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Zoya VYZHVA[1], DSc (Phys.-Math.), Prof.
ORCID ID: 0000-0002-6338-3892
e-mail: zoya_vyzhva@ukr.net

Vsevolod DEMIDOV[1], PhD (Phys.-Math.), Assoc. Prof.
ORCID ID: 0009-0003-9472-6530
e-mail: demidov@knu.ua

Andrii VYZHVA[2], PhD (Phys.-Math.), Senior Researcher
ORCID ID: 0009-0003-6699-5848
e-mail: motomustanger@ukr.net

Tetiana SHOVKOPLIAS[1], PhD (Phys.-Math.), Assist. Prof.
ORCID ID: 0009-0004-8991-0285
e-mail: 1zagmat.tetyana1@knu.ua

[1]Taras Shevchenko National University of Kyiv, Kyiv, Ukraine
[2]SE "Naukanaftogaz", Kyiv, Ukraine

THE STATISTICAL SIMULATION OF DATASET IN 3D AREA WITH PENTAMODEL TYPE VARIOGRAM TO RIVNE NPP GEOPHYSICAL MONITORING

(***Представлено членом редакційної колегії д-ром геол. наук, ст. дослідником Олександром МЕНЬШОВИМ***)

B a c k g r o u n d ***. This paper presents a statistical modeling approach for three-dimensional spatial data using a pentamodel type variogram, which provides an optimal mean-square approximation. The proposed method is applied to supplement geophysical survey data for karst-suffusion processes in monitoring the density of the chalk stratum in the Rivne Nuclear Power Plant (RNPP) area. A comprehensive set of geophysical investigations was conducted in the RNPP site area.***

Among these investigations, radioisotope measurements of soil density and moisture around the constructed facilities are of primary interest. However, the available observation dataset, derived from 29 wells using radioisotope methods, was insufficient for high-resolution density characterization.

To address this limitation, a statistical modeling technique based on the pentamodel variogram was employed, enabling the reconstruction of the random field representing the studied parameter at any point within the 3D domain of interest.

M e t h o d s ***. A statistical model of the averaged density distribution of the chalk stratum within the study area was developed using the spectral decomposition of random fields in 3D space. The algorithm allows for generating realizations of random fields with predefined correlation structures, ensuring spatial discretization consistent with the required accuracy and resolution for geophysical monitoring applications.***

R e s u l t s ***. An algorithm for statistical modeling of random fields with pentamodel type correlation functions was formulated and implemented. Using the developed software, additional realizations of the random component of the chalk density field were generated on a regular observation grid with the desired level of detail. A comparison of a set of correlation functions for one data set in mean-square was performed. A statistical analysis of the simulated results was performed, including validation against the original observation data and an assessment of the adequacy and convergence of the modeled fields.***

C o n c l u s i o n s ***. The proposed statistical modeling method, based on pentamodel type correlation functions, provides a robust framework for supplementing sparse geophysical datasets with high accuracy. This approach significantly improves the reliability of density distribution estimates and can be effectively applied to geophysical monitoring and the interpretation of spatially distributed geological parameters.***

K e y w o r d s ***: Statistical simulation, pentamodel variogram, spectral decomposition, conditional maps, Rivne Nuclear Power Plant (RNPP).***

Background

The study of hazardous natural and anthropogenic phenomena and disasters represents a critical scientific challenge that requires the implementation of comprehensive environmental monitoring systems, including geological monitoring, supported by modern mathematical methods, information technologies, and analytical tools. In the context of monitoring potentially hazardous anthropogenic facilities, several significant issues arise, such as the temporal and spatial irregularity of data, incomplete databases, insufficient data volume, and the need to supplement existing datasets with the required spatial resolution without conducting additional field investigations.

The theoretical foundations of statistical modeling methods based on spectral decomposition of random fields for solving various applied problems have been extensively discussed in the literature (Yadrenko, 1983; Guyon, 1993; Chiles, Delfiner, 2012; Vyzhva, 2003, 2011, 2021).

In several studies by the authors, practical investigations were carried out using measured chalk density data within a three-dimensional domain at the Rivne Nuclear Power Plant (RNPP) site. Various correlation functions were applied, including the Bessel correlation function (Vyzhva, Demidov, & Vyzhva, 2013), the Cauchy correlation function (Vyzhva et al., 2014b), the spherical correlation function (Vyzhva, Demidov, & Vyzhva, 2020), the "cubic" correlation function (Vyzhva, Demidov, & Vyzhva, 2024), and the pentamodel type correlation function (Vyzhva et al., 2023).

In this study, we propose an enhanced method and algorithm for numerical modeling of random field realizations using pentamodel type correlation functions. It is worth noting that statistical modeling methods for three-dimensional random fields applied in Earth sciences have been developed by numerous researchers, including Mantoglou, & Wilson (1981), Wackernagel (2003), Emery (2006), Webster, & Oliver (2007), Chiles, & Delfiner (2012), and Tolosana-Delgado, & Mueller (2021), among others.

Current challenges in monitoring karst-suffusion Processes at the Rivne NPP. The problem of modeling random fields in a three-dimensional domain arises when addressing critical tasks of ecological and geophysical monitoring. Over the years, a comprehensive series of geophysical studies has been conducted in the area of the Rivne Nuclear Power Plant (RNPP). Among these monitoring activities, the most significant are radioisotope investigations of soil density and moisture around the perimeter of constructed facilities at the site. Soil density was determined using the gamma-gamma logging method, while soil moisture was measured by neutron-neutron logging.

Geophysical monitoring studies are conducted periodically over an extended time within the industrial zone of the Rivne NPP (Vyzhva et al., 2010). For the monitoring program described in Vyzhva, Demidov, & Vyzhva (2013, 2014a), a key challenge was the need to supplement the dataset obtained from radioisotope-based control of chalk density variations within the industrial testing site using a grid of 29 wells. A schematic representation of the measured chalk density values and the well locations at the RNPP site is presented in Fig. 1. These data are insufficient to fully characterize the state of the chalk strata in the study area, where karst-suffusion processes have been significantly intensified by aggressive groundwater activity.

