

ГЕОЛОГІЧНА ІНФОРМАТИКА

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STATISTICAL SIMULATION OF RANDOM FIELD ON 2D AREA WITH GENERALIZED GNEITING TYPE CORRELATION FUNCTION IN THE GEOPHYSICAL PROBLEM OF ENVIRONMENT MONITORING

(Представлено членом редакційної колегії д-ром геол. наук, ст. дослідником О.І. Меньшовим)

Due to the increasing number of natural and technogenic disasters the development of geological environment monitoring system is actual using modern mathematical tools and information technology.

The local monitoring of potentially dangerous objects is an important part of the overall environment monitoring system.

Complex geophysical research was conducted on Rivne NPP area. Among these monitoring observations radioisotope study of soil density and humidity near the perimeter of buildings is of the greatest interest.

In this case a problem was occurred to supplement simulated data that were received at the control of chalky strata density changes at the research industrial area with use of radioisotope methods on a grid that included 29 wells.

This problem was solved in this work by statistical simulation method that provides the ability to display values (random field on a plane) in any point of the monitoring area. The chalk strata averaged density at the industrial area was simulated using the built model and the involvement optimal in the mean square sense correlation function generalized Gneiting type.

In this paper the method is used and the model and procedure were developed with enough adequate data for generalized Gneiting type correlation function.

The model and algorithm were developed and examples of karst-suffusion phenomena statistical simulation were given in the problem of density chalk strata monitoring at the Rivne NPP area. The statistical model of averaged density chalk strata distribution was built in the plane and statistical simulation algorithm was developed using generalized Gneiting type correlation function based on spectral decomposition. The research subject realizations were obtained with required detail and regularity at the observation grid based on the developed software. Statistical analysis of the numerical simulation results was done and tested for its adequacy.

Keywords: Statistical simulation, generalized Gneiting type correlation function, spectral decomposition, conditional maps.

Introduction. Due to the increasing number of dangerous natural and technogenic disasters the development of geological environment monitoring system is actual using modern mathematical tools and information technology.

The local monitoring of potentially dangerous objects is an important part of the overall environment monitoring system.

When monitoring of such objects a lot of problems were raised, for example, such as the lack of some data in the database, or insufficient quantity or necessity to supplement the database without conducting additional research.

The Department of Geophysics at Institute of Geology and involved experts from Faculty of Mechanics and Mathematics of Taras Shevchenko National University of Kyiv in recent years developed theoretical and methodological application basics of statistical simulation in the development of geological environment monitoring.

Theoretical aspects of capacity use of statistical simulation of solving problems in the work of Geophysics are considered in (Yadrenko, 1983; Grikh (Vyzhva) et al., 1993; Vyzhva, 2003, 2011). Practical testing on real data density chalky strata on the territory of the Rivne NPP was carried out for the fields on the plane - in the (Vyzhva et al., 2004), but using only Bessel correlation function and Cauchy functions (Vyzhva et al., 2014, 2017) and the Whittle-Matern type correlation function (Vyzhva et al., 2019). In this paper, the method and the model and procedure involving enough adequate *in the mean square sense* data correlation function generalized Gneiting type (Gneiting, 1997; Gneiting et al., 2010; Vyzhva et al., 2021) are used.

We should note, that methods of random field's statistical simulation were used in geosciences problems in works:

(Mantoglov, Wilson, 1981; Chiles, Delfiner, 1999; Gneiting, 1997; Gneiting et al., 2010; Wackernagel, 2003; Vyzhva et al., 2010, 2017) and other.

Problem of karst-suffusion phenomena monitoring at Rivne NPP area. The complex geophysical research was conducted on Rivne NPP area. Among these monitoring observations radioisotope study of soil density and humidity near the perimeter of buildings is of the greatest interest. The soil density was determined by gamma-gamma well logging, soil humidity - by neutron-neutron logging.

