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Original Research

Extraction and Mapping of Soil Factors Using Factor Analysis and Geostatistical Analysis on Intensively Manured Heterogenous Soils

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Abstract

To investigate both natural variability and anthropogenic inputs, a small lake catchment that collects water from slurry-irrigated (~300 $m^3 \cdot ha^{-1}$ annual application) natural meadows was explored. Analysis of the distribution of heavy metals suggests that concentrations of Ni, Zn, Pb, and Cu are closely associated with the geochemical signatures of soil parent material and, to a lesser extent, with soil organic matter. The data set of selected soil parameters was subjected to factor analysis (FA), which reduced the dataset into two major components (Factors 1 and 2) representing the different elemental sources. Geostatistical analysis showed interrelationships between heavy metal accumulations and soil genetic properties. Contour mapping of these variables identified the areas where anthropogenic processes are especially evident. Such visual information allowed spatial identification of the optimum number of 'tipping points' for soil monitoring.

Keywords: grassland, heavy metals, statistical analyses, contour maps

Introduction

Concerns about degradation of natural resources and the sustainability of agricultural production enhance the need for environmentally-oriented policy measures and monitoring programmes. Consequently, increasing demand from policy-makers and regulators in establishing the current status of the soil and monitoring changes require optimal sampling approaches and statistical procedures in order to collect maximum relevant reliable information with limited resources in a cost-efficient way. Ecosystem and land use studies often require specific sampling and statistical procedures, especially in heterogeneous landscapes under high anthropogenic pressure. Agricultural land used to utilize swine factory farm slurry is permanently under high, and usually rather uneven, loads of organic matter, as well as pollutants such as heavy metals. Livestock manures could be a major source of many metals where these materials are applied [1]. Cu and Zn are the most frequent metals in soils experiencing applications of pig slurry [2]. For soil organic carbon (SOC) inventories such complex soils need to be adequately categorized to represent soil heterogeneity, the different SOC pools, topsoil characteristics and SOC, and pool and flux data for deeper mineral-soil com-

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partments [3]. The same also applies to heavy metals. Currently, there are extensive databases on heavy metals, especially those listed in the Sewage Sludge Directive of the European Union (Council Directive 86/278 EEC).

Organic materials improve soil fertility, increase plant production and change heavy metal availability [4, 5]. Increased total metal concentrations are often partly reflected in soil solution. Certain edaphic properties relate in characteristic ways with dissolved organic carbon (DOC). DOC concentrations in soil solution typically decrease as soil depth increases [6]. Mobile Pb, Mn, and Cd concentrations have stronger correlations with SOC than with total soil metal concentrations, which might be explained by the fact that mobile metals have more direct inhibitory effects on micro-organism activity than total concentrations [7].

SOC chemical stabilization by adsorption is often considered of particular importance due to increasing evidence showing strong positive correlations between SOM and clay content, surface area, and metal oxide contents [8]. SOM adsorption varies considerably depending on the particle sizes of metal oxides. But the interpretation of SOM loading on oxides directly based on mass can be incorrect, because the same total mass with surface area of 1 nm diameter spheres is 200 times the surface area of 200 nm-diameter spheres [9, 10].

There is potential to study the spatial distribution of elements in the context of covariance with other elements [11]. On the European scale, factor analyses (FA) and cluster analyses (CA) revealed in topsoil one cluster with soil total organic carbon linked with chalcophilic elements, which are typical of pollution. The regions with the highest factor scores in soil samples are situated in central Europe, Great Britain, Ireland, southern Fennoscandia, and the Baltic States [12].

Rawlins et al. [13] analyzed five topsoil indicators in UK soils (total metal concentrations of copper, nickel, and zinc, plus soil pH, and SOC content) and found that each were significantly correlated with parent material, land use and region. At the landscape, catena or poly-pedon level, heavy metal accumulation and relations with SOM are rather complex due to various natural and anthropogenic drivers. Taking into account widely held, but largely untested, assumptions that physical habitat heterogeneity exerts control over ecosystem level processes [14], we can postulate that patterns of heavy metal accumulation connected with anthropogenic factors play important roles in areas under permanent pig manure loads. As suggested by Langhans et al. [15] for river-floodplain ecosystems, knowledge of natural variance should be integrated in future restoration approaches, which to date have often been site-specific and therefore do not consider the heterogeneous character of such systems.

