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A new method for estimating sedimental integrated toxicity of heavy metal mixtures to aquatic biota: a case study

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Abstract
The existing methods of measuring combined toxicity of heavy metal mixtures in environment do not fully consider three major factors (i.e., number of heavy metal species, aquatic biota, all investigated sites as an entity). Herein, a new method named joint probabilistic risk (JPR) method is proposed for evaluating the combined toxicity of heavy metal mixtures to aquatic biota. In this new method, the above three factors are fully taken into account. In order to evaluate the feasibility of the new method, the Pearl River Estuary (PRE) is selected as a case study. Concentrations of heavy metals (Cd, Pb, Cr, Ni, Cu, and Zn) in surface sediments of PRE are investigated and toxic equivalent factors (TEFs) of these heavy metals are calculated. Based on TEFs, sedimental concentrations of heavy metals of PRE are converted to Cd toxic equivalent concentration (Cd_{eq}), while the Cd toxicity data (Cd_{to}) are extracted from the literature. The probability density curves for Cd_{eq} and Cd_{to} are constructed and the overlap area is quantified as 0.2497. This indicates that the surface sediments of PRE have a 24.97% probability of toxic effect towards aquatic biota. Finally, this new method is validated by two indirect methods of mERMq and mPELq.

Keywords Heavy metals · Sediments · Toxic response factors · Cd toxic equivalent concentration · Probability risk assessment

Introduction

Heavy metals, which are metals having densities above 5.0 g/cm^3, have received significant attention because of their toxicity, non-degradability, bioaccumulation, and widespread pollution (McConnell and Edwards 2008; Fu and Wang 2011). Heavy metals contributed by natural and anthropogenic sources can enter the aquatic ecosystems and mainly bind with the sediments (Acevedo-Figueroa et al. 2006; Souza Machado et al. 2016). Due to various chemical, physical and biological processes, sedimental heavy metals can be released back to the water column (Eggleton and Thomas 2004; Ip et al. 2007; Gu and Lin 2016). Therefore, the heavy metal accumulation in sediments can have severe negative environmental implications for the surrounding ecosystem (Bryan and Langston 1992; Gao and Chen 2012). Furthermore, heavy metals in sediments would adversely affect the water quality and the physiological functions of aquatic organisms, resulting in potential negative impacts on ecosystem and humans (Wang and Fisher 1999; Pejman et al. 2015; Wang et al. 2018). Therefore, it is important to study the sedimental toxicity of heavy metal mixtures to aquatic biota to develop strategies for the protection of the aquatic ecosystem and human health.

Several techniques have been used to evaluate the combined toxicity of heavy metal mixtures to aquatic biota in the environment, which can be divided into two categories based on their characteristics. In the first category of methods, the number of aquatic and heavy metal species is limited. For example, some models have been extensively

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used in environment and are based on biotic ligand model (BLM), concentration addition (CA), independent addition (IA), quantitative structure–activity relationship (QSAR), and their modified methods (e.g. Vijver et al. 2011; Backhaus and Faust 2012; Balistrieri and Mebane 2014; Wu et al. 2016; Le and Peijnenburg 2017; Qin et al. 2018; Peter et al. 2019; Koppel et al. 2020). However, these methods of analyzing the combined toxicity of heavy metal mixtures in environment are mainly constructed for evaluating integrated toxicity of mixtures with less than five metals to less than three biological species.

In the second category of methods, there is a paucity of suitable site-by-site assessment methods. For example, the mean-effects-range-median quotient (mERMq) and mean-probable-effects-levels quotient (mPELq) methods were introduced by Long et al. (2006) based on values of ERM and PEL. These two methods have been established by a large amount of data collected by numerous toxicity tests, field investigations, and alterations in aquatic biota (Long et al. 1995; Carr et al. 1996; Macdonald et al. 1996) and are extensively applied in the sediment assessment (e.g. Gao and Chen 2012; Gu 2018; Garmendia et al. 2019). The two methods can evaluate the combined toxicity of heavy metal mixtures to aquatic biota confined by the number of heavy metal species.

It is meaningful for aquatic ecosystem protection and related decision-making that assessment of integrated toxicity of heavy metal mixtures in sediments considers the number of heavy metal species, aquatic biota and all investigated sites as an entity. Accordingly, a new approach named joint probabilistic ecological risk method was developed herein for estimating the combined toxicity of heavy metal mixtures to aquatic biota in sediments to address the above challenges.