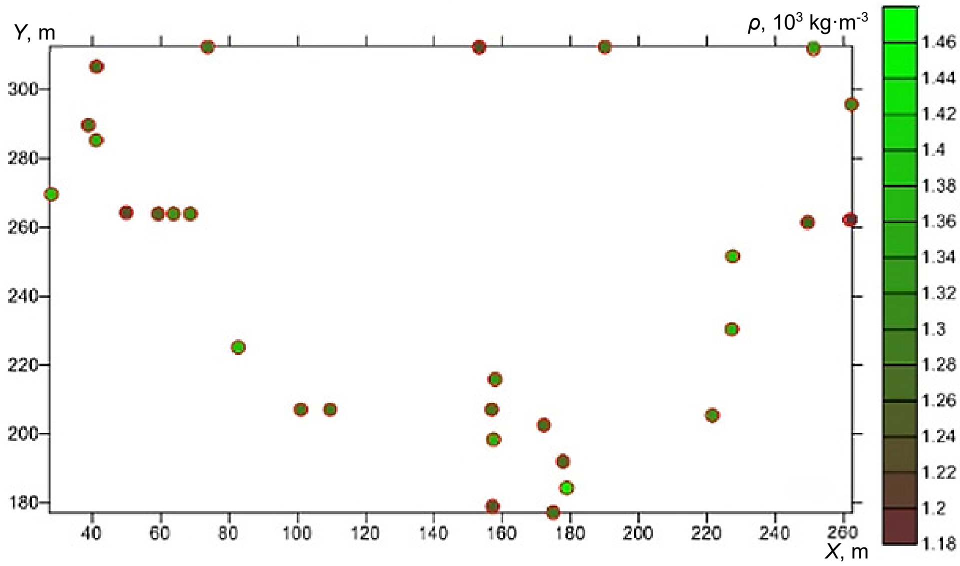

Fig. 1. Observation points and chalk strata averaged density at industrial area of Rivne NPP

In this study, we continue the development of three-dimensional statistical modeling methods based on correlation functions, specifically employing the pentamodel type correlation function, which is well established in geostatistical research (Chiles et al., 2005, Chiles, Delfiner, 2012; Vyzhva et al., 2023). This approach was applied to a dataset of chalk density measurements collected from 1984 to 2002 across 29 wells at the RNPP industrial site at depths of 28, 29, and 30 meters below the surface. The difference between the density values from the input map and the trend was primarily characterized as a stationary, homogeneous, isotropic random field in three-dimensional space (Vyzhva, Demidov, & Vyzhva, 2014a, 2014b, 2019).

In this paper, authors propose modeling the random component within the three-dimensional domain using spectral decomposition (Vyzhva, 2003, 2011) in combination with a pentamodel type correlation function.

Statistical simulation of chalk density data at the Rivne NPP. In this study, statistical simulation of chalk density data at the Rivne Nuclear Power Plant (RNPP) site was carried out for three depth levels: 28 m, 29 m, and 30 m from the surface. During the analysis of chalk density data at each level, it was found to be appropriate to separate the deterministic and random components of the field. The deterministic component was extracted using a curve approximation method to identify the underlying trend. The difference between the initial density map and the trend generally represents a realization of a homogeneous isotropic random field, which is a fundamental assumption in this approach.

The input data for each of the three levels can be expressed as realizations of a random field in 3D space: $\eta(x, y, z_i)$, $i = 1,2,3; z_1 = 28\text{m}$, $z_2 = 29\text{m}$, $z_3 = 30\text{m}$, where $\eta(x, y, z_i) = \eta_i(r, \theta, \varphi)$ in spherical coordinates (r, θ, φ), and i – level numbers. For each level, the trend $f_i(r, \theta, \varphi)$ and the random component $\xi_i(r, \theta, \varphi)$ (commonly modeled as a homogeneous isotropic random field in 3D space, also referred to as "noise") were identified as follows:

$$\eta_i(r, \theta, \varphi) = f_i(r, \theta, \varphi) + \xi_i(r, \theta, \varphi), \qquad i = 1,2,3.$$

Using statistical simulation, an extensive set of random field realizations $\xi_i(r, \theta, \varphi)$ $(i = 1,2,3)$ was generated for additional points within the three-dimensional observation domain. These simulated random components were superimposed onto the corresponding trend functions $f_i(r, \theta, \varphi)$, $i = 1,2,3$ to obtain refined estimates of chalk density. As a result, the final stage of modeling provided a more detailed and continuous representation of chalk layer density within the study area at RNPP.

The adopted approach is based on statistical simulation of homogeneous isotropic random fields in 3D space using spectral decomposition (Vyzhva, 2003). This method enables accurate reconstruction of the random component of the data across the entire observation domain, thereby producing realistic representations of chalk density variations.

Prior to constructing the model and implementing the simulation procedure, a statistical analysis of the input data was performed. If the three-dimensional data distribution approximates a Gaussian law, the simulation procedure developed in several works (Vyzhva, Demidov, & Vyzhva, 2013; Vyzhva, 2011) can be applied, in which realizations of the random field are generated from sequences of standard normal random variables.

The statistical analysis of the chalk density data at RNPP, obtained from 29 wells, demonstrated that the histogram of the density distribution is approximately Gaussian (Fig. 2). The proposed simulation methodology also includes preliminary statistical processing to determine the key statistical characteristics of the data, including the correlation function model. When the Gaussian hypothesis for the data field is confirmed, the mathematical expectation and correlation function completely define the random field in 3D space, enabling the construction of an adequate statistical model based on spectral decomposition.

The principles of constructing statistical models and simulation procedures for pentamodel type correlation functions have been described in detail in work (Vyzhva et al., 2023) and are further discussed below.

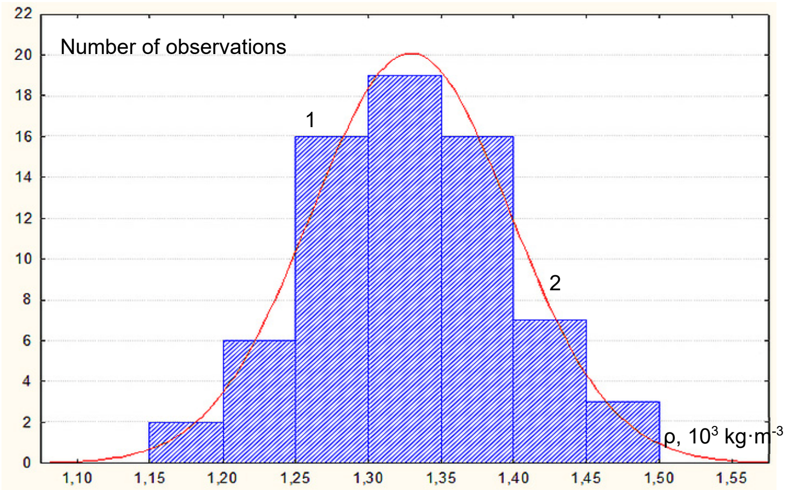

Fig. 2. Histogram of the chalky strata density (averaged data for all years of observation):
1 – the number of observations in a separate range of density, 2 – theoretical Gaussian curve

For the data correlation function $B(\rho)$, where ρ is the distance between the vectors $x, y \in R^3$ $(x = (r_1, \theta_1, \varphi_1), y = (r_2, \theta_2, \varphi_2))$, statistical models were selected to describe the density distribution of chalk strata within the three-dimensional observation domain. The correlation function was determined by comparing the root-mean-square approximation between the empirical and theoretical variograms derived from chalk density data.

