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An investigation of location continuity of Arsenic metal using the successive Gaussian simulation method

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ABSTRACT

In this article, the hydrochemical effects of the heavy element arsenic in the Ardestan region of Isfahan province have been investigated and described using geostatistical methods. For; this purpose, using the information of 105 sampling locations in the area, preliminary statistics and exploratory-spatial information were obtained, and using the interpolation method of distance squared photo, spatial continuity, and estimation of heavy metal concentration in unknown points were evaluated. Then; taking into account the specific grid in the region and following the modeling and drawing the variogram of the normalized values, consecutive Gaussian simulations were performed so that the results were the closest to reality. The; obtained results show that in the middle part of the study area in two places (well and spring), the amount of arsenic in the underground water is high. In the southwest and middle parts of the region, arsenic is less concentrated, but in the southeast and northeast parts. In; the area towards Ardestan city, the concentration of this metal in water has increased.

1 .Introduction

In spatial statistic methods, each sample is related to its surrounding pieces at a specific distance. According to Geostatistics assumptions, the possibility of similarity between the closer samples is higher. Therefore; it is expected that Geostatistics methods have more estimation considering correlation, location structure of data, and the ability to use equations between variables [1]. Based; on the classical statistics model, the obtained samples from the community are considered random, and the measured value of a specific quantity is not indicative of the value of the same amount in other models within the community. While; in Geostatistics, the importance of a portion can be related to the distance and direction of representatives [2].

Water quality in agriculture is crucial regarding its effect on soil and plants. This; impact is due to chemical and physical impurities in water, which are increased or decreased due to environmental factors. The; waters used for agriculture highly affect the quality of soil and agricultural products [3]. Considering; that removing pollutions of groundwater is costly and time-consuming, and it is diagnosed when almost impossible to be removed from the aquifer, the best solution is determining the quality, preventing pollution, and preventing reducing the quality of these water resources [4]. In; conceptual terms, water quality is properties that affect its proportion for specific uses [5]. The; water used for agriculture is affected

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by the type and value of salts. Hydrogeology; and water resource quality studies have extensively used the Geostatistics method, including [7], [8], [9], and [10].

2. Material and Methods

2.1. Studied area

The study area is a small area located in the Ardestan plane and the structural height and width of Sanandaj-Sirjan, southwest of Ardestan. The; elevations in Ardestan are oriented northwest-southeast toward Shahin Peak in Natanz. The; highest elevation in the study area is Dorochin mountain, with 2947 meters in height, and the most inflated point is in the north of the Ardestan plane, with 978 m in height. Fig; 1 shows the location of the study area.

Fig 1. The location of the study area, Ardestan, in Isfahan province.

1. Results and Discussions

1.1. Primary statistic of data

Statistical parameters are the basis for interpreting the environmental behavior of heavy metals in water. This; research investigated the statistical analysis results of the used sample based on the minimum, maximum, average, variance, standard deviation, skewness, and kurtosis in Minitab 19 software, as shown in Table 1. When; conducting Geostatistics analysis, data should be expected. The; first step in achieving this goal was to sketch the histogram of the elements and then transform the data to a normal distribution using the Gaussian normalization method. Fig 2-A shows the histogram of the central values. It; is evident that the data did not have a normal distribution and had a positive skewness. Also; Fig 2-B shows the standard possibility diagram of the primary data. The; data did not correspond with a one-to-one line, but after normal distribution, they did, and Gaussian transformation was performed appropriately for normalization.

Table 1. Exploratory and preliminary statistics of sampled data.

kurtosis	skewness	variance	standard deviation	Average	Maximum	Minimum	Number	Variable
47.25	6.28	358.28	18.93	7.11	161.17	0.12	105	As

