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PROBABILITY MAPPING OF CONTAMINANTS

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ABSTRACT

Exhaustive characterization of a contaminated site is a physical and practical impossibility. Descriptions of the nature, extent, and level of contamination, as well as decisions regarding proposed remediation activities, must be made in a state of uncertainty based upon limited physical sampling. The probability mapping approach illustrated in this paper appears to offer site operators a reasonable, quantitative methodology for many environmental remediation decisions and allows evaluation of the risk associated with those decisions. For example, output from this approach can be used in quantitative, cost-based decision models for evaluating possible site characterization and/or remediation plans, resulting in selection of the risk-adjusted, least-cost alternative. The methodology is completely general, and the techniques are applicable to a wide variety of environmental restoration projects.

The probability-mapping approach is illustrated by application to a contaminated site at the former DOE Feed Materials Production Center near Fernald, Ohio. Soil geochemical data, collected as part of the Uranium-in-Soils Integrated Demonstration Project, have been used to construct a number of geostatistical simulations of potential contamination for parcels approximately the size of a selective remediation unit (the 3-m width of a bulldozer blade). Each such simulation accurately reflects the actual measured sample values, and reproduces the univariate statistics and spatial character of the extant data. Post-processing of a large number of these equally likely, statistically similar images produces maps directly showing the probability of exceeding specified levels of contamination (potential clean-up or personnel-hazard thresholds).

INTRODUCTION

Cost-effective remediation of a contaminated site is partially dependent upon the accuracy of site characterization. Without a reasonable understanding of where contaminants are located and where they are not, the only remediation alternatives available are to treat the entire region or to incur what may be an unacceptably high risk of failing to meet regulatory requirements, followed by consequent fines and other penalties. An understanding of the location, magnitude, and spatial variability of contamination may also be important in designing an effective remediation program and in developing appropriate personnel-protective measures.

However, complete characterization of a contaminated site is never possible. Inevitably, descriptions of the nature, extent, and level of contamination are incomplete, and decisions regarding what areas to clean up and what technology to use must be made in a state of uncertainty, based upon limited physical sampling. Because sampling and the resulting factual knowledge are limited, it is important not only to make use of the information contained in the actual data values themselves, but also to extract significant other information that is contained in the spatial relationships between and among the individual sample values. Geostatistical simulation is a relatively new technique that can provide powerful tools for investigating contaminant levels, and in particular, for identifying and using the spatial interrelationships among a set of isolated sample values. This additional information can then be used to assess the likelihood of encountering contamination at unsampled regions within a site. A quantitative assessment of this risk can then be used to allocate resources between additional site characterization work and the restoration of areas identified as "likely" to be contaminated. The objective is to achieve the minimum cost combination of site characterization and site remediation for a given level of risk.

THE FERNALD SITE

Past operation of the DOE Feed Materials Production Center near Fernald, Ohio, has resulted in extensive contamination of surficial soils by natural uranium. Soil geochemistry and other non-invasive techniques are being used to characterize the nature and extent of the surficial contamination as part of the Uranium-in-Soils Integrated Demonstration Project. (1)

Numerous individual areas within the Fernald site have been identified as contaminated, and these form the focus of an on-going restoration effort. In this paper, we have evaluated the spatial correlation patterns and uranium concentration levels existing at a site referred to as the drum baling area using only the soil geochemical data. We have then produced a set of geostatistical simulations (stochastic images) that are *equally likely and indistinguishable from one another* based upon what is currently known about the site. Any one of these simulations could represent the actual distribution of uranium contamination in the drum baling area. However because of their individual and collective similarity to the sample data, there is little basis for choosing among the set of alternative, replicate images. Yet it is within this uncertain context that the site manager will need to designate certain regions to be excavated and treated while other areas will be left as-is. To assist in this decision (on a preliminary basis), we have produced maps showing the expected uranium values and the probability of exceeding several different levels of contamination for individual 3 m-square parcels that may represent the smallest individually treatable region (a selective remediation unit).