The aim of this study is to determine the level of variability of SOC and relevant heavy metals in the topsoil of agricultural land under long-term applications of pig slurry and highlight statistical methods capable of analysing heterogeneity and visualizing contamination 'hot-spots.'

Experimental Procedures

Site description: The study site is located in the Middle Lithuanian lowlands, in the basin of the River Neris. The site is adjacent to the small Lapoja Lake (latitude 54º49'07"-54º49'31"N, longitude 24º46'33"-24º45'46"E, elevation 113-123 m above sea-level). This site was chosen because since 1978 the Lapoja Lake basin has collected water from a slurry-irrigated natural meadow and represents a small catena typical of the Lithuanian landscape (the Neris Lower Course Plateau). The area belongs to the Nemoral environmental zone with climatic conditions characterized by the vegetation growth season (≥10ºC) lasting on average 183-191 days per year, and +6.2ºC mean annual air temperature and 661 mm mean annual precipitation.

The dominant soil types are Luvisols, Podzols and Gleysols, with small spots of Histosols, developed on a suite of Pleistocene glacial, proglacial, and Holocene parent materials (Fig. 1). Soil pH ranges from 4.7-6.8, C/N ratio 4.5-12.4, soil available P_2O_5 27-700 mg·kg^{-1}, and K_2O varies between 79-793 mg·kg^{-1}. According to plant taxonomy, the largest part is comprised of ruderal and semi-ruderal plant communities and only negligible parts of plant communities are characterized as fertile meadows. Braun-Blanquet cover-abundance varies from 30-100%.

Average annual application of slurry is ~300 m^3·ha^{-1}. Slurry is sprayed on the land during several short cycles from April-August (with negligible quantities applied in

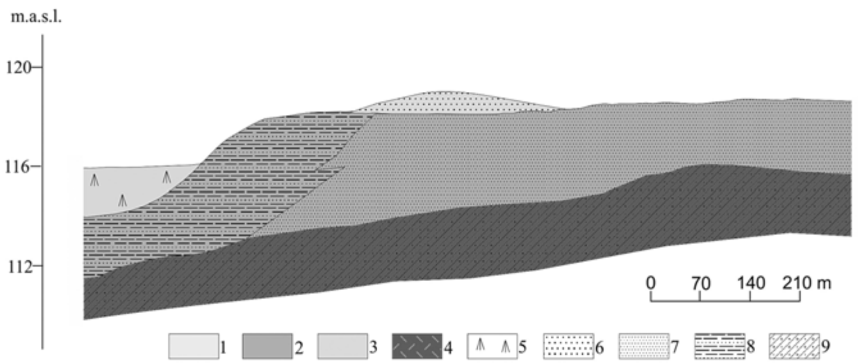

Fig. 1. Schematic cross-section of parent materials.
1 – biogenic sediments, 2 – limnoglacial sediments, 3 – fluvioglacial sediments, 4 – glacial sediments, 5 – peat, 6 – sand, 7 – fine sand, 8 – aleuritic clay, aleurits, and sands layers, 9 – morain loam, sandy loam.

June). Other anthropogenic activities are limited to mowing and grazing by cows. However, the land subjected to such management is rather limited and without a clear formal management plan.

Field Studies and Sampling

Nutrient-loading and pollution studies are most often performed in geographically-defined catchments. Therefore, the agricultural sector of Lapoja Lake basin was selected for studies and 33 soil sampling sites were chosen, based on summarized morphological site characteristics. A Garmin Ique3600 GPS unit was used to identify the location of each sampling point (WGS84). At each sampling site a composite soil sample of ~0.5 kg (using auger at 0-20 cm depth) was collected randomly from a 50-100 m^2 area.

