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The weight-of-evidence approach to the development of sediment quality guidelines (SQGs) was modified to support the derivation of biological effects-based SQGs for Florida coastal waters. Numerical SQGs were derived for 34 substances, including nine trace metals, 13 individual polycyclic aromatic hydrocarbons (PAHs), three groups of PAHs, total polychlorinated biphenyls (PCBs), seven pesticides and one phthalate ester. For each substance, a threshold effects level (TEL) and a probable effects level (PEL) was calculated. These two values defined three ranges of chemical concentrations, including those that were (1) rarely, (2) occasionally or (3) frequently associated with adverse effects. The SQGs were then evaluated to determine their degree of agreement with other guidelines (an indicator of comparability) and the percent incidence of adverse effects within each concentration range (an indicator of reliability). The guidelines also were used to classify (using a dichotomous system: toxic, with one or more exceedances of the PELs or non-toxic, with no exceedances of the TELs) sediment samples collected from various locations in Florida and the Gulf of Mexico. The accuracy of these predictions was then evaluated using the results of the biological tests that were performed on the same sediment samples. The resultant SQGs were demonstrated to provide practical, reliable and predictive tools for assessing sediment quality in Florida and elsewhere in the southeastern portion of the United States.

Keywords: sediment quality guidelines; contaminants; biological effects; marine; estuarine.

Introduction

Sediment chemistry data indicate that Florida coastal sediments in several areas are contaminated (Long and Morgan 1990, Delfino et al. 1991, FDEP 1994). For example, sediments in Tampa Bay, Pensacola Bay and Biscayne Bay are contaminated with trace metals, polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs) and certain pesticides. Additionally, Choctawhatchee Bay and St Andrews Bay sediments are contaminated with metals, PAHs and pesticides and elevated levels of PCBs have been

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detected in St Andrews Bay, Apalachicola Bay, Charlotte Harbor, Naples Bay, Rookery Bay and the St Johns River (Long and Morgan 1990).

While sediment chemistry data are essential for evaluating sediment quality, they do not provide a comprehensive basis for classifying or managing contaminated sediments (Long et al. 1995). Interpretive tools are also required to relate sediment chemistry data to the potential for adverse biological effects. Various toxicity and bioaccumulation tests can be performed to evaluate the biological significance of sediment-associated contaminants (Burton 1992). In addition, numerical sediment quality guidelines (SQGs) can be used to help interpret the significance of chemical concentrations in sediments, identify contaminants of concern and prioritize areas for regulation or restoration (Long and Morgan 1990, Di Toro et al. 1991, Persaud et al. 1992, MacDonald et al. 1992).

A variety of approaches have been developed to support the derivation of numerical SQGs in the United States and Canada (see Chapman 1989, Adams et al. 1992, MacDonald et al. 1992, USEPA 1992, MacDonald, 1994 for reviews). The procedures used for deriving the SQGs and the philosophy behind their development are approach specific. Consequently, each approach has certain advantages and limitations that affect the applicability of the resultant guidelines. Presently there is little agreement as to which approach provides the most reliable guidelines, therefore, each of the major approaches was evaluated to determine which would best address Florida's unique requirements for SQGs (MacDonald 1994). The results of this evaluation indicated that the weight-of-evidence approach, developed to provide informal guidelines for evaluating data collected under the National Status and Trends Program of the National Oceanic and Atmospheric Administration (NOAA; Long and Morgan 1990, Long 1992), would provide scientifically defensible and broadly applicable guidelines for assessing sediment quality. The evaluation by MacDonald (1994) also indicated that some modifications to the original approach could potentially increase the applicability of the procedure for deriving SQGs for Florida's coastal waters.

The objectives of this study were to (1) describe the modifications made to the weight-of-evidence approach to support the development of SQGs for Florida coastal waters, (2) present the SQGs that were derived and (3) evaluate the applicability of these SQGs for Florida coastal waters. The comparability of the SQGs was assessed by comparing them with those derived using other data or other methods. The reliability of the guidelines was evaluated by determining the percent incidence of adverse effects within each of three ranges of contaminant concentrations. The predictability of the SQGs was assessed using several independent data sets from Florida and the Gulf of Mexico, which contain both sediment chemistry and biological effects data.

Methods

The weight-of-evidence approach to the development of numerical sediment quality guidelines has been described in detail elsewhere (Long and Morgan 1990, Long 1992, Long and MacDonald 1992, Long et al. 1995), so only an overview of the approach and the modifications that were adopted in Florida will be presented here. The derivation of numerical guidelines using the weight-of-evidence approach consists of three main steps. First, all of the available information which described associations between contaminant concentrations and adverse biological effects in sediments was collected and evaluated. These data were collated in a biological effects database for sediments (BEDS;

MacDonald et al, 1994). N effects level (PEL), were intended to define three occasionally and frequently were evaluated to determine

Development of a biological The first step in the derivat database for sediments (BE numerous studies conducted and critically evaluated for equilibrium-partitioning mastudies used to investigate the and estuarine sediments. Exand/or biological effects ob duration (if applicable and reproduction TOC concentrations (if report a dry weight basis). More (1992), Long and MacDona (1995).

Derivation of sediment qual The BEDS was used as the sediment-associated contami coastal waters were retrieved in ascending order of th summarized all available inf effects on aquatic organisms was then sorted into two data of the 'effects' data entries (i. in association with at least reference conditions; Long ei of the 'no effects' data entries observed or an effect was c relative to reference conditic were derived for each substar 'no effects' category.

In this study, the original a PEL for each analyte. Origin the effects data set were Morgan 1990, Long 1992, Lowas similar to the procedure water quality standards in Ca of aquatic toxicity data effect data points on the resultant a procedure did not utilize a Nonetheless, data on the cor

Naples Bay, Rookery

liment quality, they do ontaminated sediments ediment chemistry data d bioaccumulation tests of sediment-associated ality guidelines (SQGs) entrations in sediments, on or restoration (Long lacDonald et al. 1992). derivation of numerical , Adams et al. 1992, views). The procedures /elopment are approach d limitations that affect little agreement as to re, each of the major Idress Florida's unique valuation indicated that formal guidelines for rogram of the National gan 1990, Long 1992), uidelines for assessing indicated that some the applicability of the

ifications made to the Gs for Florida coastal te the applicability of SQGs was assessed by nods. The reliability of nce of adverse effects predictability of the orida and the Gulf of effects data.

rical sediment quality gan 1990, Long 1992, w of the approach and ere. The derivation of ts of three main steps. between contaminant llected and evaluated. It sediments (BEDS; MacDonald et al. 1994). Next, two SQGs, a threshold effects level (TEL) and a probable effects level (PEL), were derived for each chemical substance. These guidelines were intended to define three ranges of contaminant concentrations that were rarely, occasionally and frequently associated with adverse biological effects. Finally, the SQGs were evaluated to determine their applicability to Florida coastal waters.

Development of a biological effects database for sediments

The first step in the derivation of SQGs involved the development of a biological effects database for sediments (BEDS) to compile matching chemical and biological data from numerous studies conducted throughout North America. Over 350 reports were reviewed and critically evaluated for this purpose. These reports provided information from equilibrium-partitioning models, laboratory spiked-sediment toxicity tests and field studies used to investigate the toxicity and/or benthic community composition of marine and estuarine sediments. Each record in the database included the citation, type of test and/or biological effects observed or predicted approach that was used, study area, test duration (if applicable and reported), species tested or the benthic community considered, TOC concentrations (if reported) and the concentration(s) of each chemical (expressed on a dry weight basis). More detailed descriptions of the BEDS are provided in Long (1992), Long and MacDonald (1992), CCME (1994), MacDonald (1994), Long et al. (1995).