In this case (Vyzhva et al., 2017) a problem occurred to supplement simulated data that were received at the control of chalky strata density changes at the research industrial area with use of radioisotope methods on a grid that included 29 wells. Schematic representation of the measurement results at the object that was investigated, and the well locations are shown on Fig. 1. These data are obviously not enough to represent the overall picture of the chalk strata, where due to the aggressive water action the karst-suffusion processes were significantly intensified.

This problem was solved in works (Vyzhva et al., 2004) and (Vyzhva et al., 2017) by statistical simulation method that provides the ability to display values (random field on a plane) in any point of the monitoring area. The chalk strata averaged density at the industrial area was simulated using the built model and the involvement of the Bessel type correlation function (Vyzhva et al., 2004), Cauchy correlation function (Vyzhva et al., 2016, 2017) and the Whittle-Matern type correlation function (Vyzhva et al., 2019).

This work continues development of methods for statistical simulation, involving optimal in the mean square

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sense correlation function generalized Gneiting type that is well-known in geostatistic works (Chiles, Delfiner, 1999; Gneiting, 1997; Gneiting et al., 2010).

This operation was done for data array of density chalk strata in 1984-2002 years' for 29 wells at Rivne NPP industrial area and depth is 28 m below the surface.

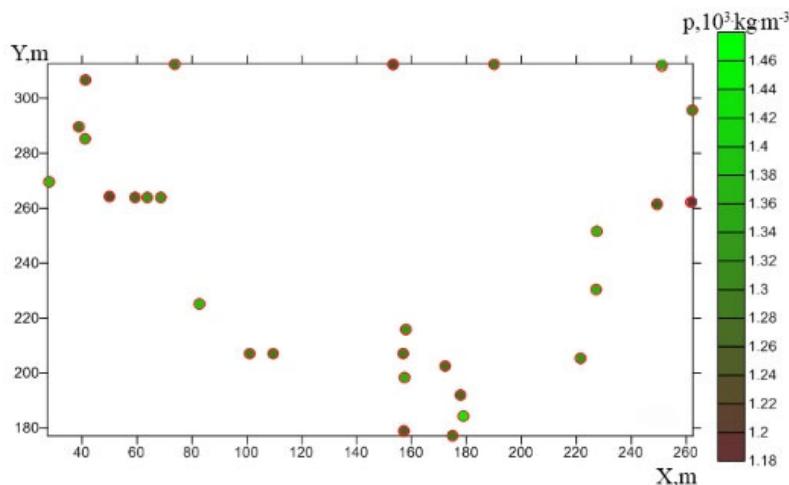


Fig. 1. Observation points and chalk strata averaged density at industrial area of Rivne NPP

The method of solving the problem. Data of density chalky strata was divided (Vyzhva et al., 2017) into deterministic and random components. Deterministic function can be selected by the method of approaching the minimum curve (separation of the trend). The difference between the map of input density values and the trend is in most cases a homogeneous isotropic random field. With the assumption that the input data is a random field $\eta(\bar{x})$, then we express them through a random component $\xi(\bar{x})$ (so-called "noise" random field) and trend $f(\bar{x})$ as a deterministic function as follows:

$$\eta(\bar{x}) = f(\bar{x}) + \xi(\bar{x})$$

Thus, the problem has been reduced to simulation of random component $\xi(\bar{x})$, which in most cases is a homogeneous and isotropic.

Consider the same approach as in (Grikh (Vyzhva) et al., 1993; Vyzhva et al., 2004; Vyzhva, 2011). We use the method of statistical simulation of random fields, which are homogenous and isotropic, based on their spectral decomposition. By means of the obtained values of realizations, this technique allows to find the perfect image of these isotropic fields in the whole observation interval.

It is necessary to make the statistical analysis to build the model and procedure of statistical data simulation at observation area. If the verified data has distribution density with approximately Gaussian type, then procedure can be used, which is developed in (Grikh (Vyzhva) et al., 1993; Vyzhva et al., 2004; Vyzhva, 2011) to generate on the computer realizations of the simulated data by means of standard normal random variable sequences.

