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INDUSTRIAL EXPERIENCE FEEDBACK OF A GEOSTATISTICAL ESTIMATION OF CONTAMINATED SOIL VOLUMES

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ABSTRACT

Geostatistics meets a growing interest for the remediation forecast of potentially contaminated sites, by providing adapted methods to perform both chemical and radiological pollution mapping, to estimate contaminated volumes, potentially integrating auxiliary information, and to set up adaptive sampling strategies. As part of demonstration studies carried out for GeoSiPol (Geostatistics for Polluted Sites), geostatistics has been applied for the detailed diagnosis of a former oil depot in France.

The ability within the geostatistical framework to generate pessimistic / probable / optimistic scenarios for the contaminated volumes allows a quantification of the risks associated to the remediation process: e.g. the financial risk to excavate clean soils, the sanitary risk to leave contaminated soils in place. After a first mapping, an iterative approach leads to collect additional samples in areas previously identified as highly uncertain. Estimated volumes are then updated and compared to the volumes actually excavated. This benchmarking therefore provides a practical feedback on the performance of the geostatistical methodology.

INTRODUCTION

Several investigation campaigns conducted after the closure of an oil depot in France, highlighted the existence of high hydrocarbons grades in the lower part of a backfill layer covering almost entirely the former oil depot. Given the future use envisaged for the site, potential health risks led to the definition of a remediation threshold for Total Hydrocarbon (‘THC’) grades of 2500 ppm by proper authorities.

As a consequence, areas presenting hydrocarbons grades above the remediation threshold had to be characterized in order (i) to quantify and locate the contamination and (ii) to estimate the volumes to be excavated.

The key points of this study are:

- the consideration of all available data;
- the geostatistical recommendation for additional boreholes;
- the uncertainty quantification;
- the consideration of remediation constraints such as the remediation support.

MATERIAL

High hydrocarbon grades are occurring in the lower part of a backfill layer covering an area of 43 709 m² and corresponding to approximately 75 000 m^3 of soil.

In 2002, a remediation threshold of 2 500 ppm was decided after the detailed risk evaluation of the site. An evaluation of the contaminated areas led to a suspected contaminated surface of 7 775 m² (in yellow on Figure 1), corresponding to a volume estimated to lie between 11 650 and 15 550m^3.

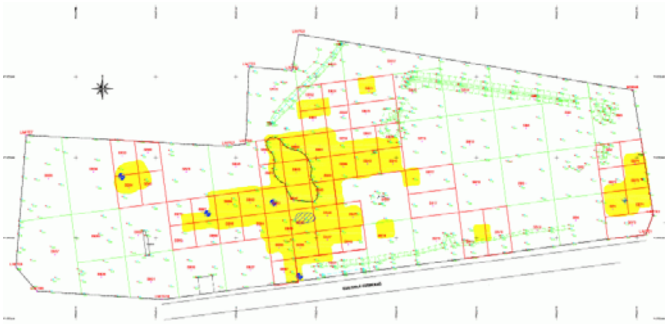

Figure 1: Overview of the former oil depot.

In December 2005, a systematic sampling of potentially contaminated areas was carried out using a 15 m mesh (whilst the rest of the site was sampled using a 30 m grid). During this first sampling campaign, eighty-two boreholes were drilled (green crosses in Figure 2) each of them containing two samples. Depending on organoleptic observations, these samples were generally taken between 0 and 1 m and 1 and 2 m. In the presence of visual indication of pollution, a first sample is taken in the upper part of the backfill (usually clean) and the second sample in the lower part (visually contaminated). The advantages of this sampling scheme are the effective delineation of the contamination with a reduced cost assuming that THC is the only target compound and that the level of correlation between the visual aspect of the sample and the actual risk of exceeding the threshold remains acceptable. However it leads to a sampling strategy which is neither systematic nor regular. Moreover the practical selection of samples inside the borehole is difficult and not always reliable.