Derivation of sediment quality guidelines

The BEDS was used as the sole source of information about the potential effects of sediment-associated contaminants. Data for each of the chemicals of concern in Florida coastal waters were retrieved from the database, incorporated into data tables and sorted in ascending order of the chemical's concentration. Each ascending data table summarized all available information that related the concentrations of the chemical to effects on aquatic organisms (MacDonald et al. 1994). The information in these tables was then sorted into two data sets, including (1) an 'effects data set', which included all of the 'effects' data entries (i.e. those for which an adverse biological effect was observed in association with at least a 2-fold elevation in the chemical concentration above reference conditions; Long et al. 1995) and (2) a 'no effects data set', which included all of the 'no effects' data entries (i.e. those for which either no adverse biological effect was observed or an effect was observed but the chemical concentration was not elevated relative to reference conditions; less than a 2-fold elevation). Both a TEL and a PEL were derived for each substance that had at least 20 data entries in both the 'effects' and 'no effects' category.

In this study, the original derivation procedures were modified to develop a TEL and a PEL for each analyte. Originally, the 10th (ER-L) and 50th (ER-M) percentile values in the effects data set were used to establish sediment quality guidelines (Long and Morgan 1990, Long 1992, Long and MacDonald 1992, Long et al. 1995). This method was similar to the procedure used by Klapow and Lewis (1979) to establish marine water quality standards in California. These authors reasoned that the use of percentiles of aquatic toxicity data effectively minimized the influence of single (potentially outlier) data points on the resultant assessment values (e.g. Barrick et al. 1988). The original procedure did not utilize the information in the no effects data set, however. Nonetheless, data on the concentrations of contaminants that are not associated with

adverse effects may provide additional information for defining the relationships between contaminant exposure and biological effects and was, therefore, used in this investigation.

In the present study, two SQGs were derived for each analyte using the information in both the effects and the no effects data sets, with the distributions of these data sets determined using percentiles (Byrkit 1975). For each analyte, a TEL was derived by calculating the geometric mean of the 15th percentile of the effects data set and the 50th percentile of the no effects data set. Similarly, a PEL was developed for each chemical by determining the geometric mean of the 50th percentile of the effects data set and the 85th percentile of the no effects data set. These arithmetic procedures were established by testing a variety of options using data for cadmium, copper, fluoranthene and phenanthrene and, subsequently, evaluating the resultant guidelines relative to their narrative objective. In this respect, the TEL was intended to estimate the concentration of a chemical below which adverse effects only rarely occurred (i.e. a minimal effects range; Fig. 1). Similarly, the PEL was intended to provide an estimate of the concentration above which adverse effects frequently occurred (i.e. probable effects range). Therefore, the TEL and PEL were intended to define three concentration ranges for a chemical, including those that were rarely, occasionally and frequently associated with adverse effects (Fig. 1). The extent to which the tested options satisfied these narrative objectives was determined by calculating the percent incidence of adverse effects below the TEL and above the PEL (Long et al. 1995).

The arithmetic procedures used to derive the SQGs in Florida were similar to those that have been used in other applications. For example, the Canadian Council of Ministers of the Environment (CCME, 1992) calculated the geometric mean of the lowest-observed-effect concentration (LOEC) and the no-observed-effect concentration (NOEC) to establish effects-based soil quality criteria. Similarly, Rand and Petrocelli (1985) calculated maximum acceptable toxicant concentrations (MATCs) from LOECs and NOECs from aquatic toxicity tests. The Canadian Council of Resource and Environment Ministers (CCREM, 1987) established a protocol that utilizes an analogous method for deriving water quality guidelines for the protection of agricultural water uses. In each of these cases, the geometric mean, rather than the arithmetic mean, was calculated due to uncertainty regarding the distributions of the data sets (i.e., the data were not expected to be normally distributed; Sokal and Rohlf 1981). The arithmetic procedures used in this study recently were adopted for deriving national SQGs in Canada (CCME 1994).

Evaluation of sediment quality guidelines

The SQGs developed in this study were evaluated using three procedures. The comparability of the SQGs was evaluated by comparing the TELs and PELs with similar assessment tools that have been derived using different approaches or procedures. The reliability of the SQGs was evaluated by calculating the percent incidence of adverse effects within ranges of contaminant concentrations defined by the TELs and PELs, using the information contained in the BEDS (MacDonald 1994, Long et al. 1995). Finally, the predictability of the SQGs was assessed using independent sediment chemistry and biological effects data sets from areas throughout the southeastern portion of the United States (MacDonald 1994).

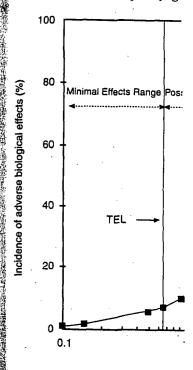


Fig. 1. Conceptual representation the potential for observing adversarial for observing adversar

Comparability. The SQGs guidelines, objectives and s (Tables 1 and 2). Guidelines were considered to be comdeveloped in this study (Lo

We interpret the threshol adverse biological effects r high level of protection for were identified for compari NOAA effects range-low v (PSDDA-SL) developed fc (USACOE 1988), (3) the Lyman et al. 1987, Pavlot quality objectives SQOs) developed for the comparison of the comparison

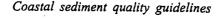
We interpret the probable adverse biological effects frolower level of protection for compared to the PELs inc. Long et al. 1995), (2) the (LAETs; Barrick et al. 19

fining the relationships, therefore, used in this

te using the information utions of these data sets a TEL was derived by effects data set and the was developed for each entile of the effects data ithmetic procedures were um, copper, fluoranthene uidelines relative to their stimate the concentration ed (i.e. a minimal effects de an estimate of the ed (i.e. probable effects hree concentration ranges and frequently associated d options satisfied these ent incidence of adverse i).

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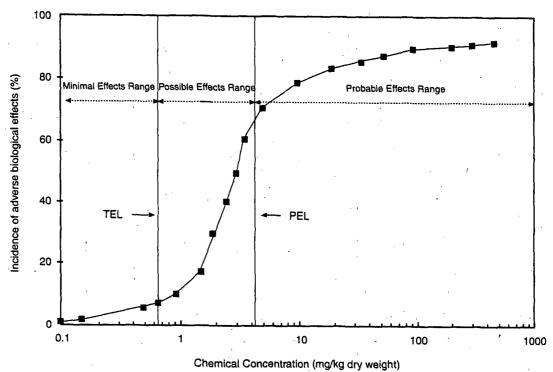


Fig. 1. Conceptual representation of the ranges of contaminant concentrations defined by SQGs and the potential for observing adverse effects within these ranges.

Comparability. The SQGs were compared to a variety of sediment quality criteria, guidelines, objectives and standards that were developed for use in other applications (Tables 1 and 2). Guidelines developed using different approaches or different procedures were considered to be comparable if they agreed within a factor of three of the SQGs developed in this study (Lorenzato et al. 1991).

We interpret the threshold effects levels (TELs) as the concentrations below which adverse biological effects rarely occur. Hence, the TELs are considered to provide a high level of protection for aquatic organisms. A total of four sets of similar guidelines were identified for comparison with the TELs derived in this study, including (1) the NOAA effects range-low values (ER-Ls; Long et al. 1995), (2) the screening levels (PSDDA-SL) developed for the Puget Sound Dredged Disposal Analysis Program (USACOE 1988), (3) the USEPA chronic sediment quality criteria (SQC-chronic; Lyman et al. 1987, Pavlou 1987, Hansen et al. 1993a,b,c,d,e) and (4) the sediment quality objectives SQOs) developed for Burrard Inlet (Swain and Nijman 1991).

