Supplementary Data

Heavy Metals in Sediments of Hulun Lake in Inner Mongolia: Spatial-Temporal Distributions, Contamination Assessment and Source Apportionment

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Section S1. Potential ecological risk index model

As a method to evaluate the ecological risk of heavy metals in soil or sediment from the perspective of sedimentology, the PERI has been widely used in environmental risk assessment. The PERI value was calculated in Eq. (1):

$$TI_{PER} = \sum {I_{PERr}}^{i} = \sum T_r^i C_f^i = \sum T_r^i C_n^i / C_r^i \quad (1)$$

where TI_{PER} is the total ecological hazard index value of all trace metals, ${I_{PERr}}^{i}$ is the single ecological hazard index value of each individual trace metal, T_r^i is the toxic response factor for the trace metal, C_f^i is the contamination factor, C_n^i is the concentration (mg/kg) and C_r^i is the geochemical background concentration (mg/kg). The toxicity response coefficients of Cd, As, Cr, Cu, Pb and Zn are 30, 10, 2, 5, 5 and 1 [33].

Section S2. PMF-PERI model

In this study, a PMF-PERI model was developed to quantitatively apportion the ecological risks of the identified trace metal sources by combining the PMF model and the PERI model. Three steps are needed in this model. First, the contributions of trace metals from various potential sources were apportioned by the PMF model. Then, the trace metal content in one sediment sample contributed by each source was calculated by multiplying the estimated source contribution of the trace metal in the sediment sample by the total concentration of this trace metal from the corresponding source. Last, the ecological risk attributed to each source in each sediment sample was obtained with the PERI model with the source based trace metal content in the sediment. The trace metal content contributed by each source was calculated according to Eq. (2):

$$C_{ij}^{k} = P_{ij}^{k} \times C_{j}^{k} \quad (2)$$

where C_{ij}^{k} is the concentration (mg/kg) of the j_{th} trace metal from the k_{th} source in the ith sample, P_{ij}^{k} is the estimated contribution of the j_{th} trace metal in the i_{th} sample from the k_{th} source and C_{j}^{k} is the total concentration (mg/kg) of the j_{th} trace metal from the k_{th} source. The mathematical expression of source-based potential ecological risk can be described by Eq. (3):

$$SI_{PER,k} = \sum SE_{r}^{i} = \sum T_{r}^{i} SC_{f}^{i} = \sum T_{r}^{i} C_{ij}^{k} / C_{r}^{i} \quad (3)$$

where SI_{PER} is the comprehensive PERI of all trace metals from the k_{th} source, SE_{r}^{i} is the single ecological hazard index value of each individual trace metal from the k_{th} source and SC_{f}^{i} is the contamination factor from the kth source [47].

Table S1. The evaluation standard of Geo-accumulation index (Igeo).

Geo-accumulation index (Igeo)	Evaluation grade
Igeo≤0	Uncontaminated
0 < Igeo < 1	Uncontaminated to moderately contaminated
1 < Igeo < 2	Moderately contaminated
2 < Igeo < 3	Moderately to heavily contaminated
3 < Igeo < 4	Heavily contaminated
4 < Igeo < 5	Heavily to extremely contaminated
Igeo > 5	Extremely contaminated