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Journal of Environmental Monitoring

Supplementary materials

Polycyclic aromatic hydrocarbons and ecotoxicological characterization of sediments from the Huaihe River, China

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Contents:

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Description of sampling sites

Table S1 Sampling sites and description

Sampling sites		Description
Name	Location	
XY	Lat 32º18'50", Long 114º04'04"	The river was narrow and affected by domestic effluent from the nearby village. The samples were drab and hard plastic with aquatic weeds.
HN	Lat 32º40'14", Long 117º01'45"	There were many dredgers on the river and oil stain on the surface of river. Location affected by the industrial effluent from nearby chemical plant and power plant. The samples were black and flow plastic with no organisms.
BB	Lat 32º57'50", Long 117º25'09"	There were some aquatic weeds and solid waste on the river. The water was turbid and affected by the industrial effluent from nearby chemical plant. The samples were dark brown and flow plastic with a few of shellfish.
XuY	Lat 32º02'21", Long 118º29'40"	The river was narrow and affected by the effluent from a nearby hospital. The samples were grey and flow plastic with some shellfish.
FY	Lat 32º53'29", Long 115º50'32"	The river was gentle and a number of plants were on the bank. The samples were yellow and hard plastic with a few of shellfish.
MC	Lat 33º11'14", Long 116º41'52"	There were a few boats at riverside and some aquatic plants on the surface of river. The samples were drab and flow plastic with aquatic weeds.
ZZ	Lat 34°85'38", Long 113°63'75"	There is a bridge on the river with two garbage dumps at the bridge heads. A resident family was under the bridge. A food factory was nearby with a sewage outfall into the river. The river bank was semi-stony and semi-terrene.

Source of PAHs

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Table S2 Parent PAH ratios in the sediment samples from the Huaihe River, China

Sample	Parent PAH ratios		
	Fla/Pyr	Phe/Ant	Fla/(Fla + Pyr)
XY	1.29	10.06	0.56
HN	2.27	1.88	0.69
BB	1.87	1.20	0.65
XuY	3.20	0.27	0.76
FY	1.93	0.79	0.66
MC	1.56	10.43	0.61
ZZ	1.82	0.33	0.64

Principal component analysis (PCA) analysis

PCA as the multivariate analytical tool is used to reduce a set of original variables (measured PAHs content in the sediment samples) and to extract a small number of latent factors (principal components, PCs) for analyzing relationships among the observed variables. As a result of an effective ordination process, the first PC accounts for the greatest proportion of the original variance, while the second as well as the following PCs progressively explain smaller amounts of data variation.

In this study, concentrations of 16 PAHs as active variables and 7 samples as subjects were selected. The majority of the variance (88.92%) of the scaled data was explained by three eigenvectors-principal components. The first principal component (PC1) can explain 51.47% of the total variance, and the second (PC2) and the third (PC3) explained 27.78% and 9.67% of the total variance, respectively.

The principal component plot (Fig. S1) shows the loadings for the individual PAHs. Fang et al. [S1] reported that high loadings of Pyr, Flu, BghiP, Fl, Chr, BaP indicated incomplete combustion, pyrolysis of fuel and oil burning. Basically, factors heavy-weighted by BkF, BaP, BghiP, InP, Pyr, Chr, Flu, and BaA were identified as pyrolytic origin, whilst the compounds of Nap, Phe, Ant, Ace and Acy were indicative of petrogenic origin of PAHs. [S2] In this study, heavy-weighted PAHs, DahA, BaP,

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BghiP, InP, BaA, BkF, BbF and Fl, constituted the first cluster. This confirms the results obtained from the ratios of specific PAH compounds that the PAH contamination in the sediments mainly resulted from a pattern of pyrolytic sources.