Laboratory Analyses

All soil samples were air-dried and sieved to <2.0 mm (to analyze SOC) and <1.0 mm (to analyze heavy metals). Analyses of the soil samples were performed using the following methods: organic C by dry combustion; and total soil Al, Fe, Ca, Mg, Cu, Ni, Pb, and Zn by atomic emission spectrography (AES) in <1.0 mm material. A DFS-13 spectrograph was used for examining samples. The spectrum lines were deciphered using a DM-100 microdensitometer.

Datasets

Data of chemical analyses were stored in a dataset according to its geographical co-ordinates. Datasets contained concentrations of heavy metals reported to be present in the highest mean concentrations in Lithuanian pig manures (Cu, Ni, Pb, and Zn), elements important for pedogenic implications (Al, Fe, Ca, and Mg); and the main soil quality parameter (SOC). The derived parameters (Al+Fe: sorption pool and Ca+Mg: total alkalinity) were calculated from the primary measurements of these elements. Selection was based on the assumptions that soil sorption properties are reflected in Al and Fe concentrations, and Ca and Mg indicate the amount of carbonates in the soil matrix and influence soil fertility, erodibility and available water capacity.

Data Analysis

Descriptive statistics, factor analysis (FA), and geostatistical interpolation using Kriging methods were used to analyze the soil data. Descriptive statistics (mean, median, minimum, maximum, standard deviation, kurtosis, and skewness) were performed using routine methods [16]. In order to detect the relationship between the studied parameters, Pearson's correlation coefficients ($p<0.01$ and $p<0.05$) were calculated.

The factors were extracted using principal component analysis (PCA) and eigenvalues >1 were retained. To increase the interpretability of the results, the variance maximizing (Varimax) normalized factor rotation was applied. Maximum iterations for convergence was set to 25. FA was performed using Statistica 6.0 (StatSoft, Inc) for Windows.

Geostatistical interpolation was accomplished using Kriging methods with a linear variogram to show the spatial variation of variables and to produce contour maps. For geostatistical calculations and modelling of the datasets, 'Surfer 8' software was used.

Results

Descriptive Statistics

Results of descriptive statistical analysis demonstrated substantial variability in topsoil metal and SOC concentrations (Table 1). Variability of SOC, soil total Fe, Ca, Mg, Cu, Ni, and Pb was moderate and characterized by coefficients of variation (CV) from 25.5-57.7%. Only Al demonstrated low spatial variability in the soil, with CV 16.4%. (Value of CV <25% is classified as low variability, 25-75% moderate variability, and >75% high variability). It is probable that spatial variability of SOC and Al, Fe, Ca, and Mg concentrations mainly reflect pedological or site characteristics. However, it is probable that the long history of arable land use and especially slurry applications (which has lasted for several decades), will have strongly influenced accumulation processes and contributed to increased variability of heavy metal concentrations in topsoil.

Distribution patterns of the datasets were evaluated by assessing skewness and kurtosis. Skewness values show that the distribution of Cu, Al, and Al+Fe is particularly influenced by the higher values. The remaining parameters have skewness values >0 and their distribution is influenced more by lower values (Table 1). According to kurtosis values, most investigated parameters (Cu, Ni, Zn, Al, Ca, Fe, Al+Fe, Ca+Mg) have relatively high variability. Kurtosis values for Pb and Mg were >0 and showed lower variability. Higher kurtosis values for SOC suggests low variability. However, CV for SOC is high (57.7%) (Table 1).

Factor Analysis (FA)

FA was used to investigate interrelationship among tested parameters. FA is a technique that helps reduce multidimensional datasets to interpretable sizes [17, 18] by identifying factors that contain most of the variance of the associated variables [19].

Soil metals and SOC relationships were analyzed using a correlation matrix (CM) (Table 2). Strong correlations among the concentration of metals in the soil, especially among Cu, Ni, Pb, Zn, Ca, Fe, and Mg and, conversely, weak correlations among metals and SOC were found ($r=0.01-0.42$). Specifically, soil organic carbon seems to play some role in Cu ($r=0.42$) and Ca ($r=0.35$) mobility. The observation that SOM is a secondary variable affecting the spatial distribution of heavy metals contradicts numerous findings, especially that humic substances form geochemical barriers and are an active regulator of heavy metal mobility in ecosystems [20].