As result, the input data was most adequately described using of 3 types of correlation functions: the Bessel correlation function (1) at the value of parameter $c = 5$, the Cauchy correlation function (2) at the value of parameter $a = 1$, the spherical correlation function (3) at the value of parameter $a \approx 1,25 * 10^{-2}$, the "cubic" correlation function (4) at the value of parameter $a \approx 1,25 * 10^{-2}$ and the pentamodel type correlation function (5) at the value of parameter $a \approx 2{,}4 * 10^{-2}$ (Vyzhva, Demidov, & Vyzhva, 2024).

The selection of these correlation functions was based on their ability to minimize the discrepancy between empirical and theoretical variograms, thereby ensuring the best statistical fit to the observed chalk density data. The Bessel and Cauchy functions demonstrated strong performance in modeling long-range spatial correlations, while the spherical and cubic functions effectively described medium-range structures. The pentamodel type correlation function has been explored to represent both local variations and larger scale spatial continuity.

$$B(\rho) = \sqrt{\frac{\pi}{2\,cr}}\, J_{\frac{1}{2}}(c\rho),\ c = 5, \quad (1)$$

where $J_k(x)$ is the Bessel function of the first kind of order $k = 1/2$,

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

$$B(\rho) = \begin{cases} 1 - \frac{3}{2}\,\frac{\rho}{a} + \frac{1}{2}\left(\frac{\rho}{a}\right)^3, & \rho \le a; \\ 0, & \rho > a. \end{cases} \quad (3)$$

$$B(\rho) = \begin{cases} 1 - 7\left(\frac{\rho}{a}\right)^2 + \frac{35}{4}\left(\frac{\rho}{a}\right)^3 + \frac{7}{2}\left(\frac{\rho}{a}\right)^5 + \frac{3}{4}\left(\frac{\rho}{a}\right)^7, & \rho \le a; \\ 0, & \rho > a. \end{cases} \quad (4)$$

$$B(\rho) = \begin{cases} 1 - \frac{15}{8}\,\frac{\rho}{a} + \frac{5}{4}\left(\frac{\rho}{a}\right)^3 - \frac{3}{8}\left(\frac{\rho}{a}\right)^5, & \rho \le a; \\ 0, & \rho > a. \end{cases} \quad (5)$$

It is well established that a homogeneous isotropic random field is characterized by a variogram $\gamma(\rho)$. In this case, the variogram (Chiles, & Delfiner, 2012) is related to the correlation function $B(\rho)$ through the following expression:

$$\gamma(\rho) = B(0) - B(\rho). \quad (6)$$

This relation reflects the dependence of the variance of the difference between random field values at two points on the distance between them. For $\rho = 0$, the variogram is zero, and as ρ increases, it grows, indicating a decrease in correlation between the random field values. Therefore, knowledge of $B(\rho)$ enables the construction of a variogram, which is essential for modeling the spatial structure of the data.

Thus, the variogram of a homogeneous isotropic random field is bounded by 2 $B(0)$. Equation (6) demonstrates that if the correlation function is known, the variogram can also be determined. Conversely, if the variogram of a homogeneous isotropic random field is bounded by a finite value, then $\gamma(\rho)$ follows the form given in equation (6). If the variogram has a sill, the value of $B(0)$ must be chosen equal to or greater than this sill. Therefore, knowing $\gamma(\rho)$ is equivalent to knowing $B(\rho)$.

The variograms of the three-dimensional chalk density data at the RNPP were constructed using the *R* software environment and the geoR package. The results correspond to the following correlation functions: Bessel (1) correlation function (the mean square approximation is 0,0008599), Cauchy (2) correlation function (the mean square approximation is 0,002816), spherical (3) correlation function (the mean square approximation is 0,000480) and "cubic" correlation function (4) (the mean square approximation is 0,001360). Variograms plots were presented at Fig. 3(a), that according to Bessel type of correlation function, at Fig. 3(b), that according to Cauchy type of correlation function, at Fig. 3(c), that according to spherical type of correlation function for the random component of investigation 3D data.

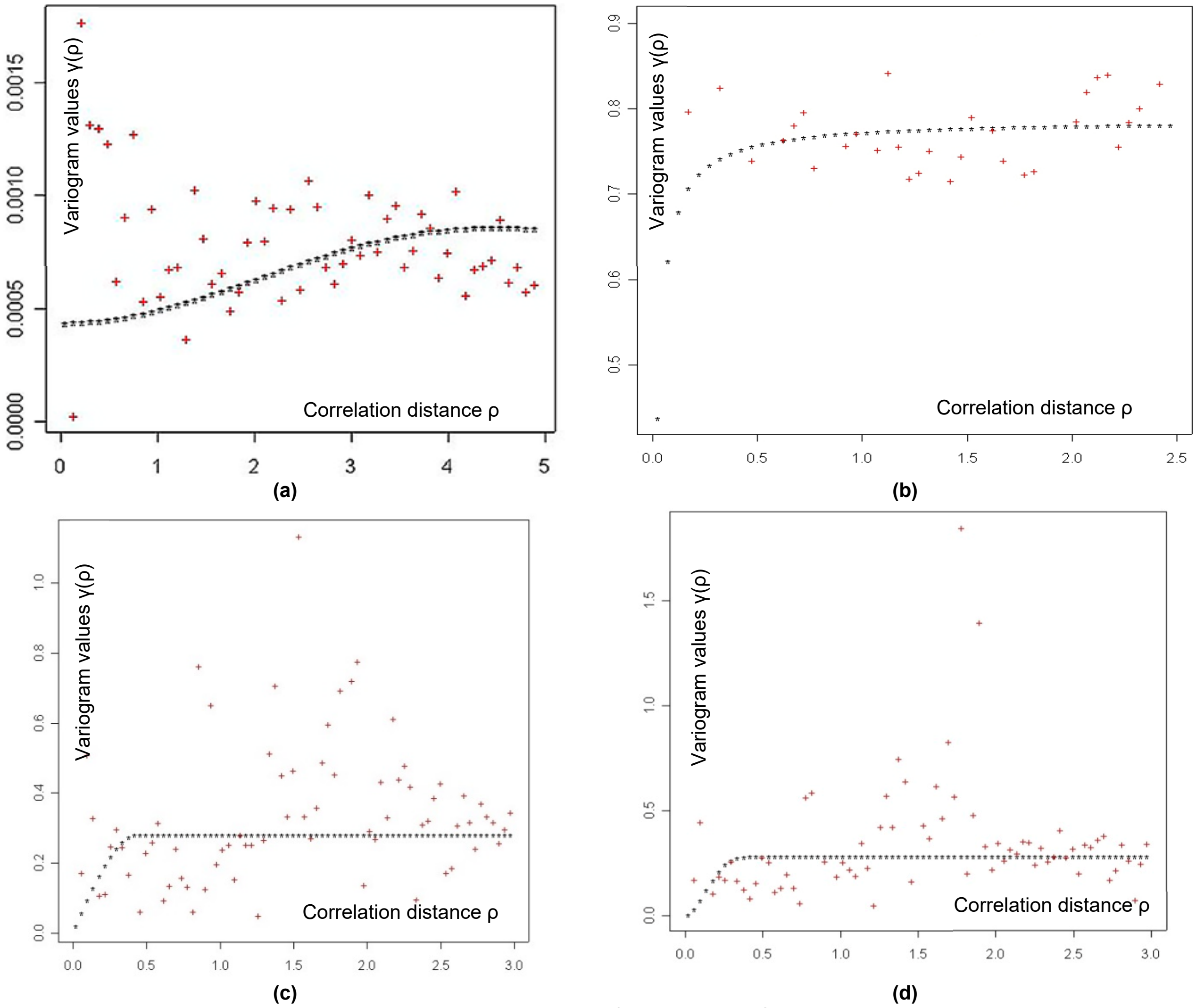

Fig. 3. Empirical (crosses) and theoretical (curve) variograms for input data of the chalky strata, that corresponding to the:
(a) the Bessel (1) correlation function; (b) the Cauchy (2) correlation function;
(c) the spherical (3) correlation function; (d) the "cubic" (3) correlation function

