Ecological risk analysis of heavy metals in farmland soil based on Monte Carlo simulation

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Abstract. This study is aimed to analyze ecological risk for heavy metals in farmland soil. In order to solve the problem of uncertainty in the risk assessment process, the potential ecological risk analysis based on Monte Carlo is established. The evaluation results showed that the probability of As belonging to low risk level was 100%; that of Pb belonging to low risk and medium risk were 34% and 66%; that of Cd belonging to extremely high risk and high risk were 97.44% and 2.56%. The risk of the three heavy metals was ranked as Cd > Pb > As. The probability of total risk belongs to extremely high risk and high risk was 99.48% and 0.52%. The method established in this study can reduce the error caused by a small sample. This study can put forward an objective evaluation methodology for the risk management of farmland pollution by heavy metals.

1. Introduction

The safety of farmland soil environment directly affects food security, so the soil security is very important [1-3]. In order to strengthen the management and prevention of soil pollution, the “Action Plan for Prevention and Control of Soil Pollution” was promulgated on May 28, 2016. In 2018, the People’s Republic of China issued “Soil Environmental Quality Risk Control Standard for Soil Contamination of Agricultural Land (GB15618-2018)”. And the soil environmental quality standard(GB15618-1995) was abolished, which indicated that soil security has received unprecedented attention.

Heavy metal contamination in soil is the most common. But the treatment of heavy metal pollution is very difficult due to the properties of heavy metal, such as difficult degradation and migration, with high cost [4, 5]. Soil ecological risk analysis is one of the important means of soil pollution control and management[6,7]. Before pollution control, the risk level of the region can be classified through ecological risk analysis, to select the region with a higher risk for priority management and control. The potential ecological risk index is commonly used in soil contamination risk analysis, which is used to evaluate the ecological risk of heavy metals in soil or sediment. This method was originally proposed by Hakanson and widely used [8]. In the evaluation process, the average concentration of heavy metal pollutants is often used to analyze. To some extent, the uncertainty of heavy metal concentration is ignored.

Monte Carlo is a kind of statistical simulation experiment method and an important one of random simulation method. Based on the theory of statistical sampling, using the random number, through the statistics of random variables, sampling experiments, or random simulation, to obtain the statistical
eigenvalue as the numerical solution of the problem, is a numerical calculation method for solving the approximate solution of engineering and technical problems [9]. Monte Carlo can obtain the sampling data of the function through many independent simulation experiments, and determine the probability distribution characteristics of the function. In the uncertain and complex environment, the prediction results given by Monte Carlo simulation are more accurate and scientific[10]. Therefore, Monte Carlo simulation has become one of the important methods of random analysis in uncertainty analysis[11]. Considering the uncertainty of sampling, this study used Monte Carlo simulation to generate random number instead of average concentration to reduce the uncertainty in the evaluation process. It can put forward an evaluation methodology for risk assessment of heavy metals in soil.

In this research, the farmland soil near a lead smelter was sampled and analyzed, and the ecological risks of As, Pb, and Cd in the soil were evaluated.

2. Research area and methods

2.1. Research area
The survey region is about 2000m away from the west of a lead smelting plant in a central province of China, and the range of sampling farmland is 100m × 48m. The sampling area is divided into 120 samples of 5m × 8m on average, and 5 soil samples are randomly collected from each sample for mixing and standby, with the sampling depth of 0 ~ 20cm. The sampling diagram of the study area is shown in Figure 1.

![Figure 1. Sampling diagram of the study area](image)

2.2. Experimental method
The soil samples were sealed and stored in a sealed bag, cleaned, sieved and ground in the laboratory, sieved 0.149mm, and prepared for testing. Two soil samples were taken from each of 120 soil samples. After one soil sample was digested by electric heating plate, the Pb and Cd were determined by atomic absorption method; the other samples were added with aqua regia, and the content of As was determined by atomic fluorescence method (AF7550, Beijing East West analysis) after water bath digestion.

