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Modeling release and distribution of harmful substances in river

Dilnoz Muhamediyeva[1*], and *Otabek* Khujaev[2]

[1]"TashkentInstitute of Irrigation and Agricultural Mechanization Engineers" National Research University, Tashkent, Uzbekistan
[2]Urgench Branch of Tashkent university of Information Technologies Named After Muhammad al-Khwarizmi, Urgench, Uzbekistan

Abstract. The development and analysis of a computational algorithm for mathematical models of the release and spread of harmful substances is an important area of research that can help mitigate the impact of pollution on the environment and human health. Mathematical models of the distribution of harmful substances in the river are useful for predicting the spread of pollutants and identifying potential environmental and public health risks. The computational algorithm for the problem of diffusion of harmful substances can help researchers and policymakers to understand the mechanisms of pollutant dispersion and identify effective strategies for mitigating the impact of pollution. The algorithm can simulate the release and spread of harmful substances in various scenarios, including accidental spills, industrial discharges, and natural disasters. The results of a computational experiment can provide valuable insights into the behavior of pollutants in different environmental conditions and help identify potential risks and areas of concern. By analyzing the results of a computational experiment, researchers can develop effective strategies for managing and mitigating the impact of pollution on the environment and public health.

1 Introduction

The ecological problem is a global concern that affects the well-being of every living being on Earth. It is essential to promote environmental priorities to ensure sustainable development and protect the planet for future generations. The increasing pollution and environmental degradation threaten human health, biodiversity, and ecosystem services [1].

The rise in pollution indicators such as carbon dioxide, nitrogen oxides, sulphur, and other atmospheric pollutants is a result of human activities, including industrialization, urbanization, and the use of fossil fuels. These activities have led to deforestation, land degradation, climate change, and biodiversity loss, among other environmental problems [2].

Addressing these issues requires a collective effort from governments, businesses, and individuals worldwide. Implementing policies and regulations that promote sustainable

* Corresponding author: dilnoz134@rambler.ru

practices, such as renewable energy, conservation of natural resources, and waste reduction, is essential. Additionally, individuals can make a difference by adopting environmentally friendly behaviors, such as reducing energy consumption, recycling, and using public transportation.

A thorough investigation and assessment of atmospheric pollution are crucial for understanding and mitigating the impact of pollution on the environment and public health. The distinction between passive and active impurities is important for determining the behavior and fate of pollutants in the atmosphere. Passive impurities tend to follow a straightforward path from the emission source to the Earth's surface and can directly impact the environment and public health. In contrast, active impurities can undergo chemical reactions and atmospheric transformations, making them more challenging to predict and manage [3].

The dissemination of industrial emissions into the atmosphere can occur through various processes, including advective transfer and diffusion. The behavior of the emitted particles depends on their size and physical properties. Larger particles tend to settle under the influence of gravity at a constant rate. In comparison, smaller particles can remain suspended in the atmosphere longer and travel long distances. Understanding the behavior and fate of pollutants in the atmosphere is essential for developing effective strategies for managing and mitigating the impact of pollution. This can include reducing emissions, implementing air quality regulations, and promoting sustainable practices. In summary, a thorough investigation and assessment of atmospheric pollution, including the distinction between passive and active impurities, is necessary for mitigating the impact of pollution on the environment and public health. Heavy impurities primarily settle due to the gravitational field, while light ones undergo diffusion. Gaseous impurities such as oxides are the most hazardous to the environment, and we will only consider light compounds [4].

We will now present the most significant outcomes of the authors' previous investigations.

The article [5] proposes numerical techniques for solving the diffusion equation and some hydrodynamic problems with peculiar initial or boundary conditions and singularities that arise in the solution due to the differential operator's characteristics. One-dimensional nonstationary diffusion equations, advection equations, and the "shallow water" theory equations serve as examples. The solution of irregular problems demands the close correspondence of the spectral properties between the differential operator of the examined equation and the operator of the numerical method approximating it. The paper introduces the concept of spectral efficiency and explores the relationship between spectral efficiency and method precision. It also examines the spectral efficiency of the Lagrange and Hermite space finite element and finite difference techniques.