The built empirical variogram (Fig. 4) of input chalky strata density 3D data at the Rivne NPP has the best approximation by theoretical variogram which is connected to the pentamodel type correlation function (5) with parameter $a \approx 2,4 * 10^{-2}$.

We have, that the constructed variogram of realizations in the studied territory (Fig. 5) has sufficiently adequate approximation by the theoretical variogram, which is associated with a pentamodel type correlation function (a mean square deviation is $9,35 * 10^{-4}$).

Methods

Model, the spectral representation of homogeneous isotropic random fields in the 3D area, approximation theorem. Some theorems from the spectral theory of random fields now we present. We consider a real-valued homogeneous isotropic random field $\xi(r,\theta,\varphi)$ in the three-dimensional area, here r,θ,φ are spherical coordinates. It was previously proven (Yadrenko, 1983; Vyzhva, 2003; Vyzhva, 2011, p. 208) that square-mean continuous real-valued isotropic random field $\xi(r,\theta,\varphi)$, that is in 3D Euclidean space *R*^{3}, admit the spectral decomposition by spherical harmonics.

The correlation function $B(\rho)$ of the homogeneous isotropic random field $\xi(r,\boldsymbol{\theta},\varphi)$ in three-dimensional area depends on distance ρ between the vectors x and y, where $x,y \in R^3$, these vectors are given as follows $x,y \in R^3$, $x = (r_1,\theta_1,\varphi_1)$, $y = (r_2,\theta_2,\varphi_2)$:

$$\boldsymbol{\rho} = r\sqrt{2(1-\cos\boldsymbol{\psi})} = r\sin(\boldsymbol{\psi}/2),$$

where $\cos\boldsymbol{\psi}$ is angular distance between vectors x and y, where $x,y \in R^3$:

$$\cos\boldsymbol{\psi} = \cos\boldsymbol{\theta}_1\cos\boldsymbol{\theta}_2 + \sin\boldsymbol{\theta}_1\sin\boldsymbol{\theta}_2\cos(\boldsymbol{\varphi}_1 - \boldsymbol{\varphi}_2).$$

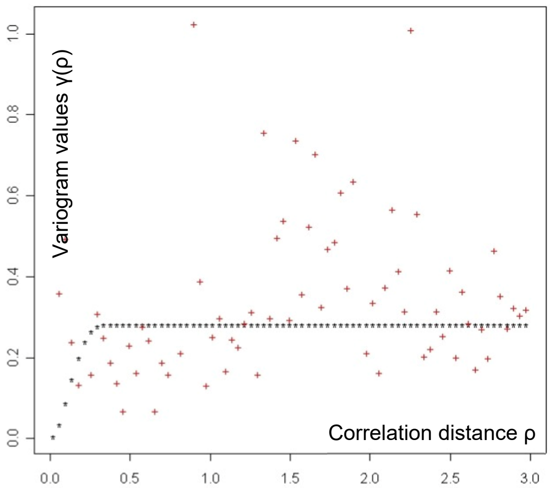

Fig. 4. Empirical (crosses) and theoretical (curve) variograms of input data arrays of chalk layer density, corresponding to pentamodel type correlation function ($a \approx 2,4 * 10^{-2}$)

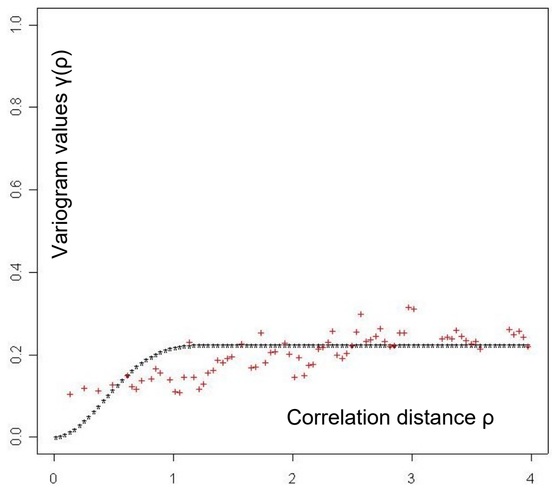

Fig. 5. Empirical (crosses) and theoretical (curve) variograms of simulated data arrays of chalk layer density, corresponding to pentamodel type correlation function ($a \approx 2,4 * 10^{-2}$)

However, the spectral decomposition of considered random field is used to solve the problems of statistical modeling of realizations of a random field in three-dimensional space, where real-valued random variables occur. Let us present a theorem where the considered spectral distribution is applied.

Theorem 1. Let a mean square continuous realvalued homogeneous isotropic random field $\xi(r,\theta,\varphi)$ is in 3D space with zero mean. Then this random field admits (Vyzhva, 2011, p. 210) such decomposition:

$$\xi(r,\theta,\varphi) = \\ =\sum_{m=0}^{\infty} \sum_{l=0}^{m} \tilde{c}_{m,l}\, P_m^l(\cos\theta)\ [\varsigma_{m,\,1}^l(r)\cos l\varphi + \varsigma_{m,\,2}^l(r)\sin l\varphi], \quad (7)$$

in the spectral decomposition (7) the symbols P_m^l, m, $\tilde{c}_{m,l}$ mean: P_m^l is associated Legendre functions of degree m, $\tilde{c}_{m,l}$ are constants sequences and are calculated by the formula:

$$\tilde{c}_{m,l} = \frac{1}{2}\sqrt{\frac{v_l}{\pi}\,\frac{(m-l)!}{(m+l)!}\,(2m+1)}\ ,\ v_l = \begin{cases}1, & l \neq 0,\\ 2, & l = 0;\end{cases} \quad (8)$$

random processes sequences $\{\varsigma_{m,\,k}^l(r)\}$, $k = 1, 2$:

$$\varsigma_{m,\,k}^l(r) = \int_0^{\infty} \frac{J_{m+\frac{1}{2}}(\lambda r)}{(\lambda r)^{\frac{1}{2}}}\ Z_{m,k}^l(d\lambda)\ ,$$

such that satisfying the following conditions:

