

## Mathematical modeling of impurity diffusion process under given statistics of a point mass sources system. II

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Modeling of the impurity diffusion process in a layer under the action of a system of random point sources is carried out. Mass sources of different power are uniformly distributed in a certain internal interval, that may also coincide with the entire region of the layer. The statistics of random sources is given. The solution of the initial-boundary value problem is found as the sum of the homogeneous problem solution and the convolution of the Green's function with the system of the random point sources. Averaging of the solution is performed on the internal subinterval and in the entire body region. The formulas for the variance, correlation function of the concentration field and coefficient of correlation are expressed in terms of the second moment of random mass sources. Software modules are developed for simulating the behavior of the averaged concentration, variance and correlation function. Their numerical analysis also is performed. General properties of the considered function are determined depending on the problem parameters.

**Keywords:** *mathematical modeling; diffusion; random point source; correlation function; variance; correlation coefficient.*

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### 1. Introduction

In practical applications today, significant emphasis is placed on the challenges of accurately describing the impact of random point mass sources on the concentration of migrating impurity components in both homogeneous and heterogeneous media. The insights gained from such research are important, offering practical applications across a range of scientific disciplines and related industries including physics, chemistry, ecology and engineering. These studies are instrumental in developing formalized models that delineate the relationships between individual system components or distinct processes occurring within them [1]. In this context, examining the second moments of the field is key [2,3], as it enhances our understanding of the transport and interaction of impurity substances in various media.

A key aspect of this study is its practical contribution towards addressing pressing environmental pollution issues, particularly those related to pollution and quality control in manufacturing processes. By analyzing the interactions between random point mass sources and impurity substances, this research promises to enhance the prediction and management of pollution levels. For instance, the study [4] employs cumulative functions generated in Monte Carlo modeling to monitor the efficiency of observed welding procedures.

In [5], a statistical mathematical model of radionuclide migration in an underground nuclear waste repository was developed, based on a linear partial differential equation of the diffusion-convection type. This partial differential equation has a large number of locally equally spatially distributed sources on the median plane of the porous area. The model is obtained by extending a model with a deterministic averaged source. Similarly, in [6], the time dependence of the concentration of a pollutant carried by diffusion and convection from a large number of similar local sources was studied. A mathematical

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model describing the global evolution of such a system was studied, and numerical modeling was carried out assuming a random distribution for each local source.

The authors [7,8] constructed and investigated a mathematical model of the mass exchange process taking into account the local structure of the medium and the cascade decay of impurity particles, and obtained key systems of model equations for double- and tripple-heterodiffusion. In [9], an exact solution of the contact initial-boundary value problem for the diffusion of impurity particles in a body with a two-phase periodic layered structure was constructed, and the regularities of concentration distribution depending on different values of the substance decay intensity coefficient were analyzed.

Problems with point mass sources can arise in various fields, for example, in analyzing the motion and stability of systems of point masses, in the presence of radioactive radiation in a body, and when it is necessary to consider the gravitational interaction of point masses, etc. In this case, the specific location of the point source may be unknown.

In [10], the mathematical model has been developed for the diffusion of impurity particles in a layer under the action of a system of randomly located point mass sources within a given internal interval. The field of migrating particles concentration averaged over uniform distribution has been found and investigated. This article is a continuation of [10] focused on finding and studying the second moments of the field within the scope of the same mathematical model, and aimed at development of advanced mathematical apparatus for describing random transport processes.

## 2. Mathematical model

The diffusion process of impurity substances in a layer with thickness  $x_0$  under the action of a system of randomly located point mass sources  $\omega_i(\delta(x - \hat{x}_i))$ , where  $\omega_i$  is the power of the  $i$ -th source, and  $\delta$  represents the Dirac delta function [11], within a certain internal interval, is described by the boundary problem of mass transfer (1)–(3) in the article [10]. It is assumed, that the points  $x = \hat{x}_i$  of the located internal mass sources are random and uniformly distributed within the body region, as shown in Figure 1 of the article [10], and that contribution of each source to the system is equally probable. The statistics of the random sources are also defined, where  $N$  is the number of point sources included in the system.

The solution to the stochastic diffusion problem with the first-order initial and boundary conditions has been found as a sum of the solution to the homogeneous boundary problem solution and the convolution of the Green's function with the system of random point sources. Following the formal averaging procedure, the concentration function takes the form

$$\langle c(t, x) \rangle = c^h(t, x) + \sum_{i=1}^N \omega_i \int_{\bar{x}_1}^{\bar{x}_2} \int_0^t \int_0^{x_0} f(\hat{x}_i) G(t, t', x, x') \delta(x' - \hat{x}_i) dx' dt' d\hat{x}_i, \quad (1)$$

where  $c^h(t, x)$  is the solution of the homogeneous problem,  $G(t, t', x, x')$  is the Green's function and  $f(\hat{x}_i)$  is the density of the distribution function of the location of the  $i$ -th source.

Based on the obtained formulas for the averaged field of the concentration of impurity particles diffusing in a layer under the action of the point mass sources system within the internal interval  $[\bar{x}_1, \bar{x}_2]$ , we search for the second moments of the field, namely the variance and the correlation function of the field, as well as the correlation coefficient.

## 3. The second moments of the random concentration field

Let us find the variance  $\sigma_c^2(t, x)$  of the impurity concentration field and the correlation function (auto-correlation) under the action of a system of random point mass sources. By definition, the variance of the field  $\sigma_c^2(t, x)$  is [12,13]

$$\sigma_c^2(t, x) = \langle c^2(t, x) \rangle - \langle c(t, x) \rangle^2.$$

For the average of the product of concentration fields, the following relation holds [13]

$$\langle c(t_1, x_1)c(t_2, x_2) \rangle = \langle c(t_1, x_1) \rangle \langle c(t_2, x_2) \rangle + \psi_c(t_1, x_1; t_2, x_2), \quad (2)$$

where  $\psi_c(t_1, x_1; t_2, x_2)$  is correlation (auto-correlation) function of the concentration field  $c(t, x)$  at points  $(t_1, x_1)$  and  $(t_2, x_2)$ .