In [6], a new approach for directly computing heat and diffusion fluxes at the interface between media, without the need for pre-determining fields, is presented. This method extends the range of problems for which solutions can be obtained in the form of formulas, making it practically significant. The paper provides examples of the solution to various crucial problems in the heat and mass transfer theory, including those involving chemical transformations.

In [7], the article examines the diffusion of particles of one type placed in a medium with particles of another type. The study investigates the problem's existence and the uniqueness of the solution in a broader context than the previous research and discusses the solution's properties in specific cases.

2 Methods

Consider the transport of pollutants in the river section using a three-dimensional model [8-10].

$$\frac{\partial q}{\partial t}+u\frac{\partial q}{\partial x}+v\frac{\partial q}{\partial y}+w\frac{\partial q}{\partial z}=\frac{\partial}{\partial x}k_x\frac{\partial q}{\partial x}+\frac{\partial}{\partial y}k_y\frac{\partial q}{\partial y}+\frac{\partial}{\partial z}k_z\frac{\partial q}{\partial z}-\alpha q\,. \tag{1}$$

Initial condition:

$$q(x,y,z,o)=q_0(x,y,z),\ 0\le x\le l_1,\ \ -l_2\le y\le l_2,\ \ 0\le z\le l_3\,. \tag{2}$$

Boundary conditions:

$$q(0,y,z,t)=q_0(y,z,t);\ \ 0\le z\le l_3;\ \ -l_2\le y\ \le l_2;\ \ 0\le t\le T\ . \tag{3}$$

$$\frac{\partial q(x,y,z,t)}{\partial x}\Big|_{x=l_1}=0,\ 0\le z\le l_2,\ \ -l_2\le y\le l_2,\ \ 0\le \mathrm{t}\le \mathrm{T}\,; \tag{4}$$

$$\frac{\partial q(x,y,z,t)}{\partial y}\Big|_{y=-l_2}=\frac{\partial q(x,y,z,t)}{\partial y}\Big|_{y=l_2}=0,\ 0\le x\le l_1,\ \ 0\le z\le l_3,\ \ 0\le \mathrm{t}\le \mathrm{T}; \tag{5}$$

$$\frac{\partial q(x,y,z,t)}{\partial z}\Big|_{z=0}=\frac{\partial q(x,y,z,t)}{\partial z}\Big|_{z=l_3}=0,\ \ 0\le x\le l_1,-l_2\le y\le l_3,\ \ 0\le \mathrm{t}\le \mathrm{T}; \tag{6}$$

The characteristic data provided in [11] for modeling water pollution in a river are as follows:

q is concentration of the propagating substance;

t is time;

axis x and y are located in a horizontal plane;

axis z is located vertically;

u is average speed along the x-axis: This component represents the average speed of impurities in the x-direction;

v is average speed along the y-axis: This component represents the average speed of impurities in the y-direction;

w is average speed along the z-axis: This component represents the average speed of impurities in the z-direction.

k_x, k_y – are horizontal exchange coefficient;

k_z – is vertical exchange coefficient;

α – is transformation coefficient, which determines concentration changes due to impurity transformations;

l_1 – is average length of the watercourse;

l_2 – is average width of the watercourse;

l_3 – is depth of the watercourse.