In June 2006, following a first geostatistical study, seventeen additional boreholes were drilled in areas indicated as uncertain by the geostatistical analysis (see Figure 2).

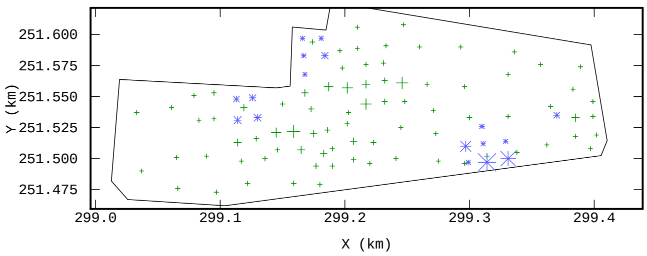

Figure 2: Sampling campaigns (green crosses: 82 initial boreholes, blue stars: 17 complementary boreholes).

The statistical distribution of grades is very asymmetrical (Figure 3), with many low values and a few extremely high grades. Median and mean values are therefore very different.

Using all the data, a first evaluation based on analytical results without geostatistics led to the estimation of 8 300 m^3 of contaminated soil.

In the summer of 2006, remediation took place, leading to the excavation and sorting of 22 347 m^3 of soil, out of which 13 171 m^3 were contaminated. The contaminated volumes estimated from the analytical results clearly underestimate the amount of pollution.

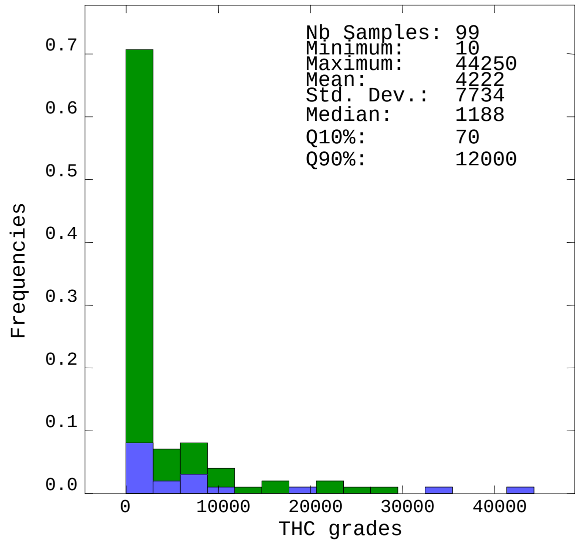

Figure 3: Histogram of THC grades (green crosses: 82 initial boreholes, blue stars: 17 additional boreholes). Statistics are reported in the top right part.

METHODOLOGY

Reminders about geostatistics and its application to soil pollution can be found in Chilès & Delfiner (1999), Goovaerts (1997) or Jeannée et al. (2003). A brief description of the methodology, derived from Desnoyers et al. (2009), is also reported in Appendix A.

Because of the sampling strategy, a two step procedure has been adopted for the geostatistical methodology. Firstly the geometry of the potentially contaminated layer is estimated, then grades are estimated inside this 2D layer to assess the contaminated volume.

Data processing

As described in the previous part, vertical sampling was not carried out using regular intervals and was oriented depending on organoleptic observations. To account for this particular scheme, a preliminary data processing is necessary in order to synthesize the two samples taken in each borehole. A 1000 ppm threshold is chosen to consider whether samples belong to the potentially contaminated layer or not.

Therefore, to determine the potentially contaminated layer, only the samples with a grade exceeding 1 000 ppm are kept. The length, Z_{min} (minimal depth) and Z_{max} (maximal depth) corresponding to each sample are reported to get the thickness of the potentially contaminated layer. In case both grades in a same borehole are greater than 1 000 ppm, a weighted average is performed to compute the borehole grade and the total length of the borehole is used for estimating the thickness of the potentially contaminated layer.

