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Dataset Development on Heavy Metals and Its Potential Ecological Risk in Multiple Media of Shimen Realgar Mine (2015)

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Abstract: The Shimen Realgar Mine, located in Hunan Province, is the largest single-arsenic (As) mine in Asia, with a mining history spanning over 1,500 years. Long-term and large-scale mining activities, coupled with industrial operations such as phosphate fertilizer and cement production, have led to extensive and severe As contamination in the surrounding areas. In 2015, we collected 21 surface water samples, 19 sediment samples, and 28 surface soil samples along the Huangshui stream and the Zaoshi Reservoir near the mine. Water quality parameters were measured using a YSI6600V2 multi-parameter analyzer, while the concentrations of heavy metals were analyzed in the laboratory using a combination of inductively coupled plasma-optical emission spectrometer (ICP-OES) and inductively coupled plasma-mass spectrometer (ICP-MS). The dataset includes: (1) geo-information of the sampling sites for surface water, sediment, and soil samples; (2) physical and chemical properties of surface water, including pH, water temperature, dissolved oxygen, total phosphorus, and total nitrogen; (3) physical and chemical properties of sediment and surface soil, including pH and organic matter content; (4) heavy metal concentrations (As, Cr, Cd, Pb, Zn, Ni, Mn, etc.) in surface water, sediment, and soil; and (5) heavy metal pollution assessment for soil, including geo-accumulation, single-pollution, Nemerow, and potential ecological risk indices. The dataset is archived in .kmz, .shp, and .xlsx formats, and consists of 25 data files with data size of 122 KB (Compressed into one file with 98 KB).

Keywords: Shimen Realgar Mine; surface water; sediment; soil

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Dataset Availability Statement:

The dataset supporting this paper was published and is accessible through the *Digital Journal of Global Change* Data Repository at: https://doi.org/10.3974/geodb.2024.11.08.V1.

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1 Introduction

The Shimen Realgar Mine, located in northwestern Hunan Province, is the largest realgar (As_4S_4) deposit in Asia. It has been mined for over 1,500 years, resulting in elevated metal concentrations in the surrounding environment[1]. As an independent arsenic deposit, the mine has an average arsenic grade of 75% and an ore reserve of 730,000 tons[2]. Large-scale mining and smelting operations began in 1958, with an annual ore processing capacity of 15,000 tons and the production of approximately 3,000 tons of raw ore[3]. Over time, the 300,000 tons realgar reserve has nearly been depleted, and resources are now nearing exhaustion. The arsenic smelting plant was closed in 1978, and the mine itself was officially shut down in 2001. Years of mining and smelting activities have resulted in significant As contamination of the local water and soil, causing persistent environmental pollution[4]. In response, the "12th Five-Year Plan for Comprehensive Prevention and Control of Heavy Metal Pollution" was lauched in 2012 to address this issue. The plan focuses on cleaning up historical As slag and treating the contaminated surrounding soil and river channels. Given the extent of contamination, monitoring and investigation the physical and chemical properties of water, sediment, and soil in the area is crucial. This will provide a comprehensive understanding of the current pollution levels in the Shimen Realgar Mine and aid in controlling further environmental degradation. In May 2015, a dataset was gathered through on-site monitoring of surface water samples, sediments, and soil from upstream to downstream along the Huangshui stream to the Zaoshi Reservoir. Multiple pollution assessment methods were employed to evaluate the ecological risks posed by the heavy metals.

2 Metadata of the Dataset

The metadata of Heavy metals and its environment risk assessment on Shimen Realgar Mine, Hunan Province of China[5] is summarized in Table 1. This includes the dataset full name, short name, authors, year of the dataset, data format, data size, data files, data publisher, and data sharing policy, etc.

3 Methods

In May 2015, we collected 21 surface water samples, 19 sediment samples and 28 surface soil samples from upstream to downstream along the Huangshui stream to the Zaoshi Reservoir. The sampling network was intensified surrounding the stone-representative zones of the Shimen Realagr Mine (Figure 1), with on-site monitoring conducted for surface water, sediment, and soil samples at all locations.

