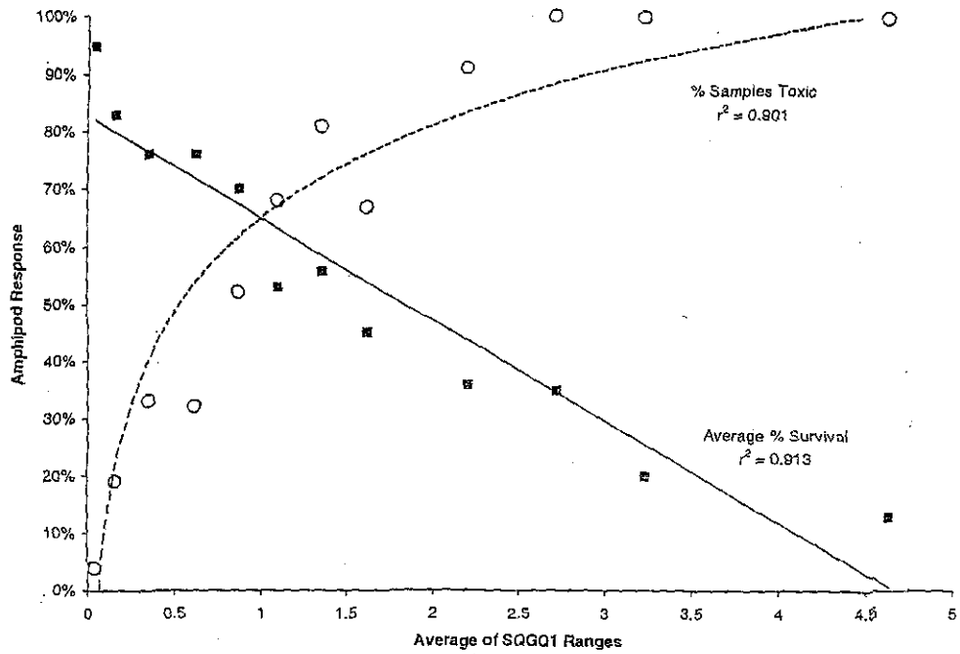

Fig. 1. Amphipod response over the range of average sediment quality guideline quotients (SQGQ1) values. Values were calculated from 1,692 samples for which all 18 chemical combinations could be calculated from the combined National Oceanic and Atmospheric Administration/Bay Protection and Toxic Cleanup Program (NOAA/BPTCP), Biscayne Bay databases. Logarithmic fit equation for percent of samples toxic versus SQGQ is $y = 0.2352 \ln(x) + 0.6487$ ($r^2 = 0.901$, $p < 0.001$). Linear fit equation for average % survival versus SQGQ is $y = -0.1774(x) + 0.8277$ ($r^2 = 0.913$, $p < 0.001$).

of chemicals and SQGs used in the calculation. This relationship becomes clear from the wide range of predictive success observed among derivation methods presented here. It is also clear that use of different data to assess mean SQGQ calculation influences the estimates of predictive ability for sediment toxicity. This demonstrates that calculation methods for mean SQGQs must be refined and standardized using a method for which predictive ability and interstudy comparability are not compromised. This point is critical to our future use of mean SQGQs and will directly impact their utility as assessment tools.

To refine calculation of mean SQGQs, a major assumption must be made that chemical analytes used in the mean SQGQ calculation are indeed representative of, or surrogates of, the toxicologically significant chemical mixture in the samples regardless of which chemicals were quantified in the analyses. This is a simplistic approach because of the seemingly infinite number of chemical combinations present in field-collected sediments. In addition, each research or monitoring program that generates sediment chemistry data has its own objectives and resultant analyte lists, based on economic and regional environmental considerations. Use of chemicals that occur most commonly across many programs will maximize data use and allow development of mean SQGQs more applicable to a wide range of environmental conditions and objectives. The choice of toxicologically representative chemicals is limited, however, by current analytical methodologies and our knowledge of those chemicals in the literature for which sediment quality guidelines have been established. This operational limitation mandates the assumption that those few published SQG chemical analytes are representative of anthropogenic contamination in the sample or that they serve well as covarying surrogates. It is constructive, though, because, as demonstrated, limiting the number of chemicals in the calculation allows more data to

vation that only 4% of samples were toxic when toxicity was not predicted (i.e., mean SQGQ1 < 0.1; Table 6) suggests that chemicals for which analyses were not performed, or for which there are no individual SQGs, infrequently occur at toxicologically significant concentrations in otherwise uncontaminated samples.