1) $M\varsigma_{m,\,k}^l(r) = 0$;

2) $M\varsigma_{m,\,k}^l(r)\ \varsigma_{m',\,k'}^{l'}(r) = \delta_l^{l'}\ \delta_m^{m'}\ \delta_k^{k'}\ b_m(r)$, (9)

in the conditions 1) and 2) of the form (9) $\delta_m^{m'}$ is Kronecker symbol, $b_m(r)$ are the spectral coefficients and $\{Z_m^l(.)\}$ is a sequence of orthogonal random measures on Borel subsets from the interval $[0,+\infty)$, i.e.

$$E\ Z_m^l(S_1)\ Z_{m'}^{l''}(S_2) = \delta_l^{l'}\ \delta_m^{m'}\ \Phi(S_1 \cap S_2)\ ,$$

for any Borel subsets S_1 and S_2, here $\Phi(\lambda)$ is the bounded nondecreasing function so-called spectral function of random field $\xi(r,\theta,\varphi)$.

The spectral density of homogeneous isotropic random field $\xi(r,\theta,\varphi)$ is determined by formula $f(\lambda) = d\Phi(\lambda)/d\lambda$ and also it is obtained by correlation function of this random field as integral:

$$f(\lambda) = \frac{2}{\pi}\int_0^{\infty} \rho\lambda \sin(\lambda\rho)\, B(\rho)\, d\rho. \quad (10)$$

The spectral coefficients $\boldsymbol{b_m(r)}$ of random field $\boldsymbol{\xi(r,\theta,\varphi)}$ considered in three-dimensional space are defined by the spectral density $\boldsymbol{f(\lambda)}$ of this random field in the way:

$$b_m(r) = \int_0^{\infty} \frac{J^2_{m+\frac{1}{2}}(\lambda r)}{\lambda r} f(\lambda) d\lambda. \quad (11)$$

The statistical simulation of homogeneous isotropic random fields in the 3D space on the basis the spectral decomposition (7) coefficients (11) are considered further.

$$\xi_N(r,\theta,\varphi) = \sum_{m=0}^{N} \sum_{l=0}^{m} c_{ml}\, P_m^l(\cos\theta)\big[\zeta_{m,\,1}^l(r)\cos l\varphi + \\ + \zeta_{m,\,2}^l(r)\sin l\varphi\big],\ N \in \mathrm{N}. \quad (12)$$

Further we used mean square estimate from the paper (Vyzhva, Demidov, & Vyzhva, 2018). The following theorem is based on the results obtained in (Vyzhva, Demidov, & Vyzhva, 2018).

Theorem 2. Let a mean square continuous realvalued isotropic random field $\xi(r,\theta,\varphi)$ on the sphere $S_3(r)$ in 3D space with zero mean (r – radius of sphere). If $\mu_3 < +\infty$, then the mean square approximation of this random field by model (10) is such that

$$M\ [\xi(r,\theta,\varphi) - \xi_N(r,\theta,\varphi)]^2 \leq \frac{5\pi r^3}{2N^2}\mu_3, \quad (13)$$

where

$$\mu_3 = \int_0^{\infty}\ \lambda^3 \Phi\ (d\lambda)\ . \quad (14)$$

If we proposed, that r (radius of sphere) is not fixed, then the random field $\xi(r,\theta,\varphi)$ is in 3D Euclidean space R^3.

Based on the model (12) and estimate (13), the algorithm for the statistical simulation of realizations of Gaussian homogeneous isotropic random fields $\xi(r,\theta,\varphi)$ in 3D Euclidean space R^3 was constructed. We have described this algorithm.

In this paper we constructed the algorithm for the statistical simulation of Gaussian homogeneous isotropic random fields on three-dimensional space with pentamodel type correlation function of the form (5).

The spectral density is obtained for pentamodel type correlation function (5) by means the formula (10) and then we have:

$$f(\lambda) = \frac{2}{\pi}\Big[\Big(\frac{5a}{2} + \frac{105}{a^3\lambda^4} - \frac{270}{a^5\lambda^6}\Big)\cos(\lambda a) - \Big(\frac{51}{a^2\lambda^3} - \\ - \frac{270}{a^4\lambda^5}\Big)\sin(\lambda a) + \frac{30}{a^3\lambda^4} - \frac{270}{a^5\lambda^6}\Big]. \quad (15)$$

The spectral coefficients, which correspond to the pentamodel type correlation function (4) of homogeneous isotropic random field $\xi(r,\theta,\varphi)$, are calculated by the formula (11) and we have:

$$b_m(r) = \frac{2}{\pi r}\int_0^\infty \frac{J^2_{m+\frac{1}{2}}(\lambda r)}{\lambda}\left[\left(\frac{5a}{2}+\frac{105}{a^3\lambda^4}-\frac{270}{a^5\lambda^6}\right)\cos(\lambda a) - \left(\frac{51}{a^2\lambda^3}-\frac{270}{a^4\lambda^5}\right)\sin(\lambda a) + \frac{30}{a^3\lambda^4}-\frac{270}{a^5\lambda^6}\right]d\lambda. \quad (16)$$

These spectral coefficients $b_m(r), m = 0,1,2,\dots N$ from (16) are calculated by Mathematica software for density chalky strata data.

Results

The statistical simulation procedure of random field in 3D area with the pentamodel type correlation function. In this paper we generated the realizations of homogeneous isotropic random field in 3D area with the pentamodel type correlation function (5) at the values of parameter $a \approx 2,4 * 10^{-2}$. By the technique of spectral decomposition and finding of spectral coefficients the statistical simulation of density chalky strata data at the Rivne NPP object was performed.

By means of the abovementioned model (12), which is described in (Vyzhva et al., 2023), the procedure of numerical simulation the realizations of the 3D data field random component with the pentamodel type correlation function was conducted.

For the constructed model the value of number N is determined by the inequality, which is the estimate of the mean square approximation of random field $\xi(r,\theta,\varphi)$ by partial sums $\xi(r,\theta,\varphi)$. This number N corresponds to the prescribed small number ε (approximation accuracy). The mentioned inequality was obtained in theorem 2. Consequently, the estimate of the mean square approximation of the random field $\xi(r,\theta,\varphi)$ with the pentamodel type correlation function (5) by the partial sums $\xi(r,\theta,\varphi)$ has the following representation:

$$M[\xi(r,\theta,\varphi) - \xi_N(r,\theta,\varphi)]^2 \le \frac{5\pi r^3}{2N^2}\mu_3,$$

where

$$\mu_3 = \frac{2}{\pi}\int_0^K \left[\left(\frac{5a\lambda^3}{2}+\frac{105}{a^3\lambda}-\frac{270}{a^5\lambda^3}\right)\cos(\lambda a) - \left(\frac{51}{a^2}-\frac{270}{a^4\lambda^2}\right)\sin(\lambda a) + \frac{30}{a^3\lambda}-\frac{270}{a^5\lambda^3}\right]d\lambda, \quad K = \text{const}. \quad (17)$$

We define the dependence of the number N on r and ε in the case of correlation function of the pentamodel type (5) in the form of an inequality:

$$N(r,\varepsilon) \ge \sqrt{\frac{5\pi r^3}{2\varepsilon}\mu_3}. \quad (18)$$

The statistical simulation procedure of Gaussian homogeneous isotropic random field $\xi(r,\theta,\varphi)$ in 3D area with the pentamodel type correlation function (5) was built by means of the model (10) and the estimate (16). This random field is determined by its statistical characteristics: the mathematical expectation and the pentamodel type correlation function $B(\rho)$ of form (5) at the value of parameter $a \approx 2,4 * 10^{-2}$.

