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Estimating Source Apportionment of Heavy Metals Contamination in Surface Soil based on Positive Matrix Factorization (PMF) model around Cerrito Blanco in San Luis Potosi, Mexico

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Introduction

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- One of the most serious environmental issues facing the world today is soil contamination. The heavy metal contaminants in the soil spread to other parts of the ecosystem and pose a direct or indirect threat to human health.
- Industrial emissions, illegal dumping, municipal disposal of wastes, and the improper use of agrochemicals collectively contribute to the concentration and absorption of heavy metals in the environment.
- Heavy metal contamination has been linked to serious health consequences in humans, including cardiac diseases, skeletal illnesses, infertility as well as neurological disorders.
- For the purposes of detecting locations with significant levels of concentrations and correlating the levels with potential sources of contamination, soil mapping has been carried out in many countries to investigate the spatial distribution of heavy toxic metals in the contaminated soils.
- The most prominent and widely used receptor models for source apportionment are principal component analysis/absolute principal component scores (PCA/APCA), positive matrix factorization (PMF), and UNMIX.
- GIS has become a valuable tool for monitoring environmental pollutants. To fill in any voids in the cognitive design model, interpolation of data can be utilised to forecast values in unsampled areas using adjacent observed values.



Research Objectives

IECG 2022 The specific objectives of this study are as follows:

- a) to estimate the heavy metal concentrations in the surface soil around Cerrito Blanco, Matehuala, San Luis Potosi, Mexico,
- b) to identify the possible pollution sources of the heavy metals using PMF model.
- c) to analyse the spatial distribution patterns of source factors of heavy metals.



Study Area

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- The soil sampling sites were located in the Joya Verde soccer sports club, Cerrito Blanco, around 6.8 km from the municipality of Matehuala in the northern part of the state of San Luis Potosi, Mexico.
- It covers a total land area of around 4.84 hectares and is located between 23°40'30"N latitude and 100°35'27" W longitude.
- The area has semi-arid weather, and the predominant vegetation is a microphallus shrub that supports modest cow grazing, mixed with maize croplands.
- The types of soil in this area include Calcisol and Gypsisol, and the area receives limited precipitation, ranging from 300 to 500 mm per year.



Study area



Units: Degree



Materials and Methods

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Soil Sampling and Chemical Analyses

- A total of 39 surface soil samples were collected with an auger at a depth of 0–5 cm from soccer fields and scrub areas around the fields.
- A Garmin Etrex Personal navigator global positioning system receiver was used to geo-locate all the soil sampling locations.
- A proportion less than 2 mm was obtained by sieving the soil samples after they were air-dried at room temperature.
- Inductively coupled plasma optical emission spectroscopy (ICP-OES) was used to estimate the elements in the digestion of soil samples. One gram of soil was combined with 250 mL of deionised water and stirred in an orbital shaker for two hours at 25°C to evaluate the solubility of different metals.



Materials and Methods

IECG 2022 Positive matrix factorization model (PMF) model

- □ PMF is a receptor model that the United States Environmental Protection Agency has recommended to analyse the different types of sources of environmental pollution.
- □ This model was developed by Paatero and Tapper, (1994).
- □ In this research, PMF 5.0 model was implemented to source identification of heavy metals in the surface soils.

$$x_{ij} = \sum_{k=1}^{p} g_{ik} f_{kj} + e_{ij}$$

where x_{ij} is a quantitative matrix for the *j*th heavy metal component in *i* samples; g_{ik} denoted a contribution matrix of the *k*th source factor; for the *k*th source factor, f_{kj} represents a source factor of the *j*th heavy metal component, and the residual value for the *j*th metal element over *i* numbers of samples is denoted by the symbol e_{ij} .



Materials and Methods

IECG 2022 Positive matrix factorization model (PMF) model

$$Q = \sum_{i=1}^{n} \sum_{j=1}^{m} \left(\frac{e_{ij}}{u_{ij}}\right)^2$$

where *Q* is the difference (i.e., e_{ij}) between the x_{ij} and the output of $g_{ik}f_{kj}$, weighted by the uncertainty measurement u_{ij} .

Two input files are needed for the PMF model: soil sample concentration values and soil sample uncertainty values. The following equation was used to estimate the uncertainty values:

 $\begin{aligned} u_{ij} &= 5/6 \times MDL \ (\text{for } c \leq MDL) \\ u_{ij} &= \sqrt{(error \ fraction \ \times c)^2 + MDL^2} \ (\text{for } c > MDL) \end{aligned}$

where *c* is the concentration values of soil samples, *MDL* is the species-specific method detection limit, and the error fraction represents the uncertainty measurement percentage.