Table 1. Descriptive statistics of element concentrations in soil (mg·kg^{-1} or %), n=33 samples.

Parameter		Mean	Median	Minimum	Maximum	Std. Dev.	Skewness	Kurtosis	CV, %
Cu	mg·kg^{-1}	9.64	11.0	3.00	17.0	3.94	-0.162	-0.990	40.9
Ni		11.9	11.5	5.00	22.0	4.28	0.328	-0.269	36.0
Pb		10.5	10.0	6.60	18.0	2.68	0.788	0.419	25.5
Zn		34.3	33	10.0	64.0	12.9	0.157	-0.343	37.6
Al	%	3.83	3.80	2.40	4.80	0.628	-0.753	-0.044	16.4
Ca		0.571	0.580	0.210	1.10	0.239	0.464	-0.060	41.9
Fe		1.61	1.60	0.700	2.90	0.588	0.023	-0.685	36.5
Mg		0.157	0.160	0.020	0.350	0.0796	0.507	0.190	50.7
Al+Fe		5.44	5.60	3.10	7.10	0.993	-0.491	-0.400	18.3
Ca+Mg		0.728	0.720	0.260	1.44	0.305	0.324	-0.108	41.9
SOC		2.22	1.89	0.654	6.84	1.28	1.55	3.954	57.7

Table 2. Correlation matrix (CM) of elements analyzed in soil.

	SOC	Cu	Ni	Pb	Zn	Al	Ca	Fe	Mg	Al+Fe
Cu	0.42*									
Ni	0.18	0.63**								
Pb	0.29	0.68**	0.61**							
Zn	0.22	0.65**	0.87**	0.72**						
Al	0.01	0.30	0.72**	0.46**	0.61**					
Ca	0.35*	0.73**	0.76**	0.68**	0.71**	0.70**				
Fe	0.32	0.63**	0.71**	0.53**	0.65**	0.33	0.52**			
Mg	0.13	0.51**	0.90**	0.55**	0.80**	0.78**	0.77**	0.64**		
Al+Fe	0.19	0.56**	0.88**	0.61**	0.77**	0.83**	0.75**	0.80**	0.87**	
Ca+Mg	0.31	0.70**	0.83**	0.68**	0.77**	0.75**	0.99**	0.57**	0.87**	0.82**

*p<0.05; **p<0.01; n=33

Table 3. Component matrix of factor analysis with eigenvalues – two components extracted.

Components	Factor loading of each variable											Egenvalues
	SOC	Cu	Ni	Pb	Zn	Al	Ca	Fe	Mg	Al+Fe	Ca+Mg	
1	-0.073	0.457	**0.894**	**0.57**	**0.795**	**0.901**	**0.772**	**0.57**	**0.928**	**0.908**	**0.848**	7.39
2	**0.839**	**0.755**	0.292	**0.553**	0.391	-0.09	0.466	**0.527**	0.169	0.254	0.41	1.3

Extraction method: principal component analysis; bold characters are similar sources in factors.

To identify the statistical factors that capture most of the variance and explains the distribution of elements in the manure-treated soil, two factors (FAC1 and FAC2) were derived based on the eigenvalues >1 (Table 3). This shows that almost all variables load positively on the first component, except SOC. Furthermore, most variables load positively on the second component, except Al.

FA extracted two factors that explained ~79% of total variance. Factor 1 (FAC1) included seven variables, had an eigenvalue of 7.39 and accounted for 67.19% of variance. Factor 2 (FAC2) included one variable, had an eigenvalue of 1.30 and accounted for only 11.82% of variance. The remaining factors accounted for the remaining 20% of variance. Pictorial representation of results from cluster analysis (CA) is provided in Fig. 2.

The following general distribution patterns of soil elements were revealed by FA, which identified four factor groups. The first factor group is composed of SOC; the second of Cu, Pb and Fe; the third of Ca, Zn, Ca+Mg, Ni, Al+Fe and Mg, and the fourth Al.