From this, we obtain the correlation function of the field  $\psi_c(t, x; t, x)$  at the point  $(t, x)$

$$\psi_c(t, x; t, x) = \langle c^2(t, x) \rangle - \langle c(t, x) \rangle \langle c(t, x) \rangle. \tag{3}$$

Then, the average of the square of the field can be expressed as the sum of the products of the averages and the corresponding correlation function,

$$\langle c^2(t, x) \rangle = \langle c(t, x)c(t, x) \rangle = \langle c(t, x) \rangle \langle c(t, x) \rangle + \psi_c(t, x; t, x).$$

Let us substitute the expressions for  $c(t, x)$  (4) and  $\langle c(t, x) \rangle$  (15) in [10] into the formula (3). Firstly, we find  $\langle c^2(t, x) \rangle$ ,

$$\begin{aligned} \langle c^2(t, x) \rangle &= (c^h(t, x))^2 + 2c^h(t, x) \left\langle \sum_{i=1}^N \omega_i \int_0^t \int_0^{x_0} G(t, t', x, x') \delta(x' - \hat{x}_i) dx' dt' \right\rangle \\ &+ \sum_{i=1}^N \sum_{k=1}^N \omega_i \omega_k \int_0^t \int_0^{x_0} \int_0^t \int_0^{x_0} G(t, t', x, x') G(t, t'', x, x'') \langle \delta(x' - \hat{x}_i) \delta(x'' - \hat{x}_k) \rangle dx' dt' dx'' dt''. \end{aligned} \tag{4}$$

Taking into account (4), correlation function of the field  $\psi_c(t, x; t, x)$  in the point  $(t, x)$ , i.e. variance of the field, is expressed as

$$\begin{aligned} \psi_c(t, x; t, x) &= (c^h(t, x))^2 + 2c^h(t, x) \left\langle \sum_{i=1}^N \omega_i \int_0^t \int_0^{x_0} G(t, t', x, x') \delta(x' - \hat{x}_i) dx' dt' \right\rangle \\ &+ \sum_{i=1}^N \sum_{k=1}^N \omega_i \omega_k \int_0^t \int_0^{x_0} \int_0^t \int_0^{x_0} G(t, t', x, x') G(t, t'', x, x'') \langle \delta(x' - \hat{x}_i) \delta(x'' - \hat{x}_k) \rangle dx' dt' dx'' dt'' \\ &- \langle c(t, x) \rangle^2, \end{aligned} \tag{5}$$

where the square of the averaged concentration field is found in the form

$$\begin{aligned} \langle c(t, x) \rangle^2 &= (c^h(t, x))^2 + c^h(t, x) \frac{4\Omega}{dx_0 N (\bar{x}_2 - \bar{x}_1)} \sum_{n=1}^{\infty} S_{12}(y_n) (1 - e^{-dy_n^2 t / \rho}) \sin(y_n x) \\ &+ \frac{4\Omega^2}{d^2 x_0^2 N^2 (\bar{x}_2 - \bar{x}_1)^2} \left( \sum_{n=1}^{\infty} S_{12}(y_n) (1 - e^{-dy_n^2 t / \rho}) \sin(y_n x) \right)^2. \end{aligned} \tag{6}$$

Let us consider the second term of relation (5). We denote the double integral in this term as  $I_1(t, x)$ . Taking into account formulas (15) and (16) in [10], we obtain

$$I_1(t, x) = 2c^h(t, x) \frac{2\Omega}{dx_0 N (\bar{x}_2 - \bar{x}_1)} \sum_{n=1}^{\infty} S_{12}(y_n) (1 - e^{-dy_n^2 t / \rho}) \sin(y_n x).$$

Now let us find the third term in the relation (5), denoting it as  $I_2(t, x)$ . Allowing for the assumption that the system of  $N$  random point mass sources has the uniform distribution over the interval  $[\bar{x}_1, \bar{x}_2]$  we deduce

$$\langle \delta(x' - \hat{x}_i) \delta(x'' - \hat{x}_k) \rangle = \frac{1}{N^2 (\bar{x}_2 - \bar{x}_1)^2}.$$

Thus, after averaging, we obtain

$$I_2(t, x) = \frac{\Omega^2}{N^2 (\bar{x}_2 - \bar{x}_1)^2} \int_0^t \int_0^{x_0} \int_0^t \int_0^{x_0} G(t, t', x, x') G(t, t'', x, x'') dx' dt' dx'' dt''.$$

In the case when the random point mass sources are of equal power, we get

$$I_2(t, x) = \frac{\omega^2}{(\bar{x}_2 - \bar{x}_1)^2} \int_0^t \int_0^{x_0} \int_0^t \int_0^{x_0} G(t, t', x, x') G(t, t'', x, x'') dx' dt' dx'' dt''.$$

Taking into account, that  $t'$ ,  $x'$  and  $t''$ ,  $x''$  are independent variables, we obtain

$$I_2(t, x) = \frac{\Omega^2}{N^2(\bar{x}_2 - \bar{x}_1)^2} \left( \int_0^t \int_0^{x_0} G(t, t', x, x') dx' dt' \right)^2. \quad (7)$$

After substituting the Green's function (12) in [10] into relation (7)  $I_2(t, x)$  is

$$I_2(t, x) = \frac{4\Omega^2}{N^2 d^2 x_0^2 (\bar{x}_2 - \bar{x}_1)^2} \left[ \sum_{n=1}^{\infty} \sin(y_n x) \frac{1 - (-1)^n}{y_n^3} (1 - e^{-dy_n^2 t / \rho}) \right]^2.$$

In the case when sources are of equal power  $\omega$ , we get

$$I_2(t, x) = \frac{4\omega^2}{d^2 x_0^2 (\bar{x}_2 - \bar{x}_1)^2} \left[ \sum_{n=1}^{\infty} \sin(y_n x) \frac{(1 - (-1)^n)}{y_n^3} (1 - e^{-dy_n^2 t / \rho}) \right]^2.$$