Modeling the geometry of the target layer

Following the previous step, the thickness of the potentially contaminated layer is available at 99 locations. To help delineate and characterize the uncertainty attached to the potentially contaminated layer, geostatistical simulations are performed.

Spatial structure of the top of the layer (after Gaussian anamorphosis) is presented in Figure 4 and used to compute the simulations; the thickness variogram is also calculated.

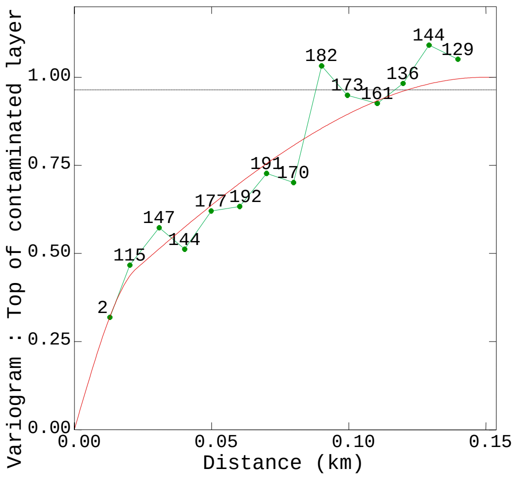

Figure 4: Experimental variogram and fitting for the top of the contaminated layer.

Geostatistical simulations using the turning bands algorithm are performed for the top and the thickness of the layer. Assuming the two variables are independent, the bottom of the layer can be deduced from these two sets of simulations.

This methodology allows quantifying the uncertainty associated to the geometry of the layer. For instance, Figure 5 presents the most probable scenario for the thickness of this layer.

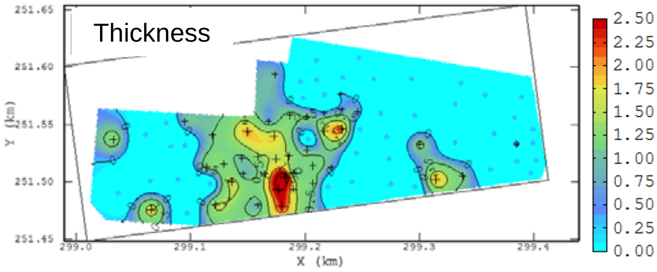

Figure 5: Median of thickness simulations (legend in meters).

Modeling THC grades

Inside the potentially contaminated layer, a 2D modeling of THC grades is performed to estimate areas exceeding the 2 500 ppm threshold.

The first step is again to calculate and model the variogram of the grades (Figure 6). Due to the multi-Gaussian assumption required for performing simulations, grades are first transformed using a Gaussian anamorphosis, which helps revealing the underlying spatial structure of the otherwise asymmetrical distribution of the grades.

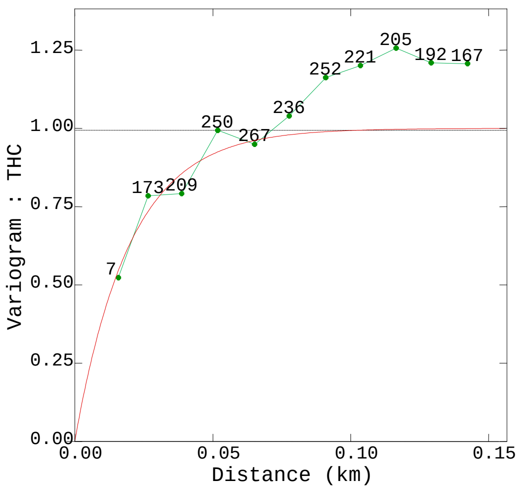

Figure 6: Experimental variogram and fitting for the THC grades.

Several maps can be produced using the geostatistical simulations such as the probability to exceed a threshold. In this case, the probability map of exceeding 2 500 ppm is of major interest to assess areas associated to high grades and which should be excavated.