We interpret the probable effects level (PELs) as the concentrations above which adverse biological effects frequently occur. Hence, the PELs are considered to provide a lower level of protection for aquatic organisms. The four sets of guidelines that were compared to the PELs included (1) the NOAA effects range-median values (ER-Ms; Long et al. 1995), (2) the lowest Puget Sound apparent effects threshold values (LAETs; Barrick et al. 1988), (3) the USEPA acute sediment quality criteria (SQC-

Table 1. A comparison of the TELs to other sediment quality guidelines for coastal and marine waters

Substance	TEL ^a	ER-L ^b	PSDDA-SL°	SQC-Chronic ^d	SQOe	Number of SQGs ^f comparable to TEL
Metals (SQGs in mg kg ⁻¹)	-					
Arsenic	7.24	8.2*	70	8.2*	20	2
Cadmium	0.68	1.2*	0.96*	7.7	1*	-3
Chromium	52.3	81*	NG^g	NG	60*	2
Copper	18.7	34*	81	34*	100	2 .
Lead	30.2	46.7*	66*	33*	30*	4
Mercury	0.13	0.15*	0.21*	0.01	0.15*	3
Nickel	15.9	20.9*	NG	NG	45*	2
Silver	0.73	1*	1.2*	- NG	NG	2
Zinc	124	150*	160*	190*	150*	3 2 2 4
Polychlorinated biphenyls (PCBs; So	QGs in µgkg ⁻¹)			•	
Total PCBs	21.6	22.7*	130	NG	30*	2
Pesticides (SQGs in µg kg ⁻¹)			-	•	٠.	·
Chlordane	2.26	0.5	NG ,	0.3	NG	0
Dieldrin	0.72	0.02	NG	200	NG	0 5
p,p'-DDD	1.22	2*	NG	NG	NG	1
p,p'-DDE	2.07	2.2*	NG	NG	NG	1
p,p'-DDT	1.19	1*	NG	1.6*	NG	^
Total DDT	3.89	1.58*	NG	1.6*	NG	2 2
Lindane (gamma-BHC)	0.32	NG	NG	3.1	NG	
Phthalates (SQGs in µg kg ⁻¹)		•	e e			0
Bis(2-ethylhexyl)phthalate	182	NG	3100	NG	NG	0

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Phthalates (SQGs in µg kg ⁻¹) Bis(2-ethylhexyl)phthalate	182	NG	3100	NG	NG	0
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Polycyclic aromatic hydrocarbons (PA	Hs; SQGs in	$\mu g k g^{-1}$)				
Acenaphthene	6.71	16*	63	2400	50	. 1
Acenaphthylene	5.87	44 -	64	NG	60	0
Anthracene	46.9	85.3*	130*	190	10	2
Fluorene	21.2	19*	64	59	50*	2
Naphthalene	34.6	160	210	500	200	ō
2-Methylnaphthalene	20.2	70	67	NG ·	NG	Õ
Phenanthrene	. 86.7	240*	320	2400	15	1
Total low molecular weight PAHs	312	552*	610*	NG	NG	2
Benz(a)anthracene	74.8	261	450	1600	130*	. 1
Benzo(a)pyrene	88.8	430	680	18 000	160*	1
Chrysene	108	384	670	1200	140*	1
Dibenz(a,h)anthracene	6.22	63.4	120	12 000	: 60	0
Fluoranthene	113	600	630	1600	170*	. 1
Pyrene	153	665	430*	850	260*	2

NG

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0.72

1.22

2.07

1.19

3.89

0.32

NG

NG

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NG

NG

NG

NG

0.3

1.6*

1.6*

3.1

850

NG

NG

260*

NG

NG

200

NG

NG

Total high molecular weight PAHs

655

1684

1700*

4022*

Total PAHs

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Dieldrin

p,p'-DDD

p,p'-DDE

p,p'-DDT

Total DDT

Lindane (gamma-BHC) Phthalates (SQGs in µg kg⁻¹)

aTEL, threshold effect level (this study).

^bER-L, effects range low (Long and Morgan 1990; Long et al. 1995).

cPSDDA-SL, screening level used in the Puget Sound Dredged Disposal Analysis Program (USACOE 1988).

dSQC-chronic, chronic sediment quality criterion (assuming 1% TOC; EqPA; Lyman et al. 1987, Pavlou 1987, Hansen et al. 1993a,b,c,d,e).

SQO, sediment quality objective (Swain and Nijman 1991).

SQG, sediment quality guideline.

^gNG, no guideline available.

^{*}Indicates that the SQGs are within a factor of three of the TEL.

Table 2. A comparison of the PELs to other sediment quality guidelines for coastal and marine waters

Substance	PEL ^a	ER-M ^b	LAET°	SQC ^d -acute	SLC	Number of SQGs ^f comparable to PEL
Metals (SQGs in mg kg ⁻¹)		 				
Arsenic	41.6	70*	57*	. 16	NG^g	2
Cadmium	4.21	9.6*	5.1*	24	NG	2
Chromium	160	370*	260*	NG	NG	Ź
Copper	108	270*	390	54	NG	1
Lead	112	218*	450	840	NG	1 .
Mercury	0.7	0.71*	0.41*	0.15	NG	.2
Nickel	42.8	51.6*	>140	NG	NG	1
Silver	1.77	3.7*	>0.56	NG	NG	1
Zinc	271	410*	410*	560*	NG	2 1 1 3
Polychlorinated biphenyls (PCBs; S	SOGs in ugkg ⁻¹)	ı			i	
Total PCBs	189	180*	130*	NG .	36.6	. 2
Pesticides (SQGs in µg kg ⁻¹)		,	•		• .	
Chlordane	4.79	6*	NG	NG	NG	1
Dieldrin	4.3	. 8*	NG	NG	NG	~ 1
p,p'-DDD	7.81	20*	16*	NG	NG	2
p,p'-DDE	. 374	27*	9	NG	NG	2 0
p,p'-DDT	4.77	7*	34	NG	NG	•
Total DDT	51.7	46.1*	NG	210	505	1
Lindane (gamma-BHC)	0.99	NG	NG	NG	NG	0
Phthalates (SQGs in µg kg ⁻¹)				•		0 1
Bis(2-ethylhexyl)phthalate	2647	NG	1900*	NG	NG	1 .
		-	-300,			

500

NG

Polycyclic aromatic hydrocarbons (PAHs; SQGs in μg kg⁻¹) Acenaphthene 88.9 500

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210

olycyclic aromatic hydrocarbons (PA Acenaphthene	88.9	500	500	NG	NG	0	
Acenaphthylene	128	640	>560	NG	47.4*	1	
Anthracene	245	1100	960	NG	163*	1	
Fluorene	144 -	540	540	NG	101*	i	
Naphthalene	391	2100	2100	10 500	414*	1	
2-Methylnaphthalene	201	670	670	NG	NG	0	
Phenanthrene	544	1500*	1500*	14 000	368	. 2	*
Total low molecular weight PAHs	1442	3160*	5200	NG	NG	. 1	
Benz(a)anthracene	693	1600*	1300*	55 000	261	2	•
Benzo(a)pyrene	763	1600*	1600*	450 000	397	2	
Chrysene	846	2800	1400*	115 000	. 384	1	
Dibenz(a,h)anthracene	135	260*	230*	NG	NG	2	
Fluoranthene	1494	5100	1700*	9000	644*	2	
Pyrene	1398	2600*	2600*	49 500	665	2 .	
Total high molecular weight PAHs	6676	9600*	12 000*	NG	NG	2	
Total PAHs	16 770	44 792*	NG	NG	NG	1	

NG

NG

NG

NG

16*

34

1900*

8*

20*

27*

7*

46.1*

NG

NG

4.79

4.3

7.81

4.77

0.99

51.7

374

2647

Chiordane

Dieldrin

p,p'-DDD

p,p'-DDE p,p'-DDT

Total DDT

Lindane (gamma-BHC) Phthalates (SQGs in µg kg⁻¹)

Bis(2-ethylhexyl)phthalate

^aPEL, probable effect level (this study). ^bER-M, effects range median (Long et al. 1995, Long and Morgan 1990).