Materials and methods

Study setting and sampling

As the second largest river in China based on discharge amount, the Pearl River winds for 2320 km and flows through 446,768 km^2 of drainage area into the PRE and finally reaches the South China Sea (Fig. 1; CAS Chinese Academy of Sciences (2012)). The PRE is located in one of the most industrialized and urbanized areas in China and receives 14,000,000 tons of sewerage per day (Pintado-Herrera et al. 2017).

Samples of surface sediments were collected in June 2018 from eighteen investigated stations distributed throughout PRE via a Peterson-grab sampler (Fig. 1). To facilitate

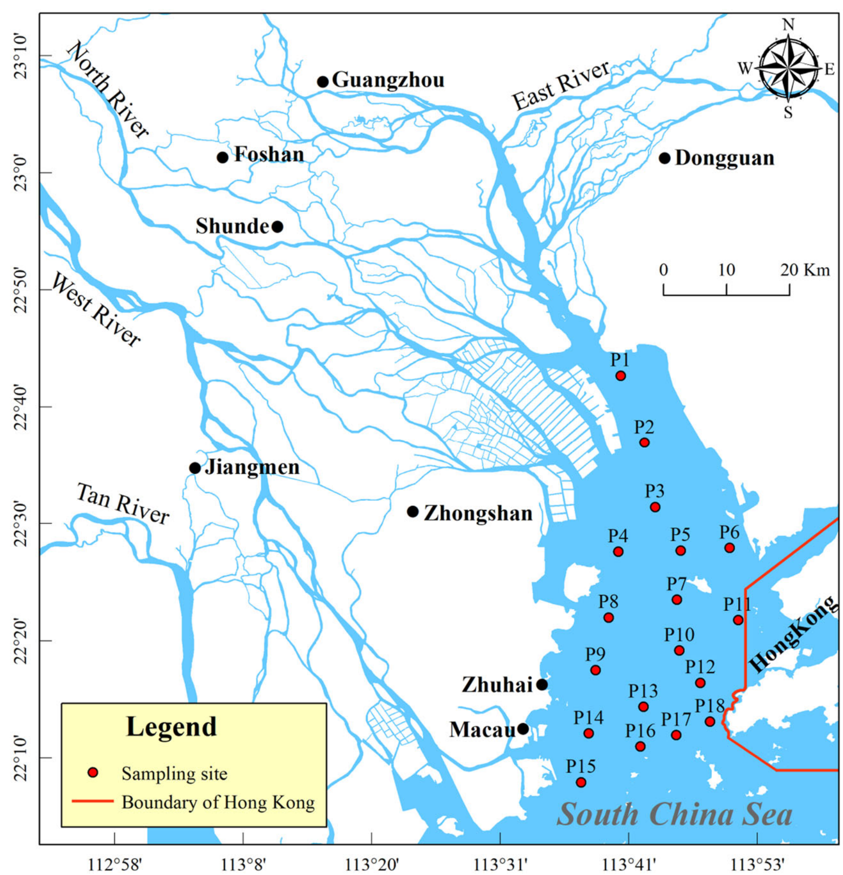

Fig. 1 Location of the study area and sampling sites in the Pearl River Estuary, South China

representative spatial coverage, the sampling stations were evenly distributed across the PRE. Sediment samples from each site were placed in zippered plastic bags and transported to the laboratory. Then, they were placed in an oven and dried at 50 °C until they reached a stable weight. Subsequently, they were homogenized (ground and passed through a 63-µm mesh nylon sieve), and stored at −20 °C in zippered plastic bags until the heavy metal analysis.

Analytical methods

The microwave digestion procedures were performed in compliance with the EPA Method 3050B using an Italy Milestone Ethos Plus Microwave Labstation. The sediment heavy metal recoveries were estimated according to the Chinese National reference material standard (GBW 07314). The recoveries of heavy metals were in the range of 96%–107%.

Joint probabilistic risk (JPR) estimation

The proposed novel procedure for evaluating the JPR of sedimental heavy metals is presented in Fig. 2 and is described below:

Step 1: data collection

The exposure data are the measured heavy metal concentrations in sediments collected during the field investigation. The Cd toxicity data were extracted from the related literature on the effects of sediment-associated Cd. The acute toxicity data of Cd (LC50 or EC50) for 11 aquatic species comprising phytoplankton, zooplankton, fish and benthic invertebrates were also collected in this study, as shown in Table 1.

Step 2: Cd toxic equivalent concentration

First, the toxic equivalent factors (TEFs) for heavy metals were established. Second, concentrations of heavy metals were transformed to the Cd toxic equivalent concentration (Table 3).

Step 3: data treatment

The exposure data of Cd toxic equivalent concentration and the Cd toxicity data were tested for normality. Non-normal data were log-transformed.

