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EVALUATION OF EFFICIENCY SELECTED SECONDARY SAMPLING METHODS IN SOIL STUDIES

OCENA SKUTECZNOŚCI WYBRANYCH METOD OPRÓBKOWANIA WTÓRNEGO W BADANIACH GLEB

Abstract: The purpose of the work was to compare effectiveness of common secondary sampling methods for assessing the distribution of soil pollution. The study case is based on an example of assessing the spatial distribution of soil contamination with lead in Slawkow area (Upper Silesian Industrial Region). This comparison was made in regard to both precision of the spatial estimation and minimization the cost of measuring campaign. The special attention was given to the often applied secondary sampling designs such as threshold radial (also known as adaptive cluster sampling) and adaptive fill sampling. These two methods were tested in typical municipal and suburban environment in Slawkow area. The work contains also detailed statistical and geostatistical analysis of above-mentioned contamination, and elaboration of series of its spatial distributions using numerous alternative sampling designs. The determined sampling plans make it possible to find compromise between ecological and financial aspects. A combination of the obtained results with the legal regulations in force concerning concentrations of heavy metals in soils are the basis for reliably estimation the ecological hazard arising from the soil contamination with lead in the Slawkow area.

The results of performed analyses show that better efficiency in terms of cost and precision of measuring campaign gives rather coarser preliminary sampling design followed by appropriate secondary sampling then use the one-stage very dense measuring grid. However, the effectiveness of both threshold radial and adaptive fill secondary sampling designs is much worse than secondary sampling designs based on geostatistical methods using eg minimization of maximum or mean kriging variance criterion.

However, it was also found that the effectiveness of both threshold radial and adaptive fill secondary sampling designs is significantly worse than secondary sampling designs based on geostatistical methods. Therefore, when a larger environmental research is envisaged the collaboration with experienced geo-statisticians is always the right choice.

Keywords: secondary sampling designs, heavy metals, soils, ecological risk, geostatistics

The choice of appropriate sampling design is essential in different soil related surveys. This arises from the fact, that our knowledge on soil in their natural state is never fully known and collecting samples as well as laboratory analysis is expensive and time consuming, especially when investigations are performed on large areas. Secondary sampling is very important stage of many environmental studies, which can

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significantly improve the analysis by relatively low cost. Secondary sampling design can refine a model, get a deeper insight into studied phenomenon, clarify situation and thus make right decision.

The goal of the work was a case-study based evaluation of effectiveness of commonly used secondary spatial sampling designs such as threshold radial design (also known as adaptive cluster sampling) and adaptive fill design for delineation of the extent of the area polluted with heavy metals.

Site description and data collection

Study area was located in Slawkow city and its vicinity (Upper Silesian Industrial Region). The studies were performed using soil samples from the archives of the Polish Geological Institute [1, 2]). The whole measuring campaign led to the collection of 2672 soil samples and 330 samples of water sediments. All samples were collected on the basis of a very dense grid pattern. The sampling points were placed in an regular way and the average distance between the neighbouring points was almost constant reaching about 250 [m]. The aim of the analysis was to determine the concentrations of Ag, Al, As, Ba, C_{org}, Ca, Cd, Co, Cr, Cu, Fe, Hg, Mg, Mn, Ni, P, Pb, S, Sr, Ti, V and Zn, as well as pH. (For our analysis only 1393 Pb samples were used.) These measurements resulted in the preparation of "Detailed Geochemical Map of Upper Silesia in the scale 1:25 000, a promotional sheet Slawkow". Soil samples weighing about 0.5 kg were collected with a penetrometer of 8 cm in diameter, at a depth of 0.0 to 0.2 cm. The samples were dried at room temperature and then sieved through a 1 [mm] sieve. Finally, analytical samples weighing (100 g) were obtained by quartering, and then concentrations were determined analytically. Lead concentrations in samples collected from the Slawkow area were determined by the ICP-AES method, using a Philips 8060 emission spectrometer with plasma excitation. The details of measurements campaign as well as of analytical methods are given in [1, 2].

All values of lead concentrations in soils were expressed in [mg/kg]. A detailed map of sample point locations was shown in Fig. 1.