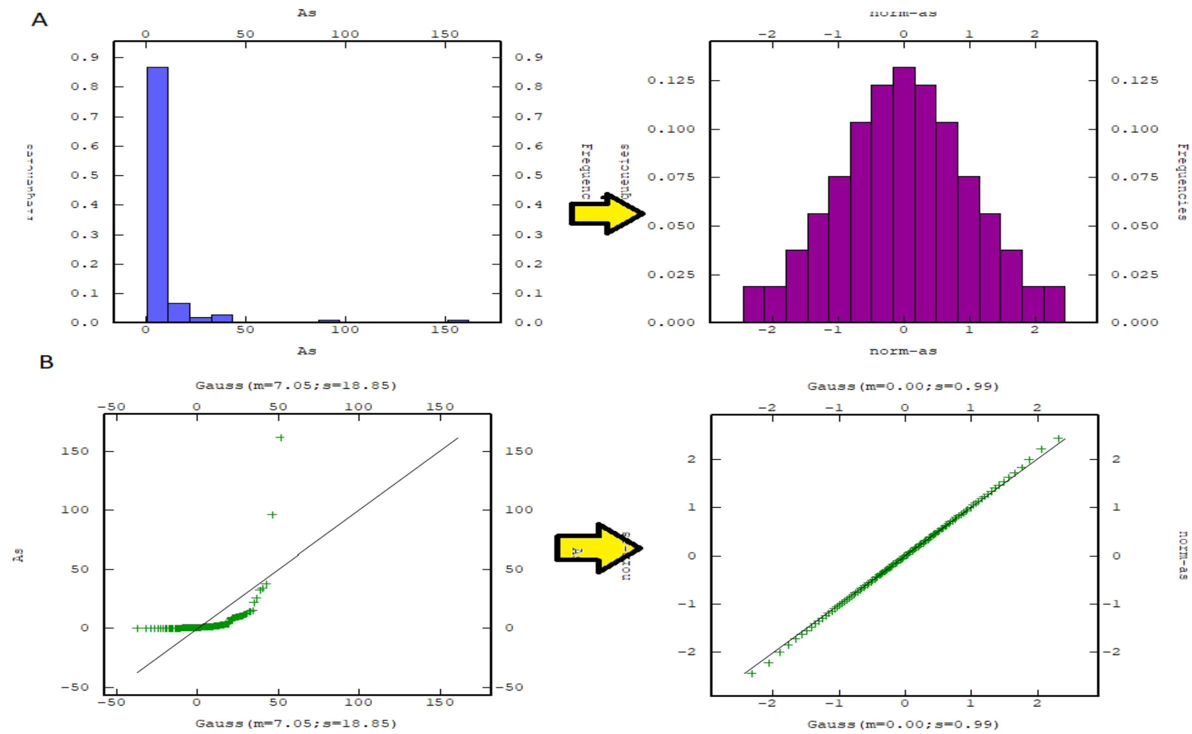

Fig 2. A) Histogram of the central and standard data using the Gaussian transformation, B) Possibility diagram of the regular and central data.

3.2. Discuss and interpretation

To evaluate time-spatial variations in the density of studied heavy metals, a dispersion map of the sampling points' locations was first drawn (Fig 3-A). In; an addition to having an overall vision of the region considering sampling data, Inverse Distance Interpolation was conducted (Fig 3-B). According to data from analyzing groundwater samples, the minimum density of arsenic was 0.12, and its maximum was 161 micrograms/lit. Regarding; the dispersion distribution map (Fig 3-A) and interpolation; of the Arsenic density (Fig 3-B), the arsenic in groundwater has increased in two locations, including the southeast and northeast of the region to the Ardestan city. In contrast, the density of arsenic is lower in the southwest and middle parts of the area. In; To obtain a more accurate analysis, successive Gaussian simulations were conducted. The location exceeding allowable values was determined based on the diagram depicting the possibility of values exceeding the 0.05 mg/lit threshold.

3.3. Arsenic spatial distribution (As)

A better understanding of the spatial distribution of the arsenic density and its variation requires cartography and successive Gaussian simulation in the study area. Fig; 4-A shows the Variogram to study the location continuity of the arsenic. In; this regard, the empirical model was fitted with cubic, spherical, and exponent models, and the model with minimum error, best fitting, and the minimum difference from the experimental model was selected for modeling. A; correlation diagram of estimated values versus primary values should be drawn to verify the Variogram. As; shown in Fig 4-B, the correlation value is 0.79, a high amount. Fig; 4-C shows that the histogram of the remaining error is non-skewed and has a normal distribution. The; information from this step is used for the Gaussian simulation.