Consequently, the variance takes the form

$$\sigma_c^2(t, x) = \frac{4\Omega^2}{d^2 x_0^2 N^2 (\bar{x}_2 - \bar{x}_1)^2} \left[ \sum_{n=1}^{\infty} \frac{\sin(y_n x)}{y_n^3} (1 - e^{-dy_n^2 t / \rho}) (1 - (-1)^n - \cos(y_n \bar{x}_1) + \cos(y_n \bar{x}_2)) \right]^2. \quad (8)$$

Let us find the correlation function of a random field of the impurity substance concentration under the action of the system of random point mass sources. From formula (2) we get

$$\psi_c(t_1, x_1; t_2, x_2) = \langle c(t_1, x_1) c(t_2, x_2) \rangle - \langle c(t_1, x_1) \rangle \langle c(t_2, x_2) \rangle.$$

Let us determine the product of the averaged concentration fields at points  $(t_1, x_1)$  and  $(t_2, x_2)$

$$\begin{aligned} \langle c(t_1, x_1) \rangle \langle c(t_2, x_2) \rangle &= c^h(t_1, x_1) c^h(t_2, x_2) + \frac{2\Omega}{dx_0 N (\bar{x}_2 - \bar{x}_1)} \sum_{n=1}^{\infty} S_{12}(y_n) \\ &\times \left[ c^h(t_1, x_1) (1 - e^{-dy_n^2 t_2 / \rho}) \sin(y_n x_2) + c^h(t_2, x_2) (1 - e^{-dy_n^2 t_1 / \rho}) \sin(y_n x_1) \right] \\ &+ \frac{4\Omega^2}{d^2 x_0^2 N^2 (\bar{x}_2 - \bar{x}_1)^2} \sum_{n=1}^{\infty} S_{12}(y_n) (1 - e^{-dy_n^2 t_1 / \rho}) \sin(y_n x_1) \\ &\times \sum_{m=1}^{\infty} S_{12}(y_m) (1 - e^{-dy_m^2 t_2 / \rho}) \sin(y_m x_2), \end{aligned} \quad (9)$$

where  $y_m = \pi m / x_0$ .

Then the averaging of the product of the concentration field at points  $(t_1, x_1)$  and  $(t_2, x_2)$  is the next:

$$\begin{aligned} \langle c(t_1, x_1) c(t_2, x_2) \rangle &= c^h(t_1, x_1) c^h(t_2, x_2) + \frac{2\Omega}{dx_0 N (\bar{x}_2 - \bar{x}_1)} \sum_{n=1}^{\infty} S_{12}(y_n) \\ &\times \left[ c^h(t_1, x_1) (1 - e^{-dy_n^2 t_2 / \rho}) \sin(y_n x_2) + c^h(t_2, x_2) (1 - e^{-dy_n^2 t_1 / \rho}) \sin(y_n x_1) \right] \\ &+ \frac{4\Omega^2}{d^2 x_0^2 N^2 (\bar{x}_2 - \bar{x}_1)^2} \sum_{n=1}^{\infty} \frac{1 - (-1)^n}{y_n^3} (1 - e^{-dy_n^2 t_1 / \rho}) \sin(y_n x_1) \\ &\times \sum_{m=1}^{\infty} \frac{1 - (-1)^m}{y_m^3} (1 - e^{-dy_m^2 t_2 / \rho}) \sin(y_m x_2). \end{aligned} \quad (10)$$

Taking into account expressions (9) and (10), we obtain the correlation function of the impurity concentration field, which diffuses in the layer under the action of the system of random point sources, in the form

$$\begin{aligned} \psi_c(t_1, x_1, t_2, x_2) &= \frac{4\Omega^2}{d^2 x_0^2 N^2 (\bar{x}_2 - \bar{x}_1)^2} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(y_n x_1) \sin(y_m x_2)}{y_n^3 y_m^3} (1 - e^{-dy_n^2 t_1 / \rho}) (1 - e^{-dy_m^2 t_2 / \rho}) \\ &\times \left[ (1 - (-1)^n) (1 - (-1)^m) - (\cos(y_n \bar{x}_1) - \cos(y_n \bar{x}_2)) (\cos(y_m \bar{x}_1) - \cos(y_m \bar{x}_2)) \right]. \end{aligned} \quad (11)$$

If the powers of the sources are equal, then formula (11) can be reduced to

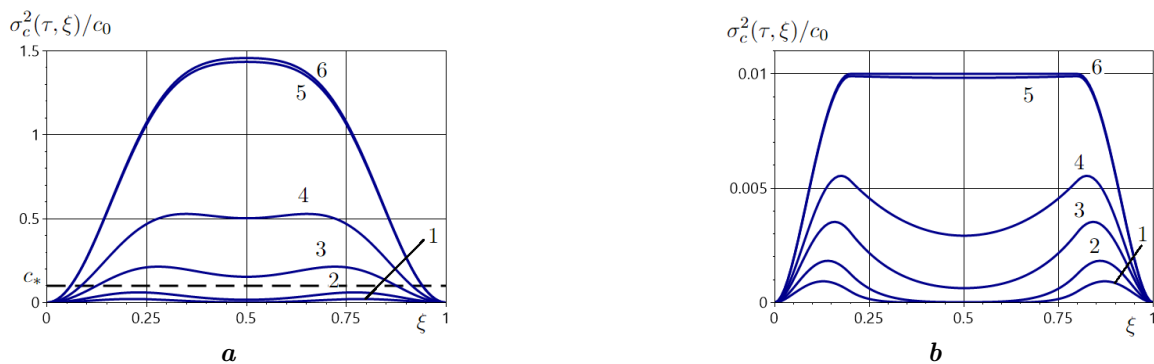
$$\psi_c(t_1, x_1, t_2, x_2) = \frac{4\omega^2}{d^2 x_0^2 (\bar{x}_2 - \bar{x}_1)^2} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(y_n x_1) \sin(y_m x_2)}{y_n^3 y_m^3} (1 - e^{-dy_n^2 t_1 / \rho}) (1 - e^{-dy_m^2 t_2 / \rho}) \times [(1 - (-1)^n)(1 - (-1)^m) - (\cos(y_n \bar{x}_1) - \cos(y_n \bar{x}_2))(\cos(y_m \bar{x}_1) - \cos(y_m \bar{x}_2))].$$

It should be noted that the correlation function  $\psi_c(t_1, x_1; t_2, x_2)$  is directly proportional to the square of the total power of the point sources included in the system and inversely proportional to the square of the number of sources.