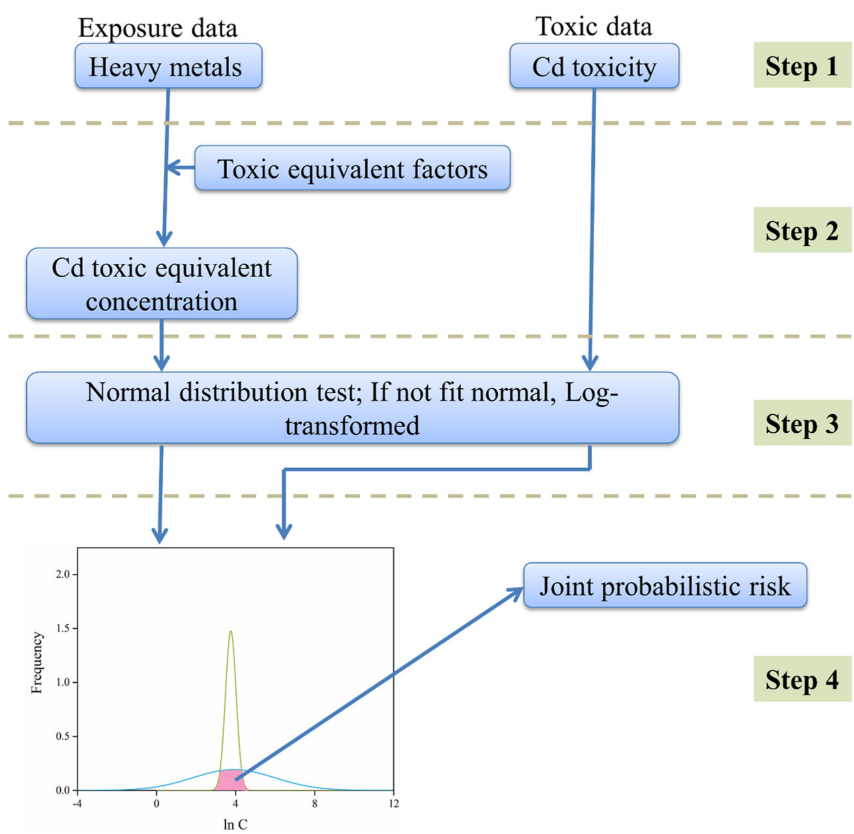

Fig. 2 Flow chart showing the steps for estimating joint probabilistic risk of sedimental heavy metals

Table 1 Acute toxicity data of sediment-associated Cd for 11 aquatic species (mg/kg, dry weight)

Group	Species	LC50	EC50	Exposure time (day)	Reference
Phytoplankton	*Cylindrotheca closterium*		79	3	(Moreno-Garrido et al. 2003)
Zooplankton	*Daphnia magna*	707.14		3	(Li et al. 2017)
	Amphiascus tenuiremis	37.9		4	(Green et al. 1993)
	Rhepoxynius abronius	9.81		10	(Long and Morgan 1990)
	Ampelisca abdita	2580		10	(Di Toro et al. 1990)
	Corophium volutator	2.83		1	(Ciarelli et al. 1997)
Fish	*Pimepheles affinis*	11		446	(Long and Morgan 1990)
Benthic invertebrates	*Ruditapes philippinarum*	4.09		10	(Riba et al. 2004)
	Monopylephorous limosus	281		21	(Shen et al. 2014)
	Chironomus tentans	26.3		21	(Shen et al. 2014)
	Chironomus tentans (larvae)	28.0		1	(Sae-Ma et al. 1998)
	Chironomus dilutus	170		10	(Chen et al. 2015)

Step 4: probability risk assessment

The probability density curves for the sedimental Cd_{eq} exposure and toxicity data were constructed. The overlap area is the JPR.

Results and discussion

Descriptive statistics

Table 2 provides the mean, median, standard deviation and range of heavy metals in the sediments of the PRE and sums up the number of samples in various grades of sedimentary quality on the basis of the National Marine Sediment Quality Standard of China (GB 18668−2002). The sedimental heavy metals notably exceed the background values in PRE sediments in terms of the one-sample t test ($p <$ 0.01), clearly indicating human enrichment.

Based on the National Marine Sediment Quality Standard of China (GB 18668 − 2002), the concentrations meet the class II standards in 6 sites (33.33%) for Cd, 15 sites (83.33%) for Pb, 17 sites (94.44%) for Cr, 13 sites (72.22%) for Cu, and 12 sites (66.67%) for Zn, suggesting the potential ecological risk of sedimental heavy metal pollution of PRE.

