Study on pollutant model construction and three-dimensional spatial interpolation in soil environmental survey

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Abstract. In site soil investigation, the construction of three-dimensional (3D) geological model and spatial three-dimensional distribution model of pollutants can help investigators to clearly and intuitively understand the morphology distribution and spatial relationship of pollutants. Four 3D interpolation methods (Krige, IDW-Shepard, FastRBF and Nearest Neighbor) are compared and studied, based on the Sb (antimony) data in soil of a polluted plot in Tianjin by using EVS-Pro. The results show that the selection of interpolation method is quite different for the calculation results of 3D interpolation model, and the cross-verification results show that the interpolation accuracy of Krig-3D interpolation model is the highest. The pollution distribution model of Sb based on interpolation results can truly reflect the actual pollution of the site and accurately help to calculate earthwork, and 3D model and visualization technology have more intuitionistic and clear display. It provides a reference and framework for the subsequent remediation and treatment of contaminated sites.

1. Introduction

In recent years, with the adjustment of urban functional layout, some industrial enterprises in the central urban area have gradually relocated and stopped production, resulting in more contaminated sites, so it is necessary to carry out site environmental investigation and risk assessment[1-5]. In the investigation of contaminated sites, because the construction project involves underground space, geological information and monitoring data are numerous, in the face of a large number of two-dimensional map data, it is difficult to understand the geological situation and pollutant distribution pattern of underground space comprehensively and accurately, which brings difficulties and even mistakes for the detailed investigation of plots and the later soil restoration and construction. Moreover, geological information and spatial monitoring data are essentially 3D[6-8]. It is necessary to analyze and solve the problems in the process of soil environmental investigation and restoration more intuitively on the basis of local geological condition parameters and with the help of 3D geological modeling and visualization.

With the development of spatial information technology, 3D geological modeling technology emerges as the times require[9-19]. It is a new subject based on computer technology, which combines geostatistics, geographic information data management, spatial analysis technology, 3D visualization and spatial prediction. It has powerful data statistics function and clear 3D graphics and image visualization functions. In the site environment survey, all types of original data (geological data, detection and analysis data) are integrated, and based on the sampling point data, the spatial...
interpolation of the characteristic data of other unknown areas in the research area is carried out[20-23]. Then the digital models, such as the site formation model and the pollution distribution model, are established. The spatial geological information and the pollutants distribution can be obtained clearly and intuitively, which provides the basis for the decision-making and planning of site investigation.

2. Materials and methods

2.1. Overview of the study area

The site of the research area has been a chemical plant in history, covering an area of 30000 m², the original products are hydrofluoric acid, copper naphthalate, freon, and new water reducer. Since 2000, the original site has been built in succession to produce glycerol products, plastic products, fertilizer products, petroleum products, mechanical and electrical equipment maintenance. Through pollution identification (the first stage of site environmental investigation), the characteristic pollutants in the block include fluoride, heavy metals, petroleum hydrocarbons, BTEX (benzene series) and other volatile organic compounds and semi-volatile organic compounds such as polycyclic aromatic hydrocarbons (PAHs).

2.2. Data acquisition and monitoring

According to the genetic type and sedimentary age of the site, the soil layer within the maximum exploration depth of the site (13.0m) is divided into artificial accumulation layer and Quaternary loose sedimentary layer. According to the genetic age, the foundation soil can be divided into the following four layers, Layer 1 is artificial fill soil layer, the upper part of the layer is brick slag, ash slag, cinder, broken stone, silty clay, containing a small amount of ash, with the thickness of 1.5-2.7 m.; Layer 2 is the continental alluvium of the Upper Holocene formation, with the total thickness of 3.1-4.5 m, which is mainly composed of clay, silty clay and silt, and the distribution of this layer is continuous and stable in the site. Layer 3 is the marine sedimentary layer of the Holocene formation, with a total thickness of 6.4-6.9 m, which is mainly composed of silty clay and silt. Layer 4 is the continental alluvium of the lower Holocene formation. The maximum depth reached, because of the limited exploration depth, only reveals the roof of the layer, so its thickness is not defined. The distribution of the deepest layer is mainly composed by silty clay with clay.

In the preliminary investigation stage, a total of 10 soil monitoring points were set up. The detection parameters are 13 heavy metal elements (zinc, lead, arsenic, chromium, antimony, cadmium, copper, vanadium, mercury, nickel, beryllium, cobalt, hexavalent chromium), VOCs, SVOCs (including organic pesticides), fluoride, TPH and cyanide. In the detailed investigation stage, 31 soil monitoring points were set up in the plot as shown in the Figure 1, and the detection parameters were 10 heavy metal elements (lead, arsenic, cadmium, copper, mercury, nickel, hexavalent chromium, zinc, antimony), VOCs, SVOCs (organic pesticides), petroleum hydrocarbons (C10–C40), pH, cyanide and fluoride.

