

An automated monitoring system of urban pollution using geochemical and magnetic parameters

Un sistema automatizado de monitoreo de la contaminación urbana con el uso de parámetros geoquímicos y magnéticos

Francisco Bautista^{1,*}, Dorian Bautista-Hernández¹, Aristeo Pacheco², Avto Goguitchaichvili³, Juan Morales³, Ángeles Gallegos-Tavera¹

¹Laboratorio Universitario de Geofísica Ambiental, Centro de Investigaciones en Geografía Ambiental, Universidad Nacional Autónoma de México, Michoacán, Mexico.

²Acts with Science. Morelia, Michoacán, Mexico.

³Laboratorio Universitario de Geofísica Ambiental, Instituto de Geofísica, Universidad Nacional Autónoma de México, Michoacán, Mexico.

* Corresponding author: (F. Bautista)
leptosol@ciga.unam.mx

ABSTRACT

The World Health Organization (WHO) estimates that environmental pollution causes seven million premature deaths annually, equivalent to one in eight deaths worldwide. To combat this, the organized implementation of reliable indicators is critical, and these indicators should be monitored over short, medium, and long terms. The principal industrial and economic activities at Mexico's national level are concentrated in the Mexico City Metropolitan Area. Urban expansion, with unmeasured and essentially unplanned growth, has been accompanied by a notable increase in environmental pollution. The software discussed herein quantifies and analyzes the contents of potentially toxic elements in soils, dust, and plants to monitor how environmental pollution contributes to the ill-health of the population of Mexico City and how these adverse effects could potentially be reduced. The software can analyze conventional geochemical data and alternative proxies such as magnetic parameters and color variations for three environmental matrices: soils, dust, and plants in urban areas.

Keywords: urban soils, urban dust, urban plants, magnetic properties, color, FRX.

RESUMEN

La Organización Mundial de la Salud (OMS) estima que la contaminación ambiental causa siete millones de muertes prematuras al año, lo que equivale a una de cada ocho muertes en todo el mundo. Para combatir esto, la instrumentación organizada de indicadores confiables es crítica, y estos indicadores deben ser monitoreados a corto, mediano y largo plazo. Las principales actividades industriales y económicas a nivel nacional en México se concentran en la Zona Metropolitana de la Ciudad de México. La expansión urbana, con un crecimiento desmedido y esencialmente no planificado, ha ido acompañada de un notable aumento de la contaminación ambiental. El software discutido aquí cuantifica y analiza el contenido de elementos potencialmente tóxicos en suelos, polvos y plantas para monitorear cómo la contaminación ambiental contribuye a la mala salud de la población de la Ciudad de México y cómo estos efectos negativos podrían reducirse potencialmente. El software se puede utilizar para analizar datos geoquímicos convencionales junto con indicadores alternativos, como parámetros magnéticos y variaciones de color para tres matrices ambientales: suelos, polvos y plantas en áreas urbanas.

Palabras clave: suelos urbanos, polvo urbano, plantas urbanas, propiedades magnéticas, color, FRX.

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1. Introduction

The urbanization and industrialization of cities have produced increased emissions of heavy metals into the environment. In large urban populations such as Mexico City, London, Beijing, Madrid, and New York City, more than seven million deaths yearly due to cancer and other pollution-related diseases have been detected (WHO, 2014). In recent years there have been many findings worldwide of heavy metal pollution in soil (Aguilar *et al.*, 2013a; Ihl *et al.*, 2015), urban dust (Aguilar *et al.*, 2013a, Cortés *et al.*, 2017; Aguilera *et al.*, 2019; Delgado *et al.*, 2019; Morales *et al.*, 2020) and urban plants (Aguilar *et al.*, 2013a, 2013b). However, heavy metal pollution monitoring systems are not systematically implemented globally; only isolated disclosures have been made.

Pollution monitoring is complex and expensive due to the need to process large quantities of samples and information, and chemical analyses are a further cost. Efforts have therefore been made to find high-speed, inexpensive technologies called “proxies” that promote the study of heavy metal pollution, elements of which are magnetic properties (Cejudo *et al.*, 2015; Sánchez-Duque *et al.*, 2015) and the color of soils and dust (Cortés *et al.*, 2015; Marín *et al.*, 2018). These elements can be inexpensively acquired and are considered to provide reliable proxy indicators.

Many developing countries cannot count on many experts in heavy metal contamination, so the generation of technological tools that can analyze large quantities of information quickly and effectively is required. This work aimed to create software to save, sort, and analyze chemical information and relate it to proxy technologies with magnetic and color parameters in studying three environmental matrices: soils, dust, and tree leaves.

2. Materials and Methods

2.1. SOFTWARE DESIGN

The design and development of the software were based on the Mexican Standard NMX-I-12207-

NYCE-2011 (Secretariat of the Economy, 2011), using the “waterfall model” with its methodological focus on ordering the activities of software development from beginning to end, finalizing each activity before beginning a new one. The tools utilized in our study were: Java 1.8 as the programming language, the Integrated Development Environment Eclipse Photon 4.7 (IDE), and the relational database management system H2 1.4.195 Database Engine with the syntax of the consulted language structure (SQL). These tools were selected for their free access, flexibility, robustness, high performance, and to accommodate the large community of users who volunteered their support.

The Model-Vision-Controller (MVC) software construction architecture divides software development into three areas. The model is in charge of requesting the data from the database manager (DBMS) through defined mechanisms and delivering the data to persist over time. The view is in charge of interacting with the user and collecting the input and output data to be processed by the controller (Pop and Altar, 2014; Ishihara and Funabiki, 2017). The controller, that acts as a judge, is in charge of validating the data, requests, controls and deliberating whether or not they are sent to the model to be stored or to consult details. With this architecture, business rules can be separated from interfaces, language functions, and development environment, thus creating a more precise, more modular construction and structure that embraces change and is not closed by strong dependencies among interfaces, language, and business rules.

The algorithmic structures and interfaces were perfected to utilize a minimum quantity of information sources to meet the following minimum requirements: processor of 1.0 GHz or higher; 256 MB of RAM (Random-Access Memory) dedicated to optimizing performance; a VGA (Video Graphics Array) screen with a recommended resolution of 1024x768 and 32 MB of graphic memory with a dedicated hard disc of 100 MB or higher; JVM 1.8 (Java Virtual Machine) software installed in the equipment; operating system Windows 7 or

higher; Linux with JVM 1.8 support; and Mac OS with JVM 1.8 support.