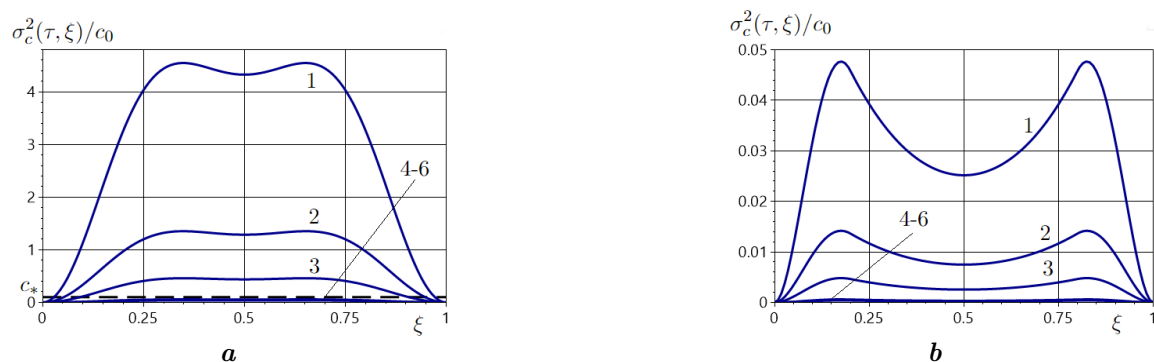
### 4. Numerical analysis of the variance and correlation function

In Figures 1 and 2 the characteristic distributions of the variance of field of the impurity concentration in the layer under the action of the point source system are illustrated. Calculations have been carried out in the dimensionless variables (19) in [10] for the same basic values of the problem parameters. Figure 1 demonstrates the distribution of variance at different moments of dimensionless time  $\tau = 0.01, 0.02, 0.05, 0.1, 0.5, 1$  (curves 1–6) for the following intervals of action of point sources  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  (Figure 1a) and  $[\bar{\xi}_1, \bar{\xi}_2] = [0, \xi_0]$  (Figure 1b).

In Figure 2 the variance of the impurity concentration field in the presence of one source with a power significantly different from the other sources in the system is shown. Figure 2a is created for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$ , and Figure 2b is built for  $[\bar{\xi}_1, \bar{\xi}_2] = [0, \xi_0]$ . Curve 1 corresponds to the system  $\{1, 1, 1, 1, 50\}$ , curve 2 corresponds to the system  $\{1, 1, 1, 1, 40\}$ , curve 3 corresponds to the system  $\{1, 1, 1, 1, 20\}$ , curve 4 corresponds to the system  $\{1, 1, 1, 1, 10\}$ , curve 5 corresponds to the system  $\{1, 1, 1, 1, 1\}$ , curve 6 corresponds to the system  $\{1, 1, 1, 1, 0.1\}$ .



**Fig. 1.** The variance of the concentration field at different moments of dimensionless time for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  (a) and  $[\bar{\xi}_1, \bar{\xi}_2] = [0, \xi_0]$  (b).

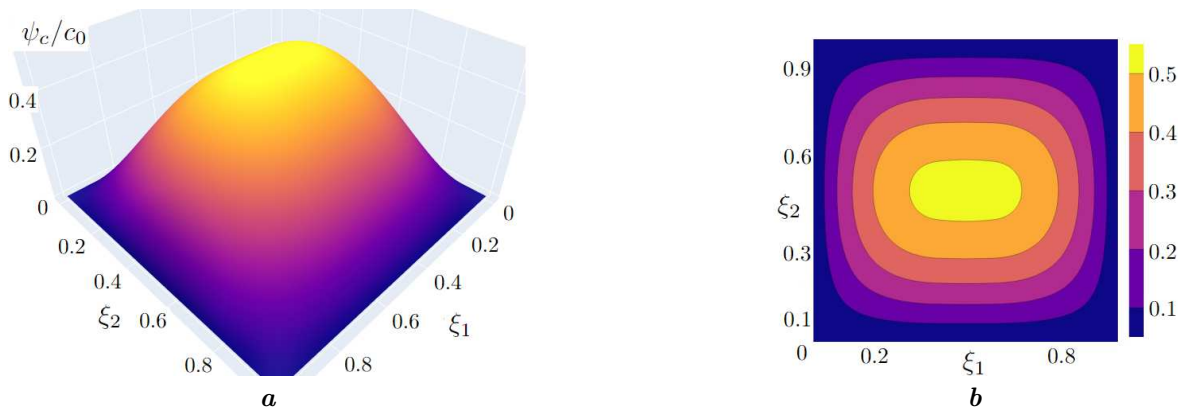


**Fig. 2.** The variance of the concentration field in the presence of a dominant source with varying power in the system for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  (a) and  $[\bar{\xi}_1, \bar{\xi}_2] = [0, \xi_0]$  (b).