Algorithm:

1. Natural number N (border of summation) is chosen according to necessary accuracy $\varepsilon > 0$ of approximation the model (12) mentioned below:

$$\frac{5\pi r^3}{2N^2}\mu_3 \le \varepsilon, \quad (19)$$

where

$$\mu_3 = \frac{2}{\pi}\int_0^K \left[\left(\frac{5a\lambda^3}{2}+\frac{105}{a^3\lambda}-\frac{270}{a^5\lambda^3}\right)\cos(\lambda a) - \left(\frac{51}{a^2}-\frac{270}{a^4\lambda^2}\right)\sin(\lambda a) + \frac{30}{a^3\lambda}-\frac{270}{a^5\lambda^3}\right]d\lambda, \quad K = \text{const}.$$

The spectral coefficients $b_m(r),\ m = 0,1,2,\dots N$ are calculated for the pentamodel type correlation function (5) as integral (16).

2. Simulate the sequences of independent Gaussian normal random variables:

$\{\varsigma^l_{m,k}(r)\}$,

$k = 1, 2;\ m = 0, 1, 2,\dots N;\ l = 1,\dots, m;$

that satisfying the conditions (9) with spectral coefficients (16).

3. Calculate the realization of the stochastic random field $\xi(r,\theta,\varphi)$ by formula (12) in given point (r_i,θ_j,φ_p), $i = 1,2,\dots,I;\ j = 1,2,\dots,G;\ p = 1,2,\dots,P$ in the 3D observations area by means of substituting in it values numbers N and sequences of Gaussian random variables from the previous items 1, 2 and 3.

4. Check whether the realization of the random field $\xi(r,\theta,\varphi)$ generated in step 4 fits the data by testing the corresponding statistical characteristics (distribution and correlation function).

By means of this algorithm the statistical simulation of realizations of the Gaussian isotropic random fields $\xi(r,\theta,\varphi)$ with pentamodel type correlation function can be done.

Note that the procedure can be applied to random fields with different type of distribution. Then the sequences of random variables $\{\zeta_{k,i}(r), i = 1,2; k = 0,1,2,\dots,N(r,\varepsilon)\}$ must be distributed according to the appropriate distribution type.

The original Spectr software, developed in Python, was designed to generate realizations of random fields in a three-dimensional domain based on the results of statistical data processing and the described simulation algorithm. In this software, the pentamodel type correlation function (5) with the parameter $a \approx 2,4 * 10^{-2}$ was applied. Using Spectr, realizations of the random field $\xi(r,\theta,\varphi)$ were computed for 100 points at each of the three observation levels (r_i,θ_j,φ_p), $i = 1,2,\dots,I;\ j = 1,2,\dots,G;\ p = 1,2,\dots,P$ within the three-dimensional study area. Based on these realizations, a statistical estimate of the correlation function was obtained. This estimate was compared with the predefined pentamodel type correlation function (5), which allowed for a statistical assessment of the adequacy of the generated realizations. The constructed variogram of these realizations for the study area (Fig. 6) demonstrated a close fit to the theoretical variogram associated with the pentamodel-type correlation function. These results confirm that the selected statistical model for the chalk density data at the RNPP site is sufficiently accurate. Furthermore, the Spectr software developed for generating such random field realizations ensures high precision in the modeling process.

The results obtained using additional modeling procedures are presented in Fig. 6. Fig. 6(a) shows an example of a chalk density map constructed from well observation data (averaged over several years for 29 wells at a depth of 28 m) using the Surfer software. However, due to the limited number of measurements, the accuracy of such a map is insufficient to provide a reliable characterization of the chalk strata condition.

Fig. 6(b) illustrates the contours of equal chalk density values generated based on simulation results, which include the anchor borehole data obtained by calculating the spectral coefficients of the pentamodel type correlation function. Furthermore, the inclusion of 100 simulated values in the intervals between observation points provides a more accurate approximation of the density distribution. This improvement allows for more informed decision-making regarding the state of the chalk strata and helps identify locations that require testing or additional research.

Similarly, the results of the simulation procedure for borehole observation data (averaged over several years for 29 boreholes at a depth of 29 m) are presented in Fig. 7. Fig. 7(a) displays a chalk density map created from observation data using the Surfer software. Fig. 7(b) shows contours of equal density values derived from the simulation data, which also incorporate the anchor borehole values. The integration of 100 simulated values between the observation points improves the approximation quality, thus enabling a more accurate assessment of the chalk strata condition and supporting better-informed decisions for further investigations.