Cd toxic equivalent concentration (Cd_{eq})

The potential ecological risk index (RI) originally established by Hakanson (1980) is commonly used to investigate the ecological risk of heavy metals. This method provides a better potential risk assessment of heavy metal pollution with the index level because it considers both ecological risks and environmental effects (Hakanson 1980). This index has been extensively used in the solid phase environment such as sediments, soils, dust, and sludge (Duodu et al. 2016; Jin et al. 2016; Karak et al. 2017; Keshavarzi et al. 2015).

The toxic response factors (TRFs) for Cd, Pb, Cr, Ni, Cu, and Zn are listed in Table 3. These TRFs were divided by 30, i.e. toxic equivalent factor (TEF) of Cd, to obtain the corresponding TEFs (Table 3). The Cd toxic equivalent concentration (Fig. S1) varies from 24.11 to 66.93 with the average of 44.38 ± 11.75 mg/kg.

Joint probabilistic ecological risk

The probability risk assessment (PRA) procedure is an effective approach to estimate the pollutant risk (Solomon et al. 2000; USEPA 2001; Wang et al. 2009; Wang et al. 2002). Herein, PRA was conducted to evaluate the overall heavy metal probabilistic ecological risk based on Cd_{eq} of each sample. The Kolmogorov–Smirnov method was carried out to test the distributions of exposure data and toxicity data. The results reveal that the data are log-normally distributed ($p > 0.05$) and the results are tabulated in Table S1. Thus, in terms of the means and standard deviations of exposure and toxicity data of Cd_{eq} and Cd, the probability-risk distribution curves are established and illustrated in Fig. 3. The overlap area of 0.2497 was calculated using MASS package in R software version 3.4.1, indicating a 24.97% probability of a toxic effect (Computational codes are given in Supplementary material).

Method validation

The mERMq and mPELq methods were implemented to further determine the combined biological effects of heavy metal mixtures via calculating mean quotients for

Table 2 Descriptive statistics for sedimental heavy metal concentrations (mg/kg dry weight) in the study area ($n = 18$) and their grades

Metal	Mean, SD	Median	Range	CV%	BV[a]	No. of sites in each class of sediment quality[b]		
						I	II	III
Cd	0.53** ± 0.46	0.44	0.02–1.48	85.71	0.2	12	6	0
Pb	76.06** ± 23.22	68.82	42.50–125.49	30.53	44	3	15	0
Cr	105.92** ± 17.45	107.11	70.14–137.22	16.48	81.1	1	17	0
Ni	52.57** ± 11.80	51.48	32.48–73.25	22.45	30.3	n.a.	n.a.	n.a.
Cu	53.40** ± 22.88	51.43	14.50–97.34	42.84	38.6	5	13	0
Zn	183.02** ± 47.18	176.21	101.51–260.48	25.78	100.7	6	12	0

Note: $**p < 0.01$ means significant level; CV: Coefficient of variation

[a]Background values of Cd, Pb, Cr, Cu and Zn (Gan et al. 2010) and background value of Ni (Ma et al. 2014) in sediments from the PRE

[b]According to the Chinese National marine sediment quality standards, class I is considered as uncontaminated, classes II and III are moderately contaminated and severely contaminated, respectively (CSBTS China State Bureau of Quality and Technical Supervision (2002)). The standard for Ni in the Chinese National marine sediment quality standards (GB 18668-2002) is not available (n.a.)

Table 3 TRF, TEF, ERM, and PEL for Cd, Pb, Cr, Ni, Cu, and Zn

	Cd	Pb	Cr	Ni	Cu	Zn
TRF[a]	30	5	2	5[b]	5	1
TEF	1	0.17	0.07	0.17	0.17	0.03
ERM[c] (mg/kg)	9.6	218	370	51.6	270	410
PEL[d] (mg/kg)	4.21	112	160	42.8	108	271

[a]Hakanson (1980)

[b]Kulkarni et al. (2018)

[c]Long et al. (1995)

[d]Macdonald et al. (1996)