2.2. SAMPLE SITES AND ENVIRONMENTAL MATRICES

The processing of the information in the software is based on the relational database model that relates the sample sites with the country, city, and state, and to the environmental soil, dust, and urban plant matrices, with each of these sites being associated with data blocks of color, magnetics, and chemical properties. In this way, each sample site is associated with an environmental matrix, forming pairs of registers where one sample site is related to a matrix of soils, dust, and plants; thus, each environmental matrix is, in turn, associated with each data block of properties of color, magnetics, and chemical properties (Figure 1).

The soil matrix contains information on the type of soil sample (superficial or control), sampling time (daily, weekly, biweekly, monthly, or annual), site, date, photograph, and observations. For soil sampling, a 2.5-inch diameter polyvinyl chloride (PVC) cylinder is used; the sample is dried for two weeks in the shade and then pulverized and sieved with a 2-mm mesh to carry out the analysis of the elements' concentrations, for which X-ray fluorescence can be used (Bautista *et al*, 2011; Ihl *et al*, 2015).

The dust data matrix shows the type of swept surface (paving stone, cement, cobblestone, paving, soil, or dirt road), sample weight, temporality sampling, site, date, photograph, and observations. Dust sampling is done by delimiting one square meter on the surface to be swept; then, the sample is swept and stored in a plastic bag. The

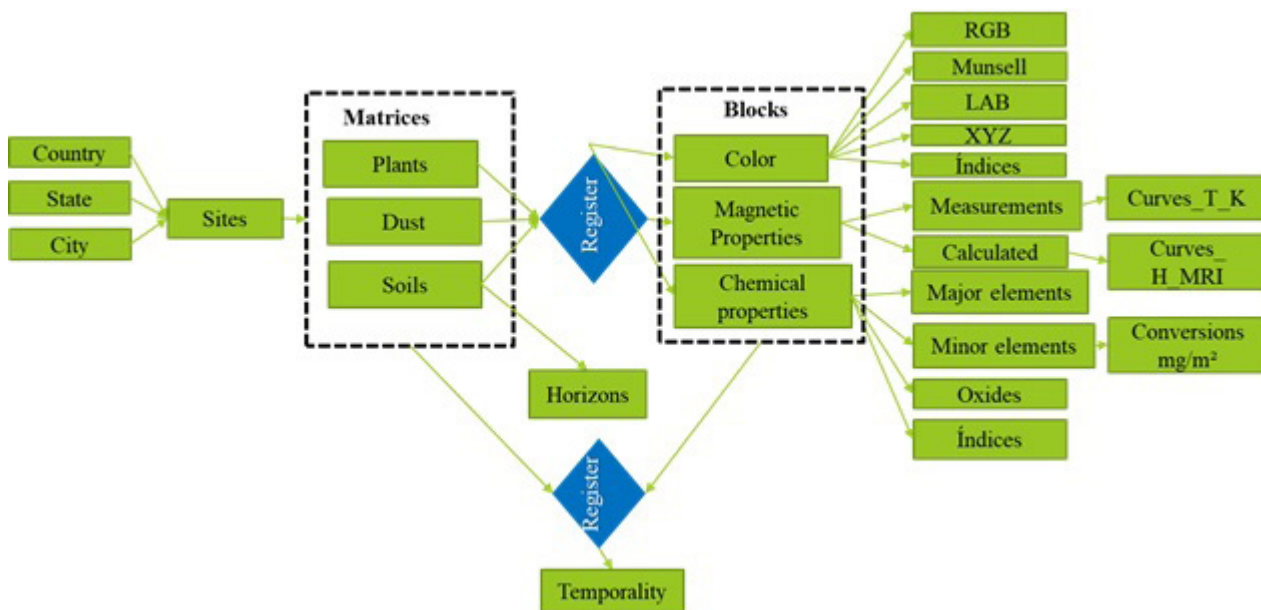


Figure 1 The architecture of the Heavy Metals Software.

samples are labeled and weighed; They are dried in the shade for two weeks, ground, and sieved with 10, 30, or 60 mesh to analyze the concentrations of the elements (Aguilar *et al.*, 2011; Aguilera *et al.*, 2018).

The plant data matrix shows the common and scientific name of the plant, life form (tree, shrub, grass, palm), the height of leaves, type of leaves (young, mature or old), state of the plant (healthy, pruned, damaged, diseased), sedimentation period of the dust on the plant leaf (days, months or years), tree stump size (small, medium or large), damage to sidewalks, the timing of sampling, site, date, photography, and observations (Aguilar *et al.*, 2013a). The plant data is recorded by measuring tree stump width and height, and height and diameter on all trees; the tree species that presented or not dust particles deposited on the leaf surfaces are recorded; a qualitative estimate of the state of health and maturity of the trees is made, and damage to the infrastructure is sought (Benavides *et al.*, 2002; Flores and Álvarez-Sánchez, 2011).

2.3. CHEMICAL PROPERTIES AND INDICES OF CONTAMINATION

The chemical properties registered by the software are the major elements of oxide types such as MgO, Al₂O₃, SiO₂, P₂O₅, K₂O, CaO, TiO₂, MnO, Fe₂O₃; major elements such as Al, Ca, Fe, Mg, P, Na, K, Mn, Ti; and heavy metals and other potentially toxic elements such as Rb, Si, Y, Ag, As, Ba, Be, Cd, Co, Cr, Cu, Mo, Ni, Pb, Se, V, Zn, Li, B, and Hg.

The indexes calculated from the concentrations of these elements are contamination factor, level of contamination, contaminate load, and geoaccumulation index (Cejudo-Ruíz *et al.*; 2015), (Delgado, *et al.*; 2015), (Ihl *et al.*; 2015), (Sánchez-Duque *et al.*; 2015).