The simplified form of the equation (1) for practical problems, where the axis x is oriented in the direction of the average wind speed and vertical motions in the atmosphere are small $v=0$, is given by $w\approx 0$. For a heavy impurity gradually settling down, the term $\frac{\partial q}{\partial t}$ represents the settling rate and enters the equation with a minus sign. In prognostic problems, a nonstationary term $\frac{\partial q}{\partial t}$ is necessary to account for changes in concentrations in the atmosphere with time. Still, it can be eliminated by setting it equal to zero if the changes are quasi-stationary in nature. When studying the process of steady diffusion under conditions of horizontally homogeneous terrain, the term $\frac{\partial q}{\partial t}$ is excluded, and the resulting simplified equation takes the form given in [12].

$$u\frac{\partial q}{\partial x}+w\frac{\partial q}{\partial z}=\frac{\partial}{\partial y}k_y\frac{\partial q}{\partial y}+\frac{\partial}{\partial z}k_z\frac{\partial q}{\partial z}-\alpha q. \tag{7}$$

In the equation mentioned above, the second term on both sides vanishes when dealing with a light impurity ($w\approx 0$), while for a conserved impurity ($\alpha=0$), the last term on the right-hand side also disappears. Conservative impurities refer to substances that do not undergo any degradation. In contrast, non-conservative ones do, either through degradation or transformation into different forms, for instance, in the case of water pollution. One way to quantify this reduction in concentration resulting from these processes is to utilize non-conservative coefficients that account for the total transformation rate of substances. The non-conservative coefficients for pollutant decay are negative, and further elaboration can be found in [11]. When vertical currents are present in the atmosphere, the term w includes the vertical component of the air velocity $w\frac{\partial q}{\partial z}$. In complex hilly terrains where wind direction is not horizontal and varies with distance, the term $\frac{\partial}{\partial x}k_x\frac{\partial q}{\partial x}$ should be considered.

Due to the complexity of the problem, obtaining an analytical solution is challenging. Thus, to tackle the problem, we will employ the finite difference method, where we discretize the range of change and the desired variables into a grid [12-15].

To integrate the problems (1)-(6), we will use the finite difference method and develop a computational algorithm using the method of fractional steps. To accomplish this, we represent equation (1) in the operator form:

$$\frac{\partial q}{\partial t}+\alpha q=(L_1+L_2+L_3)q\ , \tag{8}$$

where

$$L_1 q=-u\frac{\partial q}{\partial x}+\frac{\partial}{\partial x}k_x\frac{\partial q}{\partial x}, \tag{9}$$

$$L_2 q=-v\frac{\partial q}{\partial y}+\frac{\partial}{\partial y}k_y\frac{\partial q}{\partial y}, \tag{10}$$

$$L_3 q=-w\frac{\partial q}{\partial z}+\frac{\partial}{\partial z}k_z\frac{\partial q}{\partial z}. \tag{11}$$

The time step is entered as follows: $t=n\Delta t,\ n=\overline{1,N}$, and problem (8), (1)-(6) for each n-th step is solved in three stages; the approximation in fractional time steps has the form [12]:

$$\frac{q^{n+1/3}-q^n}{\Delta t/3}+\alpha q^{n+1/3}=L_1 q^{n+1/3}+(L_2+L_3)q^n\ , \tag{12}$$

$$\frac{q^{n+2/3}-q^{n+1/3}}{\Delta t/3}+\alpha q^{n+2/3}=L_2 q^{n+2/3}+(L_1+L_3)q^{n+1/3}\ , \tag{13}$$

$$\frac{q^{n+1}-q^{n+2/3}}{\Delta t/3}+\alpha q^{n+1}=L_3 q^{n+1}+(L_1+L_2)q^{n+2/3}\ , \tag{14}$$

further for each moment of time t_n, the difference equation is solved in the grid domain:

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$$D_h = \begin{cases} x_i = \Delta x i, i = 1,...,N_1+1; \Delta x = \dfrac{L_x}{N_1+1}; \\ y_j = \Delta y j, j = 1,...,N_2+1; \Delta y = \dfrac{Ly}{N_2+1}; \\ z_l = z_{l-1} + \Delta z_l, \Delta z_l = z_l - z_{l-1}, l = 1,2,...,K. \end{cases} \quad (15)$$