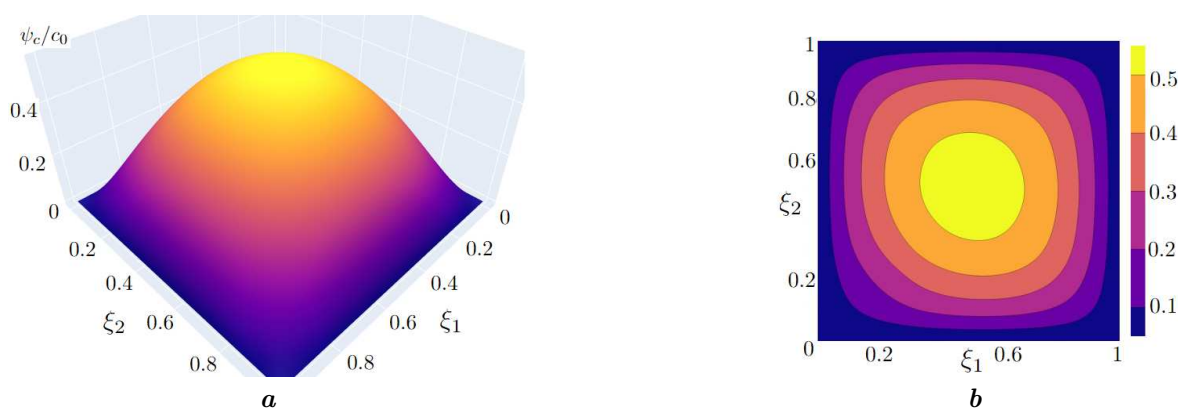
Note that the function  $\sigma_c^2(\tau, \xi)$  is symmetric within the body region (Figures 1 and 2). From the beginning of the diffusion process in the layer in which the system of point sources acts, the variance starts to increase in the neighborhoods of points  $\xi = 0.2$  and  $\xi = 0.8$  for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  and  $\xi = 1.5$  for  $\xi = 8.5$  when  $[\bar{\xi}_1, \bar{\xi}_2] = [0, \xi_0]$ . At the same time, there is a local minimum of the function  $\sigma_c^2$  at the point  $\xi_{\min} = 0.5$  (Figure 1). Over time, the variance increases, its local maxima shift into the body middle, they are leveled off. Eventually, in the vicinity of the steady-state regime (curves 5 and 6 in Figure 1) the point  $\xi = 0.5$  evolves into the maximum point of variance for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  (Figure 1a) and into the interval  $[0.25, 0.75]$  of constant maximum values  $\sigma_c^2$  for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  (Figure 1b).

We also note that for all  $\tau$ , the longer is the interval of action of the point source system, the smaller the variance becomes (Figures 1a and 1b). For instance, the difference in the values  $\sigma_c^2$  for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  and for  $[\bar{\xi}_1, \bar{\xi}_2] = [0, 1]$  is two orders of magnitude.

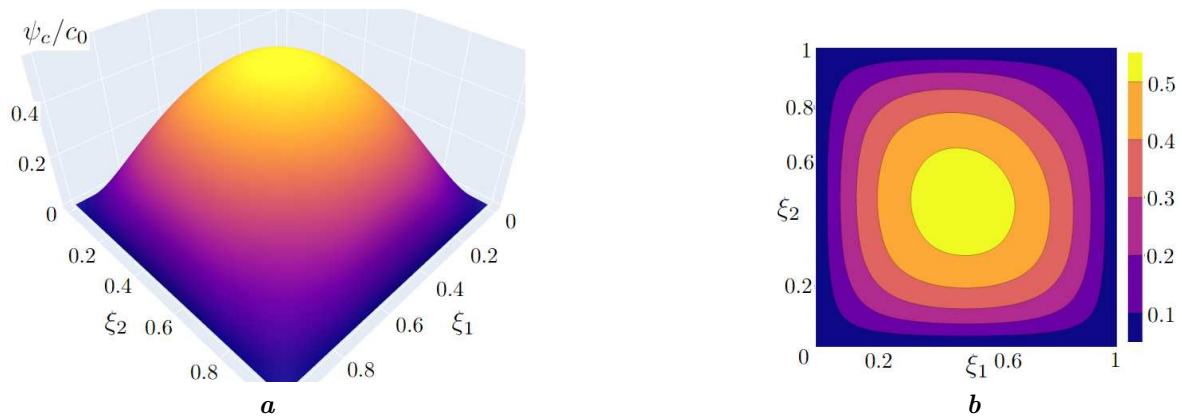
Figures 3–10 show the characteristic surfaces formed by the correlation function  $\psi_c(\tau_1, \xi_1, \tau_2, \xi_2)$  (Figures a) and the corresponding 2D-plots (Figures b) for the basic values of the problem parameters. For values  $\tau_1$  and  $\tau_2$  of small time interval  $[0.05, 0.06]$  3D- and 2D-plots of the correlation function are demonstrated for the following intervals of action of the point source system:  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  in Figure 3,  $[\bar{\xi}_1, \bar{\xi}_2] = [0.1, 0.3]$  in Figure 4,  $[\bar{\xi}_1, \bar{\xi}_2] = [0.7, 0.9]$  in Figure 5,  $[\bar{\xi}_1, \bar{\xi}_2] = [0.2, 0.8]$  in Figure 6.



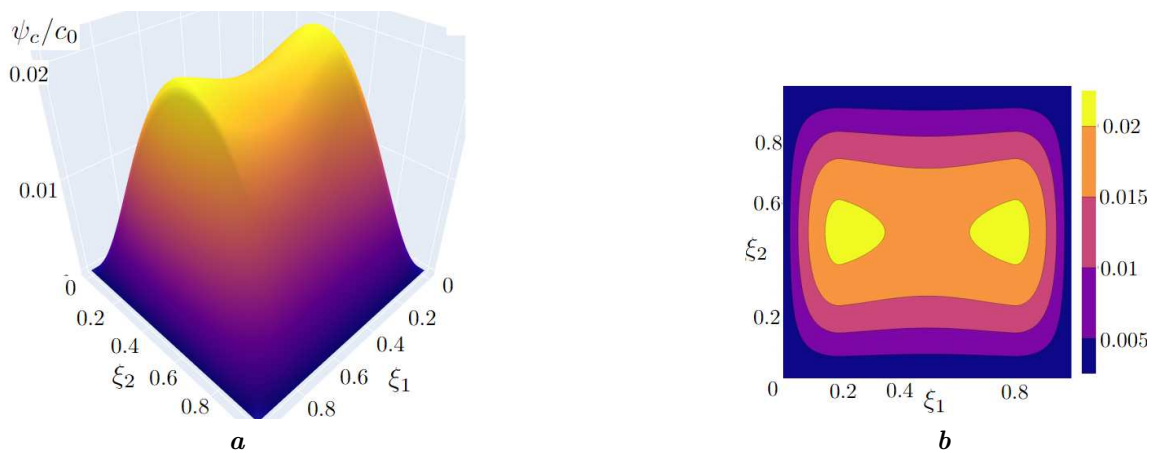
**Fig. 3.** Correlation function for the interval of action of the point source system  $[0.4, 0.6]$  at  $\tau_1 = 0.05$  and  $\tau_2 = 0.06$ .