2.3. Interpolation accuracy evaluation method

In the process of spatial interpolation, the error between the measured value and the predicted value directly determines the accuracy of spatial interpolation. In order to verify the accuracy of spatial interpolation, it is used the cross validation method. In this study, the average absolute error (ME) and root mean square error (RMSE), which are commonly used in interpolation accuracy evaluation, are selected as error statistical indexes to evaluate the accuracy of various interpolation models for cross validation. The average absolute error (ME) can evaluate the possible error range of the estimated value. The root mean square error (RMSE) can reflect the estimation sensitivity and extreme value effect of the sample points. The closer the average error (ME) is to 0, the smaller the root mean square error (RMSE) value is, and the higher the interpolation accuracy is. On the contrary, the farther the average absolute error (ME) is to 0, the larger the root mean square error (RMSE) value is, and the lower the interpolation accuracy is[24-26]. The formula is as follows:
In the equations 1 and 2, \( u(x_i) \) is the predicted value and \( u^*(x_i) \) is the measured value of the sample, and \( x_i \) is sampling point data.

2.4. Data processing platform

EVS Pro (Earth Volumetric Studio) is a 3D geological modeling and visualization software developed by C-Tech USA. C-Tech's EVS-Pro is the world's leading three-dimensional geological modeling software system, which is widely used in geology, environmental science, the processing of soil, groundwater, surface water, air and other data. [27-28].

2.5. Data preparation

A total of 104 samples were collected from 41 points in the site. The detection parameters were mentioned above. According to the test results, some samples present levels of lead, nickel, copper,
antimony, chromium, zinc and fluoride that exceeded the screening values. According to the investigation results, the heavy metal pollution in soil is serious. In this paper, the Sb element is selected as an example, and the Sb analysis data at different depth in drilling points are presented in Table 1.

Table 1. Partial drilling sampling point data.

| Bore | X     | Y     | Ground (m) | Lithology (m) | Depth-Top (m) | Depth-Bot (m) | Sb (mg/kg) |
|------|-------|-------|------------|---------------|---------------|---------------|------------|
| X12  | 96736.06 | 311347.95 | 2.34 | Layer1 | 0 | 2.8 | 5.5 |
| X12  | 96736.06 | 311347.95 | 2.34 | Layer2 | 2.8 | 5.4 | 0.5 |
| X12  | 96736.06 | 311347.95 | 2.34 | Layer3 | 5.4 | 13.5 | 0.5 |
| X12  | 96736.06 | 311347.95 | 2.34 | Layer4 | 13.5 | 14 | 0.5 |
| X13  | 96762.21 | 311346.92 | 2.16 | Layer1 | 0 | 4.7 | 0.5 |
| X13  | 96762.21 | 311346.92 | 2.16 | Layer2 | 4.7 | 6 | 0.5 |
| X13  | 96762.21 | 311346.92 | 2.16 | Layer3 | 6 | 12.8 | 2.2 |
| X13  | 96762.21 | 311346.92 | 2.16 | Layer4 | 12.8 | 13.6 | 0.5 |
| X14  | 96748.45 | 311336.66 | 2.15 | Layer1 | 0 | 1.7 | 0.5 |
| X14  | 96748.45 | 311336.66 | 2.15 | Layer2 | 1.7 | 7.8 | 17.5 |
| X14  | 96748.45 | 311336.66 | 2.15 | Layer3 | 7.8 | 12.1 | 0.5 |
| X14  | 96748.45 | 311336.66 | 2.15 | Layer4 | 12.1 | 13.5 | 0.5 |
| X15  | 96778.71 | 311319.19 | 2.23 | Layer1 | 0 | 4.8 | 0.5 |
| X15  | 96778.71 | 311319.19 | 2.23 | Layer2 | 4.8 | 8.3 | 0.5 |
| X15  | 96778.71 | 311319.19 | 2.23 | Layer3 | 8.3 | 12.6 | 418 |
| X15  | 96778.71 | 311319.19 | 2.23 | Layer4 | 12.6 | 13.5 | 358 |
| X16  | 96760.87 | 311304.13 | 2.05 | Layer1 | 0 | 2 | 0.5 |
| X16  | 96760.87 | 311304.13 | 2.05 | Layer2 | 2 | 3 | 0.5 |
| X16  | 96760.87 | 311304.13 | 2.05 | Layer3 | 3 | 13.7 | 0.5 |
| X16  | 96760.87 | 311304.13 | 2.05 | Layer4 | 13.7 | 14 | 0.5 |

EVS can show the content of analyte at different depths and represent it in different colors corresponding to the legend color mark. Figure 2 shows the concentration distribution of Sb at different depth for each sampling point. It can be seen (in Figure 2) that Sb is mainly concentrated in the upper part.