An implication of the mean SQGQ approach is that toxicological mechanism(s) of the representative chemicals are additive. Independent experimental evidence has demonstrated that acute toxicity to amphipods by some substances, such as PAHs, are similar and additive when known combinations of chemicals are spiked into clean sediment [34]. The research presented here does not provide direct experimental evidence of additivity. The results are, however, consistent with the hypothesis because sediments are toxic more frequently when chemical concentrations simultaneously exceed increasing numbers of individual SQGs. Table 7 demonstrates that, as increasing numbers of effects range median SQGs are exceeded, the incidence and magnitude of toxicity correspondingly increases. An additional observation in the current research is that associations between toxicity and mean SQGQs improve by removing chemicals with less predictive SQGs (Table 3) from the quotient calculations. This suggests that effectively representing toxicological modes of action may be more important to SQGQ predictive accuracy than simply including additional toxic chemicals to the representative chemical matrix.

Consideration of the issues discussed here and the results presented here leads to the recommendation that a standard method for combination of chemicals and respective SQGs should be adopted for the calculation of mean SQGQs to allow comparability between regions and surveys. The current research has demonstrated that, for the methods and data tested

Table 8. Chemicals and sediment quality guidelines used in chemical combination SQGQ1[a]

SQGQ1 chemicals	SQG concentration	Guideline type
Cadmium	4.21 μg/g dry wt	PEL [17]
Copper	270 μg/g dry wt	ERM [16]
Silver	1.77 μg/g dry wt	PEL [17]
Lead	112.18 μg/g dry wt	PEL [17]
Zinc	410 μg/g dry wt	ERM [16]
Total chlordane	6 ng/g dry wt	ERM [15]
Dieldrin	8 ng/g dry wt	ERM [16]
Total PAHs	1,800 μg/g OC	Consensus [20]
Total PCBs	400 ng/g dry wt	Consensus [35]

[a] SQGQ = sediment quality guideline quotients; PEL = probable effect level; ERM = effect range median; PAH = polycyclic aromatic hydrocarbon; PCB = polychlorinated biphenyl; OC = organic carbon.

porating a number of theoretical and empirical sediment quality guidelines (Table 8) from a variety of reliable sources [16,17,20,35]. As evaluated with the criteria for identification of optimal predictive ability, the incidence of toxicity increased steadily and average survival decreased steadily as mean SQGQ1 values increased. The incidence of toxicity was less than 5% and average survival was over 90% when mean SQGQ1 values were less than 0.1. The incidence of toxicity was greater than 90% and average survival was less than 50% when mean SQGQ1 values were greater than 2.3. The SQGQ1 calculation method incorporates SQGs for nine of the most commonly measured chemicals and best utilizes available data in the tested data sets. Until a more predictive method has been demonstrated, SQGQ1 is recommended to serve as the standard for calculation of mean SQGQs when comparing with acute toxicity to amphipods. SQGQ1 is calculated as

$$\text{SQGQ1} = \Big(\Big(\sum ([\text{cadmium}]/4.21)([\text{copper}]/270)([\text{lead}]/112.18) \times ([\text{silver}]/1.77)([\text{zinc}]/410)([\text{total chlordane}]/6) \times ([\text{dieldrin}]/8)([\text{total PAH}_{oc}]/1800)([\text{total PCB}]/400)\Big) \div 9\Big)$$

An additional recommendation concerns sediments where unique chemical conditions prevail or regional anthropogenic activities warrant special consideration. In these situations, investigators might adjust the mean quotient derivation method to better fit local environmental or management concerns. A unique chemical example would be in a large agricultural watershed. Where endrin has been found to be a primary chemical of concern, managers may wish to incorporate the U.S Environmental Protection Agency's EqP-based sediment quality guideline for endrin into their mean quotient derivation method. This flexibility will ensure a major component in the watershed's chemical signature is not ignored when investigating the relationship between chemical mixtures and biological effects. With this type of specific objective, the derivation method that best demonstrates associations between chemicals of interest and biological effects will be the most effective tool for utilizing probabilities of toxicity and focusing local causality studies. It is important, however, that investigators report differences in the mean SQGQ calculation methods. We recommend use of the SQGQ1 method reported here for providing method for addressing any unique local chemical mixtures or specific management objectives. The ability to exercise flexibility with derivation methods should encourage and enhance the effective use of mean SQGQ values.