At first the distribution is determined. The preliminary statistical analysis of data shows that the distribution histogram of chalky strata density at the Rivne industrial area (29 boreholes) approximately has Gaussian distribution (Fig. 2).

The use of authors' techniques of statistical simulation implies preliminary statistical data processing to determine its statistical characteristics: the mathematical expectation and the correlation function. If the hypothesis of Gaussian distribution of the investigated field is confirmed, then the mathematical expectation and the correlation function completely define this field and give us the opportunity to build the adequate statistical model, which is based on spectral decomposition of random functions. The principles of constructing the models and procedures are described below.

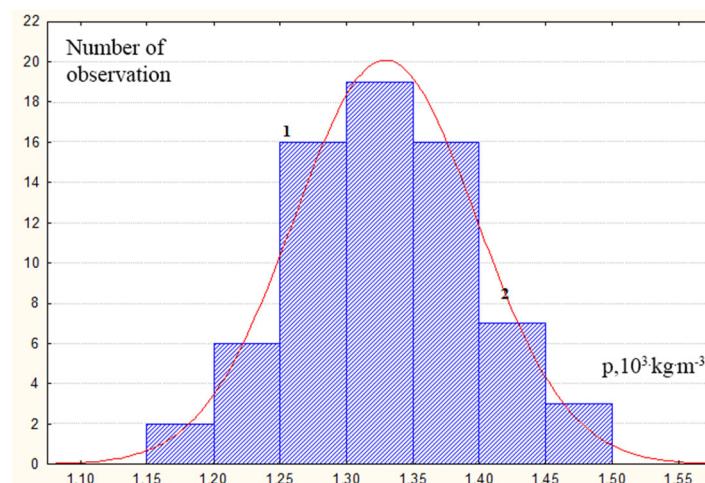


Fig. 2. Histogram of the chalky strata density (averaged data for all years of observation):
1 – the number of observations in a separate range of density; 2 – theoretical Gaussian curve

Then statistical models were chosen for the data correlation function for distribution of chalky strata density in the flat observation area. This function is defined by comparing the mean square approximation of the empirical and theoretical variograms. As result the input data was most adequately described by means of 5 types of correlation functions: the holeeffect correlation function (1) at the value of parameter $c = 1,4$, the Bessel correlation function (2) at the value of parameter $a = 5$, the Cauchy correlation function (3) at the value of parameter $a = 1$, the Whittle-Matern type correlation function (4) at the value of parameter $c = 1$:

$$B(\rho) = \exp(c\rho)\cos(c\rho), \quad c = 1,4; \quad (1)$$

$$B(\rho) = J_0(a\rho), \quad a = 5; \quad (2)$$

where $J_k(x)$ is the Bessel function of the first kind of order $k = 0$.

$$B(\rho) = \frac{a^4}{(a^4 + \rho^2)^2}, \quad a = 1; \quad (3)$$

$$B(\rho) = \frac{2^{1-\frac{3}{2}}}{\Gamma(\frac{3}{2})} (c\rho)^{\frac{3}{2}} K_{\frac{3}{2}}(c\rho), \quad c = 1; \quad (4)$$

where $K_{\frac{3}{2}}(z)$ is a modified Hankel function of order $3/2$ and c is parameter.

In this paper we used enough adequate data generalized Gneiting type correlation function:

$$B(\rho) = (1 + 7\rho)(1 - \rho)^7, \quad 1 \geq \rho \geq 0. \quad (5)$$

Note that the generalized Gneiting family model (Gneiting, 1997) is:

$$B(\rho) = (1 + (b + 1)\rho)(1 - \rho)^{(b+1)}, \\ b \geq \frac{d+2a+1}{2}, \quad d = 2, a = 1, \quad (6)$$

where a and b are parameters, d is dimension of space.