**Fig. 4.** Correlation function for the interval of action of the point source system  $[0.1, 0.3]$  at  $\tau_1 = 0.05$  and  $\tau_2 = 0.06$ .

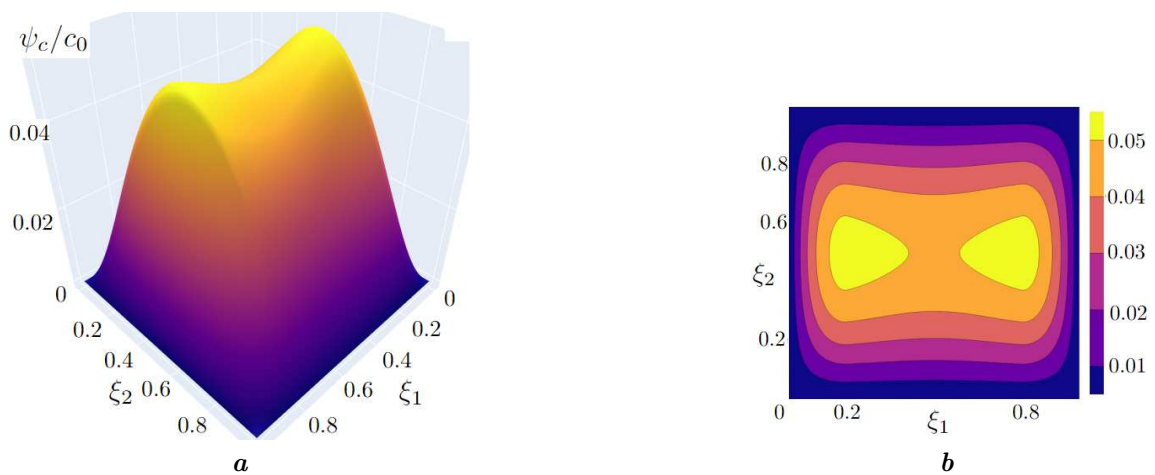


**Fig. 5.** Correlation function for the interval of action of the point source system  $[0.7, 0.9]$  at  $\tau_1 = 0.05$  and  $\tau_2 = 0.06$ .

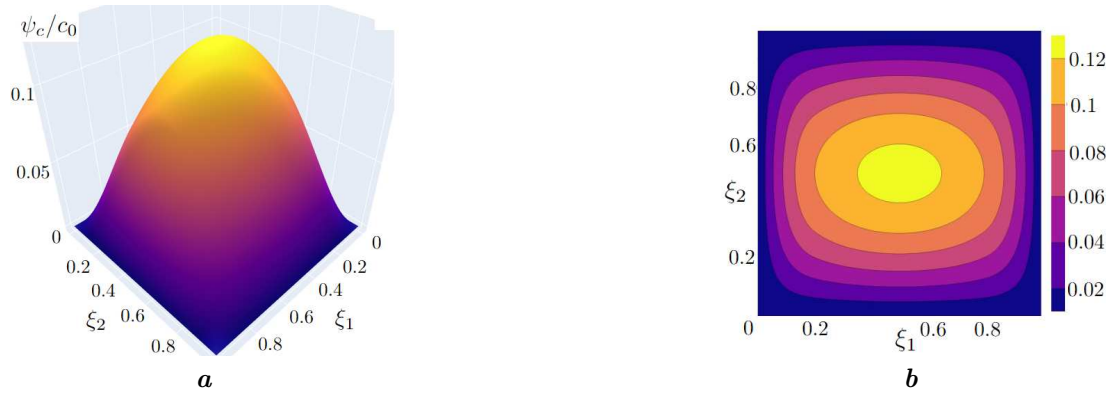


**Fig. 6.** Correlation function for the interval of action of the point source system  $[0.2, 0.8]$  at  $\tau_1 = 0.05$  and  $\tau_2 = 0.06$ .

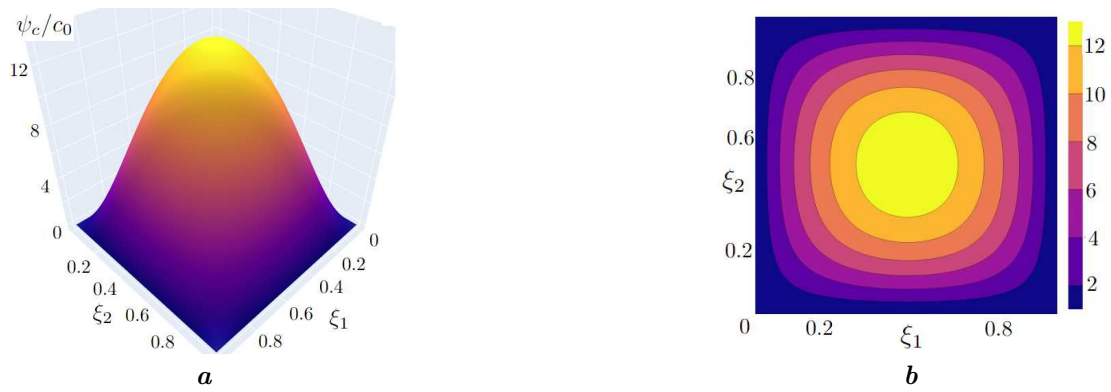
Figures 7–10 illustrate 3D- and 2D-plots of the correlation function  $\psi_c(\tau_1, \xi_1, \tau_2, \xi_2)$  for  $\tau_1 = 0.5$  and  $\tau_2 = 0.06$  with  $[\xi_1, \xi_2] = [0.2, 0.8]$  (Figures 7–8), with  $[\xi_1, \xi_2] = [0.2, 0.3]$  (Figure 9), with  $[\xi_1, \xi_2] = [0.8, 0.9]$  (Figure 10).