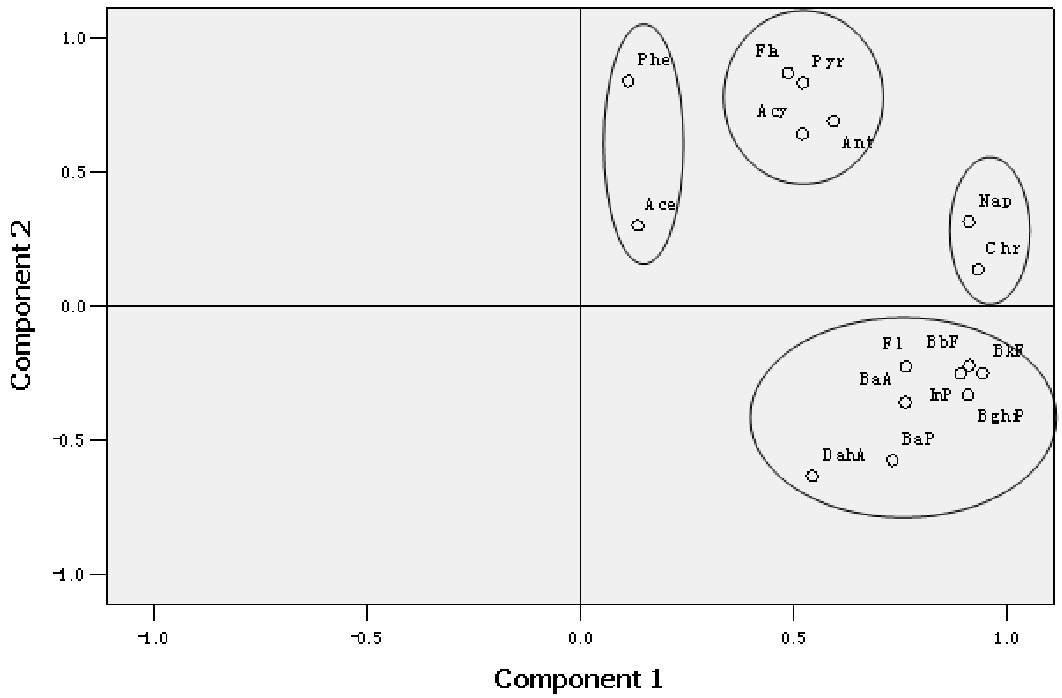

Fig. S1 The loading plot of PCA of PAHs from sediments.

Assessment of sediment toxicity

Calculation of TEQ

BaP is the only PAH for which toxicological data are sufficient for derivation of a carcinogenic potency factor among all known potentially carcinogenic PAHs. [S3] The toxic equivalency factors (TEFs) were used to quantify the carcinogenicity of other PAHs relative to BaP and to estimate BaP-equivalent doses (BaP_{eq} dose). [S5] Calculated TEFs for BaA, BaP, BbF, BkF, InP, DahA, and Chr are 0.1, 1, 0.1, 0.01, 0.1, 1, and 0.001, respectively, according to the USEPA. In this study, we converted the above mentioned seven PAH concentrations into one toxic concentration for each site using the corresponding TEFs. The total BaP toxicity equivalent (TEQ) for all PAHs was calculated as:

$$Total\ TEQ = \sum_i C_i \times TEF_i$$

where C_i was the concentrations of individual PAH (ng/g d.w.) and TEF_i was its corresponding toxic equivalency factor.

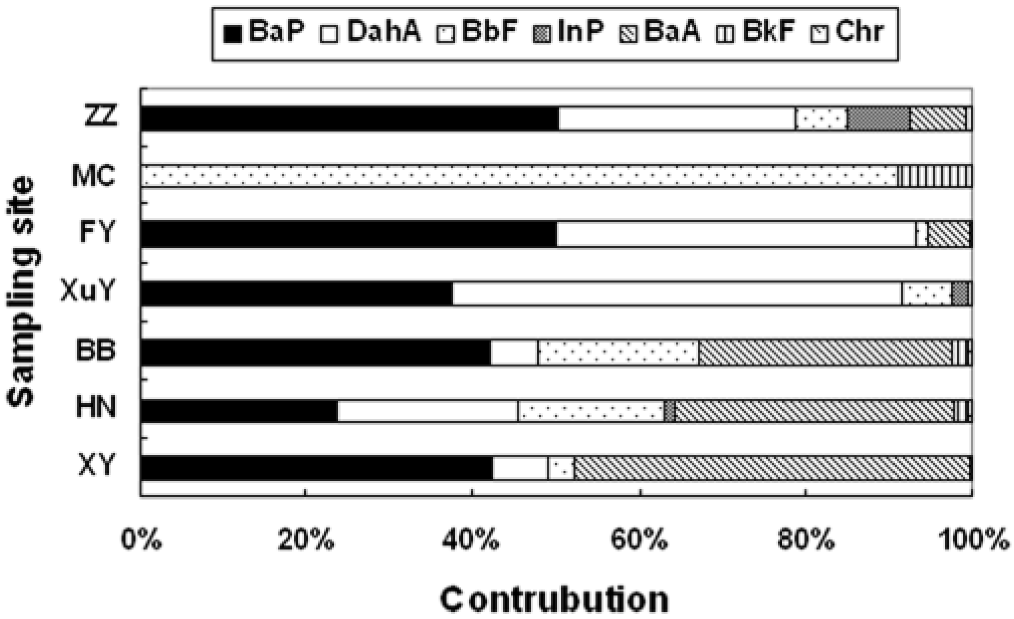

Fig. S2 Contributions of BaP, DahA, BbF, InP, BaA, BkF and Chr to the total TEQ.

Table S3 A comparison of total TEQ in sediments (ng/g d.w.)

Location	Range	Mean	Reference
Meiliang Bay, Taihu Lake, China	94-856	407	S5
Guba Pechenga, Barents, Sea, Russia	11-300	< 120	S6
Sundarban Mangrove, Wetland, India	6.95-119	59	S7
Gulf of Gemlik, Marmara Sea, Turkey	5.6-1838	134	S8
coastal lagoons in central Vietnam	2-98	21	S9
Huaihe River, China	0.01-194.1	65.9	This study

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