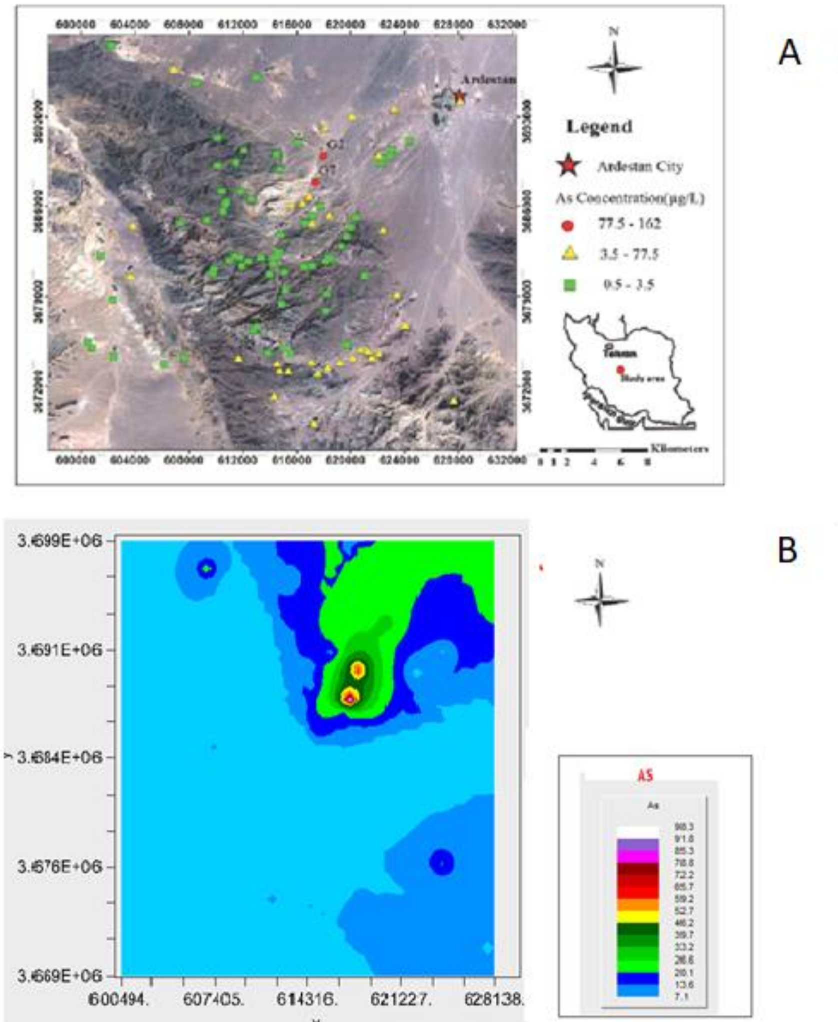

Fig 3. A) Dispersion of arsenic, B) Inverse Distance Interpolation in the study area.

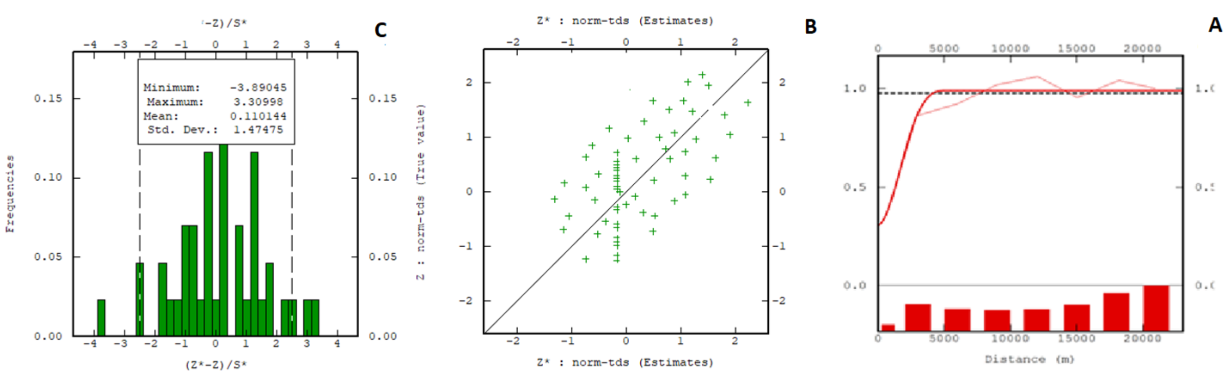

Fig 4. A) Variogram diagram of the average values of arsenic B) Correlation diagram C) Remaining values histogram.