**Fig. 7.** Correlation function for the interval of action of the point source system  $[0.2, 0.8]$  at  $\tau_1 = 0.5$  and  $\tau_2 = 0.06$ .



**Fig. 8.** Correlation function for the interval of action of the point source system  $[0.2, 0.8]$  at  $\tau_1 = 0.5$  and  $\tau_2 = 0.45$ .



**Fig. 9.** Correlation function for the interval of action of the point source system  $[0.2, 0.3]$  at  $\tau_1 = 0.5$  and  $\tau_2 = 0.45$ .



**Fig. 10.** Correlation function for the interval of action of the point source system  $[0.8, 0.9]$  at  $\tau_1 = 0.5$  and  $\tau_2 = 0.45$ .

Note that the characteristic surfaces formed by the correlation function  $\psi_c(\tau_1, \xi_1, \tau_2, \xi_2)$  are close to being symmetric ones (Figures 3–10). For small  $\tau_1$  and  $\tau_2$  (Figures 3–6) the function  $\psi_c(\tau_1, \xi_1, \tau_2, \xi_2)$  achieves its highest values in the middle of the layer. The closer the interval of action of the point source system  $[\bar{\xi}_1, \bar{\xi}_2]$  is to the surface of the body  $\xi = 0$  the slower is the decline of the correlation function (Figures 3–5). At the same time, the maximum values of  $\psi_c(\tau_1, \xi_1, \tau_2, \xi_2)$  remain the same. If the interval expands, the values of the correlation function in the middle of the layer increase and the its decline at the edges becomes sharper, moreover two maxima appear (Figure 6).

We also note that the longer is the time interval of correlation, the more probable is appearance of two local maxima of the correlation function (Figures 7 and 8). Shifting of the interval  $[\bar{\xi}_1, \bar{\xi}_2]$  to the boundary of the body  $\xi = 0$  or to the boundary  $\xi = \xi_0$  leads to a more symmetrical shape of the surface  $\psi_c(\tau_1, \xi_1, \tau_2, \xi_2)$ .



### 5. Correlation coefficient

The correlation coefficient of the concentration field  $K_c(t_1, x_1; t_2, x_2)$ , which determines the numerical measure of “dependence” of the field values at the points  $(t_1, x_1)$  and  $(t_2, x_2)$ , is defined by the expression [12, 13]:

$$K_c(t_1, x_1; t_2, x_2) = \frac{\psi_c(t_1, x_1; t_2, x_2)}{\sqrt{\sigma_c^2(t_1, x_1)\sigma_c^2(t_2, x_2)}}. \tag{12}$$

We substitute the relations for the variance (8) and for the correlation function (11) into (12). We have

$$K_c(t_1, x_1; t_2, x_2) = \frac{K_c^1(t_1, x_1; t_2, x_2)}{K_c^2(t_1, x_1; t_2, x_2)}, \tag{13}$$

where

$$K_c^1(t_1, x_1; t_2, x_2) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(y_n x_1) \sin(y_m x_2)}{y_n^3 y_m^3} (1 - e^{-dy_n^2 t_1 / \rho}) (1 - e^{-dy_m^2 t_2 / \rho}) \times [(1 - (-1)^n)(1 - (-1)^m) - (\cos(y_n \bar{x}_1) - \cos(y_n \bar{x}_2))(\cos(y_m \bar{x}_1) - \cos(y_m \bar{x}_2))], \tag{14}$$

$$K_c^2(t_1, x_1; t_2, x_2) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{\sin(y_n x_1) \sin(y_m x_2)}{y_n^3 y_m^3} (1 - e^{-dy_n^2 t_1 / \rho}) (1 - e^{-dy_m^2 t_2 / \rho}) \times [(1 - (-1)^n - \cos(y_n \bar{x}_1) + \cos(y_n \bar{x}_2))(1 - (-1)^m - \cos(y_m \bar{x}_1) + \cos(y_m \bar{x}_2))]. \tag{15}$$

It follows from the obtained formulas (13)–(15) that the correlation coefficient does not depend on the power of point sources and their number.

The values of the correlation coefficient of the concentration field at different points  $(t_1, x_1)$  and  $(t_2, x_2)$  are presented in the Table 1.

**Table 1.** Values of the correlation coefficient for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  and  $[\bar{\xi}_1, \bar{\xi}_2] = [0, 1]$ .

$\xi_1$	$\xi_2$	$\tau_1$	$\tau_2$	$K_c(\tau_1, \xi_1; \tau_2, \xi_2)$	$\xi_1$	$\xi_2$	$\tau_1$	$\tau_2$	$K_c(\tau_1, \xi_1; \tau_2, \xi_2)$
$[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$					$[\bar{\xi}_1, \bar{\xi}_2] = [0, 1]$				
0.5054	0.5044	0.5	0.45	0.9524	0.5133	0.5044	0.5	0.45	0.9520
0.1416	0.0620	0.5	0.45	0.5866	0.0353	0.0442	0.5	0.45	0.2181
0.1416	0.4956	0.5	0.45	0.8311	0.0265	0.5044	0.5	0.45	0.6194
0.0177	0.5044	0.5	0.45	0.8790	0.53097	0.0531	0.5	0.45	0.3407
0.5133	0.5221	0.05	0.06	0.9557	0.5309	0.4778	0.05	0.06	0.9363
0.1681	0.1062	0.05	0.06	0.3311	0.0354	0.0442	0.05	0.06	0.0557
0.1504	0.5044	0.05	0.06	0.7156	0.062	0.5044	0.05	0.06	0.4669
0.0880	0.4956	0.05	0.06	0.8112	0.5044	0.0619	0.05	0.06	0.1232

Note that the correlation coefficient achieves its highest values when points  $\xi_1$  and  $\xi_2$  are located in the middle of the layer both for  $[\bar{\xi}_1, \bar{\xi}_2] = [0.4, 0.6]$  and for  $[\bar{\xi}_1, \bar{\xi}_2] = [0, 1]$  (Table 1), i.e. here the relationship between the concentration field at points  $\xi = \xi_1$  and  $\xi = \xi_2$  is the strongest one. The greater is the distance between the points  $\xi = \xi_1$  and  $\xi = \xi_2$ , or the closer these points occur to the boundaries of the layer, the smaller values the correlation coefficient takes on.