Group 1: SOC content is high in soils receiving pig slurry. SOC is also the most dominant measured soil attribute [21].

Group 2: Cu and Pb are well-known pollutants in urban soils, their concentration in natural soil tends to be relatively low. Together with Fe these elements demonstrate similar features. An explanation could be that the co-precipitates of Cu and Pb with Fe oxides occur in contaminated soils [22].

Group 3: Ca, Zn, Ca+Mg, Ni, Al+Fe, and Mg; variability of these elements was less affected by slurry treatment than those of Groups 1 and 2. Ni and Zn are known to have an affinity in fixation from fertilizers [23] and are sorbed by the clay fraction (<2 μm) [24]. Marcato et al. [25] found that Ca and Mg are present on 3-25 μm slurry particles. This suggests that Group 3 describes elements that have strong sorption properties.

Group 4 consists of only Al, which occurs naturally in soil. Therefore, its distribution was less affected by soil treatment with slurry. Similar trends were exhibited by the lowest value of Al coefficient of variation (Table 1).

Geostatical Interpolation

Spatial variability assessment provides a valuable base against which subsequent and future measurements can be evaluated. Moreover, it has potential for more rapid and efficient detection of SOC differences, particularly in large areas of cultivated soil [26].

Variography and interpolation techniques have been applied to quantify the spatial variability of obtained Factor 1 and Factor 2. FAC1 and FAC2 were geostatistically interpolated using Kriging methods (point kriging type) with a linear semi-variogram model for prediction of spatially-dependent properties and visualization of the spatial variation of variables (Figs. 2 and 3). Calculated distances between data points were:

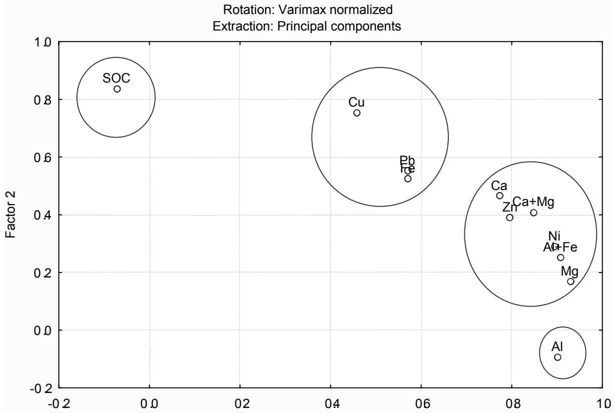

Fig. 2. Relation between FAC1 and FAC2.

NN mean distance = 49.7,
NN minimum distance = 18.3,
NN maximum distance = 99.9,
NN gamma Z = 0.31.

These distances can be used to determine new sampling locations and quantification where higher sampling density may be desired to improve map accuracy. The model for our experimental variogram appears to intersect the vertical axis at 0, so we did not apply a nugget effect (FAC1 slope = 0.00456, FAC2 slope = 0.004).

Figs. 3 and 4 show patterns of the two Factors, with FAC1 representing the most common variance in soil (67.19%) and FAC2 representing successively less variance (11.82%). The accuracy of FAC contour maps depends on complex variability of topsoil indicators: SOC and some mineral components (total soil Al, Fe, Ca, Mg, Cu, Ni, Pb, and Zn).

Visual inspection of these contour maps shows that FAC1 contours are spatially more dynamic than FAC2. The continuous high zones (black colour) and continuous low zones (white colour) are usually smaller for FAC2 contours than for FAC1. Such differences can have significant impacts on sample design, site characterization, and spatial prediction.