Then such spectral density $f(\lambda)$ for homogeneous isotropic random field $\xi(\vec{x})$ in 2D space is calculated (Vyzhva et al., 2017) by conducting the following formula:

$$f(\lambda) = \lambda \int_0^\infty x J_0(\lambda x) B(x) dx, \quad (7)$$

where $J_k(x)$ is the Bessel function of the first kind of order $k = 0$.

Thus the spectral density, which is corresponding to the generalized Gneiting type correlation function (5), is by using (7):

$$f(\lambda) = \lambda \int_0^\infty \rho J_0(\lambda\rho)(1 + 7\rho)(1 - \rho)^7 d\rho. \quad (8)$$

The spectral coefficients of generalized Gneiting correlation function, which according to correlation function (5), are determined by calculating the integral:

$$b_k(r) = \frac{2}{\pi} \int_0^\pi (1 + 14r \sin \varphi)(1 - 2r \sin \varphi)^7 \cos 2k\varphi d\varphi \quad (9)$$

Note, that we used the formula for spectral coefficients as an integral of correlation function (Grikh (Vyzhva) et al., 1993):

$$b_k(r) = \frac{2}{\pi} \int_0^\pi B(2r \sin \varphi) \cos 2k\varphi d\varphi. \quad k = 1, 2, \dots \quad (10)$$

Variograms figures of input data of chalky strata density, that correspond to the: holeeffect (1) correlation function (the mean square approximation is 0,000742); Bessel (2) correlation function (the mean square approximation is 0,0008599); Cauchy (3) correlation function (the mean square approximation is 0,002816) were given in paper (Vyzhva et al., 2019). Variograms of this input data, that correspond to the Whittle-Matern type correlation function (4) (the mean square approximation is 0,000311), were built by using the R software and geoR package. Plots were presented at Figure 3, according to this types correlation function variograms of the random component of investigation data.

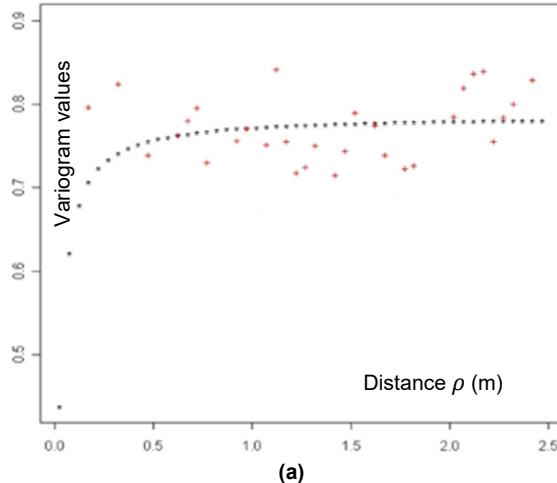


Fig. 3. Variograms of input data of the chalky strata, that corresponding to the:

(a) the Cauchy (3) correlation function at the value of parameter $a = 1$ (standard deviation - 0,002816);

(b) the Whittle-Matern type (4) correlation function at the value of parameter $c = 1$ (standard deviation - 0,000311)

$$\text{where: } v_k = \begin{cases} 1, & k = 0 \\ 2, & k > 0 \end{cases}$$

• r and φ ($r \in R_+$, $\varphi \in [0, 2\pi]$) are polar coordinates of the point x on the plane (includes observation area), and the distance ρ between the points $x_1 = (r_1, \varphi_1)$ and $x_2 = (r_2, \varphi_2)$ equals

$$\rho = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\varphi_1 - \varphi_2)};$$

• N is an integer number (the number of the summands in the model), the value of N is determined by the prescribed small number ε (approximation accuracy) by the inequality from paper (Grikh (Vyzhva) et al., 1993), which is the