### 6. Conclusion

Thus, for description of the stochastic processes of impurity diffusion caused by the presence of randomly located point mass sources the initial-boundary value problem is formulated under given statistics of random sources and solved in the case of uniformly distributed mass sources of different power acting within a certain internal interval. The random point mass sources are assembled into a system of sources, and the contribution of each source to the system is assumed to be equally probable. The solution to the problem is constructed in the form of the sum of the solution of the homogeneous

problem and the convolution of the Green's function with the system of the point sources. Such representation of the solutions allows not only to carry out a quantitative and qualitative analysis of the averaged concentration of migrating impurities, but also to find its variance, correlation function of the concentration field as well as the correlation coefficient. The formulas for the second moments of the field of the concentration of the migrating substance are obtained, they are expressed in terms of the second moment of random mass sources. Based on the obtained formulas, software modules have been developed for simulating the behavior of the averaged concentration, variance and correlation function for different lengths of intervals of action of the system of point sources and their locations in the body region, for different number of sources in the system, at the presence or absence of a source with prevailing power.

The symmetry of the field variance is shown as well as the closeness of the surfaces formed by the concentration field's correlation function to being symmetric. It is established that the variance increases with time until it reaches the steady-state regime. Particularly, growth begins in the vicinity of two different spatial points, then these maxima are leveled off and one maximum is formed in the middle of the layer. We also show that the correlation function achieves the largest values in the middle of the layer and the interval location of the point source action system near the boundaries of the body affects only the rate of the correlation function decline.

Future research could study the diffusion processes under the action of randomly located point sources of mass, when the location of each source in the body region is an independent random variable.

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- [1] Zhou T., Yongbo P. Adaptive Bayesian quadrature based statistical moments estimation for structural reliability analysis. *Reliability Engineering & System Safety*. **198**, 106902 (2020).
  - [2] Nieto-Barajas L. E. A class of dependent Dirichlet processes via latent multinomial processes. *A Journal of Theoretical and Applied Statistics*. **55** (5), 1169–1179 (2021).
  - [3] Lin G. D., Dou X. An identity for two integral transforms applied to the uniqueness of a distribution via its Laplace–Stieltjes transform. *A Journal of Theoretical and Applied Statistics*. **55** (2), 367–385 (2021).
  - [4] Montgomery D. C., Runger G. C. *Applied Statistics and Probability for Engineers*. John Wiley & Sons (2010).
  - [5] Bourgeat A., Piatnitski A. L. Averaging of a singular random source term in a diffusion convection equation. *SIAM Journal on Mathematical Analysis*. **42** (6), 2626–2651 (2010).
  - [6] Bourgeat A., Gipouloux O., Smai F. Scaling up of source terms with random behavior for modelling transport migration of contaminants in aquifers. *Nonlinear Analysis: Real World Applications*. **11** (6), 4513–4523 (2010).
  - [7] Bilushchak Y., Chernukha O. Modeling of the Processes of Heterodiffusion in Two Ways for the Cascade Decay of Admixture Particles. II. Quantitative Analysis. *Journal of Mathematical Sciences*. **256**, 482–496 (2021).
  - [8] Chernukha O. Y., Bilushchak Y. I. A Mathematical Model of Two-Way Heterodiffusion Processes with Cascade Decay of Migrating Particles. *Journal of Mathematical Sciences*. **253**, 156–167 (2021).
  - [9] Chaplya Y., Chernukha O. Mathematical modeling diffusion of decaying particles in regular structures. *Reviews on Advanced Materials Science*. **23** (1), 21–31 (2010).
  - [10] Pukach P., Chernukha Y. Mathematical modeling of impurity diffusion process under given statistics of a system of point mass sources. I. *Mathematical Modeling and Computing*. **11** (2), 385–393 (2024).
  - [11] Abramowitz M., Stegun I. A. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. New York, Dover (1972).
  - [12] Mood A. M., Graybill F. A., Boes D. C. *Introduction to the theory of statistics*. McGraw-Hill (1974).
  - [13] Chernukha O., Bilushchak Y., Chuchvara A. Modelling the diffusion processes in stochastically non-homogeneous structures. *Lviv, Rastr-7* (2016).

## Математичне моделювання процесу дифузії домішки за заданої статистики системи точкових джерел маси. II

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Проведено моделювання процесу дифузії домішки в шарі за дії системи випадкових точкових джерел. Джерела маси різної потужності розподілені рівномірно на певному внутрішньому інтервалі, який який може співпадати з усією областю шару. Задана статистика випадкових джерел. Розв'язок крайової задачі знайдено як суму розв'язку однорідної задачі і згортки функції Гріна із системою випадкових точкових джерел. Усереднення розв'язку проведено на внутрішньому підінтервалі і в усіх області тіла. Отримано формули для дисперсії, функції кореляції поля концентрації і коефіцієнта кореляції, які виражаються другі моменти випадкових точкових джерел. Розроблено програмні модулі для симуляції поведінки усередненої концентрації, дисперсії і функції кореляції.

**Keywords:** *математичне моделювання; дифузія; випадкове точкове джерело; ймовірнісний розподіл; функція кореляції; дисперсія; коефіцієнт кореляції.*