By changing the number of contours (i.e. by reducing or increasing the contour interval) we can observe the effect of sampling density used to derive contours. It is obvious that

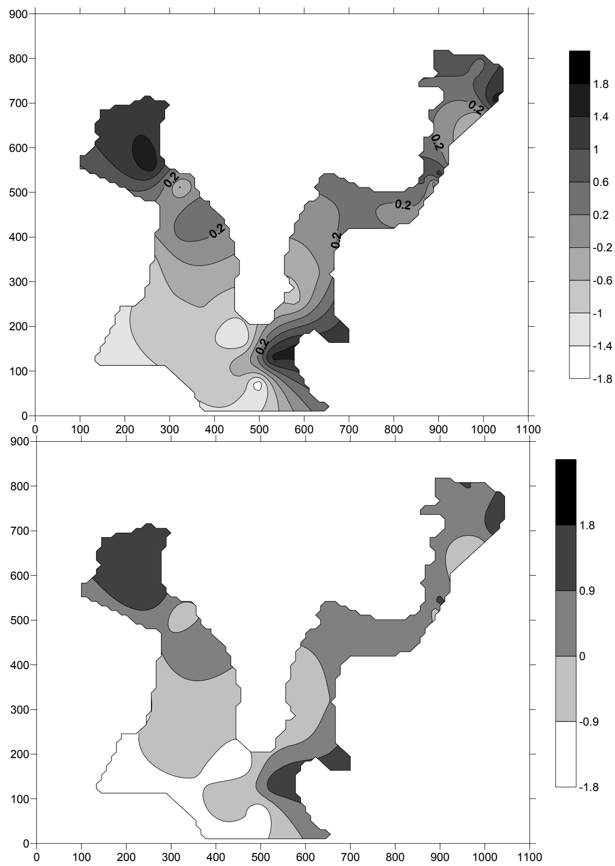

Fig. 3. Contour plot of FAC1* (10 and 5 contour intervals). FAC1*explaining 79% of total (SOC, Cu, Ni, Pb, Zn, Al, Ca, Fe, Mg, Al+Fe, Ca+Mg) variance.

reducing contours (from 10 to 5) for more rapid changing FAC1 (Fig. 3) leads to spot (x500; y50) disappearance. FAC2 continues to display similar patterns (Fig. 4).

A comparison between FAC1 and FAC2 contours shows that the number of intervals can be a critical source of identifying monitored area "tipping-points". However, the great variability of SOC distributions in soils, in conjunction with sparse sampling, can mask the spatial dependence if the number of intervals is reduced.

Discussion

Our study was on a grassland area, which forms part of a heterogeneous landscape with semi-natural pasture, forest and lakes as major components. Human-dominated environments and roads are several kilometres from the site, so that pig slurry can be treated as the only significant source of permanent pollution with heavy metals. Zn, Cu, Ni, and Pb were reported as heavy metals having the highest mean concentrations in Lithuanian pig manures [27]. However, in our study the mean topsoil concentrations of these metals showed moderate variability and were close to the background levels typical of regional soils. Although measured maximum concentrations of these elements substantially exceed background levels, they are well below maximum