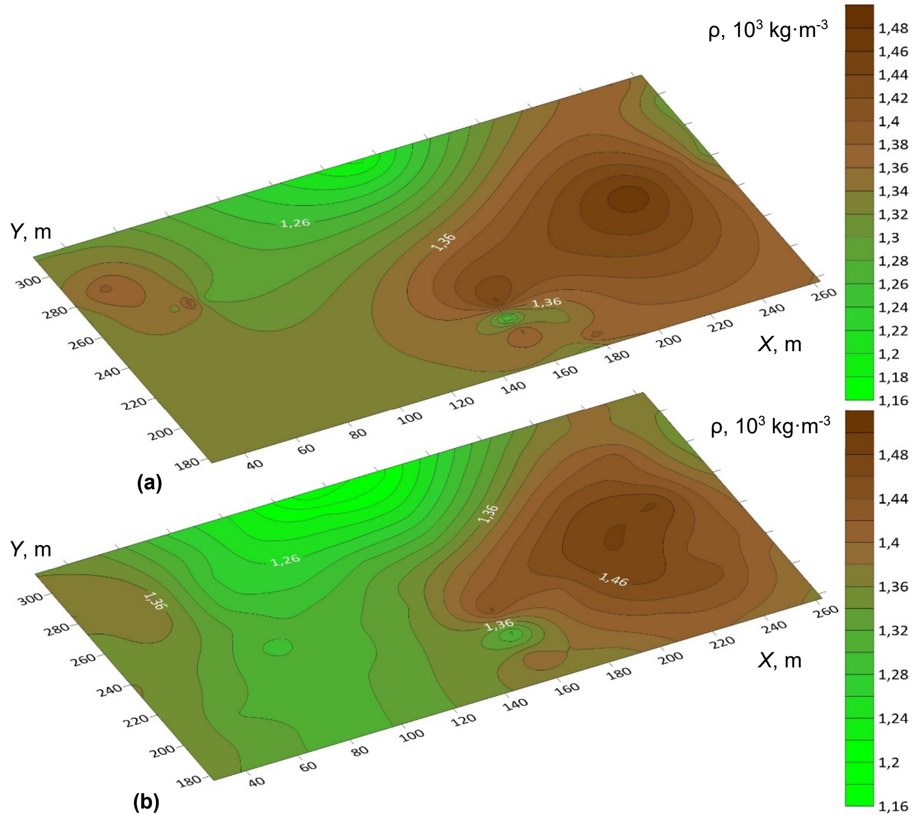

Fig. 6. The distribution of chalky strata density is on the industrial area of Rivne nuclear power plant at a depth of 28 m. from the surface, according to (a) the averaged data of 29 observational wells over 1984–2004 years, for (b) the simulated data that based on the values in secure wells by spectral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

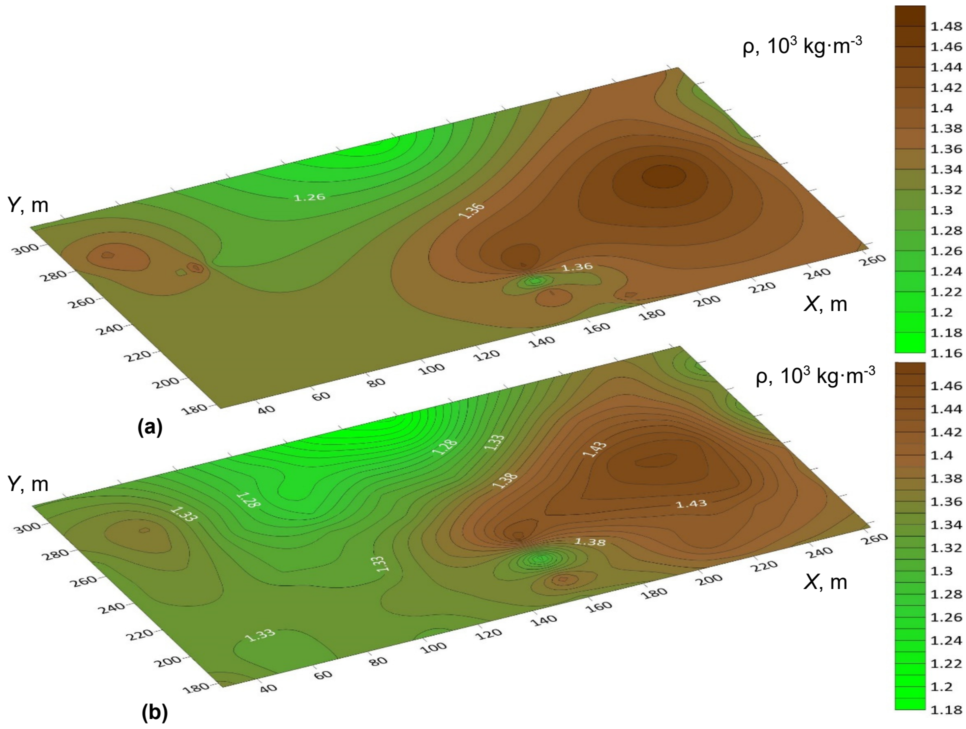

Fig. 7. The distribution of chalky strata density is on the Rivne NPP object at a depth of 29 m from the surface, according to (a) the averaged data of 29 observational wells over 1984–2004 years, for (b) the simulated data that based on the values in secure wells by spectral coefficients the pentamodel type

Finally, the results obtained using the simulation procedure for the observation wells (averaged data collected over several years for 29 wells at a depth of 30 m) are presented in Fig. 8. Fig. 8(a) shows an example of a chalk density map constructed from the observational data using the Surfer software. Fig. 8(b) displays contours of equal chalk density values derived from the simulation results, which include anchor well data. Furthermore, the addition of 100 simulated values in the intervals between the observation points provides a more reliable approximation, enabling a more accurate assessment of the chalk strata condition and supporting informed decision-making.

A statistical evaluation of the correlation function was performed for the simulated realizations of the chalk density distribution within the 3D observation domain at the RNPP site. This estimate was compared with the theoretical pentamodel type correlation function (5) with the parameter $a \approx 2,4 * 10^{-2}$, confirming the adequacy of the realizations through statistical analysis. The constructed variogram of these realizations for the study area (Fig. 5) closely matched the theoretical variogram associated with the pentamodel type correlation function. These results demonstrate that the selected correlation model for the random component of the data is sufficiently accurate and that the developed Spectr software provides reliable performance for generating random field realizations.

The pentamodel type correlation function provided the highest degree of flexibility, allowing the representation of both local variations and broader-scale spatial continuity.

The simulation process effectively supplemented sparse observational data, improving the resolution of chalk density distribution and the accuracy of geological interpretation. Statistical analysis confirmed the adequacy of the proposed model and its applicability for geophysical monitoring of potentially hazardous sites.