A one-dimensional problem is solved at each stage with the corresponding boundary conditions (2)-(6). The operator $L_1 q$ is replaced by a finite difference operator as follows:

$$\left(L_1 q\right)_l^{n+1} = \left(\frac{\partial}{\partial x} k_x \frac{\partial q}{\partial x}\right)_l^{n+1} - \left(u \frac{\partial q}{\partial x}\right)_l^{n+1}. \quad (16)$$

An approximation is presented for the cases $u_l^{n+1} \geq 0$ and $u_l^{n+1} < 0$ separately

$$\left(L_1 q\right)_l^{n+1} = \left(k(x)_{l+1/2}^{n+1} \frac{q_{l+1}^{n+1} - q_l^{n+1}}{\Delta x_l} - k(x)_{l-1/2}^{n+1} \frac{q_l^{n+1} - q_{l-1}^{n+1}}{\Delta x_{l-1}}\right) \cdot \frac{1}{\frac{\Delta x_l + \Delta x_{l+1}}{2}} + \frac{u_l^{n+1}}{\Delta x_{l-1}} q_{l-1}^{n+1} - \frac{u_l^{n+1}}{\Delta x_{l-1}} q_l^{n+1}, \quad (17)$$

at $u_l^{n+1} \geq 0$, and

$$\left(L_1 q\right)_l^{n+1} = \left(k(x)_{l+1/2}^{n+1} \frac{q_{l+1}^{n+1} - q_l^{n+1}}{\Delta x_l} - k(x)_{l-1/2}^{n+1} \frac{q_l^{n+1} - q_{l-1}^{n+1}}{\Delta x_{l-1}}\right) \cdot \frac{1}{\frac{\Delta x_l + \Delta x_{l+1}}{2}} + \frac{u_l^{n+1}}{\Delta x_l} q_l^{n+1} - \frac{u_l^{n+1}}{\Delta x_l} q_{l+1}^{n+1}, \quad (18)$$

at $u_l^{n+1} < 0$.

Merging two records:

$$\left(L_1 q\right)_l^{n+1} = \left(\frac{2k(x)_{l-1/2}^{n+1}}{\Delta x_{l-1}(\Delta x_l + \Delta x_{l+1})} + \frac{\left|u_l^{n+1}\right| + u_l^{n+1}}{2\Delta x_{l-1}}\right) q_{l-1}^{n+1} - \left(\frac{2k(x)_{l-1/2}^{n+1}}{\Delta x_{l-1}(\Delta x_l + \Delta x_{l+1})} + \frac{2k(x)_{l+1/2}^{n+1}}{\Delta x_l(\Delta x_l + \Delta x_{l+1})} + \frac{\left|u_l^{n+1}\right| + u_l^{n+1}}{2\Delta x_{l-1}} + \frac{\left|u_l^{n+1}\right| - u_l^{n+1}}{2\Delta x_l}\right) q_l^{n+1} + \left(\frac{2k(x)_{l+1/2}^{n+1}}{\Delta x_l(\Delta x_l + \Delta x_{l+1})} + \frac{\left|u_l^{n+1}\right| - u_l^{n+1}}{2\Delta x_l}\right) q_{l+1}^{n+1}. \quad (19)$$

Let's introduce an abbreviation:

$$\left(L_1 q\right)_l^{n+1} = AX^{n+1} q_{l-1}^{n+1} - BX^{n+1} q_l^{n+1} + CX^{n+1} q_{l+1}^{n+1}, \quad (20)$$

where

$$AX^{n+1} = \frac{2k(x)_{l-1/2}^{n+1}}{\Delta x_{l-1}(\Delta x_l + \Delta x_{l+1})} + \frac{\left|u_l^{n+1}\right| + u_l^{n+1}}{2\Delta x_{l-1}}, \quad (21)$$