Data

Standard soil-geochemical data (2) have been collected systematically at approximately 15-m intervals along a partial grid covering the drum baling area [Figure 1(a). As summarized in statistics associated with the histogram [Figure 1(b)], the samples are typical of those obtained in many geochemical sampling programs. The data reflect contamination levels from near background to several thousand picoCuries per gram of soil (pCi/g). Additionally, they appear somewhat log-normally distributed, with many low and a few extremely high values. However, as will be discussed below, univariate normal populations need not exhibit normal (Gaussian) multivariate spatial behavior.

Geostatistical techniques provide a method for extracting additional information from the interrelationships of the scattered data by providing a quantitative description of how a property of interest varies in space. This description, or spatial continuity model, is typically derived by computing what is known as a variogram (3, 4) from the sample values and their location coordinates. Variograms can be thought of as plots of the variance for all pairs of samples separated by a given distance, plotted as a function of that separation distance.

Sample variograms have been constructed using the soil geochemistry data from the drum baling area. Two versions of the sample variogram are shown in Figure 2. Figure 2(a) is the classical variogram computed using the actual sample values (in pCi/g). Although the figure is somewhat noisy, due in part to the small sample size, there is a definite suggestion that the variogram value increases with increasing separation between samples. At large separation distances greater than about 45-60 m (150-200 ft.),the variogram appears to oscillate somewhat erratically about the overall population variance. This distance represents the range of spatial correlation. More revealing is the indicator variogram plot shown as Figure 2(b), which uses a transformed variable (6) that emphasizes whether the sample value is above or below a particular cut-off level (here corresponding to the three quartiles of the data [from Figure 1(b)]. This transformation technique is useful with some data precisely because of its emphasis on values of similar magnitude. In effect, the question being asked is do low uranium concentrations tend to cluster together and over what distance? median values? high values? It is possible to analyze data sets using indicator transformations in which high values are correlated differently in space than low values, (5) potentially a very powerful technique in dealing with materials for which the elevated values (i.e., contaminants) were deposited by a very different physical process than the (natural) background levels. In Figure 2(b), the erratic behavior of Figure 2(a) is somewhat reduced, and there is generally a more coherent increase in the variogram value with increasing separation. The lack of symmetry between the variograms for the first and third quartiles, contrary to that expected by theory, (6) indicates that the spatial behavior of these data is not strictly as predicted by multivariate Gaussian theory (the indicator variograms for the first and third quartiles should be approximately identical and with a lower sill than that of the median). The small sample size, however, may explain some of this discrepancy, and we have assumed that Gaussian modeling techniques are adequate for the task at hand. Similar simulation methods that do not depend upon assumptions of multivariate Gaussian spatial behavior are available for use in instances of more severe non-normality. (5, 7)

The heavy solid curve in Figure 2(b) represents an isotropic, spherical variogram model (4) fitted to the sample data with a range of 55 m (180 ft.), or approximately three times the nominal sample spacing. It is this theoretical functional relationship that captures the interpreted spatial continuity patterns at the drum baling area and which is used in further modeling of uranium contamination at unsampled locations.

Simulations

A sequential, Gaussian stochastic simulation technique (7) has been used to generate 100 alternative models of the site compatible with the original soil-geochemical data. Three of these stochastic realizations are shown in Figure 3. Each realization reproduces (by construction) the original 63 conditioning data at the original sample locations. In addition, the stochastic models are essentially indistinguishable statistically from the original data. Figure 4 presents validation statistics for the simulation shown on the left in Figure 3. The histogram [Figure 4(a)] appears quite similar to the histogram presented in Figure 1(b), and the descriptive statistics are virtually identical, given that there are only 63 sample data yet 3,600 simulated values. In a similar fashion, the spatial statistics captured by the indicator variograms of Figures 2(b) and 4(b) are similar. The sample variogram is much noisier, given the small sample size, but the reproduction of the inferred spatial model (heavy line) is excellent. It is important to note that even the slightly non-Gaussian spatial behavior of the data is reproduced in the simulation, even though the variogram model provided as input to the simulation implied a purely Gaussian spatial model. These simulation techniques are sufficiently robust that many deficiencies in the model of spatial continuity can be overcome by adequate conditioning data.

Similar statistical comparisons may be obtained by evaluating any of the alternative stochastic models of the site. Because the alternative images are indistinguishable based upon any factual knowledge (data values, statistical character including spatial continuity patterns) and because the only identifiable difference between them is the initial random number seed used to begin the simulation, we may conclude that all 100 realizations are equally likely models of the unknown true contamination pattern.