LAET, lowest apparent effects threshold (PTI, 1988).

dSQC-acute, acute sediment quality criterion (assuming 1% TOC; EqPA; Lyman et al. 1987, Pavlou 1987).

SLC, national screening level concentration (Neff et al. 1987).

SQG, sediment quality guideline.

⁹NG, no guideline available.

^{*}Indicates that the SQGs are within a factor of three of the PEL.

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Reliability. The reliability of the SQGs developed in this study was evaluated using the information contained in the ascending data tables. To facilitate this evaluation, a scoring system was devised to integrate information on three distinct attributes of the SQGs, including (1) the incidence of adverse biological effects within the minimal effects range, (2) the incidence of adverse biological effects within the probable effects range and (3) the degree of concordance between the concentrations of sediment-associated contaminants and the incidence of adverse biological effects. Good concordance between these two variables is indicated by marked increases in the incidence of effects over the three ranges of contaminant concentrations (Long et al. 1995).

First, a TEL score (TS) was determined for each analyte to quantify incidence of adverse biological effects within the minimal effects range. Specifically, the number of effects data entries and the total number of data entries that were contained within the minimal effects range were determined for each substance. Subsequently, the percent incidence of adverse effects was calculated for each substance by dividing the number of effects data entries by the total number of data entries within the minimal effects range and multiplying this value by 100. A TS of 2, 1 or 0 was assigned if the incidence of adverse biological effects within the minimal effects range was <10%, 10–25%, or >25%, respectively (MacDonald 1994).

Next, a PEL score (PS) was determined for each substance for which SQGs were derived. Consistent with the procedures that were used to determine the TS, the percent incidence of adverse biological effects within the probable effects range was calculated for each substance. A PS of 2, 1 or 0 was subsequently assigned if the incidence of adverse biological effects within the probable effects range was >65%, 50-65% or <50%, respectively (MacDonald 1994).

A concordance score (CS) was determined to assess the degree of agreement between contaminant concentrations and the incidence of adverse biological effects. The CS was calculated by first determining the incidence of adverse biological effects within the possible effects range (i.e. between the TEL and PEL). Next, the percent incidence of adverse biological effects within each of the three ranges of contaminant concentrations were compared. Long et al. (1995) indicated that there should be a consistent and marked increase in the incidence of effects within the three concentration ranges. Therefore, the presence of at least a 2-fold increase in the incidence of effects between adjacent ranges of concentrations was used as an indicator of concordance. A CS of 2 was assigned if the percent incidence of adverse biological effects was a factor of 2 or more higher in the probable effects range than in the possible effects range and in the possible effects range compared to the minimal effects range. A CS of 1 was assigned if the factor of 2 difference in the incidence of effects was apparent between only two ranges. A CS of 0 was assigned if there was no apparent concordance between chemical concentrations and the incidence of adverse effects.

Finally, the overall reliability of the guidelines for each substance was evaluated by calculating a total reliability score (TRS; MacDonald 1994). The TRS was determined by calculating the sum of TS, PS and CS for each substance. The guidelines for a substance were considered to have a high degree of reliability if they had a TRS of 6 (i.e. the maximum score). A moderate degree of reliability was assigned when

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ational screening level

was evaluated using the this evaluation, a scoring attributes of the SQGs, he minimal effects range, ble effects range and (3) of sediment-associated nod concordance between dence of effects over the

to quantify incidence of recifically, the number of rere contained within the subsequently, the percent by dividing the number ithin the minimal effects: 0 was assigned if the rts range was <10%, 10—

e for which SQGs were mine the TS, the percent ects range was calculated gned if the incidence of was >65%, 50-65% or

ee of agreement between gical effects. The CS was ogical effects within the the percent incidence of intaminant concentrations uld be a consistent and ee concentration ranges idence of effects between concordance. A CS of 2 ects was a factor of 2 or effects range and in the A CS of 1 was assigned parent between only two ordance between chemical

ostance was evaluated by The TRS was determined ce. The guidelines for a if they had a TRS of 6 ity was assigned when Coastal sediment quality guidelines

intermediate scores were obtained for one or two of the parameters or when a low score was obtained for one parameter but high scores were assigned for the other two (i.e. with a TRS of 4 or 5). SQGs with a TRS that was <4 were considered to have a low degree of reliability.

Predictability. The predictability of the TELs and PELs was evaluated separately using independent data from field surveys conducted at sites in Tampa Bay, Pensacola Bay, coastal Gulf of Mexico and offshore Gulf of Mexico. First, the concentration of each substance in each sediment sample was compared to the SQGs. Sediment samples with concentrations of one or more substances that exceeded their respective PELs were predicted to be toxic. Sediment samples were predicted to be non-toxic if the concentrations of all measured substances were below the TELs. Sediment samples with concentrations of one or more contaminants above the TEL but below the PEL (i.e. within the possible effects range) were neither predicted to be toxic nor non-toxic and were not used to evaluate the predictability of the SQGs.

The accuracy of the predictions was then evaluated by comparing them with the results of the biological investigations. The predictability of the PEL was calculated as the ratio of the number of samples that were correctly predicted to be toxic and the number of samples that were originally predicted to be toxic (expressed as a percentage). Similarly, the predictability of the TEL was calculated as the ratio of the number of samples that were correctly predicted to be non-toxic and the number of samples that were originally predicted to be non-toxic (expressed as a percentage). In this assessment, toxic samples were defined as those in which one or more of the measured bioassay end-points were significantly different from control or reference samples.

Results

Numerical SQGs were derived for a total of 34 substances, including nine trace metals, total PCBs, 13 individual PAHs, three groups of PAHs, seven pesticides and bis(2-ethylhexyl)phthalate. The TELs are listed in Table 1 and the PELs are listed in Table 2. Fewer than 20 effects data records were available for a number of additional substances (e.g. tributyltin, pentachlorophenol, dioxins, furans and a suite of pesticides) that are also contaminants of concern in Florida coastal sediments (MacDonald 1994). Therefore, SQGs could not be derived for these substances.

Comparability

The evaluation of the comparability of the SQGs was impaired by the lack of guidelines for certain substances. For example, guidelines from three or more approaches were available for only 19 of the substances for which TELs have been developed and for only 18 of the substances for which PELs had been developed. An adequate number of guidelines were not available for chromium, nickel, silver, bis(2-ethylhexyl)phthalate, several PAHs and most of the pesticides. Nonetheless, the results of this evaluation indicate that many of the SQGs compare favourably to guidelines that were derived for other applications.

The TELs for 17 of the 34 substances were within a factor of three for two or more other guidelines (Table 1). The best agreement was observed for metals and the poorest

agreement was observed for high molecular weight (HMW) PAHs. The TELs were usually lower than values developed using other guidelines, indicating that the TELs could be more protective. The PELs for 14 of the 34 substances were within a factor of three for two or more of the other guidelines listed in Table 2. Once again, greatest agreement among the various guidelines was observed for metals. Relatively poor agreement was observed among the guidelines for pesticides and low molecular weight (LMW) PAHs. As was the case for the TELs, the PELs were generally lower than values developed using guidelines based on other procedures.

Reliability

Using information in the ascending data tables, the reliability of the TELs for 30 substances was found to be relatively high (TS = 2), as indicated by the low incidence of effects (<10%) within the minimal effects range (Tables 3 and 4). This group included the TELs for nine metals, 14 individual PAHs or groups of PAHs, six pesticides and bis(2-ethylhexyl)phthalate. Moderate reliability (TS = 1) was indicated for the TELs for fluorene, dibenz(a,h)anthracene and total PCBs. Low reliability (TS = 0) was indicated for only one substance (total DDT).