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$$BX^{n+1} = \frac{2k(x)_{l-1/2}^{n+1}}{\Delta x_{l-1}(\Delta x_l + \Delta x_{l+1})} + \frac{2k(x)_{l+1/2}^{n+1}}{\Delta x_l(\Delta x_l + \Delta x_{l+1})} + \frac{\left|u_l^{n+1}\right| + u_l^{n+1}}{2\Delta x_{l-1}} + \frac{\left|u_l^{n+1}\right| - u_l^{n+1}}{2\Delta x_l}, \tag{22}$$

$$CX^{n+1} = \frac{2k(x)_{l+1/2}^{n+1}}{\Delta x_l(\Delta x_l + \Delta x_{l+1})} + \frac{\left|u_l^{n+1}\right| - u_l^{n+1}}{2\Delta x_l}. \tag{23}$$

With these boundary conditions taken into account, the different schemes take the form:

$$\begin{cases} (L_1 q)_{1,j,l} = -BXq_{1,j,l} + CXq_{2,j,l}, \ \mathrm{i}=1, \\ (L_1 q)_{i,j,l} = AXq_{i-1,j,l} - BXq_{i,j,l} + CXq_{i+1,j,l}, \ \mathrm{i}=2,3,...,\mathrm{N}_1-1, \\ (L_1 q)_{\mathrm{N}_1,j,l} = AXq_{N_1-1,j,l} - BXq_{\mathrm{N}_1,j,l}, \ \mathrm{i}=\mathrm{N}_1. \end{cases} \tag{24}$$

$$\begin{cases} (L_2 q)_{\mathrm{i},1,l} = -BYq_{i,1,l} + CYq_{\mathrm{i},2,l}, \ j=1, \\ (L_2 q)_{i,j,l} = AYq_{i,j-1,l} - BYq_{i,j,l} + CYq_{i,j+1,l}, \ j=2,3,...,\mathrm{N}_2-1, \\ (L_2 q)_{\mathrm{i},\mathrm{N}_2,l} = AYq_{\mathrm{i},\mathrm{N}_2-1,l} - BYq_{\mathrm{i},\mathrm{N}_2,l}, \ j=\mathrm{N}_2. \end{cases} \tag{25}$$

$$\begin{cases} (L_3 q)_{\mathrm{i,j},1} = -BZq_{i,\mathrm{j},l-1} + CZ_{\mathrm{i,j},2}, \ l=1, \\ (L_3 q)_{i,j,l} = AZq_{i,j,l-1} - BZq_{i,j,l} + CZq_{i,j,l+1}, \ l=2,3,...,\mathrm{K}-1, \\ (L_3 q)_{\mathrm{i},j,\mathrm{K}} = AZq_{\mathrm{i,j,K}-1} - BZq_{i,j,K}, \ l=K. \end{cases} \tag{26}$$

Operators on the right side of equation (7) are similarly replaced by finite difference relations, as a result of which we obtain the difference equations:

$$AX_i Q_{j,l}^{n+1/3} = -FX_{j,l}^{n+1/3}, \tag{27}$$

$$AY_j Q_{\mathrm{i},l}^{n+2/3} = -FY_{\mathrm{i},l}^{n+2/3}, \tag{28}$$

$$AZ_l Q_{\mathrm{i,j}}^{n+1} = -FZ_{\mathrm{i},l}^{n+1}, \tag{29}$$

where

$$Q_{j,l}^{n+1/3} = \begin{pmatrix} q_{1,j,l}^{n+1/3} \\ q_{2,j,l}^{n+1/3} \\ \cdots\cdots \\ q_{\mathrm{N}_1,j,l}^{n+1/3} \end{pmatrix}, FX_{j,l}^{n+1/3} = \begin{pmatrix} (L_2+L_3)q_{1,j,l}^n + f_{1,j,l}^{n+1/3} \\ (L_2+L_3)q_{2,j,l}^n + f_{2,j,l}^{n+1/3} \\ \cdots\cdots\cdots\cdots \\ (L_2+L_3)q_{\mathrm{N}_1,j,l}^n + f_{N_1,j,l}^{n+1/3} \end{pmatrix}, \tag{30}$$