As with other empirical approaches to evaluating sediment contamination using sediment quality guidelines, limitations in the use of the mean SQGQs must be acknowledged. The SQGQ1 approach is meant to serve as a central tendency indicator (i.e., as means of multiple individual quotients) of contamination for a complex sediment matrix. The disadvantage of central tendency indicators is that they minimize the potential for impact from any one component. Therefore, when performing a sediment toxicologic evaluation, it is prudent to consider chemical exposure on an individual chemical basis in addition to the chemical matrix basis described here. Consideration of individual SQGs may help in situations when exposure to single chemicals is poorly represented by overall contamination within a sample. The point to emphasize is that mean SQGQs should not be used as the sole indicator of sediment contamination. They should be used as additional tools in our efforts to better understand the relationships between chemical exposure and biological response. Use of mean SQGQ1 should fit well in the conceptual framework of the sediment quality triad that emphasizes a weight-of-evidence approach to sediment quality assessment [36].

The current research has focused on manipulation of multiple chemical constituents to investigate their relationships with a single biological response. Critical values selected for classifying toxic biological responses are a major factor in the results presented here, and it should be noted that the critical values used as biological benchmarks for comparison over selected SQGQ ranges are themselves currently subject to investigation. New methods for determining toxicity are being examined [30,37,38] while others are reviewing current methods with more extensive data sets than have previously been assembled [28]. Results may influence the selection of critical values, such as *t* test and minimum significant difference determinates used in this study. As methods for determination of toxicity are revised, the need to revisit relationships between toxicity and chemistry also may follow.

The current research has focused on acute toxicity of sediment to marine amphipods as the sole measure of biological response. There is a need to further this research and derive optimal chemical mixtures for correlating with other test species and response parameters. Long et al. [6] reported that the incidence of toxic samples increased markedly when data from sublethal tests were added to those from the acute amphipod bioassays. Evaluation of mean SQGQs using large databases that include bioassays with reproductive, developmental, and chronic endpoints are needed to further validate use of mean SQGQs. Subsequent research should continue to expand investigation of impacts of multiple contaminants to measures in other environments and to measures of individual and community response in the field. Work with freshwater species is being reported [32], and relationships similar to those reported here are emerging between toxicity to several freshwater test species and mean SQGQs. Current efforts by Hyland et al. [14], Lowe and Thompson [39], and Fairey et al. [21] include investigations of marine benthic community response and have demonstrated increased probabilities of community impacts as mean SQGQ values increase. These efforts and the current

evidence supporting the use of mean SQGQs as interpretive tools.

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APPENDIX

Summations used in sediment quality guideline quotient (SQGQ) chemical combinations; references are given for source of summation technique

Total DDT [15,18]	$= \sum$ ([*o*,*p*'-DDD][*p*,*p*'-DDD][*o*,*p*'-DDE][*p*,*p*'-DDE][*o*,*p*'-DDT][*p*,*p*'-DDT])
Total chlordane [18]	$= \sum$ ([*cis*-chlordane][*trans*-chlordane][*cis*-nonachlor][*trans*-nonachlor][oxychlordane])
Total PCB [19][a]	$= \sum$ ([PCB8][PCB18][PCB28][PCB44][PCB52][PCB66][PCB101][PCB105][PCB118][PCB128][PCB138][PCB153][PCB170][PCB180][PCB187][PCB195][PCB206][PCB209])2)
Low molecular weight PAHs [20]	$= \sum$ ([acenapthene][acenaphthylene][anthracene][fluorene][naphthalene][phenanthrene])
High molecular weight PAHs [20]	$= \sum$([benz[*a*]anthracene][benzo[*a*]pyrene][benzo[*b*]fluoranthene]‹benzo[*k*]fluoranthene][chyrsene][fluoranthene][pyrene])
Total PAHs [20]	$= \sum$ ([low molecular weight PAHs][high molecular weight PAHs])

[a] This summation is based on work of O'Conner [19] for the National Oceanic and Atmospheric Administration's National Status and Trends Program while developing comparability between individual PCB congener summations and historic Aroclor equivalents. PCB = polychlorinated biphenyl; PAHs = polycyclic aromatic hydrocarbons; DDE = (1,1-dichloro-2,2-bis[p-chlorophenyl]ethylene).