3.1 Sampling and Preprocessing

At each site, surface water was sampled within 20 cm of the surface using a clean 500-mL polyethylene bottle. *In situ* measurements of Temperature (T), pH, dissolved oxygen (DO), and chlorophyll-a (Chl-a) were determined using a multiple water quality analyzer (Aquaread AP-2000, UK). For further analysis, approximately 400 mL of the water sample was filtered through a 0.45-μm filter. Soil and sediment samples were immediately transported to the laboratory after collection, where stone and plant debris were removed. The samples were then air-dried, sieved, and stored in clean polyethylene bags for subsequent experiments.

Table 1 Metadata summary of the Heavy metals and its environment risk assessment on Shimen Realgar Mine, Hunan Province of China

Items	Description
Dataset full name	Heavy metals and its environment risk assessment on Shimen Realgar Mine, Hunan Province of China
Dataset short name	HMsShimenRealgarMine2015
Authors	Liu, Y. X. Y., Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, lyxy@lreis.ac.cn Yang, F., Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, yangf@igsnrr.ac.cn
Geographical region	Shimen County in Hunan Province
Year	2015
Data format	.kmz, .shp, .xlsx
Data size	122 KB
Data files	(1) Information on the sampling sites for surface water, sediment, and soil samples; (2) physical and chemical properties of surface water; (3) physical and chemical properties of sediment and surface soil; (4) heavy metal concentrations in surface water, sediment, and soil; and (5) heavy metal pollution assessment for soil, and potential ecological risk indices
Foundation	National Natural Science Foundation of China (41571470)
Data publisher	Global Change Research Data Publishing & Repository, http://www.geodoi.ac.cn
Address	No. 11A, Datun Road, Chaoyang District, Beijing 100101, China
Data sharing policy	(1) *Data* are openly available and can be free downloaded via the Internet; (2) End users are encouraged to use *Data* subject to citation; (3) Users, who are by definition also value-added service providers, are welcome to redistribute *Data* subject to written permission from the GCdataPR Editorial Office and the issuance of a *Data* redistribution license; and (4) If *Data* are used to compile new datasets, the "ten percent principal" should be followed such that *Data* records utilized should not surpass 10% of the new dataset contents, while sources should be clearly noted in suitable places in the new dataset[6]
Communication and searchable system	DOI, CSTR, Crossref, DCI, CSCD, CNKI, SciEngine, WDS, GEOSS, PubScholar, CKRSC

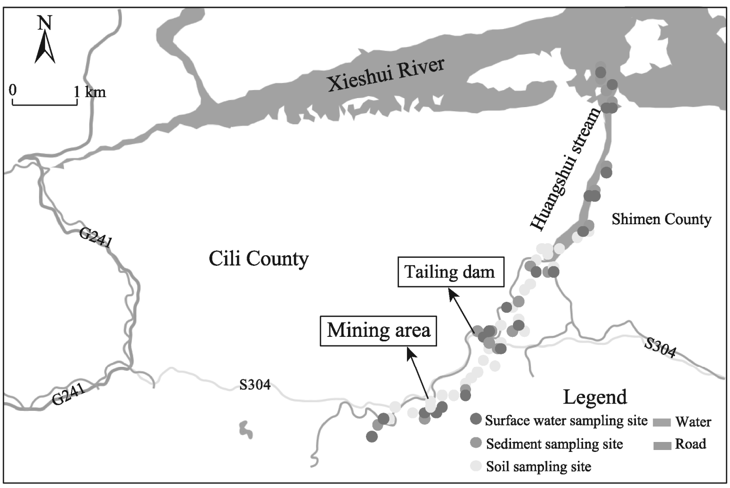

Figure 1 Map of sampling sites distribution in Shimen Realgar Mine (2015)