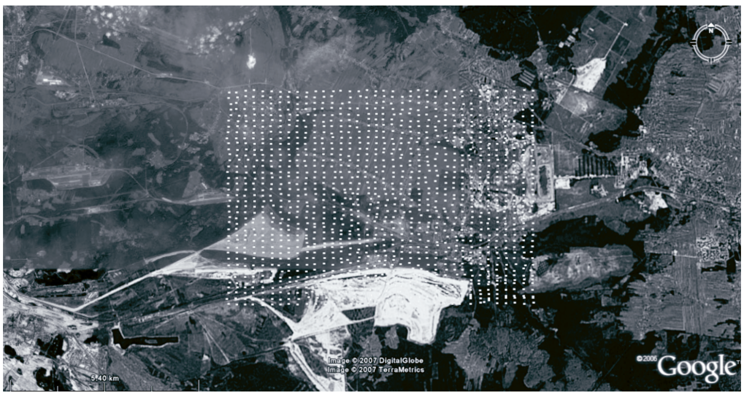

Fig. 1. Satellite view of Slawkow with sample point locations (exhaustive data set)

A satellite view of study area with sample point locations (exhaustive data set) were shown in Fig. 1, and the map of this area is given in Fig. 2.

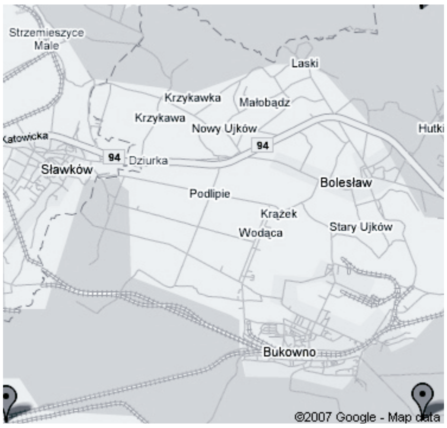

Fig. 2. Detailed map of study area

Secondary sampling strategies and geostatistical methods

In order to limit the time consuming analyses we focused in our work on two commonly used secondary sample designs [3, 4]:

1) Threshold Radial (TR) Secondary Sample Designs (also known as Adaptive Cluster Sampling) which is a straightforward secondary sample design that places samples in a radial pattern around existing data points that exceed a decision threshold. Threshold radial can be useful in situations where one have a lot of very low or undetected samples and one or two very high measurements.

2) Adaptive Fill (AF) Secondary Sample Designs. In this case, samples are placed in the largest spatial gaps among data points. Unlike Threshold Radial, this design gives no regard to the measured values, only their relative positions.

A set of new sample candidates is defined by a grid (much like a spatial model) that overlays the data points and acknowledges site boundaries, polygons, and whether layers are active or not. From this set of *N* candidates the first winning location is simply that value which has the maximum distance to its closest neighbor. The design searches for the second location among the remaining candidates by comparing with the $N + 1$ locations. If there are ties among the two locations, then the tie breaker method is used. The process repeats until one of the following becomes true:

– the total number of samples has been located,
– there are no remaining candidates,
– no remaining candidate satisfies the minimum distance constraint.

To study soil contamination with lead, it was necessary to obtain the spatial distribution of lead concentrations in soils, as well as the spatial distribution of estimation errors. This was done using geostatistical methods. The ordinary kriging was selected as the most appropriate technique for our analysis. Ordinary kriging is the most effective linear estimator as it assumes that the average value of the estimation error equals zero, and thus minimises the variance of the estimation error [5–11].

The series of spatial distribution of lead concentrations in soils were produced. In the first step preliminary coarse sampling designs (systematic or random) were chosen from the very dense exhaustive data set shown in the Fig. 1. These designs were treated as pre-information for subsequent sampling. Then above-described spatial distributions were created by careful variogram modeling and kriging technique. At this stage all modeled spatial distributions of lead concentrations in soils were validated using cross-validation methods [12]. Each of the data points was individually removed from the data set, and after that, its value was modeled and subsequently compared with the measured one. Next, the scatter plots of estimated values versus the measured ones were calculated. Using these scatter plots several estimation errors were carefully calculated. Furthermore, modeled spatial distributions were validated using true values taken from exhaustive data set.

Another important feature of sampling design is always the total cost of measuring campaign calculated on the basis of the cost of single measurement. By comparing the quality of the spatial distribution with the total cost of measurements it was possible to evaluate the efficiency of the sampling grid under investigation. Then, it was decided what type of secondary sample design should be applied, and how many additional measurements should be used. This allowed for significant reduction of uncertainty by relatively low cost. Then all above-described analyses were repeated once or twice. For clarity multistage sampling process was abbreviated. For instance, the abbreviation "200 (S) + 200 (TR)" means, that preliminary sample of 200 nodes grid was systematic (S), and furthermore 200 additional points were added using threshold radial sampling (TR) technique. Analogously, the abbreviation "100 (R) + 100 (AF)" means, that preliminary sample of 100 nodes grid was simple random (R), and furthermore 100 additional points were added using adaptive fill sampling (AF) technique.