The resulting map of Figure 7 highlights areas with low / high risk to exceed the threshold. It seems important to observe that there are also some areas presenting intermediate levels of risk. In those areas, uncertainty regarding the 2 500 ppm threshold is high. In case additional boreholes are further drilled, those areas with high uncertainties should be targeted as a matter of priority.

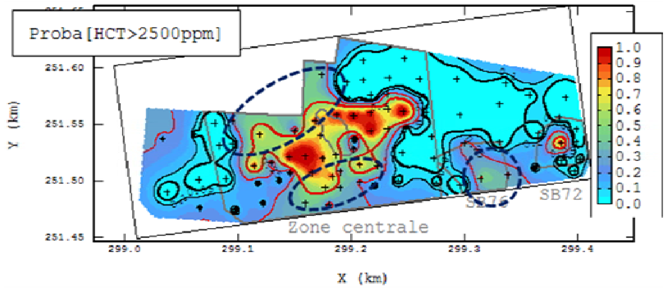

Figure 7: Probability for THC to exceed the threshold of 2500 ppm; uncertain areas circled.

Computation of contaminated volumes

Contaminated volumes are assessed by multiplying simulations of thickness by the contaminated area extent. This extent is derived from the simulations of grades: simulation by simulation, all cells exceeding the threshold are kept to determine this area.

Because of:

- the uncertainty about the depth and thickness of the contaminated layer and
- the spatial variability of the grades inside the layer,

the excavation of much more soil than what is really polluted is usually required in order to minimize the risk to leave contaminated soils in place. Once an acceptable risk level is determined, the excavation scenario might be obtained by deriving from the simulations:

- quantile maps for the geometry;
- probability maps for the grades to exceed the target threshold.

Taking the remediation support into account

Although samples are collected punctually, the soil excavation is performed using a much larger volume, called the "remediation support". In the present case, the horizontal resolution of the remediation support is 15 m x 15 m.

The knowledge of the remediation support should be taken into account when computing contaminated volumes. Indeed, the distribution of grades changes with the size of the support: though the average grade remains the same, the variability of the grades decreases when the support size increases (Figure 8). Failure to account for the impact of the remediation support on the distribution can lead to distorted estimations of the volume above a threshold.

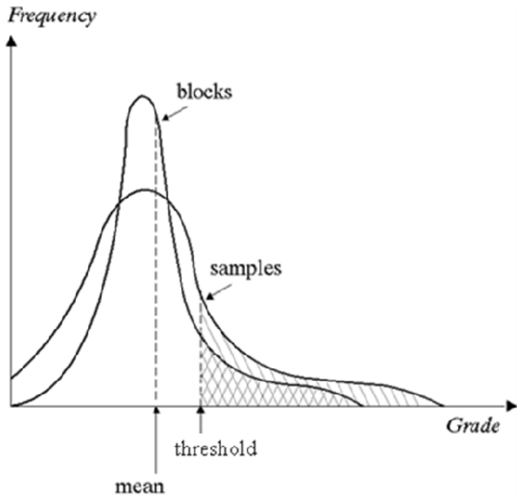

Figure 8: Difference between distributions induced by different supports.

RESULTS AND DISCUSSION

First geostatistical study

The first geostatistical study, conducted with the initial 82 boreholes, leads to a probable estimate of contaminated volumes equal to 9 217 m^3 and lying with a 90% confidence level in the interval [7 874 m^3; 11 265 m^3].

This initial volume is underestimating by 30% the real contaminated volume, equal to 13171 m^3. This result might be explained by two reasons: (i) it has been obtained without consideration of the 15 m x 15 m remediation support, and (ii) the 17 complementary boreholes were not yet integrated to the study.

Update knowing the remediation support

The estimation of contaminated volumes may be updated by considering the correct remediation support, equal to 15 m x 15 m. This leads to a probable contaminated volume equal to 11 773 m^3, lying with a 90% confidence level in the interval [9 498 m^3 – 14 726 m^3]. Though there is still an underestimation of 10.6% compared to the true value, the updated volume is now at least contained in the confidence interval.