3.2 Analytical Methods

Soil pH was measured in a 1:2.5 (soil : water) mixture, and total organic matter (TOM) content was determined using the Walkley-Black method. For heavy metal analysis, approximately 0.05 g of soil was digested with an acid mixture of HNO_3 (5 mL), HF (5 mL) and $HClO_4$ (1 mL) in 100-mL Teflon vessels[1]. For biological samples, 200–300 mg were weighed and digested with 9 mL concentrated HNO_3 and 1 mL $HClO_4$. These samples were evaporated at approximately 170 to 190 ℃ to near dryness. If necessary, 3 mL HNO_3 was added until the solution was completely cleared. The final heavy metal concentrations (Cd, Pb，Cr，Cu，Mn，Ni，Zn) were determined using ICP-OES (Avio 200, Perkin Elmer, USA)[2]. For metals like Cd, Pb and As were analyzed by using ICP-MS (PlasmaQuant MS, Analytik Jena AG, Germany)[3].

3.3 Assessment of Pollution Level

To comprehensively assess the pollution levels in surface soils, several indices were calculated: the geo-accumulation index (Igeo) (Table 2), single pollution index (PI), Nemerow integrated pollution index (NIPI) (Table 3), potential ecological risk for individual metals (EI), and potential ecological risk index (RI) (Table 4).

The index of Igeo was calculated to evaluate the degree of PTE pollution compared to background levels, using the following equation[7]:

$$I_{geo} = \log_2\left(\frac{C_n}{1.5B_n}\right) \tag{1}$$

where, C_n (mg/kg) is the metal concentration in soil, B_n (mg/kg) is the background value of the element, and 1.5 is a factor to correct for lithological influences.

Table 2 Classification of index of geo-accumulation (Igeo)

Classification	*Igeo*	Pollution degree
0	*Igeo* <0	Uncontaminated
1	0≤*Igeo* <1	Uncontaminated to moderately contaminated
2	1≤*Igeo* <2	Moderately contaminated
3	2≤*Igeo* <3	Moderately contaminated to heavily contaminated
4	3≤*Igeo* <4	Heavily contaminated
5	4≤*Igeo* <5	Heavily contaminated to extremely contaminated
6	*Igeo*≥5	Extremely contaminated

Table 3 Classification of single pollution index (PI) and Nemerow integrated pollution index (NIPI)

Classification	PI	NIPI	Pollution degree
0	PI<0.7	NIPI<0.7	Uncontaminated
1	0.7<PI<1	0.7<NIPI<1	Warning
2	1<PI<2	1<NIPI<2	Low contaminated
3	1<PI<2	1<NIPI<2	Moderately contaminated
4	PI>3	NIPI>3	Severe contaminated

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[3] Soil quality−analysis of total mercury、arsenic and lead contents in soils−atomic fluorescence spectrometry−part 2：analysis of total arsenic (GB/T 22105.2-2008). https://openstd.samr.gov.cn/bzgk/gb/newGbInfo?hcno=2B5E1AA5C CBFCB3876799A9789177DD8.

Table 4 Classification of potential ecological risk of individual factor (EI) and potential ecological risk index (RI)

Ecological risk	Low	Moderate	Considerate	Very high	Dangerous
EI	<40	40–80	80–160	160–320	>320
RI	<150	150–300	300–600	>600	

The index of PI for a single metal and the NIPI for a combination of seven metals was calculated as the following equations[8]:

$$\mathrm{PI} = \frac{C_i}{S_i} \tag{2}$$

$$\mathrm{NIPI} = \sqrt{\frac{\mathrm{PI}_{\max}^2 + \mathrm{PI}_{\mathrm{ave}}^2}{2}} \tag{3}$$

where, C_i (mg/kg) is the metal concentration in the soil, S_i (mg/kg) is the soil risk screening value from the Soil Environmental Quality Risk Control Standard for Soil Contamination of Agricultural Land (Trial) (GB15618—2018)[9], $\mathrm{PI}_{\max}$ is the maximum value of PI and $\mathrm{PI}_{\mathrm{ave}}$ is the average value of PI.

The index of EI and RI was calculated using the following equation[10]:

$$\mathrm{EI}_i = \frac{C_i}{B_i} \times CF^i \tag{4}$$

$$\mathrm{RI} = \sum_{i=1}^{n} \mathrm{EI}_i \tag{5}$$

where, EI_i and CF^i are the ecological risk factor and toxic response factor of element *i*, respectively.