The “Contamination Factor” index compares a background value with presumably contaminated samples. The background value can be an average value of world soils or a local value such as that of a subsurface horizon, the content of the element in the rock, or decile 1 of a population (Aguilera *et al.*, 2021).

$$CF = \frac{C_m}{C_{mr}} \quad (1)$$

Where CF is the contamination factor; C_m is the concentration of the potentially toxic element in the sample, and C_{mr} is the concentration of reference for the potentially toxic element.

$$Cdeg = CF_1 + CF_2 + CF_3 + \dots + CF_n \quad (2)$$

Where $Cdeg$ is the level of contamination and CF represents the contamination factor of each element potentially analyzed.

$$ICC = n \sqrt{\prod_{i=1}^n CF_i} \quad (3)$$

Where ICC is the index of contaminate load; n represents the number of potentially toxic elements, and CF is the contamination factor.

$$Igeo = \log_2 \frac{C_n}{(1.5)(B_n)} \quad (4)$$

Where $Igeo$ is the geoaccumulation index; C_n is the concentration of the chemical element in the soil; B_n is the geochemical base of reference of the elements, and 1.5 is the constant that represents the fluctuations of the substance in the environment and the anthropogenic influence.

The “geoaccumulation index” index compares an element’s background value with the presumably contaminated samples. Still, it uses base 2 logarithms and a constant of 1.5 to account for variations in the background level (Aguilera *et al.*, 2021).

$$Cdeg = CF_1 + CF_2 + CF_3 + \dots + CF_n$$

2.4. MAGNETIC PROPERTIES AS A PROXY

The values of magnetic susceptibility at frequencies of 976 Hz, 3904 Hz, 15616 Hz (available with the Kappabridge MFK1-FA equipment), and at 465 Hz and 4650 Hz (Bartington MS2B operating frequencies) are designated as K_{f1} , K_{f2} , K_{f3} ,

K_{lf} , K_{hf} respectively; NRM (Mass Normalized Natural Remanent Magnetization) in $mAm^2 kg^{-1}$; ARM (Anhysteretic Remanent Magnetization) obtained in an alternate field (AC) of 120 mT with a field of direct current (CD) of 100 μT , in units of Am^{-1} ; IRM (Isothermal Remanent Magnetization) obtained at ambient temperature and with magnetic field pulses of 1000 mT, 100 mT, 200 mT, 300 mT in units of A/m designated as IRM_{1000} , IRM_{100} , IRM_{200} , IRM_{300} respectively; specific magnetic susceptibility at frequencies of 976 Hz, 3904 Hz, 15616 Hz, 465 Hz, 4650 Hz in $\mu m^3 kg^{-1}$ designated as χ_{f1} , χ_{f2} , χ_{f3} , χ_{lf} , χ_{hf} respectively; percentage of frequency-dependent susceptibility at frequencies $X_{df1,2\%}$, $X_{df1,3\%}$, $X_{df2,3\%}$, $X_{df,hf\%}$; anhysteretic magnetic susceptibility X_{arm} ; and S_{-100} , S_{-200} , S_{-300} ratios determined by the isothermal remanent magnetization obtained at ambient temperature and with inverse magnetic field of 100, 200, 300 mT respectively, divided by the residual isothermal magnetization obtained at 1000 mT; unitless parameters.

Curves of magnetic susceptibility versus temperature permit to identify the points of inflection in the curves during the process of heating, where

the value of the function is equal to zero (Nanlohy *et al.*, 2022).

$$f'(x) = \frac{k_{i+1} - k_i}{\theta_{i+1} - \theta_i} \tag{5}$$

Where θ is the temperature, and k is the volumetric magnetic susceptibility and the opening data.

$$f''(k) = \frac{f'(k_{i+1}) - f'(k_i)}{\theta_{i+1} - \theta_i} \tag{6}$$

Where θ is the temperature, and $f'(k)$ is the value of the first derivative calculated in Equation 5.

3. Results

3.1. CAPTURE AND PROCESSING OF ENVIRONMENTAL MATRICES DATA

In the site's graphic interface, it is seen the number of samples and information about geolocalization (countries, cities, and towns), along with soil usage, types of road pavement (or lack of it), and geology (Figure 2).

The environmental matrices module corresponds to the soil, dust, and plant samples. Each

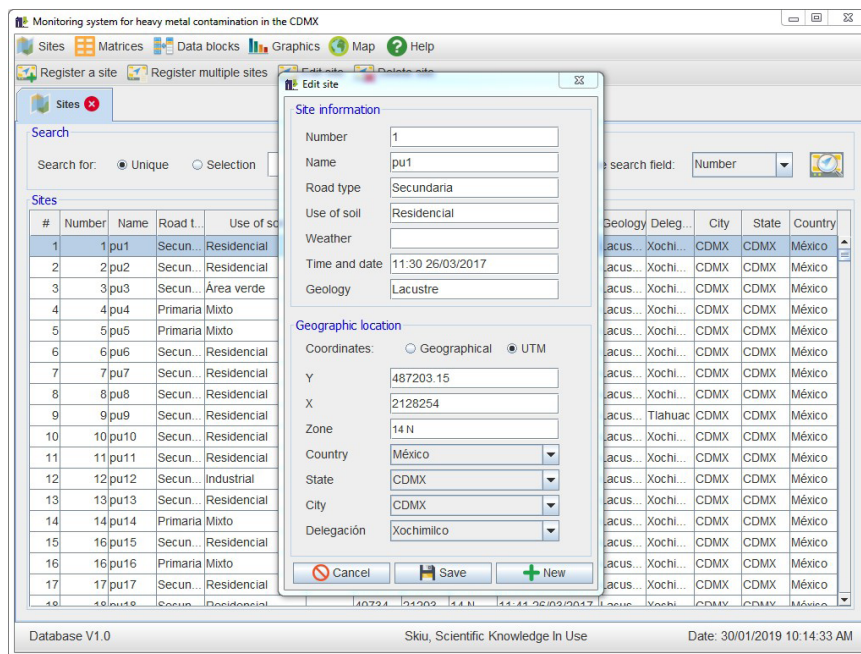


Figure 2 Screen with the main menu with the data of the study site and geographic location.

matrix shows different data; for example, in the case of urban dust, the quantity of dust per surface unit is registered, as are the types of surfaces on or near where the samples were collected, for example, those collected near cement sidewalks, paved streets, streets surfaced with cement, unpaved roads or those with paving stones or tiles (Bautista *et al*, 2011). It is essential to capture the quantity of dust from different surface areas because the contaminated load can be calculated, along with the amount of an element per square meter (Figure 3).