The set of simulations may be summarized in a manner similar to more conventional geostatistical estimation, or kriging, to present a map of the expected uranium concentrations at any particular location (Figure 5). Although this method of modeling spatially distributed data is more widely known, there are some limitations to the technique. For example, because kriging and the computational method used to produce the expected value map are essentially smoothing, or averaging algorithms, the statistical properties of the model may differ substantially from those of the data themselves. For example, the histogram [Figure 5(b)] is substantially different in shape from that of the data [Figure 1(b)] or the simulation (Figure 4). Specifically, the quasi-log-normal appearance is not present in Figure 5(b). Although the variogram of Figure 5(c) is not a particularly bad reproduction of the sample data, the probable non-Gaussian distortion of the one quartile is particularly accentuated through the averaging process. The distortion is especially noticeable for the first quartile values: the lower values (light pixels) are much more continuous spatially in the expected value model than in the simulations (Figure 3). Also, the highest contaminant values are higher (darker) in the simulations than in the expected value map. This smoothing of the data and lack of small-scale spatial variability in the expected value map seems geologically unreasonable. Furthermore, knowledge of the actual variability and maximum concentration level may be important in designing the treatment facility if an input stream of relatively constant concentration is required in processing the waste.

Uncertainty Assessment

One of the primary reasons for modeling uranium contamination at the Fernald site is to make decisions regarding the restoration of contaminated areas. The variation among the many alternative realizations, such as those in Figure 3, suggests that there may be considerable uncertainty regarding the actual contamination level of an individual pixel or selective mining unit. However, the point is not necessarily to evaluate the *actual* level of contamination. The important aspect of environmental restoration of the Fernald site is *whether or not to clean up*. The action level typically is specified by regulation or is negotiated with the responsible regulatory body. Accordingly, the uncertainty problem is actually simplified, and it reduces to describing the probability, given a particular set of sample values, that a given parcel of real estate is above (or below) a particular threshold level requiring action. For purposes of the remediation decision, it is not particularly important whether the actual contamination exceeds the action limit by 5 percent or 500 percent. The decision remains the same: clean it up.

Stochastic simulation methodology is particularly well suited to evaluation of this type of uncertainty with respect to a go/no-go decision. If there are N equally likely alternative models of a site, it is a simple matter to evaluate those alternatives pixel by pixel and to determine the fraction of the set that exceeded threshold X at any individual grid block. If the replicate simulations are, in fact, equally likely representations of the real world, this fraction should approach the actual probability of exceeding the given threshold as the number of simulations becomes large.

This post-simulation processing technique has been applied to the 100 simulations of the drum baling area, and the results are presented in the probability maps of Figure 6. Each map represents the probability, grey-scale coded from 0 to 1, that the indicated pixel exceeds the threshold. Two different threshold levels are presented. Figure 6(a) indicates the probability of exceeding the tentative remediation level of 35 pCi/g of soil. If the regulatory criterion for remediation is 35 pCi/g, virtually the entire drum baling area is contaminated and must be treated in some manner. Figure 6(b) uses a threshold level of 200 pCi/g; as anticipated, the area that must be cleaned up to a criterion of 200 pCi/g is smaller for the same probability (grey-scale level). Note that the grey-scale values in Figure 6(b) in the regions farthest removed from data (especially just east of the region occupied by some of the Fernald buildings) are medium grey corresponding to about 50-percent probability. The inference is that the existing characterization program has provided about as much information regarding whether or not these areas are above or below 200 pCi/g as tossing a coin. It then follows that the greatest gain in overall information may be had by sampling in these regions of greatest uncertainty.

An important corollary of this line of reasoning regarding probability mapping is that these *mapped probabilities translate almost exactly into the risk assumed by the project manager* in deciding whether or not to remediate a specific parcel. A parcel in Figure 6(a) that is 90-percent likely to exceed 35 pC/g presents approximately a 90-percent risk of leaving contaminated material in place if it is not treated. Because the cost of remedial treatment is a first-order function of the total area to be treated, the ability to predict uncertainty, and thereby risk, provides an important tool for cost estimation.