Analyses were performed using Arc Gis software (namely, FIELDS, Geostatistical Analyst and Spatial Analyst components) [13].

Results and discussion

Below, in Figs. 4–7 exemplary sampling designs are presented (eg systematic and random preliminary sampling design followed by threshold radial and adaptive fill secondary samplings) with the appropriate spatial distributions of lead contamination. The scale used in all figures is given in Fig. 3.

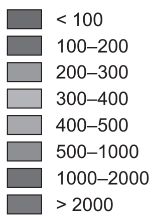

Fig. 3. The scale used in Fig. 4–7 to describe spatial distribution of lead contamination. The lead concentrations are expressed [mg/kg]

(a) (b) (c) (d) (e) (f) (g) (h)

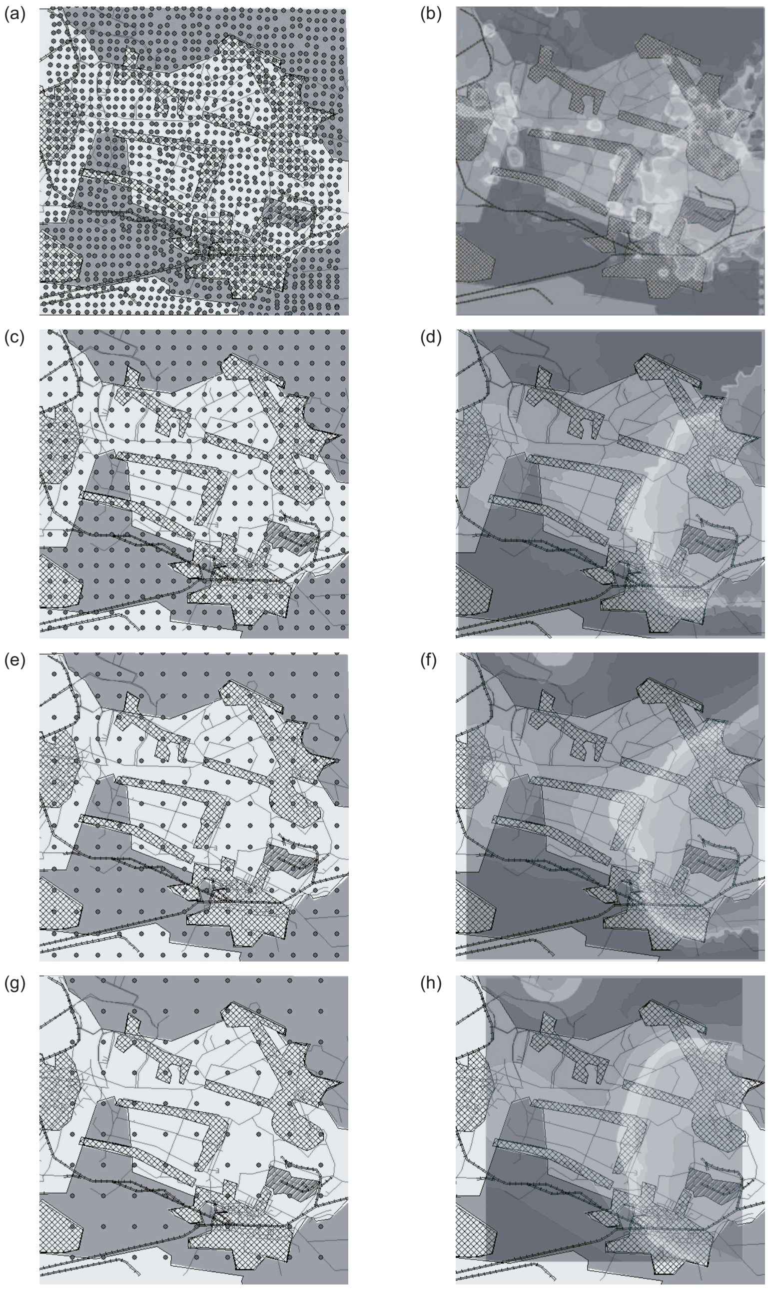

Fig. 4. Systematic sampling designs with decreasing number of observations (left) and appropriate spatial distribution of lead contamination (right): (a), (b) – 1393 measurement points (excessive dataset); (c), (d) – 400 (S) measurement points; (e), (f) – 200 (S) measurement points; (g), (h) – 100 (S) measurement points; (a) show excessive dataset; (c), (d), (e). (f), (g) and (h) shows preliminary sampling designs