$$AX_i^{n+1/3} = \begin{pmatrix} -BX_1^{n+1/3} & CX_1^{n+1/3} & 0 & \ldots & 0 & 0 \\ AX_2^{n+1/3} & -BX_2^{n+1/3} & CX_2^{n+1/3} & \ldots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \ldots & AX_{N_1}^{n+1/3} & -BX_{N_1}^{n+1/3} \end{pmatrix}. \tag{31}$$

$$Q_{i,l}^{n+2/3}=\begin{pmatrix} q_{i,1,l}^{n+2/3} \\ q_{i,2,l}^{n+2/3} \\ \dots\dots \\ q_{i,N_2,l}^{n+2/3} \end{pmatrix},\quad FY_{i,l}^{n+2/3}=\begin{pmatrix} (L_1+L_3)q_{i,1,l}^{n+1/3}+f_{i,1,l}^{n+2/3} \\ (L_1+L_3)q_{i,2,l}^{n+1/3}+f_{i,2,l}^{n+2/3} \\ \dots\dots\dots\dots \\ (L_1+L_3)q_{i,N_2,l}^{n+1/3}+f_{i,N_2,l}^{n+2/3} \end{pmatrix}, \quad (32)$$

$$AY_j^{n+2/3}=\begin{pmatrix} -BY_1^{n+2/3} & CY_1^{n+2/3} & 0 & \dots & 0 & 0 \\ AY_2^{n+2/3} & -BY_2^{n+2/3} & CY_2^{n+2/3} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots AY_{N_2}^{n+2/3} & -BY_{N_2}^{n+2/3} \end{pmatrix}. \quad (33)$$

$$Q_{i,j}^{n+1}=\begin{pmatrix} q_{i,j,1}^{n+1} \\ q_{i,j,2}^{n+1} \\ \dots\dots \\ q_{i,j,K}^{n+1} \end{pmatrix},\quad FZ_{i,j}^{n+1}=\begin{pmatrix} (L_1+L_2)q_{i,j,1}^{n+2/3}+f_{i,j,1}^{n+1} \\ (L_1+L_2)q_{i,j,2}^{n+2/3}+f_{i,j,2}^{n+1} \\ \dots\dots\dots\dots \\ (L_1+L_2)q_{i,j,K}^{n+2/3}+f_{i,j,K}^{n+1} \end{pmatrix}, \quad (34)$$

$$AZ_l^{n+1}=\begin{pmatrix} -BZ_1^{n+1} & CZ_1^{n+1} & 0 & \dots & 0 & 0 \\ AZ_2^{n+1} & -BZ_2^{n+1} & CZ_2^{n+1} & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots AZ_K^{n+1} & -BY_K^{n+1} \end{pmatrix}. \quad (35)$$

Hence, solving the problem stated in equations (1)-(6) is challenging to solve analytically. Therefore, we will employ the finite difference method to solve the problem by replacing the range of change and the desired variables with discrete grid points [16-20]. In this method, we use the method of fractional steps and write equation (1) in the operator form. Consequently, the problem's solution reduces to solving a system of linear algebraic equations at every time step. The coefficients of the difference equations concerning x and y are dependent on the height of the levels and time, while the coefficients of the difference equation concerning z are dependent on x, y, and time t.

Matrix AX_i, AY_j, AY_j represents a three-point matrix with diagonal dominance, i.e., satisfies the stability condition, and to solve it, the sweep method can be used.