3. Results and analysis

3.1. Experimental results
The concentration distributions of As, Cd and Pb in 120 soil samples are shown in Table 1.

| Heavy metal | Concentrations range (mgkg⁻¹) | Background concentration[12] |
|-------------|-------------------------------|-----------------------------|
| As          | 10.00~19.40                   | 9.4                         |
| Cd          | 1.10~3.84                     | 0.065                       |
| Pb          | 140~188                       | 20.1                        |

It can be seen from Table 1 that the concentrations of As, Pb and Cd in the farmland near the smelter exceeded the background concentration of soil in Henan Province, which is mainly caused by the
pollution of waste slag and waste water of the smelter to the soil and the sedimentation of heavy metals in the vicinity and waste gas.

3.2. Risk analysis based on traditional potential ecological risk index method

The traditional potential ecological risk index was used to analyze the concentration of heavy metals in the soil of the plot. The formula is as follows[8]:

\[ C_f^i = \frac{C_D^i}{C_R^i} \]  
\[ E_f^r = T_r^i \times C_f^i \]  
\[ RI = \sum_{i=1}^{m} E_f^i \]

Where: RI is the total potential risks of various heavy metals; \( E_f^i \) refers to the potential risks of various heavy metals; \( T_r^i \) refers to the toxicity response coefficient (As, Pb, and Cd toxicity response coefficients are 10, 5 and 30 respectively); \( C_f^i \) is the pollution factor; \( C_R^i \) is the concentration of As, Pb, and Cd; \( C_R^i \) refers to the background concentration of heavy metals in the soil before industrialization (Background concentration of soil in Henan Province refer to reference[12]).

**Table 2. Indices and grades of potential ecological metals contamination**

| Risk of single metal | Risk level | Total risk | Total risk level |
|----------------------|------------|------------|-----------------|
| [0,40)               | low risk   | [0,150)    | low risk        |
| [40,80)              | medium risk| [150,300)  | medium risk     |
| [80,160)             | equivalent high risk | [300,600) | high risk       |
| [160,320)            | high risk  | [600,+)    | extremely high risk |
| [320,+)              | extremely high risk | [600,+)    | extremely high risk |

The risk indexes of As, Cd, and Pb can be calculated, and the statistical values are shown in Table 3.

**Table 3. Statistical results of risk indexes of As, Cd, and Pb**

|       | As     | Cd     | Pb     | Total  |
|-------|--------|--------|--------|--------|
| Min   | 10.64  | 507.69 | 34.83  | 562.49 |
| Max   | 20.64  | 1772.31| 46.77  | 1834.46|
| Mean  | 15.89  | 822.50 | 40.95  | 879.34 |
| SD    | 1.87   | 135.37 | 2.34   | 136.87 |
| CV(%) | 11.79% | 16.46% | 5.72%  | 15.56% |

According to Table 3, the mean value of the potential ecological risks of As, Pb and Cd belong to low risk, high risk and medium risk, respectively.
The ecological risk distribution of As is shown in Figure 2(a). It shows that the total risk of As is in the range of 10.64~20.64. There are many peaks on the three-dimensional map. The peaks generally appear near the width of the farmland plot of 20 m and 48 m. The highest risk appears near the coordinates (70, 45), and the risk value is 20.64. The average risk value of As is 15.89, which is low risk level.

Figure 2(b) is the ecological risk distribution of Cd. The total risk of Cd is between 508~1772, and the distribution of three-dimensional map is relatively average. Most of the risks are around 800. There is a sudden steep peak near the coordinates (30, 45), and the risk value is 1772. The average Cd risk of the whole plot is 822, which is at an extremely high risk level.

The risk distribution of Pb is shown in Figure 2(c). The total risk of Pb is between 35~47. There are many peaks in the three-dimensional map. The peaks are on both sides, with the valley in the middle, and the average value of the peaks are higher than 40. The average risk of Pb is 41, which is belonging to medium level.

The risk distribution of As, Cd, and Pb within 100m×48m of the whole farmland is shown in Figure 2(d). It shows that the total risk of As, Cd, and Pb is between 562~1834, and the three-dimensional map is relatively average. Most of the risks are around 850. There is a sudden steep peak near the coordinates (30, 45), and the risk value is 1834, mainly due to the high Cd risk value. The average Cd risk of the whole plot is 879, which is far higher than the extremely high level of 600.