Figure 9 illustrates the presence of areas where large uncertainties remain (probability of exceeding the threshold close to 50%).

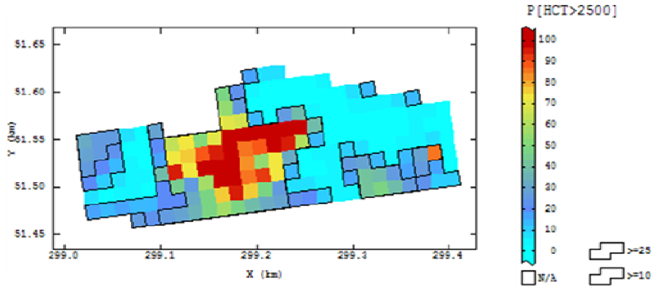

Figure 9: Probability map of exceeding 2500 ppm using a 15 x 15 m mesh.

Update using complementary boreholes

The integration of the recommended boreholes to the analysis leads to a clear decrease of the uncertainty in the newly sampled areas (Figure 10).

Updating the computation of contaminated volumes finally leads to an estimate of 12 059 m^3, contained with a 90% confidence level in the interval [10 028 – 15 421 m^3].

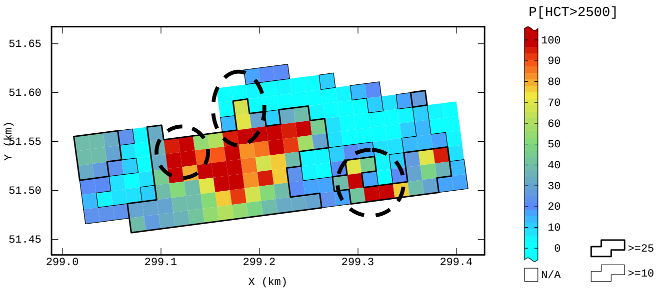

Figure 10: Probability map of exceeding 2500 ppm using a 15 x 15 m mesh and the complementary boreholes (carried out in the circled areas).

Despite the 8.4% underestimation, the true contaminated volume corresponds to the 25% quantile of the statistical distribution of contaminated volumes (Figure 11).

Therefore, given the limited knowledge of the pollution, final results integrating all boreholes and the remediation support of 15 m x 15 m are consistent. Moreover two reasons may explain the remaining difference: (i) the excavation was carried out on a 15 m basis but with some irregular blocks and (ii) the estimation takes into account the exact thickness whereas excavation has probably been done with 0.5 m vertical benches and remains unknown.

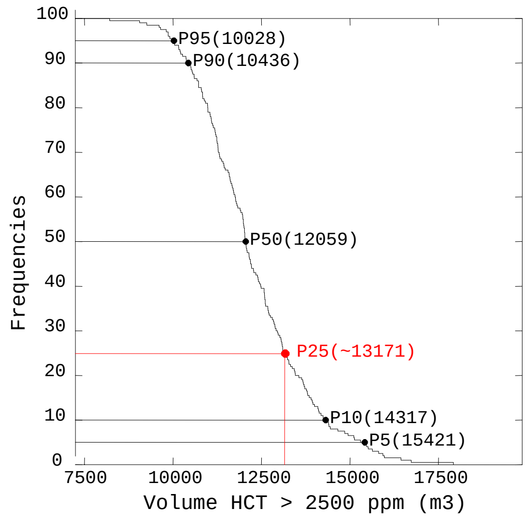

Figure 11: Inverse cumulative histogram of the global contaminated volume (in cubic meters).

These estimates can also be compared with the initial estimation of contaminated volumes, performed without geostatistics, which resulted in an estimate of 8300 m^3.

Remediation in practice

Several scenarii can then be recommended for the remediation depending on the accepted risk, as illustrated in Table 1. These volumes can be compared with the real excavated volume, equal to 22 348 m^3.