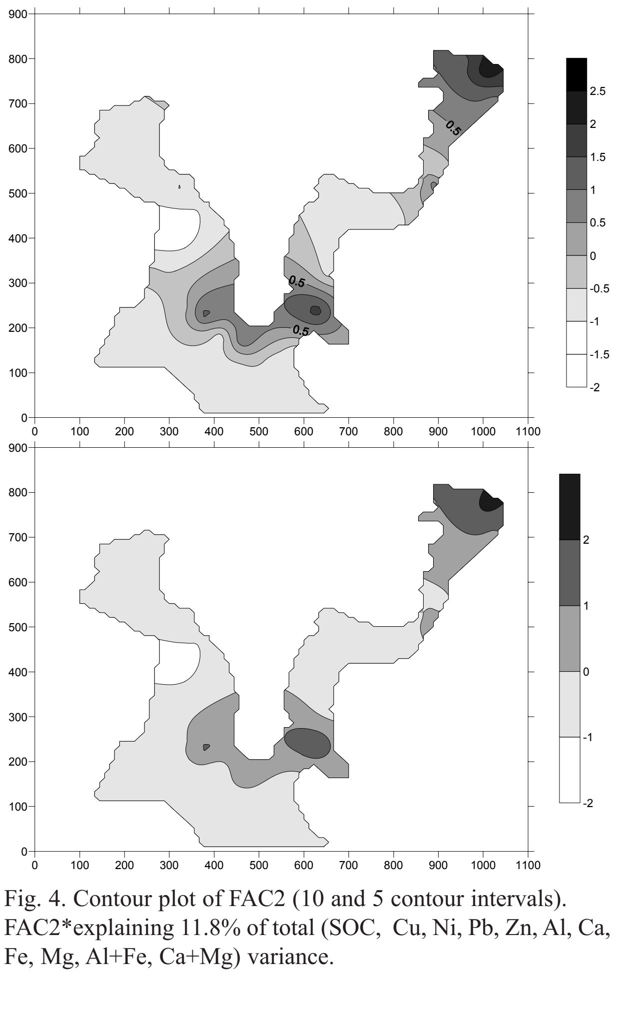

Fig. 4. Contour plot of FAC2 (10 and 5 contour intervals). FAC2*explaining 11.8% of total (SOC, Cu, Ni, Pb, Zn, Al, Ca, Fe, Mg, Al+Fe, Ca+Mg) variance.

permitted values for the soil defined by current Lithuanian legislation. As a result, we can assume that the study area is sufficiently homogeneous in terms of relevant heavy metal contents and the area can be monitored and managed as a uniform one. However, such an approach seems to be too straightforward if complexity and heterogeneity of landscape processes are considered. Due to inherent natural multi-scale space-time heterogeneity and anthropogenic factors, even small catena areas can be diverse and require specific monitoring and management targeted at risk spots, where processes of land degradation are obvious. In our study, to extract additional information on ecologically-relevant soil heterogeneity, we employed different statistical methods. Statistical assessment of heavy metal distribution suggests that concentrations of Ni, Zn, Pb, and Cu are probably more associated with soil parent material and, to a lesser extent, with SOC. Cluster analysis also suggests that the concentrations of Ni and Zn are more dependent on alkalinity (with significant positive correlations with Ca and Mg concentrations), and these findings accord with well-established patterns [28]. As in similar studies where different multivariate statistical methods were employed to identify sources of heavy metals in agricultural land [29, 30], the findings of our study provided relevant information regarding the variation of concentrations as well as indications of the major drivers of heavy metal accumulation in topsoil. However, such an approach in the case of heterogeneous terrain can mask a possible steady accumulation of heavy metals in limited plots, especially when such processes are rather uneven and slow. In order to highlight the effect of slurry application and to predict the input of heavy metals, more sophisticated studies are needed, especially those designed to estimate heavy metal mass balances and examine a complete slurry production chain, including heavy metal contents in feedstuff and additives.

Focusing monitoring efforts on the plots with the highest concentrations of anthropogenic metals seems to be expedient, even if the soil in these plots is not very polluted from the viewpoint of maximum permissible levels, and sources of pollution are not clearly proven. Polluted soil monitoring networks can provide vital information for sustainable management of soil resources. FA results in the form of readily-defined contour maps, which can be potentially powerful instruments in the hands of specialists working in pollution control. In our study, comparison of the FAC1 and FAC2 contours also showed that there is a critical source for targeting monitoring areas. Proper application and combination of various statistical methods could be a valuable approach for explaining the variability of soil data sets (SOC and soil macro-elements and heavy metals resulting from regular applications of slurries) and identifying compact and optimal number or areas of "tipping points" for soil monitoring.

Conclusions

This study revealed relatively moderate variations in heavy metals contents. However, zones of environmental concern were identified within the small lake basin. These zones were identified on the basis of topsoil indicators: SOC and some mineral components (total soil Al, Fe, Ca, Mg, Cu, Ni, Pb, and Zn) under long-term applications of pig slurry. Analysis of the distribution of heavy metals suggests that concentrations of Ni, Zn, Pb, and Cu are closely associated with the geochemical signatures of soil parent material and, to a lesser extent, with soil organic matter. Principal Component Analysis reduced the dataset into two major components (Factors 1 and 2) representing the different sources of the elements. Mapping these variables showed the areas where anthropogenic processes are evident to some degree. Combining statistical multivariate analyses with geostatistical interpolation, and especially contour maps, seems a useful tool for highlighting and visualizing areas of environmental concern in heterogenous terrain.

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