Additional Output from Post-Processing

The collective set of simulations contains additional information that may be of value in designing and executing an environmental restoration project. It is possible to modify the post-processing algorithm slightly to compute the average, or expected concentration of the contamination for those areas (and individual simulations) that exceed a particular threshold (Figure 7). This information may be useful for several purposes. First, it may be necessary to provide physical protection from radiation and/or chemical toxicity to personnel working in areas that exceed certain levels of contamination. These types of maps can be used to identify both the likelihood of encountering significant personnel hazards and the expected magnitude of that hazard. The highest absolute contaminant level to be encountered can be approximated from the simple summary statistics of the composite simulated data set.

Another use of this type of data may be in designing the physical processing facility for removing the contaminant from the soil or other natural media. Depending upon the circumstances, the efficiency of a remediation process may be dependent upon both the absolute concentration and the variability of that concentration in the feed to the treatment plant. As noted earlier, the variability in input-stream concentration implied by the maps of Figures 3 and 5(a) is significantly different, even if over the long run the "average" concentration level is very similar.

PROBABILITY MAPPING, DECISION MAKING, AND DATA WORTH

It is possible to build upon these probability mapping techniques to provide additional, quantitative information that is useful in making environmental remediation decisions. Stochastic simulation and direct probability mapping of contaminant levels provide much of the input needed to evaluate alternative approaches to a remediation problem. Because the techniques are inherently probabilistic, the information generated is closely allied with the risk of failure associated with a particular remediation approach. The probability maps also provide site-specific information that relates directly to cost of a remediation effort. The total area to be treated to achieve a 10-percent risk of failure (in Figure 6, the region subject to 10-percent risk would include all regions but those shaded very light grey) is intuitively significantly greater than that necessary to be treated if one is willing to accept a 50-percent risk of failure (includes only the area shaded dark grey to black). The mapping and evaluation techniques described above are subject to the limitations of an existing state of knowledge. To increase that level of knowledge also costs money and other resources.

If the investment of resources in increasing the knowledge level at a contaminated site results in a more than commensurate decrease in the cost of the remediation program itself, for a given level of risk, then the data that was acquired has worth. Conversely, additional data that do not change the extent of the region to be treated (and which do not change the level of risk associated with that decision) have no worth (in this context), and in fact serve only to increase the total expenditures on a site.

Building upon a conceptual decision framework developed by Freeze and others, (8) we can quantify this cost relationship, and the implied decision model related to costs, as follows:

$$\text{MINIMIZE:} \quad E[C_{total}] = C_{char} + C_{treat} + C_{fail} \times P_{fail} \tag{1}$$

where

$E[C_{total}]$ = the *expected* total cost of the project
C_{char} = the cost of the site characterization program
C_{treat} = the cost of the treatment or remediation program
C_{fail} = the cost of failure (regulatory penalties, cost to repeat work, etc.)
P_{fail} = the probability of failure[a]

The total cost of the project is uncertain principally because there is a non-zero probability of failure. Nevertheless, it is generally possible, *a priori*, to make reasonable engineering projections of the various right-hand-side costs, and, using probability mapping techniques, to estimate the probability of failing to completely remediate the site, given a set of data.[b] *In effect, P_{fail} becomes a management choice.* The objective then becomes to minimize $E[C_{total}]$ by considering a number of alternative characterization programs, and potentially a number of alternative treatment programs as well.

The decision model of Equation 1 has some important implications. First, an initial sampling program probably should be predicated on identifying broad areas of contamination across the entire region of interest and on producing a reasonable statistical understanding (both univariate and spatial) of that contamination, rather than on closely delimiting (supposedly) known contaminated regions from uncontami-

a. This expected value framework involving the value (cost) of certain outcomes multiplied by the probability of those outcomes is widely used in economics and business.(9)

b. It is simplest to treat C_{char}, C_{treat}, and C_{fail} as single-valued deterministic quantities to be identified through engineering estimates, as is assumed here. However, C_{total} is still an expectation, because of the finite probability of failure. The model is sufficiently general that the right-hand-side costs could be treated as distributions (expectations) also, thus explicitly incorporating the uncertainty in those engineering estimates.