Figure 2. Visual expression of Sb concentration data in boreholes.
3. Results and discussion

3.1. Analysis of Sb distribution in soil

The results of preliminary investigation and detailed investigation showed that 56 samples were detected and 12 samples exceeded the standard which were X7(0.5m), X8(0.5m), X11(0.5m,1.7m), X15(0.5m,1.8m,3.0m), X26(1.8m,3.0m), X30(0.5m,1.5m), X4(0.5m). In the preliminary investigation stage, 3 samples exceeded the standard, The depth of the sampling point exceeding the standard was 0.3-0.4m, ZQ4 (0.4m), ZQ2 (0.3m) and ZQ5 (0.3m). The maximum antimony concentration exceeds the soil pollution risk control standard (GB36600-2018) of construction land for soil environmental quality. There is usually an unacceptable risk to human health and risk control or remediation measures should be taken. The raw materials in the site involve Sb pentachloride, and the pollution of antimony may also be involved in the waste, which may be the cause of Sb exceeding the standard.

3.2. 3D geological modeling of contaminated sites

Drilling is the most intuitive, accurate and detailed means to obtain 3D geological information [29-30]. The geological (formation information) in the site is obtained by drilling data. Based on the drilling data, the whole site 3D formation model is constructed. By constructing the 3D formation model, we can more clearly and intuitively understand the spatial form and relationship of strata, and understand the distribution status and the distribution and migration of pollutants in different strata can also be analyzed[31-32].

In the selection of the same spatial coordinate system, boreholes and strata will be displayed in the same coordinate system, so the unified coordinate system is the basis of three-dimensional geological modeling. According to the drilling sample data of the site, the 3D strata model of the site is constructed by the method showed in Figure 3a. It can be clearly seen that the strata in the site are divided into four layers, from top to bottom, the first layer of artificial filling layer, the second layer of clay-silty layer, the third layer of silty clay-silty layer and the fourth layer of silty clay layer. The slices of geological bodies can also be intercepted in any direction showed in Figure 3b to understand the distribution characteristics of different strata in different spatial positions and the distribution of the original invisible parts of the same strata.

![Figure 3. 3D geological model of the site strata.](image)

a) Overall effect of visualization model of geological structure; b) Separation effect of visualization model of geological structure

3.3. Construction of pollutant model and selection of interpolation methods

The data source in this soil survey was obtained through 41 boreholes arranged on the site. In order to construct a geological interface, increase the realism of the geological interface and improve the visualization effect of the geological interface, it is necessary to use the denser data points to describe the geological interface, so Krige (3D Kriging interpolation), IDW (inverse distance weighted
interpolation) have been selected in the modeling system. Four three-dimensional interpolation methods, FastRBF (Radial basis function interpolation) and Nearest Neighbor (nearest Point interpolation), were used to interpolate the data obtained from the drilling sample points.

Kriging (3D Kriging interpolation), which is a spatial local estimation or spatial local interpolation, is essentially unbiased optimal estimation for sampling points. The interpolation results are affected by the simulation accuracy of variation function, the distribution of sample points and the selection number (Searching neighborhood) of adjacent sample points[33]. It can fully consider the spatial correlation of data and the spatial distribution structure of sampling in the process of interpolation[34]. The interpolation method is based on the discrete semi-variance function and is the best fitting for the experimental variation function[35]. Inverse distance weighted (IDW) interpolation method uses the value of adjacent sampling points to estimate the value of unknown points. Taking the distance between the estimated points and the actual observed sample points as the weight, the closer the sample points are to the interpolation point, the greater the weight given by the sample points, and the weight contribution is inversely proportional to the distance[25].

The radial basis function (FastRBF) is a kind of real function whose value depends on the distance between the estimated point and the actual observed sample point[36-37]. According to the drilling sampling data, the radial basis function interpolation can be expressed by the surface function constructed by independent variables relative to the Euclidean distance of the sampling point, and can make full use of the field effect of the sampling position itself. The position of the boundary point and the corresponding normal vector information of the pollutant distribution model on the hole are determined by searching, and the implicit expression function of the pollution distribution model is calculated by interpolation[38].