A possible scenario for both geometry and THC grades could be Q25/Q75/P25:

- the horizontal extension is given by the 25% isoline of the probability map to exceed 2500 ppm;
- inside those areas, depth horizons to be excavated are obtained utilizing the Q25% scenario for the top of the layer and the Q75% scenario for its bottom.

Such results are useful to optimize the planning of the excavation phase and also to better assess its related costs.

Table 1: Volume to be excavated depending on the chosen scenario for the geometry and the probability to exceed the THC threshold.

Quantile for Top of the layer	Quantile for Bottom of the layer	THC proba	Volume to be excavated
Q50 (probable)	Q50 (probable)	P50 (probable)	14 112 m^3
Q25 (safe)	Q75 (safe)	P50 (probable)	22 160 m^3
Q25 (safe)	Q75 (safe)	P25(safe)	31 239 m^3

CONCLUSION

The above study helps emphasize the following benefits of the geostatistical approach:

- data quality control leading to a two step approach;
- relevant estimates coupled with uncertainty quantification for both contaminated and excavated volumes;
- help in designing iterative sampling strategies using uncertainty maps.

The study shows that geostatistics is a well-suited approach for the remediation forecast of such contaminated sites. Moreover it provides a framework for both uncertainty assessment and cost-benefit analyses, in particular regarding the relevance of collecting additional data versus starting the remediation.

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All geostatistical calculations and graphics are realized with the ISATIS software (Geovariances, 2010).

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APPENDIX A

GEOSTATISTICAL METHODOLOGY IN SHORT

The whole point of the geostatistical methodology is to take into account the spatial continuity of the phenomenon to predict it at unsampled locations, and quantify the prediction uncertainty. The characterization of this spatial continuity, or spatial variability, is an essential stage which is performed through the variographic analysis.

The experimental variogram *γ(h)* is calculated by averaging, within classes of distance *h*, the variability contribution of each pair of points. This contribution is usually quantified by the half squared difference of the measured values:

$$\gamma(h) = \frac{1}{2} E[Z(x) - Z(x+h)]^2 \qquad (1)$$

Generally, for a structured phenomenon, the spatial variability increases with distance and tends to stabilize to a "sill" at a distance named "range". Data separated by a distance larger than the range are no longer spatially correlated.

Kriging (interpolation) and simulations procedures require the model fitting of the experimental variogram. Indeed, for the following calculations, the spatial variability should be known whatever the distance and should integrate the a priori information on the phenomenon, which is not always illustrated by the measurements.

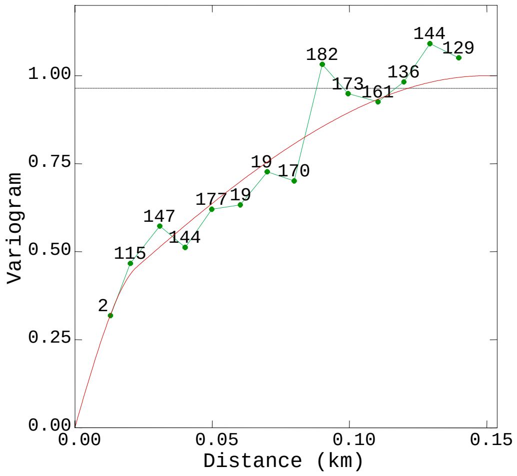

Figure 12: Experimental variogram (green) and corresponding model (red).

Kriging estimation

As for classical interpolations, kriging at a point x_0, denoted $Z^*(x_0)$, is a linear combination of the n known experimental values at measurement points:

$$Z^*(x_0) = \sum_{i=1}^{n} \lambda_i Z(x_i) \qquad (2)$$

The choice of the λ_i coefficients named "kriging weights" depends on: (i) the distances between the data and the point to be estimated (as for classical interpolators), (ii) the distances between the data (clusters…), and (iii) the spatial structure of the studied phenomenon (for example, very smooth or heterogeneous behaviour, anisotropy, etc., characterized by the variogram model).