3 Results and Discussion

Given:

Section length: $L = 11000.0$;

Average river width: $w = 7.00000$ $(m = 2)$;

Average current speed: $v = 0.68429$;

Average water consumption: $vE = 0.63966$;

Water parameters:

Average diffusion coefficients$k_x = 0.18350$; $k_y = 0.11350$;

Graphs at the initial condition for given values are shown in Figures 1-4.

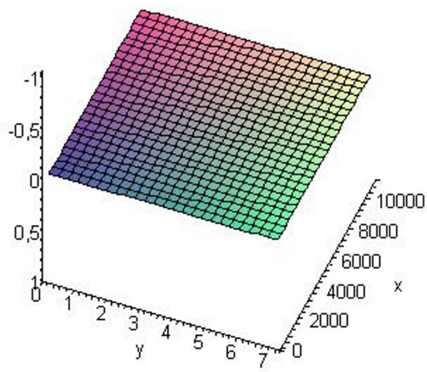

Fig. 1. Emission concentration at $t = 0, z = 0$.

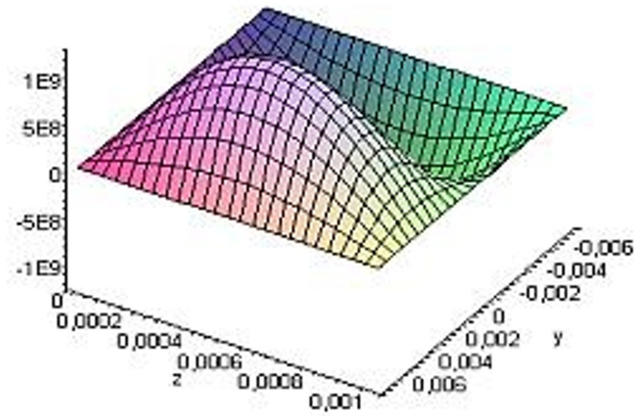

Fig. 2. Axis Emission concentration OY, OZ at $t = 0$, $x = 343.75м$.

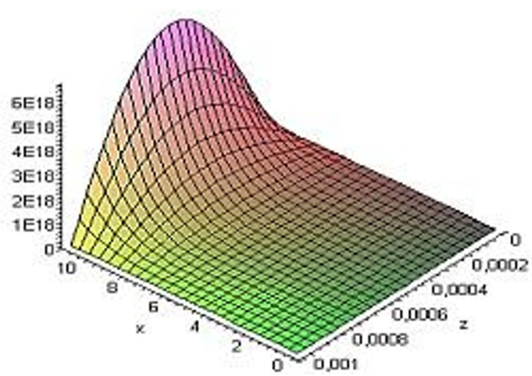

Fig. 3. Emission concentration along axes OX, OZ $t = 0$, $y = 3m$.

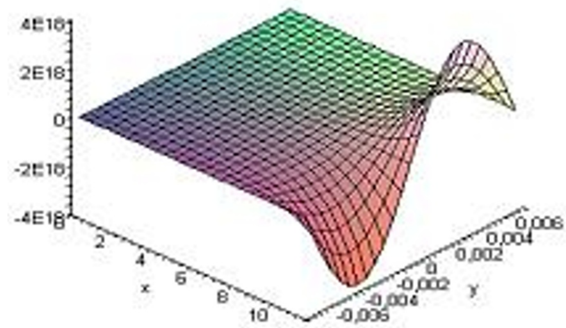

Fig. 4. Emission concentration by at $t = 0, \quad z = 0.2m$.

4 Conclusion

The study investigated various analytical and numerical methods used to determine the dispersion of harmful impurities from pollution sources. It focused on examining mathematical models for the spread of harmful impurities and water resource pollution diffusion. The research developed algorithms for one-dimensional, two-dimensional, and three-dimensional models of impurity diffusion from pollution sources. Results were presented, and it was shown that it is possible to determine the roots of the diffusion equation numerically without calculating the roots of the characteristic equation. These findings provide valuable insights into the numerical solutions to problems related to the propagation of harmful impurities and diffusion.

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