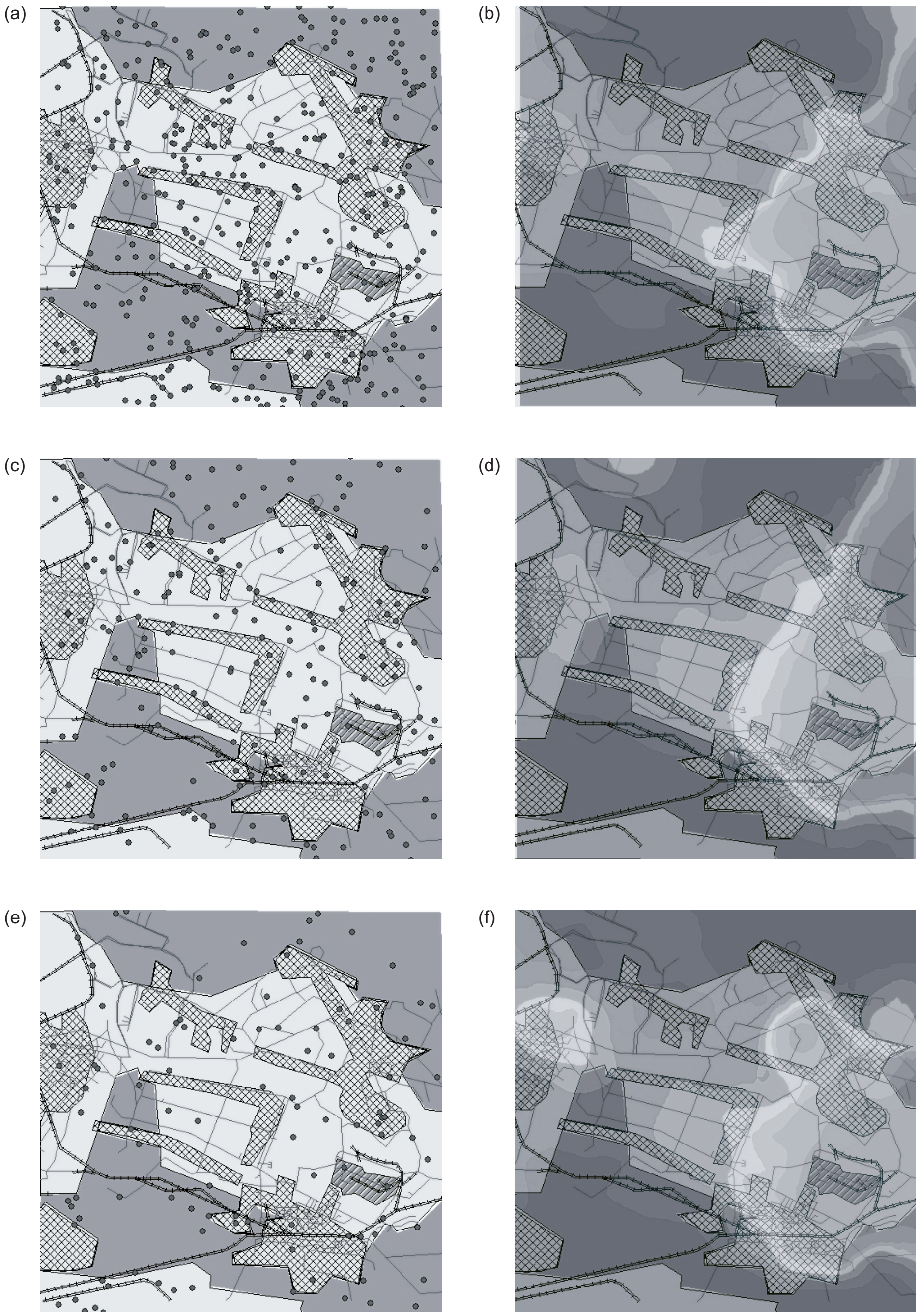

Fig. 5. Preliminary, simple random sampling designs with decreasing number of observations (left) and appropriate spatial distribution of lead contamination (right): (a), (b) – 400 (R) measurement points; (c), (d) – 200 (R) measurement points; (e), (f) – 100 (R) measurement points