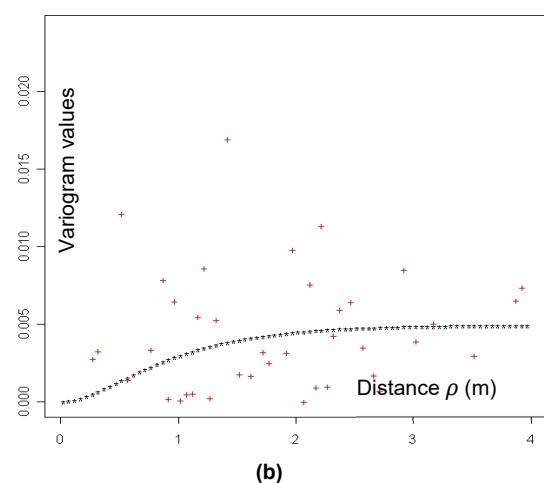
$$\rho = \sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos(\varphi_1 - \varphi_2)};$$

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The model of random field on 2D area with the generalized Gneiting type correlation function and the numerical simulation procedure. The realizations of random field $\xi(\vec{x}) = \xi(r, \varphi)$ on 2D area with the correlation function generalized Gneiting type (5) are generated. The statistical simulation was performed by the technique of spectral decomposition and finding of spectral coefficients.

From the spectral theory (Vyzhva, 2011) it follows that the model of random fields on a plane with such correlation functions is a sum of:

$$\xi_N(r, \varphi) = \sum_{k=0}^N \sqrt{v_k b_k(r)} [\zeta_k(r) \cos k\varphi + \eta_k(r) \sin k\varphi] \quad (11)$$



estimate of the mean square approximation of random field $\xi(r, \varphi)$ by partial sums $\xi_N(r, \varphi)$;

• $b_k(r)$ ($k = 0, 1, 2, \dots, N$) are the spectral coefficients in form of (9), which correspond to correlation function generalized Gneiting type (5) of random field $\xi(r, \varphi)$.

The procedure of numerical simulation the realizations of the data field random component, by means of the abovementioned model (11), was conducted by using the Spectr 2.1 software, which is described in (Vyzhva et al., 2004).

The value of number N for the constructed model is determined by the inequality, which is the estimate of the mean square approximation of random field $\xi(r, \varphi)$ by partial sums $\xi_N(r, \varphi)$. This number N corresponds to the prescribed small number ε (approximation accuracy). The mentioned inequality was obtained in work (Grikh (Vyzhva) et al., 1993) and in form of:

$$M[\xi(r, \varphi) - \xi_N(r, \varphi)]^2 \leq \frac{1}{\pi N} (r\mu_1 + r^2\mu_2), \quad (12)$$

where $\mu_k = \int_0^\infty \lambda^k f(\lambda) d\lambda$, ($f(\lambda)$ - is spectral density of the random field $\xi(r, \varphi)$). (13)

We define dependence number N on r and ε in the case of generalized Gneiting type correlation function (5). It is necessary to calculate the values of μ_k , $k = 1, 2$ for the inequality (7), by using the density of distribution (8).

Then the calculated values ($B(\rho)$ - generalized Gneiting type correlation function (5)) hold:

$$\mu_1 = \int_0^\infty \lambda f(\lambda) d\lambda = \int_0^\infty \lambda^2 \int_0^\infty x J_0(\lambda x) B(x) dx d\lambda; \quad (14)$$

$$\mu_2 = \int_0^\infty \lambda^2 f(\lambda) d\lambda = \int_0^\infty \lambda^3 \int_0^\infty x J_0(\lambda x) B(x) dx d\lambda. \quad (15)$$

Consequently, the estimate of the mean square approximation of the random field $\xi(r, \varphi)$ with generalized Gneiting type correlation function (5) by the partial sums $\xi_N(r, \varphi)$ has the following representation:

$$N(r, \varepsilon) \geq \frac{1}{\pi \varepsilon} \left(\frac{1}{2} r\mu_1 + r^2\mu_2 \right), \quad (16)$$

where μ_k , $k = 1, 2$ are the values (14) and (15).