In the case of soils, the bulk density is registered, along with the coarse fragments and the soil usage in the area (gardening, parks, wooded areas, etc.). The bulk density and the percentage of coarse fragments are used to calculate the quantity of heavy metals per surface unit, which is relevant

data in calculating the type of amendments per surface unit (Bautista *et al*, 2016; Bautista *et al*, 2017).

The environmental matrices (soils, dust, and plants) and the properties in the data blocks (oxides and heavy metals) are registered by season, allowing for monthly, seasonal, or yearly studies. The benefits of structuring the data in a relational model are a) to avoid data duplication, b) to improve referential integrity, and c) to improve data compression.

3.2. DATA BLOCKS AND GRAPHICS

The module referred to as “Data Blocks” works with the groups of data of the chemical and magnetic properties measured, such as the oxides MgO, Al₂O₃, SiO₂, P₂O₅, K₂O, CaO, TiO₂, MnO, Fe₂O₃; the major elements such as Al, Ca, Fe, Mg, P, Na,

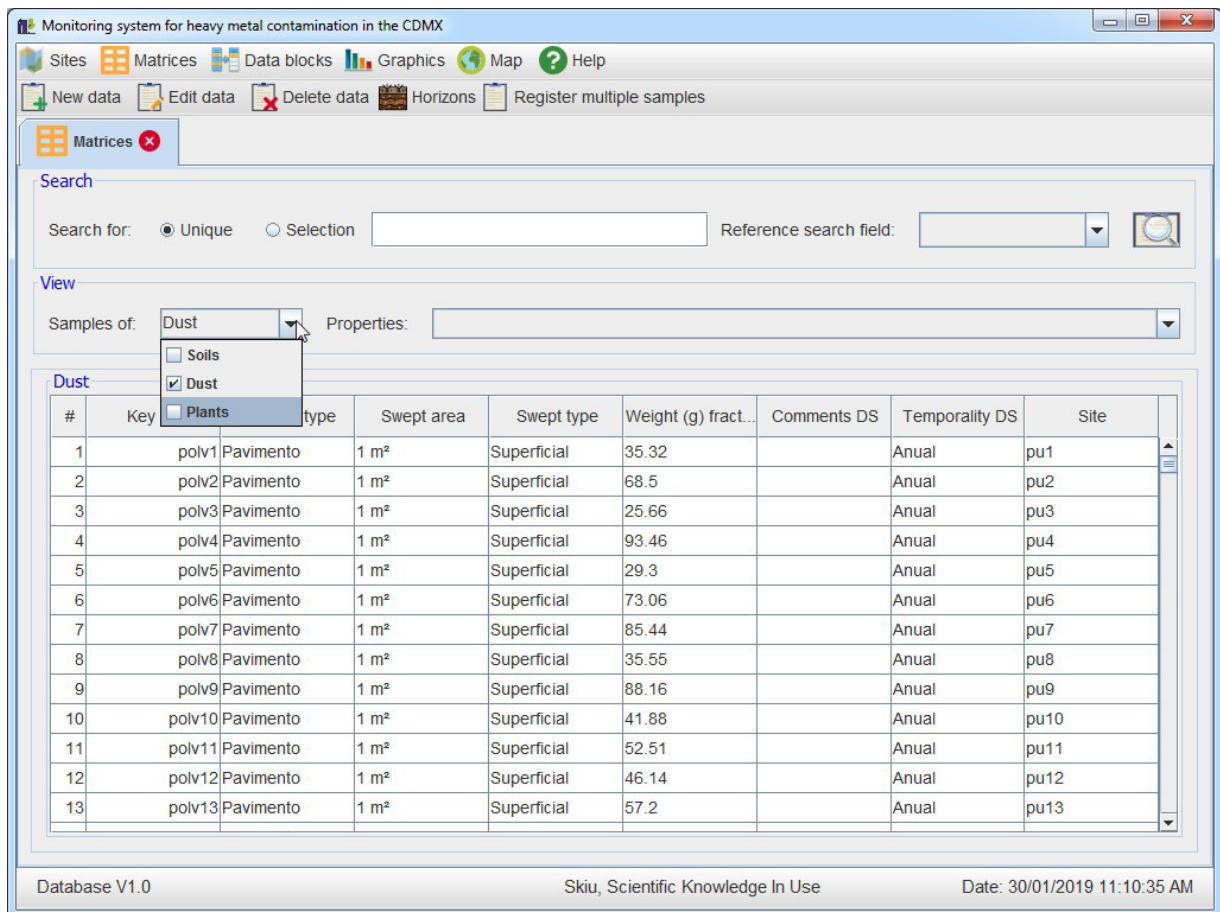


Figure 3 Matrix menu (soil, dust, plant) and information regarding the selected matrix.

K, Mn, Ti; the heavy metals, such as Rb, Si, Y; Ag, As, Ba, Be, Cd, Co, Cr, Cu, Mo, Ni, Pb, Se, V, Zn, Li, B, Hg; and the magnetic properties (Figure 4).

In this module, the index of contamination is automatically calculated, as is the index of the contaminate load, the contamination factor, the index of geoaccumulation, and the level of contamination. The option of converting the concentration units to quantity or contaminate load was included. In the case of magnetic properties, the conversion was done from the primary parameters to the calculated properties.

The “Graphics” module is divided into two submodules, “Geochemical” and “Magnetic properties”. The geochemical submodule analyses of variance can be done with the Kruskal-Wallis’s

technique, given that the data for heavy metals does not produce a Gaussian Curve (Figure 5). This type of graphics permits the identification of a median, minimum, or maximum value, inferior or superior limit, first or third quartile, the interquartile range, atypical values, notches (that represent a level of reliability of an average of 95% when this is not overlaid), and values too remote from the average in the same graphic for each element.

The graphics generated in the “Magnetic Properties” module are magnetic susceptibility, normalized magnetic susceptibility, volumetric magnetic susceptibility, terrain curves versus residual isothermal magnetization, temperature curves versus volumetric magnetic susceptibility, and S ratios (Table 1).