Kriging ensures an unbiased estimation and the minimization of the estimation error variance *Var[Z*-Z]*, which corresponds intuitively to the minimization of the error risk. Thus kriging is the best linear unbiased estimator.

In comparison to classical interpolators, the added value of geostatistical estimation lies in the quantification of the related estimation uncertainty. This quantification is possible due to the spatial variability modeling.

Uncertainty is usually described by the kriging (error) standard deviation values: it takes minimal values close to data points, where the estimation confidence is high and it increases with the distance between the target point and the data points, as a function of the chosen variogram model. Generally, the kriging standard deviation map is a good indicator of the estimation quality and is also used to help designing sampling strategies.

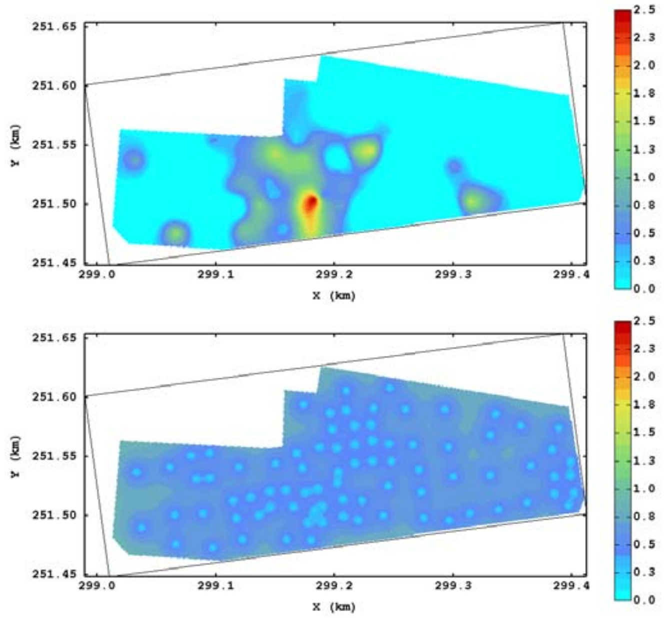

Figure 13: Kriging map and associated uncertainty.

Finally geostatistics allows a rigorous modeling of the support effect and thus takes into account the remediation support.

Risk analysis

When a delineation of areas exceeding a threshold is required or when corresponding contaminated volumes need to be computed, due to the inherent smoothing effect of kriging, one should use geostatistical simulations which reproduce the real data variability.

To perform simulations raw data should be transformed using a gaussian anamorphosis: intuitively, the raw histogram is deformed to become a Gaussian one. The resulting variogram is usually better structured, which facilitates the spatial structure determination and is required here.

Each resulting simulation corresponds to one possible scenario for the spatial distribution of the variable. All simulations are consistent with the variogram model and honor the available information (experimental values and statistical distribution).

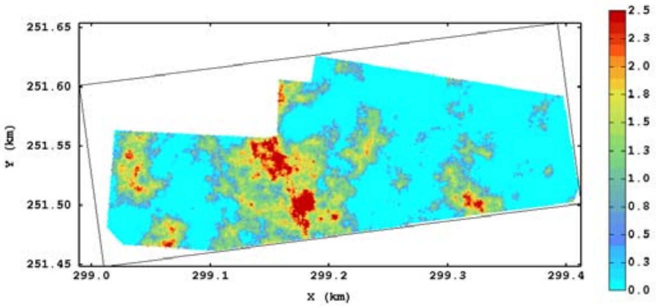

Figure 14: Example of one geostatistical simulation.

Conditional simulations allow to derive local estimates of non-linear quantities, such as quantile or probability maps of exceeding a threshold, and to estimate global statistics like contaminated surfaces or volumes.