The statistical simulation procedure of Gaussian homogeneous isotropic random field $\xi(r, \varphi)$ on the plane was built by means of the model (11) and the estimate (12). This random field is determined by its statistical characteristics: the mathematical expectation and the generalized Gneiting type correlation function $B(\rho)$ (5).

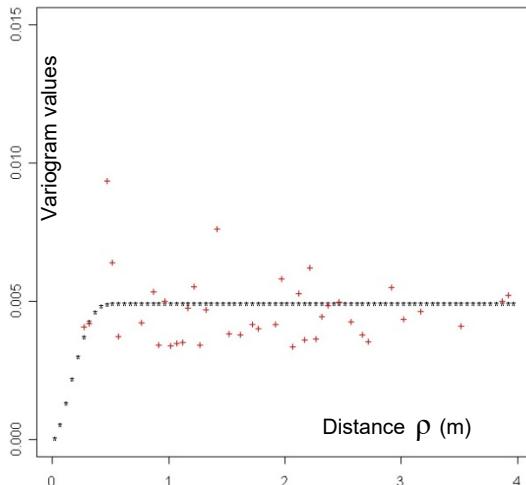


Fig. 4. Semivariogram of separated random component input data of the chalky strata density, that corresponding to the generalized Gneiting type correlation function at values of parameter $a = 1$ (standard deviation 1,51E-06)

Procedure.

1) The positive integer number N is determined corresponding to the prescribed accuracy ε and by using inequality (16), where r is a radius of the point on the plane in which the realization of the random field $\xi(r, \varphi)$ is generated. The integer number N equals 59 by using the prescribed accuracy $\varepsilon = 5 \times 10^{-2}$.

2) We calculated the spectral coefficients $b_k(r)$ ($k = 0, 1, 2, \dots, N$), $N = 59$, in form of (9), which correspond to generalized Gneiting type correlation function (5).

3) We generate values of the standard normal random variables $\{\zeta_k, k = 0, 1, 2, \dots, 59\}$ and $\{\eta_k, k = 0, 1, 2, \dots, 59\}$.

4) We calculate the realization of the random field $\xi(r, \varphi)$ in points (r_i, φ_j) , $i = 1, \dots, 10$; $j = 0, \dots, 9 \in R^2$ and evaluate the expression (11) by substituting in it values which were found in the previous steps, $r_i = 0.1 \times i$, $i = 1, \dots, 10$; $\varphi_j = j \times \frac{2\pi}{10}$, $j = 0, \dots, 9$.

5) The statistical estimate of the correlation function is obtained by the realizations of the random $\xi(r, \varphi)$. This estimate compares with a given generalized Gneiting type correlation function (5) and provides the statistical analysis the adequacy of realization.

Note that the procedure can be applied to random fields with another type of distribution. Then the random variables $\{\zeta_k(r), k = 0, 1, 2, \dots, N\}$ and $\{\eta_k(r), k = 0, 1, 2, \dots, N\}$ should be distributed by corresponding type of distribution.

The original Spectr software, based on the results of the statistical data processing and the mentioned procedure for the simulation values of such data realization in the two-dimensional case, was developed in Python, where selected generalized Gneiting type correlation function (5) was used.

The following Fig. 4 presents the semivariogram plot of the separated random data component of chalky strata density according to the generalized Gneiting type correlation functions (5).

Fig. 5 presents the variogram plot of the simulated random data component of chalky strata density according to the generalized Gneiting type correlation functions (5).