Statistical summary of heavy metal concentrations in soils

Metals	As	Cd	Со	Cr	Cu	Ni	Pb
Mean	119.44	0.95	0.76	2.96	20.65	3.20	36.95
Standard Error	17.54	0.10	0.10	0.37	1.56	0.30	3.97
Median	90.51	0.94	0.69	2.49	18.10	3.07	30.86
Standard Deviation	109.54	0.65	0.65	2.28	9.75	1.87	24.79
Sample Variance	11998.65	0.42	0.43	5.21	95.04	3.49	614.63
Kurtosis	8.37	-1.09	-0.74	4.85	3.63	0.93	5.73
Skewness	2.43	0.21	0.53	2.11	1.68	0.93	2.12
Range	578.17	2.18	2.19	10.82	47.85	8.13	126.30
Minimum	13.14	0.00	0.00	0.28	7.88	0.24	8.99
Maximum	591.31	2.18	2.19	11.10	55.73	8.37	135.29
Sum	4658.01	37.12	29.73	115.30	805.17	124.90	1440.9 9
Coefficient of variation (CV) (%)	91.71	68.06	85.77	77.22	47.22	58.32	67.10
Count	39	39	39	39	39	39	39
Confidence Level (95.0%)	35.51	0.21	0.21	0.74	3.16	0.61	8.04



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Source apportionment of heavy metals by PMF

- □ The model was running 20 times with the factors set to 3, 4, and 5.
- □ The Q value was the lowest, and the majority of the residual fell between -3 and 3 for the 3-factor analysis.
- □ The contributions of heavy metals in factor 1 increased in the following order: As < Cr < Cu < Ni < Pb < Cd < Co.
- □ The Cr, Ni, and Cd concentrations, which account for 50.76%, 32.44%, and 38.75% of factor 2, respectively, are the major contributions, with limited impact from other metal sources.
- □ Factor 3 was dominated by As (94.02%), Cu (34.74%), and Cd (23.46%).







Spatial distribution patterns of source factors

- □ Factor 1 showed a significant positive load of Co, Cd, Ni, Pb, Cu, and Cr in the source contributions and were close or below to the permissible limit standards derived from the surface soil.
- □ According to the spatial distribution mapping of factor 1, the study area's western side which is surrounded by semi-arid vegetation contains the majority of the high-value locations.
- □ The average concentrations of Co, Cd, Cu, Ni, and Pb were close to their respective permissible limits; hence they could be of natural origin. Therefore, factor 1 might be classified as a natural source.



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- □ Factor 2 was associated with Cr, Ni, and Cd. According to the results, these three metals contributed to this source factor more significantly than the other four metals.
- □ The major sources of Cd have been identified as of metallurgical origin. Industrial emissions are the only source of Cr and Ni.
- □ The spatial distribution of factor 2 shows that the middle portion of the study area of the soccer field has the majority of the high-value locations.
- □ As a result, it is possible to confirm that factor 2 represents the mining and industrial sources.





- □ Factor 3 had significant contributions of As, Cu, and Pb than the other three sources.
- □ The As is mostly associated with irrigation water and is observed in a considerable area of soccer fields and the surrounding study area.
- □ Studies conducted earlier revealed that the water in the study area had incredibly high quantities of heavy metals, which are caused by the dissolution of metallurgical waste from an abandoned smelter upstream of Matehuala.
- □ The spatial distribution pattern of factor 3 revealed that the soccer field area with high local concentrations is mostly affected by irrigation. Therefore, it might be concluded that factor 3 reflected the groundwater sources.



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Conclusions

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- □ This study measured the contamination risks by descriptive statistical analysis approach, identification of various sources of heavy metals in the surface soil using the PMF model and observed the spatial distribution patterns of source factors based on an IDW interpolation technique.
- □ This study concluded that the mean concentrations of Co, Cr, Cu, Ni, and Pb in the surface soils in Cerrito Blanco were lower than their permissible limits.
- □ But the mean concentrations of As and Cd were higher than their permissible limits.
- □ The PMF results showed that the identification of source contribution for heavy metals in the surface soil was as follows: 53% for natural sources, 23% for mining activities and industrialization sources, and 24% for irrigational groundwater sources.
- □ The spatial distribution patterns of source factors and model outcomes revealed that Co, Cd, Cu, Ni, and Pb originated from natural sources; Cr, Cd, and Ni may be obtained from past mining and industrialization; and As and Cu mainly came from groundwater sources.



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