The nearest neighbor (Nearest Neighbors) interpolation relies on the data set's own characteristic search, considering the influence of the density of spatial distribution on the number of nearest neighbors and the symmetric relation of neighbors[39]. By giving any point, the points in the index set can be used to reflect the overall situation in a small local area centered on that point[40]. In this method, the nearest node system to a certain point in geometric characteristics is defined, and the number and position of nodes only depend on the local distribution of nodes[41].

The three-dimensional pollution distribution model of heavy metal Sb is established by different spatial interpolation methods (Figure 4). It can be seen that the inverse distance weighted (IDW) interpolation method (Figure 4b) is affected by the data point cluster, and there is a "duck egg" distribution model or "cow eye" distribution model in which the outlier data is obviously higher than that in the surrounding data points[42]. The radial basis function (FastRBF) interpolation (Figure 4c) is very dependent on the distance from the origin because of its own characteristics, so the error of the deep sample points far away from the origin will increase. In contrast, Kriging (Kringe) interpolation and nearest neighbor (Nearest Neighbors) interpolation have better interpolation effect, which is closer to the actual situation, but the edge of the nearest neighbor (Nearest Neighbors) interpolation image is stacked and square. That is to say, the smoothing effect is poor, which is quite different from the actual form of pollution distribution model. Therefore, 3D krig interpolation achieved the optimal effect.

3.4. Accuracy verification of different interpolation models

Although the Kriging interpolation method is the optimal choice from the effect graph, in order to verify the accurate error of different interpolation models more accurately, the average error (ME) and root mean square error (RMSE) in the cross verification method are usually used to compare the accuracy of different interpolation models. Through cross-verification, it is possible to determine whether the relevant parameters of the interpolation method are reasonable or not, so that the different accuracy of the results obtained by different interpolation models can be compared. The cross-verification method is a method that removes the data of some known sampling points and estimates the points by using the data of other sampling points to test the interpolation accuracy.
Figure 4. Visual model of different interpolation methods of Sb in soil.

a) 3D Kriging (Krig-3D) interpolation; b) inverse distance weighted (IDW) interpolation; c) radial basis function (FastRBF) interpolation; d) nearest point (Nearest Neighbors) interpolation

In the cross-verification, the actual measured values and the predicted values obtained by the interpolation algorithm are used to cross-verify, the errors of the interpolation results are analyzed, and the accuracy of four interpolation models is compared, and the cross-verification results of the interpolation accuracy of the four interpolation models are shown in Table 2. Through the cross-verification results, it can be seen that the average error (ME) and the root mean square error (RMSE) have a positive correlation. The order of validity of the four interpolation methods is Kriging (Krig) interpolation, nearest neighbor (Nearest Neighbors) interpolation, radial basis function (FastRBF) interpolation and inverse distance weighted (IDW) interpolation. The accuracy verification of interpolation results shows that compared with the other three-dimensional spatial interpolation models, Kriging (Krig) interpolation has achieved the optimal prediction effect, and the defined pollution range can be the closest to the actual situation of site pollution, which is effective enough to guide the determination of site repair range and boundary.

Table 2. Prediction error of different interpolation models.

| Interpolation model   | ME   | RMSE  |
|-----------------------|------|-------|
| Krige                 | 3.87 | 10.46 |
| IDW                   | 28.25| 124.45|
| Nearest Neighbors     | 8.41 | 23.93 |
| FastRBF              | 4.09 | 18.68 |
4. Conclusions
In this paper, based on geological modeling and drilling pollution content data, 3D spatial interpolation is carried out. From the display of model effect, the model clearly and intuitively shows the spatial distribution of different pollutants in strata. Compared with the display of two-dimensional plane image graphics, the spatial visualization of pollutants by establishing three-dimensional pollutant spatial model not only shows the vertical position of pollutants more accurately. It can also show the relationship between different boreholes and boreholes more clearly and express the distribution of pollutants more clearly. However, different interpolation models are affected by their algorithms and site drilling data characteristics, and the interpolation results are quite different. Through comparison and cross-verification analysis, it can be seen that Kriging (Krigge) interpolation has achieved the best prediction effect and prediction accuracy, and the pollutant distribution model constructed by this method is more real and closer to the real state.

The application of 3D geological modeling technology in site environmental survey effectively improves the working efficiency and engineering quality. The spatial display of soil monitoring data based on 3D spatial data modeling can quantitatively calculate the volume and mass of a group of soil and chemical substances in geological layer specified by users, which can be used to accurately guide the range of soil remediation, and provide scientific decision support for the design and construction of subsequent work.

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