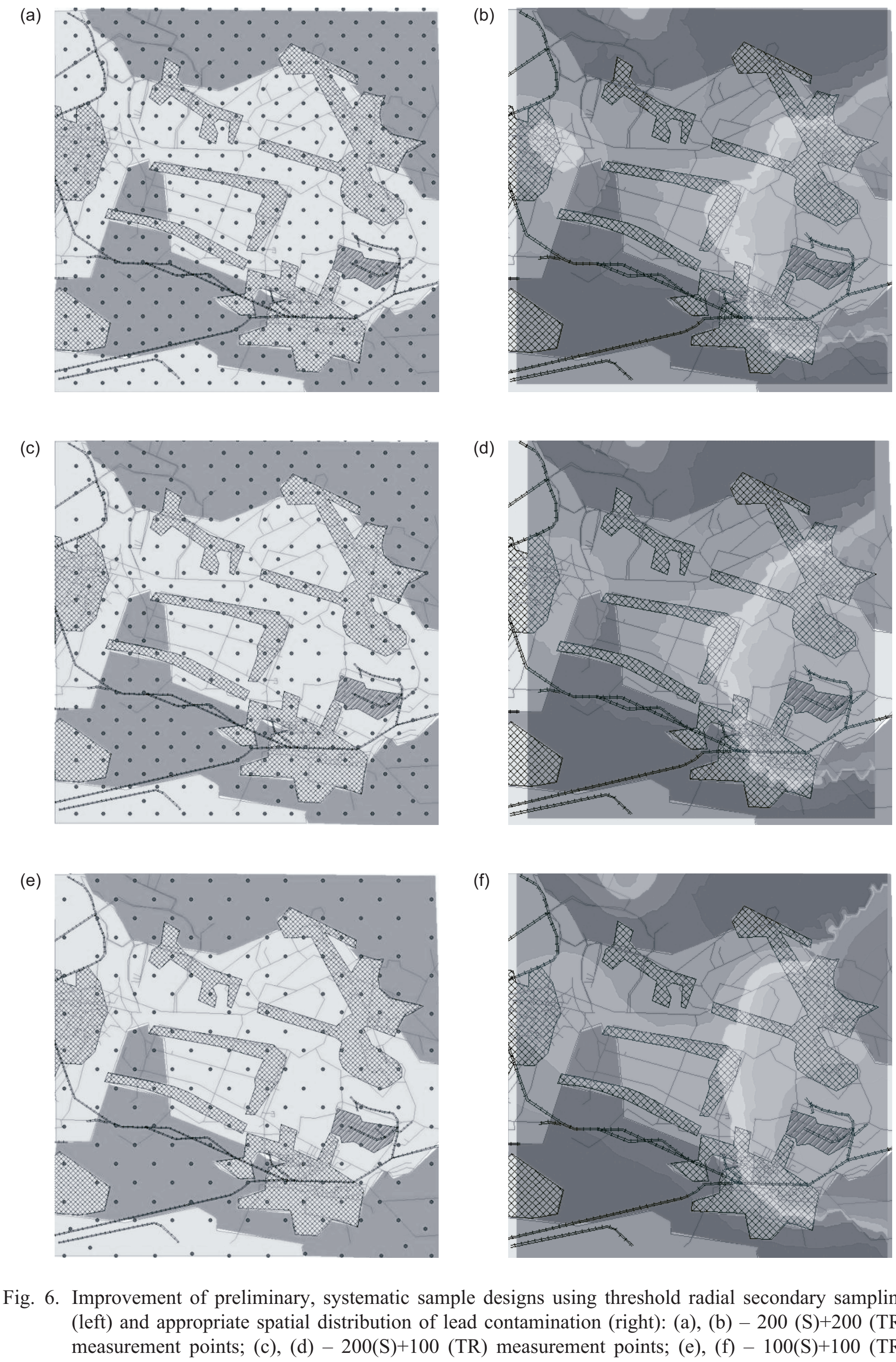

Fig. 6. Improvement of preliminary, systematic sample designs using threshold radial secondary sampling (left) and appropriate spatial distribution of lead contamination (right): (a), (b) – 200 (S)+200 (TR) measurement points; (c), (d) – 200(S)+100 (TR) measurement points; (e), (f) – 100(S)+100 (TR) measurement points