3.4. Sequential Gaussian simulation

After data normalization and drawing vario gram, the meshing of the study area is required for the successive Gaussian simulation. The; origin of the simulation mesh, the size of the mesh, the number of cells arranged in three spatial orientations, and the rotation angle toward the north should be determined when creating the simulation mesh. A; parameter that can be used to determine the dimensions of cells is the minimum computed step. In; particular, the size of the cells should be selected in a manner that includes all sampling points. The; mesh and cell dimensions of the study area are shown in Fig 5. For; a more accurate examination, the average of different created states in the Gaussian simulation should be calculated.

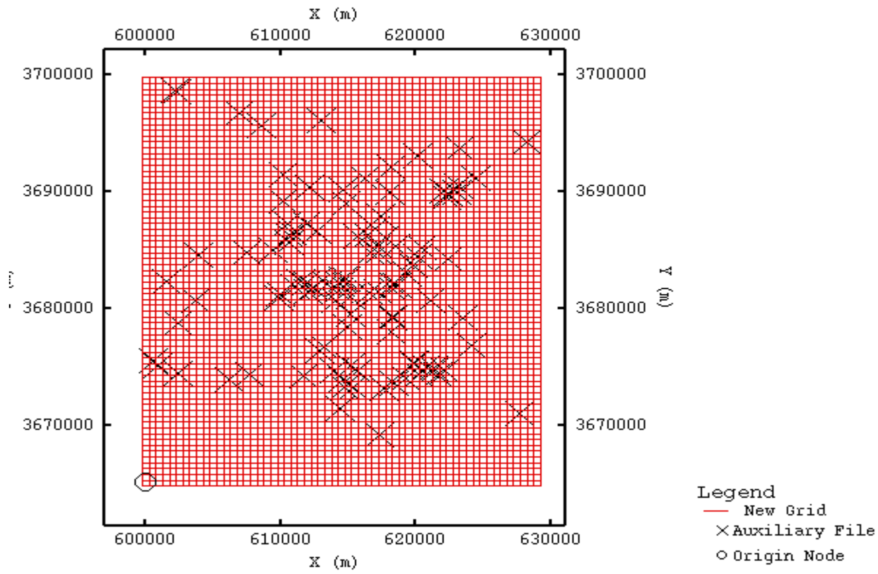

Fig 5. The study area meshing (dimension, properties, and cells number).