Monitoring system for heavy metal contamination in the CDMX

Sites Matrices Data blocks Graphics Map Help

New data Edit data Delete data Conversions Magnetic properties

Data blocks

Search

Search for: Unique Selection Reference search field: #

View

Samples of: EPT Properties: Key, Ag (mg/kg), As (mg/kg), Ba (mg/kg), Be (mg/kg), Cd (mg/kg), Co (mg/kg), Cr (mg/kg), Cu (mg/kg), M...

| # | Key | Ag (mg/kg) | As (m... | Ba (... | Be (... | Cd (... | Co (... | Cr (m... | Cu (... | Mo (... | Ni (m... | Pb (... | Se (... | Tl (m... | V (... | Zn (... | Te... | Site |
|----|--------|------------|----------|---------|---------|---------|---------|----------|---------|---------|----------|---------|---------|----------|--------|---------|-------|------|
| 1 | CDM... | 0.0 | 7.5 | 168.71 | 0.0 | 0.0 | 7.5 | 42.49 | 53.74 | 6.25 | 44.99 | 53.74 | 0.0 | 0.0 | 22.49 | 151.21 | An... | pu1 |
| 2 | CDM... | 0.0 | 0.0 | 119.91 | 0.0 | 0.0 | 8.74 | 36.22 | 58.71 | 2.5 | 62.45 | 46.22 | 0.0 | 0.0 | 22.48 | 162.38 | An... | pu2 |
| 3 | CDM... | 0.0 | 0.0 | 139.93 | 0.0 | 2.5 | 8.75 | 54.97 | 37.48 | 2.5 | 37.48 | 114.94 | 0.0 | 0.0 | 32.48 | 141.18 | An... | pu3 |
| 4 | CDM... | 0.0 | 0.0 | 139.97 | 0.0 | 0.0 | 7.5 | 42.49 | 58.74 | 2.5 | 39.99 | 106.22 | 0.0 | 0.0 | 23.74 | 176.21 | An... | pu4 |
| 5 | CDM... | 0.0 | 0.0 | 102.5 | 0.0 | 0.0 | 6.25 | 26.25 | 37.5 | 0.0 | 30.0 | 33.75 | 0.0 | 0.0 | 25.0 | 108.75 | An... | pu5 |
| 6 | CDM... | 10.0 | 0.0 | 87.46 | 0.0 | 0.0 | 7.5 | 29.99 | 24.99 | 0.0 | 34.98 | 16.24 | 0.0 | 0.0 | 29.99 | 38.73 | An... | pu6 |
| 7 | CDM... | 0.0 | 0.0 | 82.5 | 0.0 | 0.0 | 7.5 | 28.75 | 18.75 | 2.5 | 33.75 | 15.0 | 0.0 | 0.0 | 23.75 | 146.25 | An... | pu7 |
| 8 | CDM... | 0.0 | 0.0 | 111.25 | 0.0 | 0.0 | 5.0 | 32.5 | 41.25 | 2.5 | 30.0 | 37.5 | 0.0 | 0.0 | 17.5 | 92.5 | An... | pu8 |
| 9 | CDM... | 0.0 | 0.0 | 51.22 | 0.0 | 0.0 | 5.0 | 39.98 | 31.23 | 0.0 | 29.99 | 16.24 | 0.0 | 0.0 | 17.49 | 139.93 | An... | pu9 |
| 10 | CDM... | 0.0 | 0.0 | 127.47 | 0.0 | 0.0 | 5.0 | 27.49 | 32.49 | 0.0 | 28.74 | 42.49 | 0.0 | 0.0 | 13.75 | 121.22 | An... | pu10 |
| 11 | CDM... | 0.0 | 0.0 | 109.97 | 0.0 | 0.0 | 7.5 | 48.74 | 64.98 | 2.5 | 41.24 | 73.73 | 0.0 | 0.0 | 27.49 | 182.45 | An... | pu11 |
| 12 | CDM... | 0.0 | 0.0 | 78.69 | 0.0 | 0.0 | 8.74 | 82.44 | 81.19 | 7.49 | 48.71 | 271.05 | 0.0 | 0.0 | 22.48 | 188.61 | An... | pu12 |
| 13 | CDM... | 0.0 | 0.0 | 166.17 | 0.0 | 0.0 | 6.25 | 39.98 | 33.73 | 0.0 | 24.99 | 37.48 | 0.0 | 0.0 | 26.24 | 97.45 | An... | pu13 |

Database V1.0 Skiu, Scientific Knowledge In Use Current record: 1 Total records: 481 Date: 30/01/2019 10:08:58 AM

Figure 4 Block menu about physical and chemical properties (color, magnetic properties, potentially toxic elements) of soils, urban dust, and plants.

Table 1. Magnetic parameters applied in environmental samples and their possible interpretations.

| Magnetic properties | Interpretation |
|--|---|
| Magnetic susceptibility | Global estimation of the concentration of ferrimagnetic, antiferromagnetic, paramagnetic, and diamagnetic minerals. The magnetic susceptibility measurement is non-destructive, and the value depends on the form and size of the magnetic grain, the concentration and interaction with other minerals; and temperature. |
| Magnetic susceptibility dependent on the frequency | This is used to identify the presence of ferrimagnetic materials – superparamagnetic (SP), ultra-fine (<0.02 µm for magnetite, and <15 µm for hematite). |
| Saturation isothermal remanent magnetization | This magnetization is left after subjecting a material to an external magnetic field of intensity, usually more than 1 Tesla, generally at ambient temperature. This gives an estimation of the presence of ferrimagnetic and antiferromagnetic grains. |
| S _x ratio | This permit estimating the presence of minerals of high coercivity (antiferromagnetic such as hematite) against materials of low coercivity (ferrimagnetic such as magnetite). |
| NRM, Natural Remanent Magnetization, before any treatment or field laboratory tests were applied and measured in A/m. | This aids in estimating the nature of the magnetization acquired in conditions such as the initial value of magnetization before the application of artificial magnetic fields in the laboratory. |
| ARM, Magnetization acquired in the presence of alternate fields (AC) and a permanent magnetic field (DC). | This helps to determine the anhysteretic magnetic susceptibility. It also offers guidelines for the concentration of magnetic carriers and the nature of the interaction between the grains. |
| IRM ₁₀₀₀ , Isothermal Remanent magnetization obtained at ambient temperature and with a magnetic field pulse of 1000 mT. | Magnetization is acquired by a sample after subjecting it to an external magnetic field of 1000 mT at ambient temperature. This helps to discriminate between the magnetic carriers and different coercivities. |
| IRM ₁₀₀ , Isothermal remanent magnetization obtained at ambient temperature with an inverse magnetic field pulse of 100 mT. | Aids in estimating the saturation level of the residual isothermal magnetization after subjecting a material to an inverse external field of 100 mT. |
| IRM ₂₀₀ , Isothermal Remanent magnetization obtained at ambient | Aids in estimating the saturation level of the residual isothermal magnetization after subjecting a material to an external field of 200 mT. |

(Maher et al., 1986; Thompson and Oldfield, 1986; Bautista *et al.*, 2014).