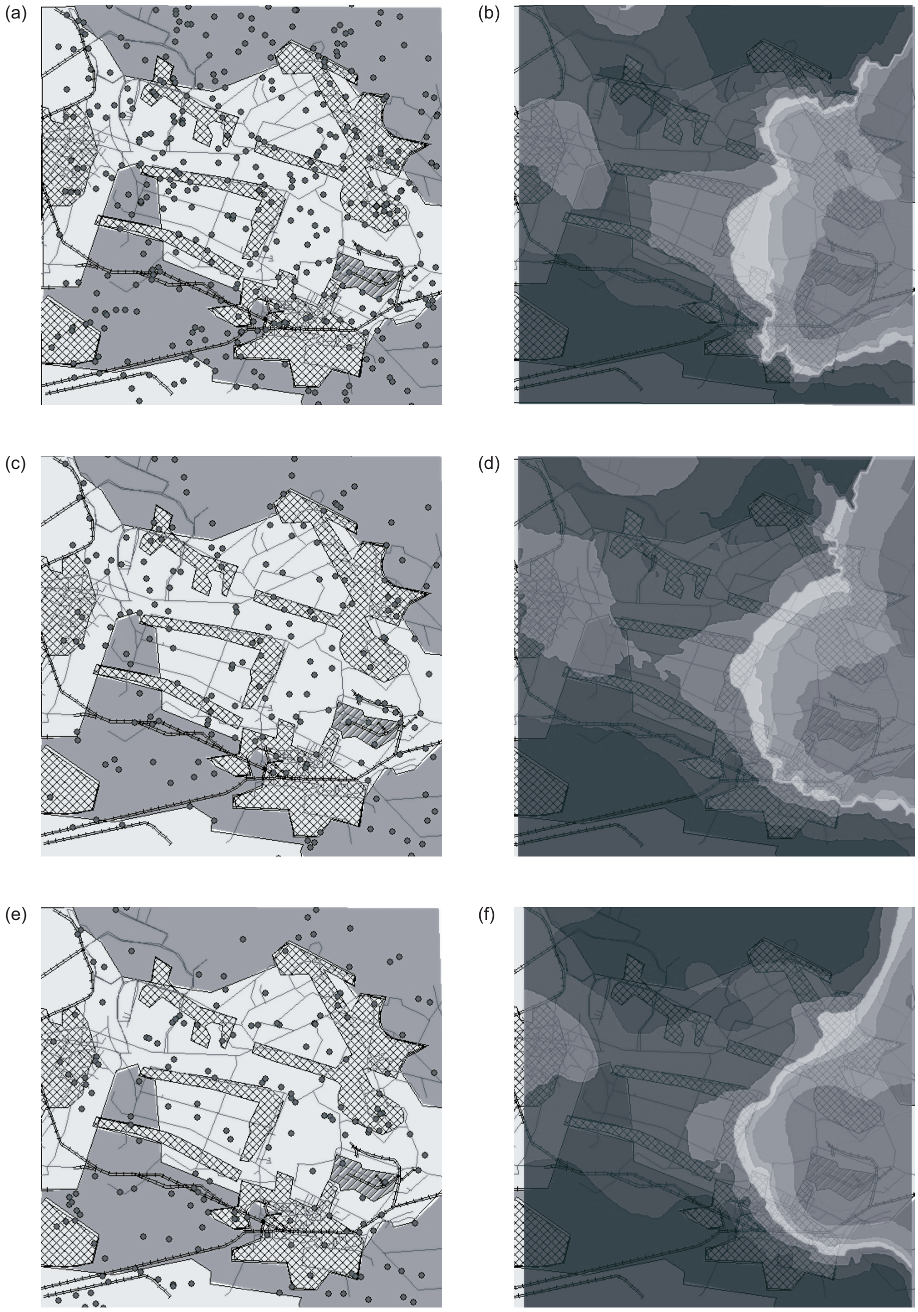

Fig. 7. Improvement of preliminary, systematic sample designs using adaptive fill secondary sampling (left) and appropriate spatial distribution of lead contamination (right): (a), (b) – 200 (R)+200 (AF) measurement points; (c), (d) – 200 (R)+100 (AF) measurement points; (e), (f) – 100 (R)+100 (AF) measurement points

Table 1

The exemplary cross-validation summaries for sampling designs obtained using adaptive fill method