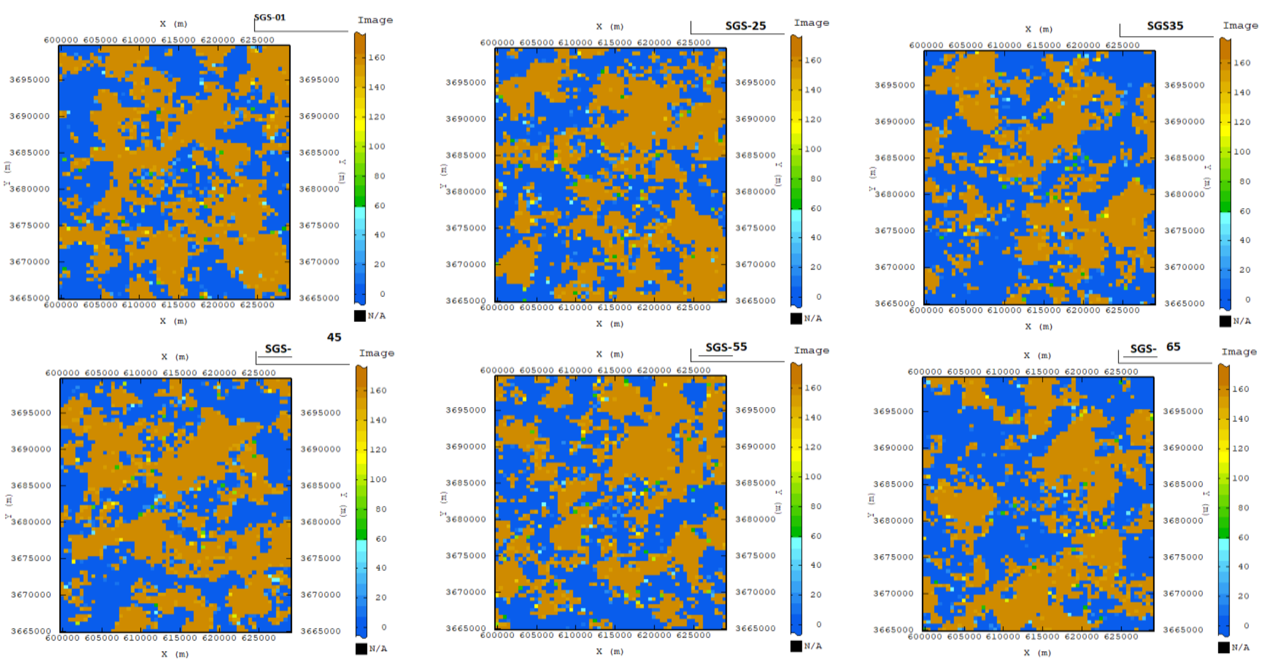

Fig 6. Different substantiations of the successive Gaussian simulation.

3.5. Expectation (simulation average) and uncertainty map

As mentioned earlier, the standard of different values of arsenic was calculated in each cell for 100 simulation substantiations. Fig; 7-A is the diagram of the Gaussian simulation in the study area.
According to the drinking water standard EPA, the maximum arsenic density in water should equal 0.05 mg/lit. According to Fig 7-B, most samples in the southwest and middle parts of the region have arsenic levels below the allowable value, with arsenic levels exceeding the EPA standard only in the southeast and northeast parts.

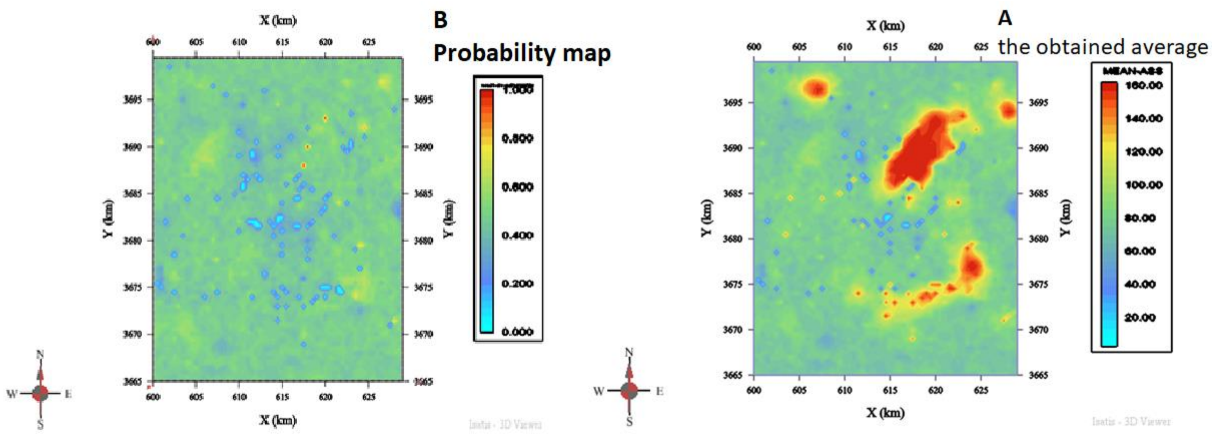

Fig 7. A) The obtained average from the Gaussian simulation B) Diagram of the uncertainty of the arsenic above the allowable value.

4. Conclusion

Geostatistics methods are appropriate for analyzing the results obtained from the decomposition of the groundwater specimen. They can be used as additional tools in decision-making spatial variation of water quality variables. In; Geostatistics methods, after data normalization, the proper model for fitting to the empirical variogram is selected based on the minimum error and the interpolation method, based on data monitoring. This; research tried to use sampling results from 105 sampling areas, including an aqueduct, spring, and deep well, to evaluate the pollution of the arsenic, and heavy metal value and determine locations where this value exceeds the limitation. Based; on the simulations by the Gaussian model for investigating the location continuity of the element in the study area, the results show that in the middle part of the study area in two places (well and spring), the arsenic value in the groundwater is high. It; is lower in the southwest and middle part of the region, while the density of this metal has increased in the southeast and northeast toward Ardestan city.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Conflicts of interest/Competing interests

No potential conflict of interest was reported by the authors.

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