Other functions of the “Heavy Metals” software are: 1) generate graphics of threshold lines, linear regression, and straight-line equation; b) estimation of the values r and r^2 ; c) identification of

anomalous values; d) filtration of data by country, state, and city; e) tabular and graphic exportation; and f) function for estimating the values directly in the graphics.

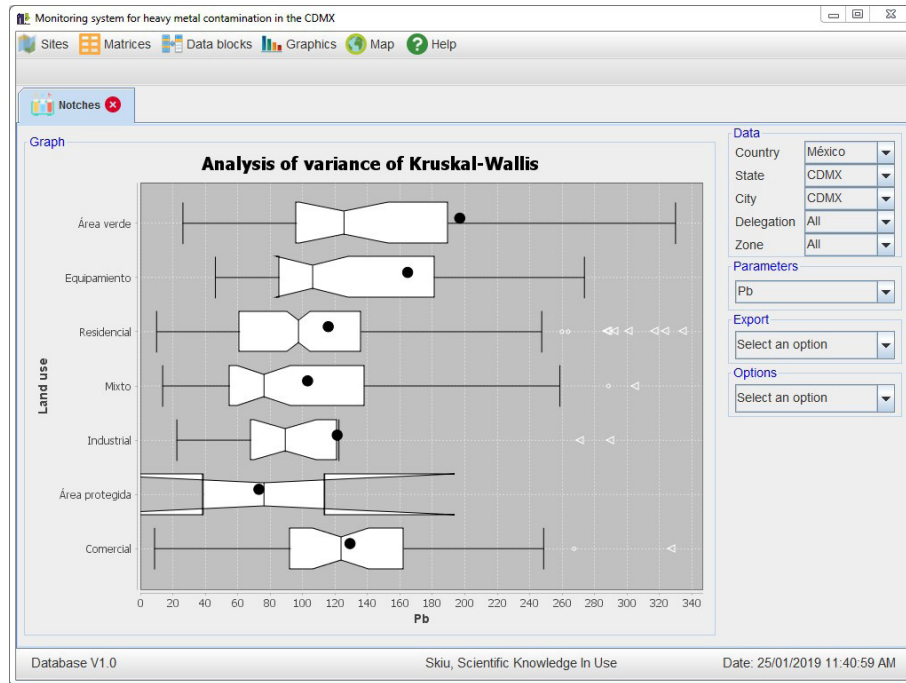


Figure 5 Example of one analysis of variance of lead by soil use.

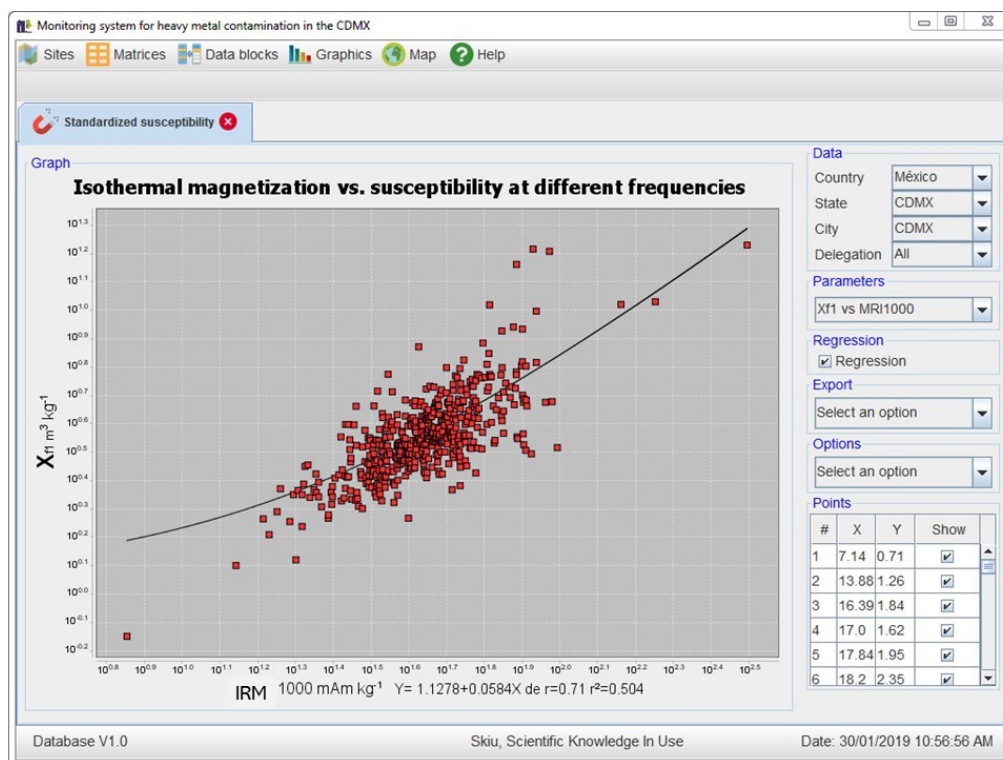


Figure 6 Example of graphic of magnetic susceptibility and isothermal remanent magnetization.

For estimating magnetic coercivity and grain size in the “Heavy metals” software, it is necessary to trace the curve of magnetic susceptibility, dependent on the frequency versus the specific magnetic susceptibility of the frequency, by pairing the groups of parameters Xdf1, 2% versus Xf1; Xdf1, 3% versus Xf1; Xdf2, 3% versus Xf2; Xdff, hf versus Xlf, and it is also possible to trace the magnetic susceptibility dependent on the frequency versus the volumetric magnetic susceptibility by pairing the groups of parameters Xdf1, 2% versus Kf1; Xdf1, 3% versus Kf1; Xdf2, 3% versus Kf2; Xdff, hf% versus Klf. “The purpose of this graphic is to permit the detection of the presence of ferrimagnetic in ultra-fine grains of sizes (superparamagnetic) smaller than $0.02 \mu\text{m}$ ” (Sánchez-Duque *et al*, 2015).