nated ones. Second, additional sampling efforts should focus on reducing the region of uncertainty, that area in which the decision to treat or not could result in the greatest cost savings from future classification as uncontaminated. The goal of each additional sampling increment should be to assign formerly uncertain territory to either the region requiring remediation or the area that will be considered "clean." The greatest benefit is obtained if analysis of each sampling increment can be conducted in near-real time, without a significant lag for laboratory measurement and office study. Third, within limits, additional sampling in regions of almost certain contamination requiring remedial efforts may not contribute value in proportion to the additional cost incurred. Refining estimates of actual contamination within an area that will be treated and cleaned-up adds sampling expense (C_{char}) without reducing the remediation expense (C_{treat}). Furthermore, including large numbers of these redundant samples may bias further statistical analyses. (10)

CONCLUSIONS

New and evolving geostatistical techniques that make use of simulation in contrast to estimation (kriging) can be used to map directly the probability of encountering contamination of various types at specific, unsampled locations given a set of isolated sample values. These techniques make use not only of the basic statistical properties of the data set, but they extract additional valuable information from the spatial continuity patterns that may be inferred directly from the locations of the data. The level for which the probability of exceedance is mapped may be set at a regulatory threshold, a concentration related to general health risk, or an exposure level significant to personnel involved in the remediation program. Additional information regarding the local variability and expected overall concentration that may be necessary in engineering a remediation program can be obtained by reprocessing the same information.

Because the probability of exceeding a specified threshold value is directly related to the risk of failure assumed by a project manager, these probability mapping techniques can be used in cost studies of alternative site characterization and treatment scenarios. A fundamental concept that results from a decision-focused modeling effort is that only data which changes a decision (or reduces risk) has worth.

The techniques and concepts described in this paper are illustrated with an example from the Fernald (Ohio) Uranium-in-Soils Integrated Demonstration Project. However, these methods form a basic framework for analysis and decision-making. As such, they should be directly applicable to a wide variety of environmental remediation activities

ACKNOWLEDGMENT

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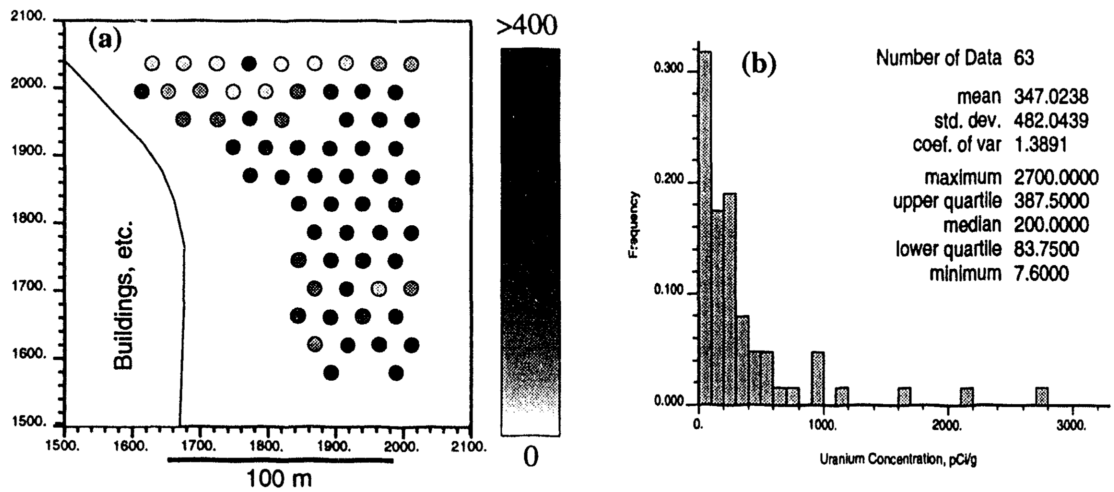

Figure 1. (a) Location map showing soil-geochemical data for the drum baling area. Uranium concentrations in pCi/g are shown as grey-scale coded dots. Grid scale in ft.; bar scale in m. (b) Sample histogram and associated statistics of soil-geochemical data. Coordinates are state plane coordinates in feet, adjusted by subtracting an arbitrary constant for plotting purposes.