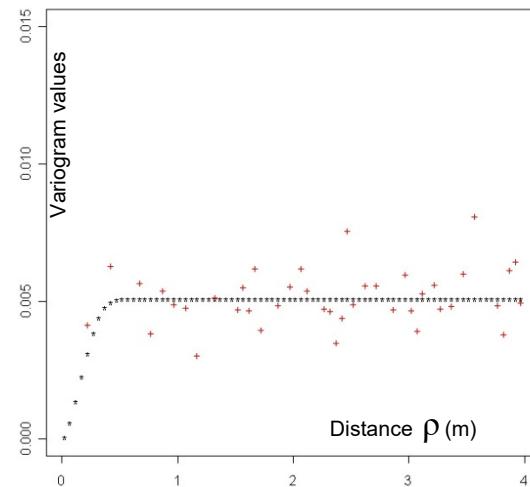


Fig. 5. Semivariogram of simulated data arrays of the chalky strata density, that corresponding to the generalized Gneiting type correlation function at values of parameter $a = 1$ (standard deviation 1,01E-06)

The results, which were obtained by the simulating procedure, are displayed in Figure 6. Figure 6 (a) presents an example of constructed map of chalky strata density according to observations data boreholes (averaged data over the years to 29 boreholes at 28 m) by Surfer software. Using available data accuracy of this construction cannot provide a reliable characteristic of the chalky strata status, because the number of measurement results is not sufficient.

Fig. 6 (b) presents the contours of equal values of chalky strata density based on simulated data including values of the anchor boreholes by means of calculating the spectral coefficients of generalized Gneiting type correlation function. Additionally, the output data (160 simulated values in intervals between the observation points of this level) can have more reliable approximation that enables more informed decisions about the status of chalky strata and determines places for testing and additional research.