The reliability of the PELs generally was lower than that of the TELs. The PELs for 16 substances had a relatively high degree of reliability (PS = 2), as indicated by a high incidence of adverse biological effects (>65%) within the probable effects ranges (Tables 3 and 4). Of the highly reliable PELs, 14 were for individual PAHs or groups of PAHs. The PELs for cadmium and bis(2-ethylhexyl)phthalate were also considered to be highly reliable. A moderate degree of reliability (PS = 1) was indicated for five of the nine metals; a low degree of reliability (PS = 0) was indicated for arsenic, mercury and nickel. The PELs for pesticides and total PCBs had either a moderate or low level of reliability.

A high degree of concordance between contaminant concentrations and the incidence of adverse biological effects was observed for the majority of the SQGs (Tables 3 and 4). The incidence of adverse effects consistently and markedly increased with increasing concentrations for all trace metals except mercury, nickel and silver. Two-fold increases in the incidence of effects between the minimal effects range and possible effects range and the possible effects range and probable effects range were also observed for ten of the 16 individual PAHs and groups of PAHs (Table 4). The concordance scores for three pesticide guidelines were high (CS = 2 for dieldrin, p,p'-DDD and p,p'-DDE), while those for four other pesticides and total PCBs were lower (CS = 0 or 1).

Overall, total reliability scores of 4 or more were calculated for the majority of the guidelines, indicating high or moderate reliability (Table 4). A high degree of reliability (TRS = 6) was indicated for one trace metal (cadmium), ten individual PAHs or groups of PAHs and bis(2-ethylhexyl)phthalate. The SQGs for 16 other substances were moderately reliable (TRS = 4 or 5), including those for six trace metals, five individual PAHs, total HMW-PAHs, dieldrin, p,p'-DDE, p,p'-DDD and p,p'-DDT. The reliability of the guidelines for mercury, nickel, total PCBs, chlordane, lindane and total DDT was lower (TRS < 4).

Predictability

The predictability of the SQGs was evaluated using four independent data sets from the southeastern portion of the United States. In Tampa Bay, Florida, matching sediment

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PAHs. The TELs were ndicating that the TELs s were within a factor of 2. Once again, greatest metals. Relatively poor nd low molecular weight are generally lower than

ity of the TELs for 30 d by the low incidence of 1 4). This group included PAHs, six pesticides and idicated for the TELs for y (TS = 0) was indicated

the TELs. The PELs for 2), as indicated by a high probable effects ranges vidual PAHs or groups of vere also considered to be indicated for five of the for arsenic, mercury and moderate or low level of

trations and the incidence f the SQGs (Tables 3 and increased with increasing silver. Two-fold increases and possible effects range also observed for ten of e concordance scores for pp'-DDD and p,p'-DDE), were (CS = 0 or 1).

ed for the majority of the high degree of reliability individual PAHs or groups 6 other substances were ace metals, five individual p,p'-DDT. The reliability indane and total DDT was

pendent data sets from the lorida, matching sediment

chemistry and biological effects data were available for 61 sediment samples (Long et al. 1994). The analytes in these samples included metals, PAHs, PCBs and a suite of pesticides. Based on a comparison of the sediment chemistry data with the PELs, 46 of these samples were predicted to be toxic (Table 5). A suite of toxicity tests was also conducted on these samples, including a 10 day amphipod (Ampelisca abdita) survival test (using bulk sediments) and a 1 hr sea urchin (Arabacia punctulata) fertilization test (using undiluted pore water). Based on the results of these toxicity tests, 40 samples were observed to be toxic (i.e. toxicity was observed in one or more tests). Therefore, the predictability of the PELs was 87% (40 out of 46 samples). Only two of the 61 sites were predicted to be non-toxic; the results of the biological tests conducted on these two samples revealed that neither sample was toxic. Thirteen samples were not classified, as the concentrations of all analytes were below the PEL but the concentrations of one or more substances exceeded the TEL (i.e. within the possible effects range).

In Pensacola Bay, data for 20 samples were available for assessing the predictability of the guidelines (E.R. Long, unpublished data). The concentrations of metals, PAHs and a suite of pesticides were measured in each of these samples. Sediment toxicity was assessed using a 10 day amphipod (A. abdita) survival test, a sea urchin (A. punctulata) fertilization (1 h) and embryo development test (48 h) and a microbial bioluminescence test (Microtox). Based on comparisons of the metals and organics data with the PELs, 12 samples were predicted to be toxic (Table 6). Of these, 11 of the samples were observed to be toxic. Therefore, the predictability of the PELs was 92%. Using the TELs, two samples were predicted to be non-toxic; both of these samples were observed to be toxic. It should be noted that these samples contained elevated levels of one or more substances that could not be identified using a range of analytical techniques and which could have caused or contributed to the toxicity.

As part of the Environmental Monitoring and Assessment Program (EMAP), administered by the US Environmental Protection Agency, matching sediment chemistry and biological effects data were collected from eight areas in the Gulf of Mexico region in 1991 (USEPA, unpublished data). The areas sampled in this survey included Galveston Bay (TX), Matagorda Bay (TX), Mississippi River (LA), Mississippi Sound (LA), Mobile Bay AL), Pensacola Bay (FL), Florida Panhandle (FL) and West Central Florida (FL). Sediment chemistry data were collected on metals, PAHs, PCBs, a suite of pesticides and several additional substances. Sediment toxicity was assessed using acute toxicity (lethality) tests with the amphipod, A. abdita (10 days) and the mysid, Mysidopsis bahia (4 days). As no statistical evaluation of the toxicity test results were reported, a 20% difference between the survival of test organisms in Gulf of Mexico sediments versus control sediments was assumed to indicate toxicity in this evaluation (USEPA/USACOE 1991, Schimmel et al. 1994). Of the 47 samples collected in this survey, three were predicted to be toxic and 16 were predicted to be non-toxic (Table 7). The results of the two toxicity tests indicated that none of the samples that were predicted to be toxic were observed to be toxic (predictability = 0%). In contrast, 15 of the 16 samples that were predicted to be non-toxic were in fact non-toxic (predictability = 94%).

As part of the Minerals Management Services (MMS) Gulf of Mexico Offshore Operators Monitoring Experiment (GOOMEX), sediment chemistry and toxicity data were collected in the vicinity of petroleum exploration and production platforms in the Gulf of Mexico (R.S. Carr, D.C. Chapman, B.J. Prestley, J.M. Biedenbach, L. Robertson

Table 3. Incidence of adverse biological effects within ranges of chemical concentrations in marine and estuarine sediments

Substance	% effects in the minimal effects range (< = TEL ^a)	% effects of the possible effects range (>TEL to <pela)< th=""><th>% effects in the probable effects range (> = PEL)</th></pela)<>	% effects in the probable effects range (> = PEL)
Metals			
Arsenic	2.7	12.9	46.8
Cadmium	5.6	20.1	70.8
Chromium	3.5	15.4	52.9
Copper	9.0	21.9	55.9
Lead	5.8	25.8	58.4
Mercury	7.8	23.6	36.7
Nickel	3.3	8.4	9.4
Silver	6.6	9.8	60.5
Zinc	3.8	27.2	64.8
Polychlorinated biphenyls (PCBs)		1.	
Total PCBs	15.7	36.9	54.9
Polycyclic aromatic hydrocarbons (PAHs)			
Acenaphthene	7.5	29.1	57.4
Acenaphthylene	7.4	13.9	51.4
Anthracene	8.7	20.5	75.0
Fluorene	11.7	20.5	70.0
2-methylnaphthalene	0.0	23.4	81.5
Naphthalene	2.6	19.3	71.2
Phenanthrene	8.0	22.8	77.8
Total low molecular weight PAHs	8.7	19.4	65.6