3.3. Potential ecological risk analysis based on Monte Carlo simulation

According to the statistical analysis, the monitoring concentrations of As and Pb are consistent with the normal distribution, and the monitoring concentration of Cd is $\gamma$ distribution. Using Monte Carlo to calculate the risk of As, Pb and Cd concentration, 10000 random numbers are generated. The total risk value was calculated by the potential ecological risk index method based on Monte Carlo simulation. The risk assessment method based on Monte Carlo simulation is as follows:
\[
\text{Rand} \left( C_i' \right) = \text{Rand} \left( C_i \right) / C_{r_i} \quad (4)
\]
\[
\text{Rand} \left( E_i' \right) = T_i' \times \text{Rand} \left( C_i \right) \quad (5)
\]
\[
\text{Rand} \left( RI \right) = \sum_{i=1}^{m} \text{Rand} \left( E_i' \right) \quad (6)
\]

The 10000 simulation results of As, Cd, Pb and total risk are all in normal distribution. According to risk assessment indicators, the probability of As pollution at low risk level is 100%; the probability of Pb at low risk level is 34%, the probability of Pb at medium risk level is 66%; the probability of Cd pollution at extremely high risk level is 97.44%, and the probability of Cd at high risk level is 2.56%. The risk levels of three heavy metals were Cd > Pb > As in turn. The probability analysis of the total risk belongs to an extremely high level of 99.48%, which belongs to a high risk of 0.52%.

The total risk of As, Pb and Cd in the farmland soil is more than 800, which is far higher than the risk limit value. Therefore, we should pay attention to heavy metal pollution, especially Cd pollution, and give priority to Cd pollution control.

The risk of As, Cd, Pb and total risk according to the above formula, and analyze the confidence interval under 95% confidence level, which was shown in Table 4.

| Risk     | Distribution         | Mean Value | Confidence Interval          |
|----------|----------------------|------------|------------------------------|
| As       | Normal distribution  | 15.92      | [12.22, 19.61]               |
| Cd       | Normal distribution  | 823.85     | [580.31,1067.40]             |
| Pb       | Normal distribution  | 40.96      | [36.36, 45.56]               |
| Total Risk | Normal distribution | 880.72     | [637.03, 1124.40]            |

Under the 95% confidence level, the confidence interval of ecological risk value of heavy metals has a large span. In particular, the confidence interval of total risk is [637.03, 1124.40], which means that under 95% confidence level, the total risk value is between 637.03 and 1124.40, while the mean value is 880.72. The traditional risk assessment method only used the mean values to analyze the ecological risk, but ignored the uncertainty in the evaluation process. However, the risk assessment method based on Monte Carlo simulation can better solve the uncertainty and more close to the real value because of the 10000 times random sampling.

4. Conclusion
1) The risks of As, Cd, and Pb in the farmland soil near the smelter were analyzed by the traditional risk assessment method, and the risk distribution differences of the area also were analyzed. The risk values of three heavy metals have obvious differences in regional distribution. The average risk of As, Pb and Cd were 15.89, 822.50 and 40.95, which belonged to the low level, extremely high level and the medium level, respectively.
2) The risk assessment method based on Monte Carlo simulation is applied to calculate single risks and total risks of As, Pb and Cd. The probability analysis of the total risk belongs to an extremely high level of 99.48%, which belongs to a high risk of 0.52%. Under the 95% confidence level, the confidence interval of total risk is [637.03, 1124.40], with the mean value 880.72. The heavy metals pollution control must be carried out immediately.
3) The probability of As pollution at low risk level is 100%; that of Pb at low risk level is 34%, that of Pb at medium risk is 66%; that of Cd at extremely high risk is 97.44%, that of Cd at high risk is 2.56%. The risk of Cd is the highest. So, giving priority to Cd pollution control is a must.
4) The coupling of Monte Carlo simulation and the traditional risk index to analyze the ecological risk of heavy metals in farmland soil can more approach the real value and reduce the error caused by too small sample. Therefore, this research can offer an objective evaluation methodology for the risk management of farmland soil pollution.
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