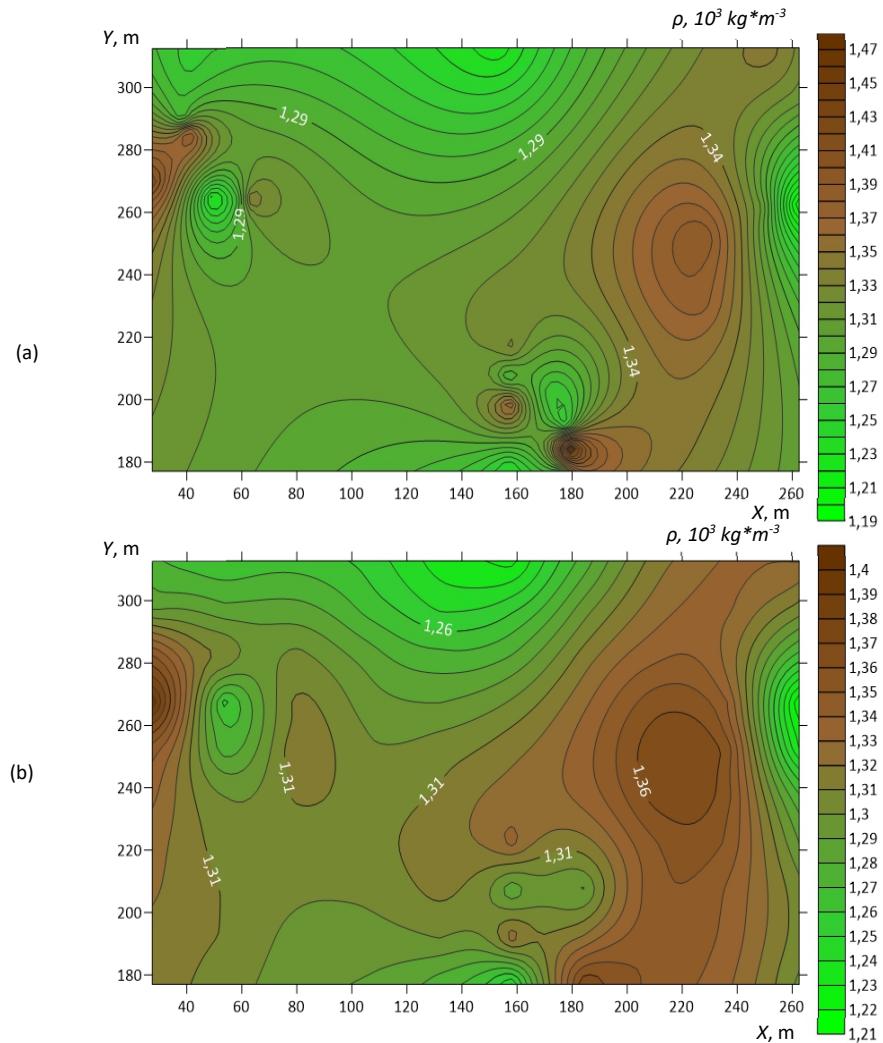


Fig. 6. The distribution of chalky strata density is on the industrial area of Rivne nuclear power plant at a depth of 28 m from the surface, according to the averaged data of 29 observational boreholes over 1984–2004 years (a), for the simulated data based on the values in secure boreholes by generalized Gneiting type spectral coefficients (b)

The results present that the chosen model of the chalky strata density data is rather adequate (standard deviation 1,01E-06). The developed Spectr2_1 software works with sufficient accuracy.

Conclusions. The theory, techniques and procedure of statistical simulation of random fields on the plane by using optimal in the mean square sense the generalized Gneiting type correlation function can significantly increase the effectiveness of monitoring observations on the territory of potentially dangerous objects. This makes it possible to simulate the values in the area between regime observation grids and abroad, adequately describe real geological processes.

The method of statistical simulation of random fields with the generalized Gneiting type correlation function allows complementing data with a given accuracy. It can also be used to detect abnormal areas.

There are several other fields of statistical simulation methods application in geosciences. Among them primary are soil science and environmental magnetism (Menshov *et al.*, 2015).

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**СТАТИСТИЧНЕ МОДЕЛЮВАННЯ ВИПАДКОВОГО ПОЛЯ В ДВОВИМІРНІЙ ОБЛАСТІ
 З КОРЕЛЯЦІЙНОЮ ФУНКЦІЄЮ УЗАГАЛЬНЕНЕГО ТИПУ ГНЕЙТИНГА
 В ГЕОФІЗИЧНІЙ ЗАДАЧІ МОНІТОРИНГУ ДОВКІЛЛЯ**

У зв'язку зі зростанням кількості природно-техногенних катастроф актуальною є розробка систем моніторингу за станом геологічного середовища з використанням сучасного математичного апарату та інформаційних технологій. У загальній системі моніторингу доведілося важливою складовою є локальний моніторинг територій розташування потенційно небезпечних об'єктів.

На території розміщення Рівненської АЕС проводиться комплекс геофізичних досліджень. Серед таких моніторингових спостережень найбільший інтерес становлять радіоізотопні дослідження густини та вологості ґрунтів по периметру збудованих споруд. Водночас виникла проблема доповнення моделюванням даних, які отримано при контролі зміни густини крейдяної товщі на території дослідженого проммайданчика з використанням радіоізотопних методів по сітці, що включала 29 свердловин. Таку проблему було вирішено у роботі методом статистичного моделювання, який надає можливість відобразжати явище (випадкове поле на площині) у будь-які точці області спостереження. При цьому моделювалися усереднені значення густини крейдяної товщі на території проммайданчика із використанням побудованої моделі та запущенням оптимальної в середньому квадратичному наближенні кореляційної функції узагальненого типу Гнейтінга.

Розроблено алгоритм та приклад статистичного моделювання карстово-суфозійних явищ у задачі моніторингу густини крейдяної товщі на території Рівненської АЕС. За спектральним розкладом побудовано статистичну модель розподілу усередненої густини крейдяної товщі на площині та розроблено алгоритм статистичного моделювання з використанням функції узагальненого типу Гнейтінга. На базі розробленого програмного забезпечення реалізації предмета дослідження на сітці спостережень отримано необхідну детальності та регулярність. Проведено статистичний аналіз результатів чисельного моделювання та їх перевірка на адекватність.

Ключові слова: статистичне моделювання, кореляційна функція узагальненого типу Гнейтінга, спектральний розклад, кондіційність карт.