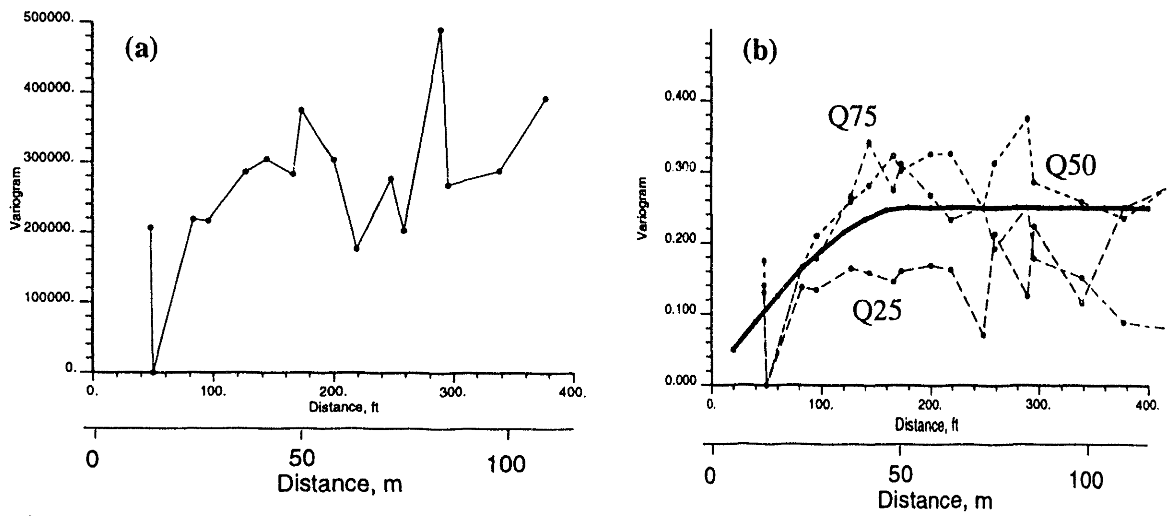

Figure 2. Sample variograms for soil-geochemical data at the drum baling area. (a) Classical variogram of sample data. (b) Equivalent indicator variograms for lower (Q25), median (Q50), and upper (Q75) quartile values.

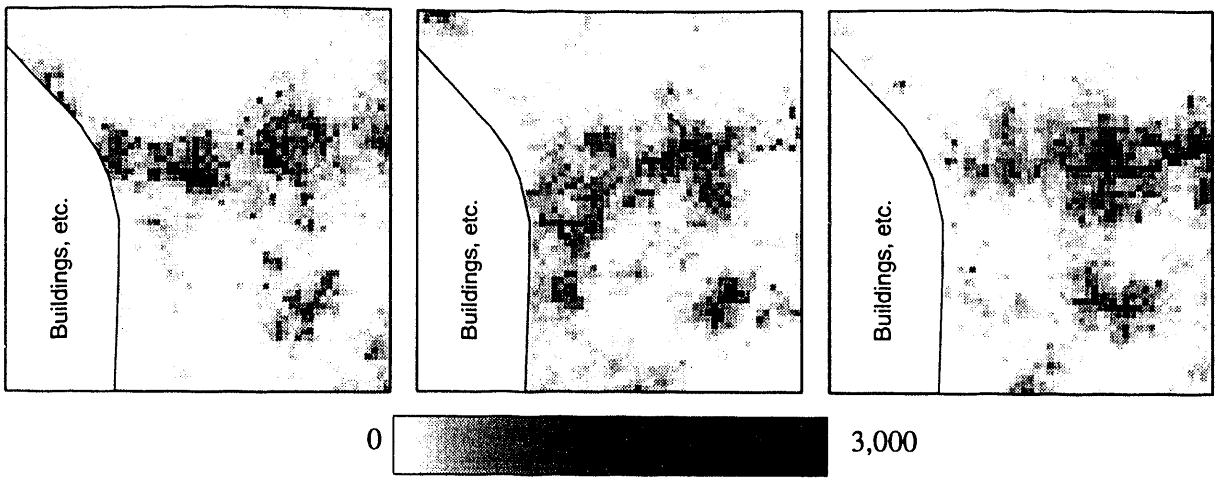

Figure 3. Three equally likely simulations of uranium concentration at the drum baling area. Concentrations of individual 3.05 m by 3.05 m (10 ft. by 10 ft.) pixels are shown as grey-scale coded values varying from 0 to 3,000 pCi/g (concentration scale bar). Each map is 183 m (600 ft.) on a side.