Stage I – Preliminary sampling: Systematic (S) or Simple Random (R)								
Sampling design / Error	100 (S)	200 (S)		400 (S)	100 (R)	200 (R)		400 (R)
Mean prediction error	0.841	1.570		1.657	–6.760	–5.101		1.013
Root-mean square prediction error	470	756		1477	553	784		648
Average kriging prediction error	449	796		1420	524	659		678
Mean standarized prediction error	0.00172	0.00156		0.00116	–0.00728	–0.00756		0.00139
Root mean square standardized prediction error	1.033	0.953		1.041	0.972	1.150		0.934
Stage II – Adaptive Fill								
Sampling design / Error	100 (S) + 100	200 (S) + 100	200 (S) + 200		100 (R) + 100	200 (R) + 100	200 (R) + 200	
Mean prediction error	–2.684	3.155	3.813		1.126	–3.842	–1.430	
Root-mean square prediction error	1252	792	699		462	677	1208	
Average kriging prediction error	1037	868	766		486	608	1216	
Mean standarized prediction error	–0.00112	0.00339	0.00486		0.00289	–0.00515	–0.00118	
Root mean square standardized prediction error	1.179	0.917	0.916		0.940	1.086	0.995	
Stage III – Adaptive Fill								
Sampling design / Error	100 (S) + 100 + 100	200 (S) + 100 + 100			100 (R) + 100 + 100	200 (R) + 100 + 100		
Mean prediction error	0.781	3.813			–0.130	–1.430		
Root-mean square prediction error	1957	699			520	1208		
Average kriging prediction error	2037	766			537	1216		
Mean standarized prediction error	0.00029	0.00486			–0.00020	–0.00118		
Root mean square standardized prediction error	0.964	0.916			0.966	0.996		

Table 2

The exemplary cross-validation summaries for sampling designs obtained using threshold radial method

Stage I – Preliminary sampling: Systematic (S) or Simple Random (R)								
Error \ Sampling design	100 (S)	200 (S)		400 (S)	100 (R)	200 (R)		400 (R)
Mean prediction error	0.841	1.570		1.657	–6.760	–5.101		1.013
Root-mean square prediction error	470	756		1477	553	784		648
Average kriging prediction error	449	796		1420	524	659		678
Mean standarized prediction error	0.00172	0.00156		0.00116	–0.00728	–0.00756		0.00139
Root mean square standardized prediction error	1.033	0.953		1.041	0.972	1.150		0.934
Stage II – Threshold Radial								
Error \ Sampling design	100 (S) + 100	200 (S) + 100	200 (S) + 200		100 (R) + 100	200 (R) + 100	200 (R) + 200	
Mean prediction error	3.505	16.45	–4.728		2.65	–8.074	–2.469	
Average kriging prediction error	1388	2765	815.8		465	927	832.4	
Average kriging prediction error	1355	2671	798.4		501	930	744.9	
Mean standarized prediction error	0.00192	0.00738	–0.00504		0.00113	–0.00821	–0.0040	
Root mean square standardized prediction error	1.026	1.254	1.013		0.893	0.988	1.11	
Stage III – Threshold Radial								
Error \ Sampling design	100 (S) + 100 + 100	200 (S) + 100 + 100			100 (R) + 100 + 100	200 (R) + 100 + 100		
Mean prediction error	0.241	17.42			–0.118	–10.44		
Root-mean square prediction error	410	2931			456.2	1461		
Average kriging prediction error	413	2572			470.1	1716		
Mean standarized prediction error	0.00078	0.00522			0.00010	–0.00646		

Tables 1 and 2 show the cross-validation errors for exemplary sampling designs obtained using adaptive fill method and using threshold radial method, respectively. At first glance, the above-shown results seem to be rather ambiguous. However, detailed analysis of estimation errors for numerous multistages sampling designs proved that better results in terms of cost and precision give very often coarser preliminary sampling designs followed by appropriate chosen secondary sampling than use of the onestage very dense measuring grid. This result arises from the fact that although mostly used dense regular sampling grids, are relatively precise, but in the same time they are very costly. (Preliminary random sampling designs give unbiased results, but in general, are less precise than systematic sampling designs.) Multistage sampling allows for treating the intermediate results as the preinformation for subsequent sampling. This make it possible to better control and tune the whole sampling process according to circumstances occurring during sampling campaign.