		, 30.9	•	lder,
			,	
Polycyclic aromatic hydrocarbons (PAHs)	7.5	29.1	57.4	Long and Ingersoll
Acenaphthene	7.5	13.9	51.4	97
Acenaphthylene	7.4	20.5	75.0	an
Anthracene	8.7	20.5	70.0	g
Fluorene	11.7	23.4	81.5	Ing
2-methylnaphthalene	0.0	19.3	71.2	jer
Naphthalene	2.6	22.8	77.8	SO
Phenanthrene	8.0	19.4	65.6	1
Total low molecular weight PAHs	8.7	****		
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Benz(a)anthracene	8.7	15.7	78.4	δ
Benzo(a)pyrene	8.5	22.1	70.9	zst.
Chrysene	9.2	18.8	70.9 72.4	al
Dibenz(a,h)anthracene	15.8	11.6	65.1	se.
Fluoranthene	9.5	20.2	79.7	din
Pyrene	9.3 7.4	19.3	83.0	7.07
	9.5	19.3	65.5	=
Total high molecular weight PAHs				nt
Total PAHs	7.3	19.3	76.7	Coastal sediment quality guidelines
Pesticides				¥ .
Chlordane	9.0	12.1	17.0	zui.
Dieldrin	3.5	. 13.2	50.0	dei
Lindane (gamma-BHC)	2.9	21.1	25.6	line
p,p'-DDD	3.6	10.9	46.2	Ŋ
p,p'-DDE	5.3	16.5	50.0	
p,p'-DDT	7.9	4.8	58.6	
Total DDT	47.6	25.6	64.0	•
Phthalates				
Bis(2-ethylhexyl)phthalate	8.5	21.2	66.7	• .

In the ascending data tables for each chemical, entries were identified as effects data entries if an adverse biological effect was reported and concordance was apparent between the observed biological response and the measured chemical concentration.

% effects = (number of effects data entries in the range/total number of data entries in the range) × 100.

aTEL, threshold effect level; PEL, probable effect level.

Predictability (using one to two

Observed number of toxic samples:

Observed number of toxic samples:

Table 4. An evaluation of the overall reliability of the sediment quality assessment guidelines for priority substances in Florida coastal waters

	TELª	PEL ^a	Concordance	Total	
	score	score	score	reliability	Overall ^b
Substance	(TS)	(PS)	(CS)	score (TRS)	reliability
Metals					
Arsenic	2	0	2	4	M
Cadmium	2	2	2	6	Н
Chromium	2	1	2	5	M
Copper	2	1	2	5	M
Lead	2	1	2	5	M
Mercury	2	0	1	3	L
Nickel	2	0	1	3	L
Silver	2	1	ī	4	M
Zinc	2	i	2	5	M
Polychlorinated biphenyls (PCBs)				• .	
Total PCBs	1	1	1	3	L
	-	-	-	*	_
Pesticides				•	
Chlordane	2	['] 0	0	2	L
Dieldrin	2	i	2	5 .	M
p,p'-DDD	2	Ô	2	4	M
p,p'-DDE	2	1	2	5	M
p,p'-DDT	2	ì	1	4	M
Total DDT	0	1	0	1	L
Lindane (gamma-BHC)	2	0	1	3	Ĺ
Phthalates			•		•
Bis(2-ethylhexyl)phthalate	2	2	2	6	Н
Polycyclic aromatic hydrocarbons (PA	Hs)				
Acenaphthene	2 [´]	. 1	1	4	M
Acenaphthylene	2	1	. 1	4	M
Antracene	2	2	2	6	H
Fluorene	1	2	1	4	M
Naphthalene	2	. 2	2	6	H
2-Methylnaphthalene	2	2	2 .	6	H
Phenanthrene	2	2	2 .	6	H
Total low molecular weight PAHs	2	2	2	6	H
•	2	. 2	1	5	n M
Benz(a)anthracene	2	4		J	IAI
Benzo(a)pyrene	2	2	2	6	H
Chrysene	2	2	2	6	H
Dibenz(a,h)anthracene	1	2 .	1	4	M
Fluoranthene	2	2	2	6	Н
Pyrene	2	2	2	6	H
Total high molecular weight PAHs	2	2	1	5	M
Total PAHs	2	2	2	6	H

 a TEL, threshold effect level; PEL, probable effect level. b H, high (TRS = 6); M, moderate (TRS = 4-5); L, low (TRS < 4).

Table 5. Predictability of the TELsa and PELsa in Tampa Bay sediments (Long et al. 1994)

Number of samples per category

Category

Table 5.	Predictability	of the TE	sa and P	PFIsa in	Tamna B	av sediments	(I ong et al	1004)
I ADIC J.	I I Cuictaviiit)	OI UNC IL	_o anu i	LLS III	Talliba D	av scumicius	ILUNE EL UL.	エフフサノ

Category	Number of samples per category	Observed number of toxic samples: amphipod test (%)	Observed number of toxic samples: sea urchin test (%)	Predictability (using one to two tests; % correct)
Actual toxicity	61	8 of 61 (13)	50 of 61 (82)	
Not toxic (<tels)< td=""><td>2 .</td><td>0 (0)</td><td>0 (0)</td><td>100 (2 of 2)</td></tels)<>	2 .	0 (0)	0 (0)	100 (2 of 2)
Possibly toxic (>TELs; <pels)< td=""><td>13</td><td>1 (8)</td><td>10 (77)</td><td></td></pels)<>	13	1 (8)	10 (77)	
Toxic (one PEL exceeded)	22	0 (0)	16 (73)	73 (16 of 22)
Toxic (two to five PELs exceeded)	3	2 (67)	3 (100)	100 (3 of 3)
Toxic (six to nine PELs exceeded)	5	1 (20)	5 (100)	100 (5 of 5)
Toxic (>10 PELs exceeded)	16 .	4 (25)	. 16 (100)	100 (16 of 16)
Toxic (one or more PELs exceeded)	46	7 (15)	40 (87)	87 (40 of 46)
Toxic (two or more PELs exceeded)	24	7 (29)	24 (100)	100 (24 of 24)

^aTEL, threshold effect level; PEL, probable effect level.

Table 6. Predictability of the TELsa and PELsa in Pensacola Bay sediments (E.R. Long, unpublished data)

Category	Number of samples per category	Number of toxic samples: amphipod test (%)	Number of toxic samples: sea urchin test (%)	Number of toxic samples: Microtox test (%)	Predictability (using one to three tests; % correct)
Actual toxicity	· -	0 of 20 (0)	13 of 20 (65)	15 of 20 (75)	_
Not toxic (<tels)< td=""><td>2</td><td>0 (0)</td><td>1 (50)</td><td>2 (100)</td><td>0 (0 of 2).</td></tels)<>	2	0 (0)	1 (50)	2 (100)	0 (0 of 2).
Possibly toxic (>TELs; <pels)< td=""><td>6</td><td>0 (0)</td><td>3 (50)</td><td>4 (67)</td><td><u> </u></td></pels)<>	6	0 (0)	3 (50)	4 (67)	<u> </u>
Toxic (one PEL exceeded)	2	0 (0)	2 (100)	2 (100)	100 (2 of 2)
Toxic (two to five PELs exceeded)	5	0 (0)	3 (60)	4 (80)	80 (4 of 5)
Toxic (six to nine PELs exceeded)	2	0 (0)	2 (100)	2 (100)	100 (2 of 2)
Toxic (>10 PELs exceeded)	3	0 (0)	2 (67)	3 (100)	100 (3 of 3)
Toxic (one or more PELs exceeded)	12	0 (0)	9 (75)	11 (92)	92 (11 of 12)
Toxic (two or more PELs exceeded)	10	0 (0)	7 (70)	9 (90)	90 (9 of 10)

^aTEL, threshold effect level; PEL, probable effect level.