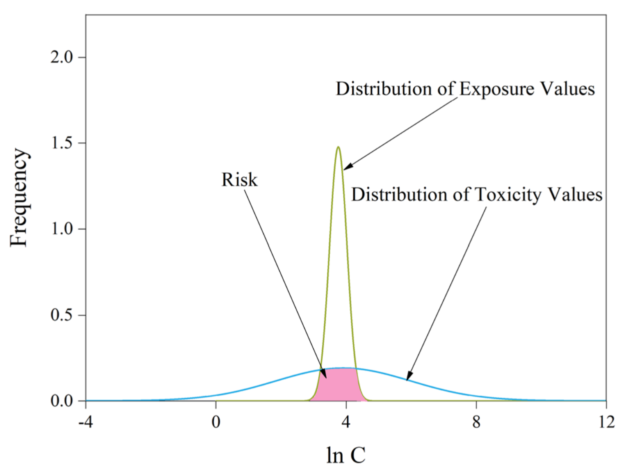

Fig. 3 Probability density curves of exposure and toxicity data of Cd_{eq} and Cd to evaluate joint probabilistic risk of sedimental heavy metals from the PRE; LnC: natural logarithm-transformation concentration

Table 4 The classification grades of mERMq and mPELq for the assessment of metals in sediments (Long et al. 2006)

Index	Category	Incidence of adverse biological effects
mERMq	mERMq ≤ 0.1	9%
	0.11≤mERMq ≤ 0.5	21%
	0.51≤mERMq ≤ 1.5	49%
	mERMq > 1.5	76%
mPELq	mPELq ≤ 0.1	8%
	0.11≤ mPELq ≤ 1.5	21%
	1.5< mPELq ≤ 2.3	49%
	mPELq > 2.3	73%

validating the proposed new method. Equations (1) and (2) were used for the calculations, which are given as follows (Carr et al., 1996; MacDonald et al., 2004; Long et al. (2006)):

$$\mathrm{mERMq} = \sum (C_x/\mathrm{ERMx})/n \quad (1)$$

$$\mathrm{mPELq} = \sum (C_x/\mathrm{PEL}_x)/n \quad (2)$$

where C_x represents the investigated content of metal x, ERM_x represents the ERM for metal x, PEL_x represents the PEL for metal x, and n represents the number of metal species.

The ERM and PEL values of the heavy metals are shown in Table 3. The grades of combined biological effects of heavy metal mixtures in sediments are listed in Table 4. The spatial variations of mERMq and mPELq values are displayed in Fig. 4. In sediments of PRE, the combination of the studied PAHs has 21% combined probability of being toxic based on the methods of mERMq and mPELq. This result is consistent with the proposed method, suggesting that the new method provides a dependable and reasonable

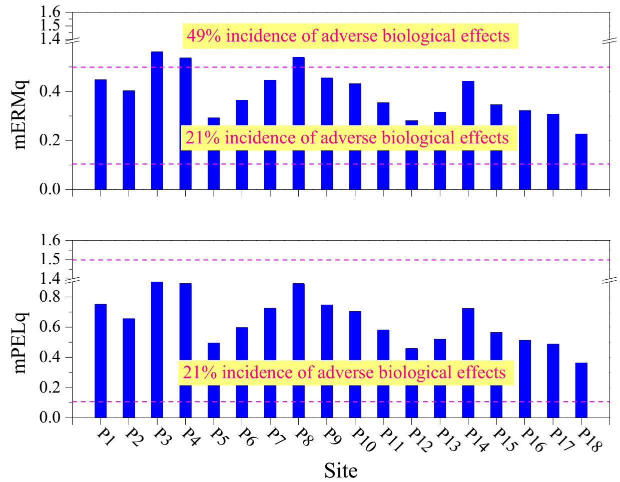

Fig. 4 Spatial variations of mERMq and mPELq values in sediments from the PRE

approach for estimating the combined toxicity of sedimental heavy metal mixtures to aquatic biota.

Conclusion

The concentrations of sedimental heavy metals from PRE were analyzed, and a new method was proposed for the estimation of the joint probabilistic ecological risks of heavy metals based on Cd_{eq} and Cd_{to}. The results showed that Cd, Pb, Cr, Ni, Cu and Zn concentrations are significantly higher than their corresponding background values, indicating anthropogenic enrichment. The Cd_{eq} in sediments of PRE is in the range of 24.11 to 66.93 mg/kg. The proposed method showed that surface sediments of PRE have a 24.97% probability of toxic effect on aquatic biota comprising phytoplankton, zooplankton, fish and benthic invertebrates. The proposed new method is a dependable and reasonable approach which was verified by two indirect methods. The normalization of toxic effects of Cd can be conveniently performed by this method, and it can possibly be adapted for other metals as well, such as Cu.

Data availability

The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

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Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

Ethical approval Animal research: This article does not contain any studies with human participants or animals performed by any of the authors.

Consent to participate Written informed consent was obtained from individual or guardian participants.

Plant reproducibility This article does not contain any studies with plant reproducibility or plant reproducibility performed by any of the authors.

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