On the other hand, graphing in the “Heavy metals” software the isothermal remanent magnetization versus susceptibility at different frequen-

cies allows to produce of a curve by pairing the groups of parameters Xf1 versus IRM1000; Xf2 versus IRM1000; Xf3 versus IRM1000; Xf3 versus IRM1000; Xlf versus IRM1000; Xhf versus IRM1000 (Figure 6).

Also, estimating the concentration of ferrimagnetic materials allows producing a curve of volumetric magnetic susceptibility versus isothermal remanent magnetization by pairing the groups of parameters Kf1 versus MRI1000; Kf2 versus MRI1000; Kf3 versus IRM1000; Klf versus IRM1000; Khf versus IRM1000. The curves of applied magnetic field versus isothermal remanent magnetization yield the curve of the applied magnetic field with groups of the series of data and correlate the magnetization value with the applied magnetic field for a set of defined groups (Figure 7). Temperature curves versus volumetric magnetic susceptibility yield the curve of gradual increase in temperature versus susceptibility, beginning

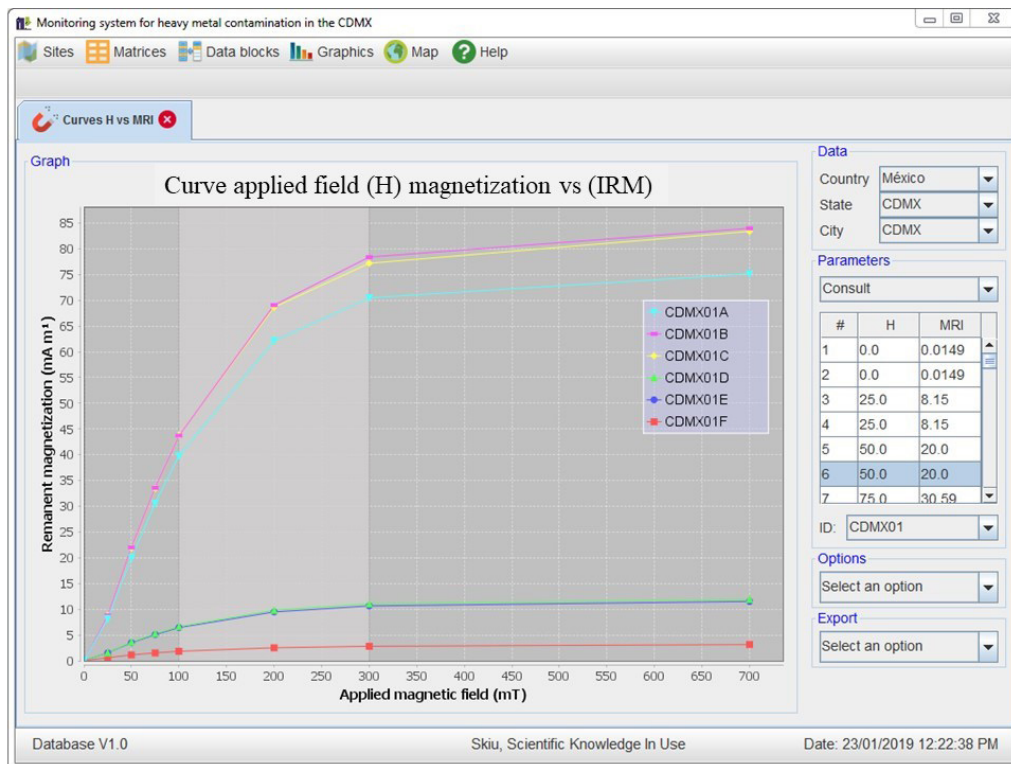


Figure 7 Example of isothermal remanent magnetization (IRM) versus applied magnetic field curves.

with the ambient temperature and reaching up to 700 °C at a rate of 10 °C min⁻¹, followed by cooling at the same rate. “The purpose of this graphic is to estimate the thermomagnetic stability and the type of the dominant magnetic mineral through the determination of Curie Temperature (T_c)” (Sánchez-Duque *et al*, 2015), as well as making it possible to identify the points of inflection in the curves with the calculation of the first and second derivatives defined in the Equations 5 and 6.

3.3. THE GEOGRAPHICAL LOCATION OF THE STUDY SITES

The “Map” module offers the visualization of the geographic localization of each sample site using Google Maps® and Google Earth®. The spatial ubication of sites can be exported as a *.kml file which can be processed in the geographic

information system to undertake a spatial analysis (Figure 8). The graphical interface of the “Map” module permits to review of the environment of each sample site, giving information about the type of road pavement (or its lack), the proximity of governmental infrastructures (schools, government service offices, parks, etc.), and also the type of factories, businesses, etc.

S ratios of the heavy metals software allow constructing a curve of values grouped in the lines of roadways and areas that have been additionally engineered, such as natural green areas, agriculture areas, residential areas, areas of mixed-use, industrial sites, protected areas, and commercial areas, to differentiate antiferromagnetic minerals from ferrimagnetic minerals with the S-100, S-200, and S-300 ratios.

The “Heavy Metals” software and some (example) input files are available from the corresponding author on reasonable request.