Table 7. Predictability of the TELsa and PELsa in coastal Gulf of Mexico sediments (USEPA, unpublished data)

Category	Number of samples per category	Number of toxic samples: amphipod test (%)	Number of toxic samples: mysid test (%)	Predictability (using one to two tests; % correct)
Actual toxicity	47	7 of 47 (15)	0 of 47 (0)	
Not toxic (<tels)< td=""><td>16</td><td>1 (6)</td><td>0 (0)</td><td>94 (15 of 16)</td></tels)<>	16	1 (6)	0 (0)	94 (15 of 16)
Possibly toxic (>TELs; <pels)< td=""><td>28</td><td>6 (27)</td><td>0 (0)</td><td>· ·</td></pels)<>	28	6 (27)	0 (0)	· ·
Toxic (one PEL exceeded)	3	0 (0)	0 (0)	0 (0 of 3)
Toxic (two to five PELs exceeded)	0	· - ·	-	·
Toxic (six to nine PELs exceeded)	0	- ` + ";*		` -
Toxic (>10 PELs exceeded)	0 .	· _ ·		~ :
Toxic (one or more PELs exceeded)	3	0 (0)	0 (0)	0 (0 of 3)
Toxic (two or more PELs exceeded)	.0		-	

aTEL, threshold effect level; PEL, probable effect level.

and S.P. Boothe submitted). Five platforms were sampled during the first cruise and three platforms were sampled during the second cruise. Twenty-five stations were sampled per platform per cruise, with the stations arranged in a radial array around each platform. The sediment chemistry data consisted of a suite of trace metals and petroleum hydrocarbons; however, no chlorinated organic compounds were measured. Both sea urchin (A. punctulata) fertilization and embryological development tests were conducted with sediment pore water from the 125 samples from the first cruise, but only the embryological development test was used for the samples collected during the second cruise, as the latter test proved to be more sensitive for assessing the effects of the contaminants present at these platforms.

In the GOOMEX study, 16 of the 200 samples tested were toxic (Kennicutt 1993). Based on comparisons of the sediment chemistry data to the guidelines, 27 of the 200 samples were predicted to be toxic and 50 were predicted to be non-toxic (Table 8). Thirty-seven percent (ten out of 27) of the samples predicted to be toxic (i.e. one or more PELs exceeded) were observed to be toxic. The predictability increased to 58% (seven out of 12) when two or more PELs were exceeded in sediment samples. All of the non-toxic samples with contaminant concentrations that exceeded one or more PELs were predicted to be toxic based on the concentrations of zinc or lead. Ninety-six percent of the 50 samples predicted to be non-toxic were observed to be non-toxic using these very sensitive toxicity tests (Carr and Chapman 1992).

Considering all of the data collected in the Gulf of Mexico region, the results of biological investigations indicated that 59 of the 88 samples that were predicted to be toxic actually were toxic (Table 9). Hence, an overall predictability of 67% was calculated for the PELs. By comparison, 66 of the 70 samples that were predicted to be non-toxic actually were non-toxic to all of the organisms tested. The predictability of the TELs was, therefore, calculated to be 94%. When data from coastal areas of the Gulf of Mexico only were considered, the predictability of the TELs and PELs were 85 and 84%, respectively. It should be noted that slightly more than one-half of the samples collected in these surveys had concentrations of one or more contaminants that fell within the possible effects range; therefore, it was not possible to predict whether or not these samples would be toxic. On average, approximately one-fifth of these samples were observed to be toxic, based on the results of a battery of tests.

Table 8. Predictability of the TELs^a and PELs^b in offshore Gulf of Mexico sediments using the sea urchin embryological development test (Carr et al. 1995)

Category	Number of samples per category	Number of toxic samples (%)	Predictability (%)
Actual toxicity	200	16 of 200 (11)	- ;
Not toxic (<tels)< td=""><td>50</td><td>2 (4)</td><td>96 (48 of 50)</td></tels)<>	50	2 (4)	96 (48 of 50)
Possibly toxic (>TELs; <pels)< td=""><td>123</td><td>11 (9)</td><td>_ ` `</td></pels)<>	123	11 (9)	_ ` `
Toxic (one PEL exceeded)	15	3 (20)	20 (3 of 15)
Toxic (two to five PELs exceeded)	12	7 (58)	58 (7 of 12)
Toxic (six to nine PELs exceeded)	0	_	_
Toxic (>10 PELs exceeded)	0 .	-	_
Toxic (one or more PELs exceeded)	27	10 (37)	37 (10 of 27)
Toxic (two or more PELs exceeded)	12	7 (58)	58 (7 of 12)

aTEL, threshold effect level; PEL, probable effect level.

Table 9. Evaluation of the predictability of the TELsa and PELsa in southeastern United States sediments

Location	Number of samples correctly predicted as not toxic (%)	Number of samples correctly predicted as toxic (%)
Tampa Bay	2 of 2 (100)	40 of 46 (87)
Pansacola Bay	0 of 2 (0)	11 of 12 (92)
Coastal Estuaries	15 of 16 (94)	0 of 3 (0)
Total coastal Gulf of Mexico	17 of 20 (85)	51 of 61 (84)
Offshore Gulf of Mexico	48 of 50 (96)	10 of 27 (37)
Gulf of Mexico (total coastal plus offshore)	65 of 70 (93)	61 of 88 (69)

aTEL, threshold effect level; PEL, probable effect level.

Discussion

The modified weight-of-evidence approach developed here is characterized by a number of attributes that make it attractive for deriving SQGs for Florida coastal waters. Unlike many other approaches to the development of SQGs, the weight-of-evidence approach does not attempt to establish absolute sediment quality assessment values. Instead, the approach delineates ranges of contaminant concentrations that are probably, possibly and not likely to be associated with adverse biological effects. This approach recognizes the uncertainty associated with the prediction of biological effects under a variety of field conditions and relies upon the evidence assembled from numerous independent studies.

One of the more important attributes of the weight-of-evidence approach is its overall practicality. Guidelines for 34 potentially toxic substances were calculated relatively quickly and inexpensively using available data. In addition, by considering matching sediment chemistry and biological effects data from studies conducted in the field, the influence of mixtures of chemicals in sediments is incorporated in the resultant SQGs. This feature increases the degree of environmental realism and, thus, applicability of the guidelines. Furthermore, the information in the BEDS is highly relevant to the guidelines derivation process because it applies to a wide range of biological organisms and end points, incorporates a large number of direct measurements on organisms that are normally associated with bedded sediments and includes many data from various studies conducted in the southeastern United States (including Florida). These attributes are likely to give the SQGs derived using the modified weight-of-evidence approach broad applicability in the southeast, increasing the probability that the guidelines would be appropriate for implementation in Florida.

In addition to the other advantages of the approach, the arithmetic procedures used in this study for calculating SQGs considered the information in both the effects and no effects data sets. Hence, the resultant guidelines were more likely to satisfy narrative objectives. And, in contrast to the apparent effects threshold approach (Barrick et al. 1988), the weight-of-evidence procedure does not rely heavily on individual data points. Therefore, outliers do not excessively influence values in the overall guidelines derivation process.

Despite the benefits associated with this approach, a number of limitations were also evident which could restrict application of these guidelines. First, the weight-of-

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Number of samples correctly predicted as toxic (%)

40 of 46 (87)

11 of 12 (92)

0 of 3 (0)

51 of 61 (84)

10 of 27 (37)

61 of 88 (69)

racterized by a number ı coastal waters. Unlike t-of-evidence approach ent values. Instead, the probably, possibly and approach recognizes the inder a variety of field us independent studies. ; approach is its overall re calculated relatively / considering matching ducted in the field, the in the resultant SQGs. hus, applicability of the nighly relevant to the of biological organisms ients on organisms that nany data from various lorida). These attributes nt-of-evidence approach at the guidelines would

netic procedures used in both the effects and no cely to satisfy narrative pproach (Barrick et al. a individual data points. the overall guidelines

of limitations were also. First, the weight-of-

evidence approach does not fully support the quantitative evaluation of cause and effect relationships between contaminant concentrations and biological responses. Although information from spiked-sediment toxicity tests and equilibrium partitioning models is included in the BEDS, the weight-of-evidence approach is still largely based on associations between contaminant concentrations and biological responses. Various factors other than concentrations of the contaminant under consideration could have influenced the actual response observed in any given investigation, including (but not limited to) the additive and synergistic effects of co-occurring contaminants. While the assembly of extensive information from numerous estuarine and marine sites across North America into a single database reduces this limitation, the level of uncertainty associated with the resultant SQGs is still not quantified. We are currently investigating the use of toxic units models to reduce uncertainty (i.e. R.C. Swartz, D.W. Schults, R.J. Ozretich, J.O. Lamberson, F.A. Cole, T.H. DeWitt, M.S. Redmond and S.P. Ferraro submitted).