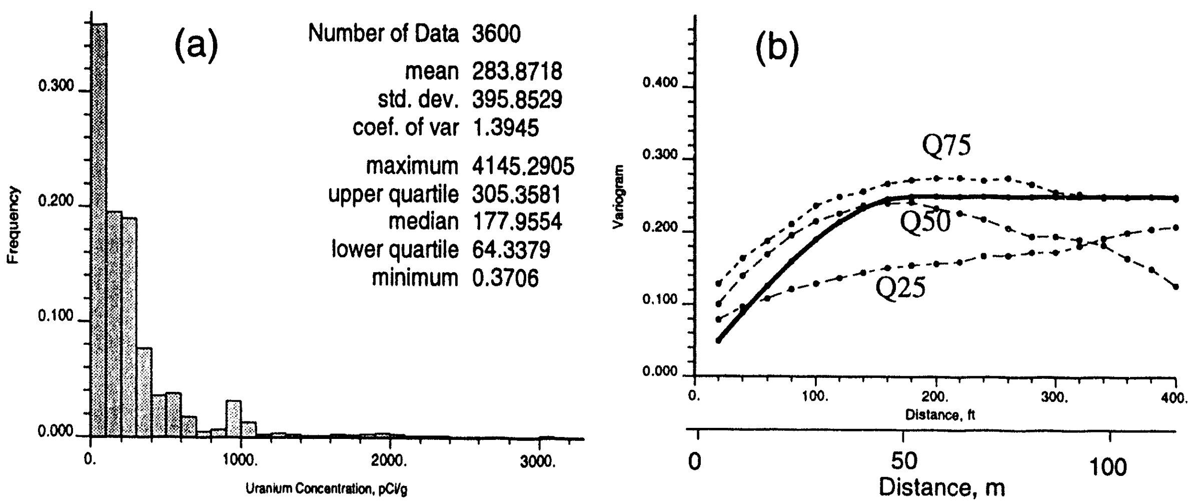

Figure 4. Validation statistics for one simulation from Figure 3. (a) Histogram of complete simulation (compare to Figure 1(b)) (b) Indicator variograms for median, first, and third quartiles compared with interpreted spatial model from Figure 2 (bold line)

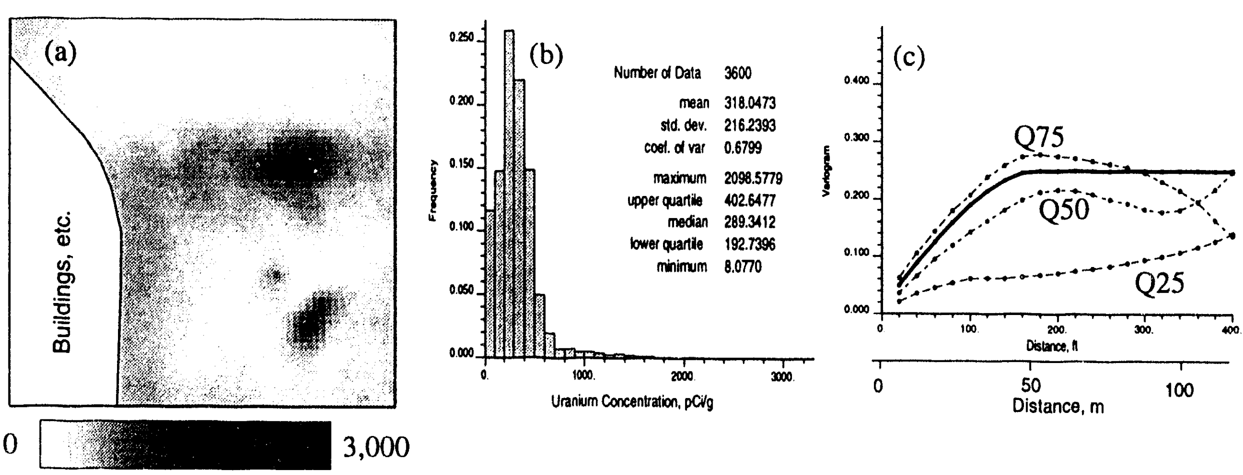

Figure 5. (a) Expected value map, grey scale in pCi/g, (b) validation histogram and statistics; (c) indicator variograms. See text for discussion.