However, we also observed that the effectiveness of both threshold radial and adaptive fill secondary sampling designs is much worse than secondary sampling designs based on geostatistical methods. These advanced methods are very flexible and use many different criteria eg minimization of maximum, or mean kriging variance [14]. The geostatistical methods take precisely into account spatial correlations that are present in spatial distributions under study. The threshold radial and adaptive fill secondary sampling designs are still derived from classical sampling theory and do not use effectively whole information present in data sets.

But these sampling designs are much simpler, and therefore easier to use. The choice of multistage sampling strategy depends on the qualifications and the experience of surveyors. Nevertheless, according to our many-years experience, we would strongly recommend use of geostatistical multistage procedures than improved sampling procedures derived from classical sampling theory. When a larger environmental research is envisaged the collaboration with experienced geostatisticians is always the right decision.

Conclusions

The choice of proper sampling design is crucial in different soil studies and in many cases even more important than high accuracy of laboratory chemical analyses. Secondary sampling is significant stage of many environmental studies, which can significantly improve the analysis by relatively low cost. This is especially important in complicated urban and suburban environment.

In this work the focus was given on secondary sampling designs such as threshold radial and adaptive fill sampling. The results of systematic analyses show that better efficiency in terms of cost and precision of measuring campaign gives coarser preliminary sampling design followed by appropriate secondary sampling then use the one-stage dense measuring grid.

The effectiveness of both threshold radial and adaptive fill secondary sampling designs can be worse than sophisticated secondary sampling designs based on geostatistical methods that make effective use of spatial correlations among measurement points. On the other hand, the secondary sampling methods considered here are often much simpler to perform and always easier to use for analyzes than geostatistical methods and therefore they are reasonable alternative for them.

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OCENA SKUTECZNOŚCI WYBRANYCH METOD OPRÓBKOWANIA WTÓRNEGO W BADANIACH GLEB

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Abstrakt: Celem pracy było porównanie efektywności wybranych metod opróbkowania dodatkowego, wykonywanego w celu wyznaczenia rozkładu zanieczyszczenia gleby. Studium przypadku zostało oparte na przykładzie wyznaczania rozkładu przestrzennego zanieczyszczenia gleby ołowiem w okolicach Sławkowa (Górnośląski Okręg Przemysłowy). Głównymi kryteriami efektywności metod opróbowania dodatkowego były oceny dokładności rozkładu przestrzennego oraz koszty kampanii pomiarowej. Szczególną uwagę zwrócono na często stosowane opróbkowanie dodatkowe metodami uzupełniania promieniowego (zwanego również adaptacyjnym opróbkowaniem klastrowym) oraz wypełniania adaptacyjnego. Te dwie metody były przetestowane w typowym miejskim i podmiejskim środowisku, na terenie i w okolicach Sławkowa. Praca zawiera również statystyczną i geostatystyczną analizę omawianego zanieczyszczenia gleby, określenie jego

ciągłości przestrzennej, jak również wyznaczenie serii rozkładów przestrzennych zanieczyszczenia gleby ołowiem przy wykorzystaniu wyżej wymienionych metod opróbkowania dodatkowego.

Wyznaczone sieci pomiarowe pozwoliły na znalezienie kompromisu pomiędzy aspektem ekologicznym i finansowym. Rezultaty analizy statystycznej i geostatystycznej wraz z obowiązującymi uregulowaniami prawnymi dotyczącymi zawartości metali ciężkich w glebie są podstawą do rzetelnego określenia potencjalnego ryzyka ekologicznego wynikającego z zanieczyszczenia gleb ołowiem w okolicach Sławkowa.

Rezultaty wykonanych analiz pokazują, że lepszą skuteczność określaną kosztem i precyzją kampanii pomiarowej daje najczęściej rzadsze opróbkowanie wstępne uzupełnione odpowiednim opróbkowaniem dodatkowym, niż jednoetapowa kampania pomiarowa z gęstą siecią pomiarową.

Jednakże zarówno metoda uzupełniania promieniowego oraz wypełniania adaptacyjnego są mniej precyzyjne niż wieloetapowe procedury opróbkowania wykorzystujące zaawansowane metody geostatystyczne. Metody te znacznie lepiej wykorzystują informację o korelacjach przestrzennych zawartą w zbiorach danych. Pomimo większej złożoności tych metod autorzy zalecają ich stosowanie lub współpracę ze specjalistami z zakresu statystyki i geostatystyki środowiska w sytuacjach, gdy planowane są znaczące badania środowiska naturalnego.

Słowa kluczowe: opróbkowanie dodatkowe, metale ciężkie, ryzyko ekologiczne, geostatystyka