Application of the recommended approach may also be restricted by other limitations on the available information. Presently, few data exist on the chronic responses of marine and estuarine organisms to contaminated sediments. Furthermore, few data are available for some potentially important contaminants of sediments in Florida, including tributyltin, pentachlorophenol, dioxins and furans and various pesticides. These data gaps impair our ability to evaluate the overall applicability of the approach to Florida.

Sediment-associated contaminants can accumulate in the tissues of aquatic organisms and thus have the potential to adversely affect human and non-human consumers of aquatic biota. However, the guidelines developed in this study do not address either the potential for bioaccumulation or the associated adverse effects of bioaccumulation on higher trophic levels.

One shortcoming of the weight-of-evidence approach is associated with the limitations on the data that describe the potential bioavailability of sediment-associated contaminants (Di Toro et al. 1990). Large differences in toxicity of sediment-associated contaminants have been reported for relatively small ranges in concentration for total organic carbon (TOC) and/or acid volatile sulphide (AVS) (Swartz et al. 1990, Di Toro et al. 1991. Adams et al. 1992). However, data on sediment grain size, levels of TOC and concentrations of AVS were not provided in most of the reports reviewed in this study. Thus, it was not possible to express the guidelines in terms of the factors that may influence the bioavailability of these contaminants. While reliance on ranges of concentrations instead of absolute values and consideration of the no effects data set reduces this limitation, sediment quality guidelines are less defensible if they do not account for the factors that control bioavailability (e.g. Di Toro et al. 1991). For this reason, the SQGs derived in this study were evaluated to determine their comparability, reliability and predictability. Sediment quality guidelines derived using other approaches and being considered for use in national or regional programs should also be thoroughly evaluated before being implemented.

The results of this evaluation indicate that the SQGs can be used with a high or moderate degree of confidence to assess sediment quality. The SQGs for approximately half of the substances were comparable to other guidelines that have been developed using different approaches or different procedures. Additionally, the SQGs for 28 substances had a moderate or high degree of reliability, as indicated by the data contained in the BEDS. Furthermore, the SQGs for 34 substances, when used

collectively, provided predictive tools for correctly classifying marine and estuarine sediments with respect to adverse biological effects. Overall, the predictability of the dry weight-normalized PELs and TELs was >67 and >94%, respectively, indicating that the potential limitations identified previously do not seriously compromise the applicability of the SQGs. Interestingly, the predictability of the PELs was higher (>80%) for sediment samples that had complex mixtures of contaminants than it was for sediment samples that were contaminated by one or two substances only (predictability = 37%). This increased ability to predict toxicity in sediments with complex mixtures is likely because the database, upon which the guidelines are based, primarily contains information from sites with sediments that contained many chemical substances. Therefore, the guidelines are particularly relevant for assessing sediment quality in areas with multiple contaminant inputs.

A critical consideration in sediment risk assessment is the potential for incorrectly classifying sediments. Based on the results of this assessment, it is apparent that there is an approximately 33% probability of incorrectly classifying non-toxic samples as toxic using the PELs (i.e. false positives). In contrast, there was a relatively low probability of incorrectly classifying toxic samples as non-toxic using the TELs (i.e false negatives). Therefore, the guidelines are considered to be conservative tools for assessing contaminated sediments (i.e. they err on the side of environmental protection; see C.G. Ingersoll, P.S. Haverland, E.L. Brunson, T.J. Canfield, F.J. Dwyer, C.E. Henke, N.E. Kemble, D.R. Mount and R.C. Fox (submitted) for a more comprehensive evaluation of type I and type II errors using SQGs). Together, the evaluations of comparability, reliability and predictability indicate that the SQGs are likely to be appropriate for use in a variety of applications and sites in Florida and, perhaps, elsewhere.

The GOOMEX study, conducted in the vicinity of offshore oil and gas exploration and production platforms in the Gulf of Mexico, provided a unique environment for testing the predictability of the SQGs. The primary contaminants of concern were metals (Cd, Cu, Hg, Pb and Zn) and the sampling design provided a gradient in contaminant concentrations along transects extending from the point source discharge. This situation was unique compared with most urban coastal environments where complex mixtures of organic and inorganic contaminants are usually present due to point and non-point sources of pollutants. Compared with the two studies in coastal areas which used the sea urchin pore water tests, the GOOMEX study had a much lower concordance between predicted and observed toxicity. This may be due to the fact that most of the data used to develop the SQGs was obtained from studies conducted near urbanized coastal areas, where complex mixtures of contaminants are more prevalent. The additive and synergistic effects of these co-occurring chemicals are of necessity incorporated into the SQGs. In this unique study in the Gulf of Mexico, where the numbers and classes of chemicals present were limited compared to urbanized coastal areas, the PELs may be overprotective due to the limited additive or synergistic effects of co-occurring contaminants. Another explanation might be that the particular forms of the metals were insoluble or ligands were present which minimized their bioavailability. The TELs, however, provided accurate predictions of non-toxicity in the GOOMEX study.

The PELs accurately predicted sediment toxicity in two out of three studies used to assess the predictability of the SQGs in coastal areas of the Gulf of Mexico. No

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of three studies used to Gulf of Mexico. No concordance was observed between predicted and observed toxicity in the EMAP study; this disparity might be explained by differences in the types of toxicity tests that were used among studies. The EMAP study utilized whole sediment toxicity tests with adult crustaceans, whereas the GOOMEX study used sea urchin pore water toxicity tests. The sea urchin fertilization and embryo development tests with pore water provide estimates of chronic toxicity and uses, as an end-point, responses of a sensitive life stage of a sensitive species. In contrast, the whole sediment assessments used in the EMAP study involved estimates of acute toxicity to adult crustaceans. The PELs appear to be more predictive of chronic, sublethal effects than the more obvious acute, lethal effects. Likewise, the TELs appear to be protective of chronic, sublethal effects, as demonstrated by the high degree of concordance between the TEL predictions and the observed toxicity with the sea urchin tests. These results emphasize the fact that the organisms used in various toxicity tests differ with respect to their ability to estimate effects of sediment-associated contaminants. Therefore, comprehensive sediment quality assessments should employ a battery of biological tests, at least one of which should be sensitive enough to detect chronic, sublethal effects in sensitive species.

The results of this investigation indicate that the SQGs generally provide reliable and predictive tools for assessing coastal sediment quality in Florida and elsewhere in the southeast. However, the SQGs should not be used as stand-alone sediment quality criteria. The applicability of these guidelines in other coastal areas of the United States has not been fully evaluated. For this reason, the predictability of the guidelines derived using the original (Long and Morgan 1990) and modified (this study) approaches will be compared using independent data sets from throughout the United States and Canada. The results of this comparison, which will be published in a subsequent manuscript, will provide additional guidance in the use and applicability of the respective SQGs.

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Disclaimer

The methods and guidelines presented in this report do not necessarily represent the policy of the National Biological Survey, the Florida Department of Environmental Protection or the National Oceanic and Atmospheric Administration.

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