4 Data Results

4.1 Dataset Composition

This dataset contains the following: (1) geographical location data for surface water, sediment, and soil sampling points; (2) physical and chemical properties of surface water pH, water temperature, dissolved oxygen, total phosphorus, and total nitrogen; (3) physical and chemical properties of sediment and surface soil, including pH and organic matter content; (4) heavy metal concentrations (As, Cr, Cd, Pb, Zn, Ni, Mn, etc.) in surface water, sediment and soil; (5) soil heavy metal pollution assessment data, including geo-accumulation index, single pollution index, Nemerow index, potential ecological risk index.

4.2 Data Products

(1) The surface water in the Huangshui stream and Zaoshi Reservoir is alkaline, with pH ranging from 8.45 to 10.11. According to Environmental Quality Standards for Surface Water (GB3838—2002)[11], the concentrations of total phosphorus and total nitrogen indicate mesotrophic to eutrophic conditions. This is attributed to the closure of the As smelting plant, which was later repurposed for sulfuric acid production for phosphate fertilizer. Consequently, the highest concentration of total phosphorus and total nitrogen were observed near the smelting and tailing areas. A total of 7 phytoplankton phyla were identified in the surface water, including *Cyanophyta*, *Bacillariophyta*, *Pyrrophyta*, *Chrysophyta*, *Cryptophyta*, *Euglenophyta*, and *Chlorophyta*. A previous study has reported

As concentration in the river water near the Shimen Realgar Mine as high as 15.8 mg/L in 1994[1]. Other study also reported that the As concentration in this area reached 40.10 mg/L[12]. In this study, the highest As concentration in the surface water was found to be 3.29 mg/L, and the As concentration decreased with increasing distance from the mine and tailing dam.

(2) The sediment is generally weakly alkaline, with pH ranging from 7.32 to 7.89. The average total organic matter content in the sediment is 17.0 g/kg. The As concentrations in the sediment ranged from 43.42 to 4,543 mg/kg, with a noticeable decrease in As level as the distance from the mine's central area increases. According to the Soil Environmental Quality Risk Control Standard for Soil Contamination of Agricultural Land (Trial) (GB15618—2018)[9], As concentrations above 40 mg/kg indicate significant contamination. This suggests that the As concentration in all collected sediments samples greatly exceeds the standard. Additionally, studying the interstitial water in sediment is essential for understanding migration of As at the water-sediment interface.

(3) The soil pH varied between 5.33 and 8.06, with organic matter content ranging from 13.12 g/kg to 77.31 g/kg. The soils collected from farmland areas contain a higher concentration of organic matter than those from the mining area, the tailings dam and the riverbed. The highest As concentration in the soil was found to be 5,008 mg/kg, significant higher than the background value of As in Hunan Province's soil (13.41 mg/kg). Previous studies have reported As concentration as high as 5,240 mg/kg in the central area of the Shimen Realgar Mine[13]. Consistent with distribution patterns of As concentration in surface water and sediment, the highest As concentrations in the soil were found near the mine's central area and tailing sites. As the distance from these area increased, As concentration in the soil decreased, highlighting mining activities as a major source of local As contamination. According to the Soil Environmental Quality Risk Control Standard for Soil Contamination of Agricultural Land (Trial) (GB15618—2018), which sets the limit for As concentrations at 40 mg/kg for Class III soil, the As levels in the collected soil samples seriously exceeds this threshold. Long-term heavy metal pollution lead to nutrients loss, damage to soil organisms, and functional degradation[14,15]. Therefore, remediation of As contamination in the soil at the Shimen Realgar Mine is essential.