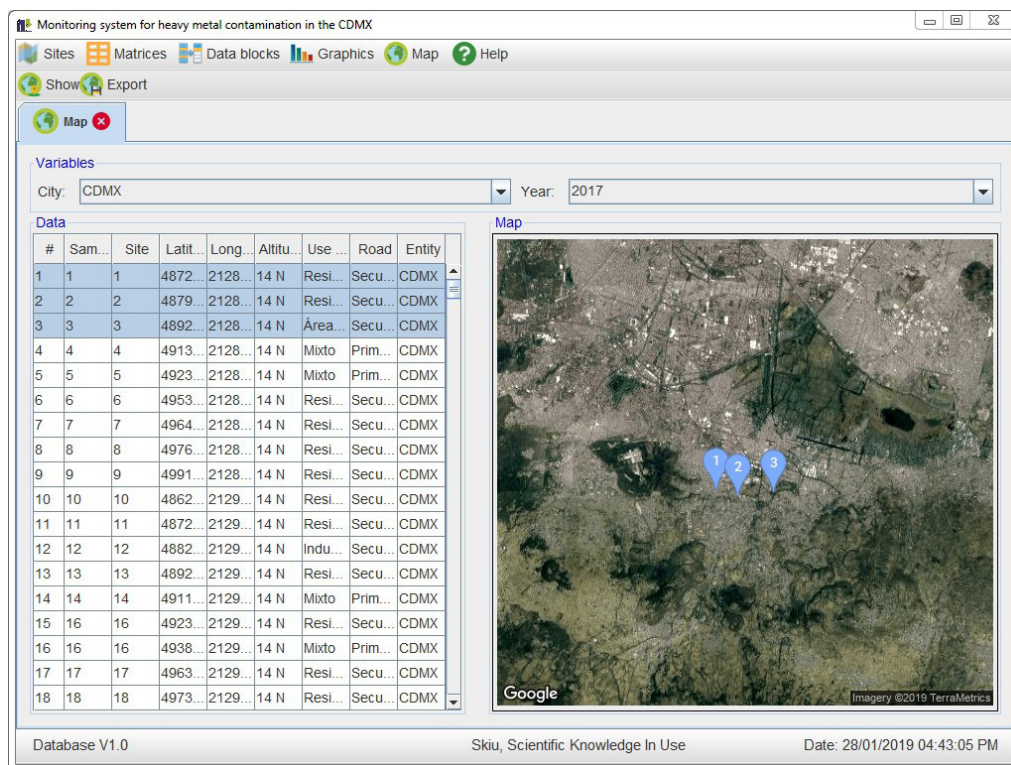


Figure 8 The geographical location of the selected study sites.

4. Discussion and conclusions

The “Heavy Metals” software is unique in its category. There are software programs that are used to evaluate the agricultural capacity of soils (De la Rosa *et al.*, 2004; Dubrovina and Bautista, 2014), and there are models of evaluation for environmental functions (Lehmann *et al.*, 2008; Lehmann and Stahr, 2010; Bautista *et al.*, 2017), and software has even been developed to evaluate the models (De la Rosa *et al.*, 2004; Gallegos *et al.*, 2014, 2016; Bautista *et al.*, 2016; Bedolla *et al.*, 2018). However, the software presented here to evaluate heavy metals in urban zones is the only one. There are no antecedents of evaluation models of the relation of heavy metals and urban dust and plants, much less any software to run them.

The “Heavy Metals” software could be improved in the areas of the index for screening heavy metals in soils (Bautista *et al.*, 2017) and with the inclusion of evaluations throughout the soil profiles, which would necessitate the measurement of the coarse fragments and the bulk density (Bautista *et al.*, 2016).

As to the architecture of the “Heavy Metals” software, it is worth mentioning that: it functions on any platform, be it Windows, Apple, Unix, or others; it is bilingual (Spanish and English), and it is user-friendly. The inclusion of magnetism as a proxy technique has made it very functional. Therefore, it would be helpful for those in charge of the environmental politics of a country with few such resources to aid in creating relevant and appropriate decisions and expenditures to correct environmental pollution issues. No computer program of this type exists in the software market worldwide, whether scientific or commercial.

Contributions of authors

Conceptualization: FB, AP, AG, (2) analysis or data acquisition: FB, AG, JM, (3) methodological/technical development: FB, AP, AGT, (4) writing of the original manuscript: FB, AP, DB, (5) writing

of the corrected and edited manuscript: FB, AG, DB, (6) graphic design: AP, AGT, (7) fieldwork: FB, AP, JM, (8) interpretation: FB, AG, JM, AGT, (9) financing: FB, AG.

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Conflicts of interest

The authors declare no competing interests.

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Annex 1. Basic operating instructions.

Site loading. Site data is loaded from the toolbar by clicking the register a site button in the pop-up window. The data to be registered is classified into site data and geographic location; starting with the site data, we must enter the site number, name, road, land use, climate (weather), geology, time, and date, followed by the geographic location section in which we must indicate the type of coordinates used to locate the sample, we must also to enter the country, state, city, and delegation to which the sample is associated.

Data capture in environmental matrices.

The capture of the environmental matrices is done from the new data function of the toolbar. To carry out the procedure, select the environmental matrix in which we want to start the data capture in the view section and click on the new data button. The pop-up window will automatically be displayed to capture a new data sample.

For example, to capture urban dust data, you must enter the key, surface area, sweep area, type of sweep, weight, observations, temporality (frequency with which sampling is performed), and site to which the sample is associated. , date, photograph, and finally, the save button of the window control options is pressed.

The data editing procedure begins with the selection of the matrix, where we must select the desired view; in the data table, we set the record to be modified, followed by clicking on the “Edit data” button, and a pop-up window will automatically be displayed with the registry data allowing each of the values to be modified. Finally, we press the save button of the window control options. The changes will automatically be reflected in the data table. To delete the record of any matrix, press the

“Delete data” button; as a general rule, we will be asked to confirm the deletion of the form.

The registration of potentially toxic elements (PTE) is done from the new data button on the toolbar in the “Register potentially toxic elements” interface, which asks us to enter the registration identification key, the concentrations of Ag, As, Ba, Be, Cd, Co, Cr, Cu, Mo, Ni, Pb, Se, Ti, V, Zn, Li, B, Hg with the associated variables of temporality, site number, name of the site to which you want to associate the concentrations of PTE, date and time. The procedure consists of ordering the source data in the tabular format of the capture interface and selecting to copy and paste the data in the interface with the help of the paste button on the toolbar. The source data will automatically be tabulated in our table capture. Finally, we press the save button from the toolbar, and the data will be stored in the software database.

In the blocks interface, from the view of potentially toxic elements (PTE), we can convert units mg/kg to mg/m² for each of the records stored in the database. The procedure we must follow is to select any record from the PTE data table and press the conversions button on the toolbar.

The calculation of the indices. The procedure begins with the selection of the records that we want to consider to calculate the index. The selection can be made directly in the conversion table using the combination of the CTRL + A keys (select all the records) or CTRL + primary mouse click. (specific selection of records), on the selection, we press the secondary mouse button, and the displayed options select the index to calculate; it is necessary to remember that to obtain the pollutant load index and geo-accumulation index, it is essential first to calculate the factor of pollution.