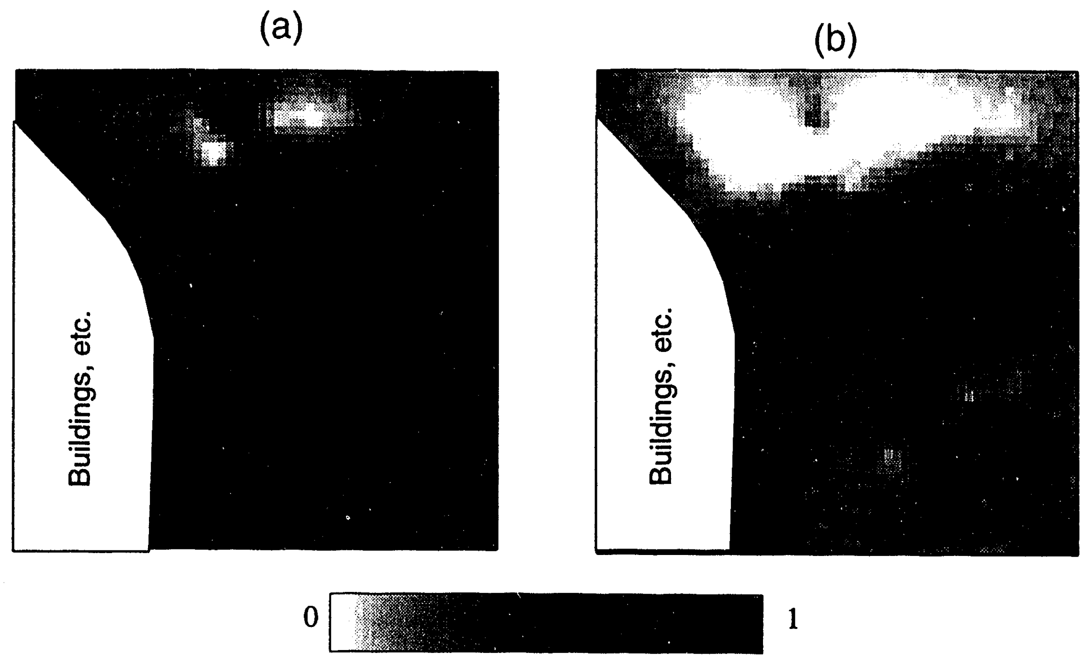

Figure 6. Maps showing the probability of exceeding (a) 35 pCi/g and (b) 200 pCi/g of uranium in soil at the drum baling area. Probability scale varies from 0 to 1.

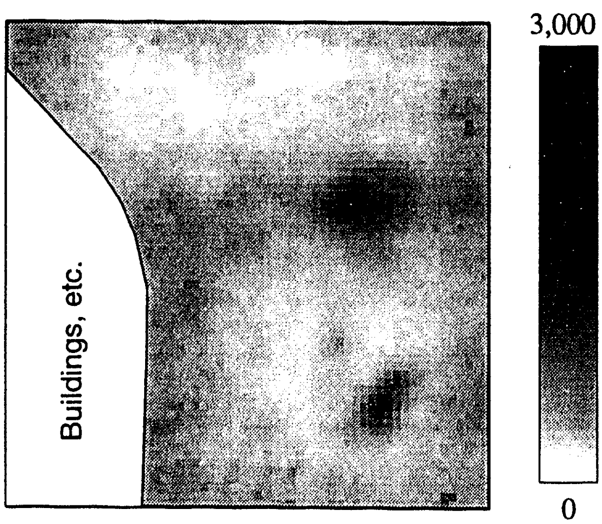

Figure 7. Average (expected) uranium concentration of parcels that exceed 200 pCi/g. Concentrations are grey-scale coded in pCi/g.

KEYWORDS

Geostatistics, Mapping, Fernald OH, Data worth, Decision making, Uncertainty analysis

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