(4) The average concentration of heavy metals in the soil surrounding the Shimen Realgar Mine are as follows: As (610 mg/kg), Cd (1.23 mg/kg), Pb (58.0 mg/kg), Cr (104 mg/kg), Cu (27.3 mg/kg), Ni (43.4 mg/kg), Zn (175 mg/kg), and Mn (738 mg/kg). The geo-accumulation index determined that some sampling sites showed a level of heavily contaminated to extremely contaminated by As and Cd (Figure 2). The Nemerow index indicates that Cr, Cu, and Ni are at non-pollution levels, Pb and Zn are slightly polluted, and As and Cd are severely polluted. The potential ecological risk assessment indicates that 43% of the soil at the Shimen Realgar Mine area has a moderate ecological risk, 39% has a strong ecological risk, and 18% has a very strong ecological risk (Figure 3). This highlights mining activities as the main factor driving environmental degradation in the Shimen Realgar Mine. It is urgent to adopt green, environmentally friendly and efficient remediation measures to reduce the heavy metal concentration in the soil. Since the remediation of heavy metals in the soil of the mining area is a long-term process, it is necessary to formulate a long-term remediation plan and monitor the environmental remediation effect in real time[16].

5 Discussion and Conclusion

Heavy metals are highly toxic, persistent, and non-biodegradable, and their accumulation in soil due to long-term mining and smelting activities has become a significant environmental concern[17,18]. The Shimen Realgar Mine in Hunan Province, the largest single arsenic mine

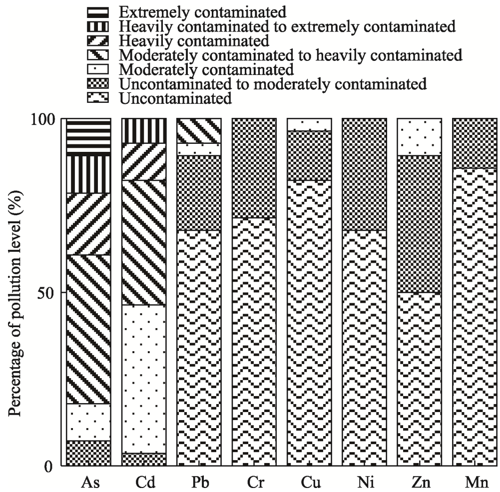

Figure 2 Assessment of pollution level (Igeo) of soil in Shimen Realgar Mine

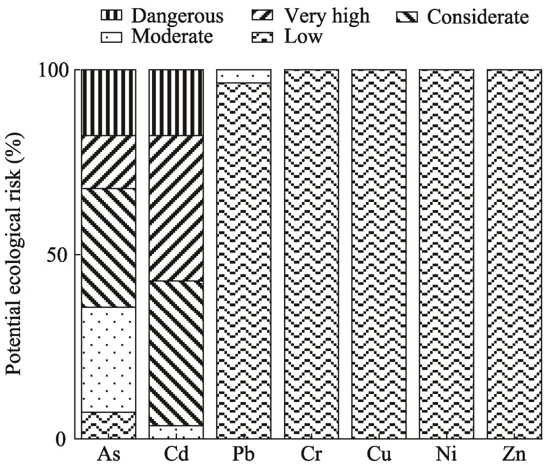

Figure 3 Potential ecological risks of the soil in Shimen Realgar Mine

in Asia, has been operational for over 1,500 years. The Huangshui stream flows through the mine and into the Zaoshi Reservoir. As an important local water source, the Zaoshi Reservoir is also contaminated by surface runoff from the mining area, tailings, and waste residue storage sites. Soil and sediment, as essential components of terrestrial ecosystems, play a direct role in shaping ecosystem structure and function. This dataset focuses on the Shimen Realgar Mine and its surrounding areas, representing the largest realgar mine in Asia. An on-site investigations was conducted in May 2015, during which comprehensive data monitoring of surface water, sediment, and soil was carried out to assess the physical and chemical properties, as well as heavy metal concentrations. As a key dataset for environmental monitoring in the Shimen Realgar Mine, this dataset offers valuable insights for ecological risk assessments in arsenic-rich mining regions. It can also serve as a basis for studying long-term As transport and distribution in the mining area. Additionally, the data provides scientific support for the development of strategies aimed at controlling environmental pollution, addressing health risks, and promoting the sustainable development of the Shimen Realgar Mine.

Author Contributions

Yang, F. designed the algorithms of dataset and contributed to the data processing and analysis. Liu, Y. X. Y. wrote the data paper.

Conflicts of Interest

The authors declare no conflicts of interest.

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