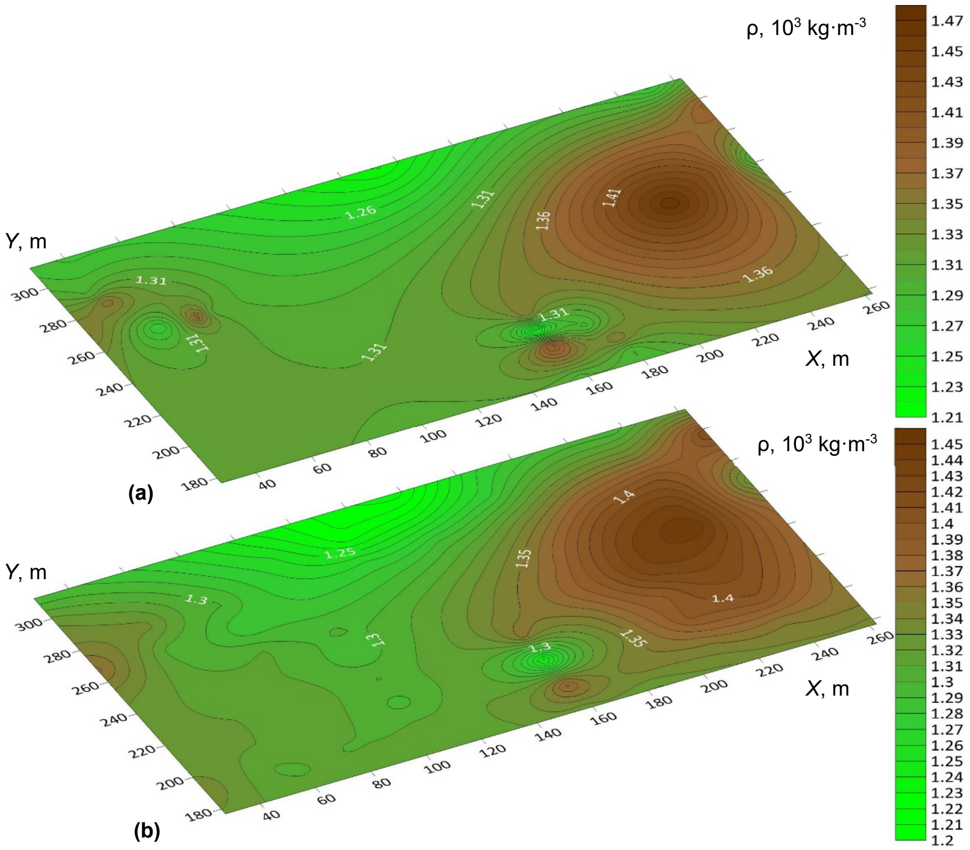

Fig. 8. The distribution of chalky strata density is on the industrial area of Rivne nuclear power plant at a depth of 30 m. from the surface, according to (a) the averaged data of 29 observational wells over 1984–2004 years, for (b) the simulated data that based on the values in secure wells by spectral coefficients the pentamodel type

Discussion and conclusions

Theoretical foundations, methodology, and procedures for statistical modeling of random fields in a three-dimensional domain using a pentamodel type correlation function, which is optimal in the mean-square sense, significantly enhance the efficiency of monitoring observations in areas of potentially hazardous facilities. This approach enables the interpolation and extrapolation of parameter values between and beyond observation grid nodes, providing a more accurate description of the three-dimensional density distribution of chalk strata within the industrial zone of the Rivne Nuclear Power Plant (RNPP).

The results presented in Vyzhva, Demidov, & and Vyzhva (2020) demonstrate that the accuracy of statistical modeling of Gaussian isotropic random field realizations using a spherical correlation function is comparable to that achieved with a pentamodel correlation function ($4.8 * 10^{-4}$). Thus, although the statistical modeling method with pentamodel-type correlation functions ensures the required accuracy, the comparable results justify the use of the spherical model as an alternative without significant loss of precision.

Previous studies by the authors (Vyzhva, Demidov, & Vyzhva, 2013, 2014a, 2014b, 2019, 2020, 2023, 2024) have shown that the proposed method can be effectively applied to detect anomalous zones in the analysis of geophysical parameters within a three-dimensional domain.

Beyond its value for geophysical investigations and environmental monitoring tasks, this approach has proven effective in identifying anomalous regions in various geological datasets, including gravimetry and magnetometry. Furthermore, statistical modeling based on random functions offers broad potential for applications in related Earth sciences disciplines, such as environmental magnetism (Menshov et al., 2015).

Authors' contribution: Zoya Vyzhva – problem formulation, development of analytical expressions for the model, selection of scientific novelty, formal analysis, methodology, review and editing; Andriy Vyzhva – statistical modeling algorithm development, editing; Vsevolod Demidov – review of publications, data processing, conclusions, refinement and editing; Tetiana Shovkoplias – improved of analytical expressions for the model.

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Зоя ВИЖВА[1], д-р фіз.-мат. наук, проф.
ORCID ID: 0000-0002-6338-3892
e-mail: zoya_vyzhva@ukr.net

Всеволод ДЕМИДОВ[1], канд. фіз.-мат. наук, доц.
ORCID ID: 0009-0003-9472-6530
e-mail: demidov@knu.ua

Андрій ВИЖВА[2], канд. фіз.-мат. наук, ст. наук. співроб.
ORCID ID: 0009-0003-6699-5848
e-mail: motomustanger@ukr.net

Тетяна ШОВКОПЛЯС[1], канд. фіз.-мат. наук, асист.
ORCID ID: 0009-0004-8991-0285
e-mail: 1zagmat.tetyana1@knu.ua

[1]Київський національний університет імені Тараса Шевченка, Київ, Україна
[2]ДП "Науканафтогаз", Київ, Україна

СТАТИСТИЧНЕ МОДЕЛЮВАННЯ ДАНИХ В 3D ОБЛАСТІ З ВАРІОГРАМОЮ ТИПУ ПЕНТАМОДЕЛЬ ДЛЯ ГЕОФІЗИЧНОГО МОНІТОРИНГУ РІВНЕНСЬКОЇ АЕС

В с т у п . ***Представлено розроблену модель та алгоритм статистичного моделювання даних у тривимірній області з використанням варіограм пентамодельного типу, що забезпечують оптимальне наближення в середньому квадратичному значенні. Як приклад продемонстровано застосування запропонованого методу для доповнення результатів геофізичних досліджень карстово-суфозійних процесів при моніторингу щільності крейдяної товщі на території Рівненської АЕС. На майданчику розміщення Рівненської АЕС було виконано комплекс геофізичних робіт. Серед проведених спостережень найбільший інтерес становлять радіоізотопні дослідження щільності та вологості ґрунтів у зоні існуючих споруд. При цьому постало завдання заповнення даних, отриманих у ході контролю зміни щільності крейдяної товщі радіоізотопними методами мережі спостережень, що включала 29 свердловин.***

Для вирішення цього завдання застосовано метод статистичного моделювання з використанням варіограми пентамодельного типу, що дає змогу відтворювати випадкове поле досліджуваного об'єкта в тривимірній області в довільних точках спостереження.

М е т о д и . ***За допомогою спектрального розкладу випадкових полів у тривимірному просторі побудовано статистичну модель розподілу усередненої щільності крейдяної товщі в межах досліджуваної території. Розроблений алгоритм забезпечує генерацію реалізацій випадкових полів із заданими кореляційними властивостями та просторовою дискретизацією, що відповідає вимогам до точності моделювання.***

Р е з у л ь т а т и . ***Сформульовано та реалізовано алгоритм статистичного моделювання випадкових полів з кореляційною функцією пентамодельного типу. На основі розробленого програмного забезпечення отримано додаткові змодельовані реалізації випадкової складової щільності крейдяної товщі на регулярній сітці спостережень з необхідним ступенем деталізації. Проведено порівняння набору кореляційних функцій для одного набору даних у середньому квадратичному значенні. Проведено статистичний аналіз отриманих результатів чисельного моделювання, включаючи перевірку їх адекватності вихідним даним спостережень та оцінку збіжності полів, що моделюються.***

В и с н о в к и . ***Запропонований метод статистичного моделювання випадкових полів з кореляційними функціями пентамодельного типу дає змогу заповнювати відсутні даних з високим ступенем достовірності та може бути ефективно застосований при вирішенні завдань геофізичного моніторингу та інтерпретації просторово розподілених параметрів геологічного середовища.***

К л ю ч о в і   с л о в а : ***статистичне моделювання, кореляційна функція типу пентамодель, спектральний розклад, кондиційність карт, Рівненська АЕС.***

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