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NUMERICAL MODELING OF THE TRANSPORT AND DIFFUSION OF POLLUTANT PARTICLES TAKING INTO ACCOUNT AIRFLOW CHARACTERISTICS AND TEMPERATURE

Nabieva I.S.
irodamubina777@gmail.com
Digital Technologies and Artificial Intelligence Development Research Institute,
17A, Buz-2, Tashkent, 100125 Uzbekistan.

The article considers the results of experimental and numerical studies of atmospheric pollution processes in industrial zones. The proposed mathematical model helps to solve problems related to monitoring and forecasting the state of the environment in industrial zones, as well as making decisions on protection against the negative impact of anthropogenic factors. studies the physicochemical properties of substances involved in the process of dispersion in the atmosphere. In the process of diffusion, the particle diameter, temperature and wind speed are taken into account. To check the adequacy of the developed mathematical model, computational experiments were carried out on a computer. Analysis of the computational experiments showed that with an increase in wind speed, the concentration of pollutants around the source is not observed, and the area of their distribution expands over time. When the speed of air masses in the atmosphere exceeds the critical value, diffusion of the substance occurs only due to the effect of transition to the atmosphere. Changes in the concentration of pollutants in the layers of the atmosphere over time depending on the actual wind speed are also noted.

Keywords: mathematical model, finite-difference scheme, heat transfer, moisture transfer, raw cotton.

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1 Introduction

Air pollution is a serious problem and it is important to understand how these pollutants move over time and distance. Air pollution from transportation, manufacturing, and technologies used for human needs and social interaction releases a variety of toxic substances into the atmosphere. The harm that these airborne contaminants do to human health is one of the biggest global problems. Air pollution from transportation, manufacturing, and technologies used for human needs and social interaction releases a variety of dangerous substances into the atmosphere. The harmful effects that these hazardous airborne chemicals have on human health are among the main global concerns.

The increase in the number of factories and industrial plants leads to an increase in emissions of substances such as carbon dioxide (CO_2), sulphur dioxide (SO_2), nitrogen oxides (NO_x) and harmful microparticles (PM2.5, PM10). The increase in the number of petrol and diesel vehicles increases air pollution as their exhaust gases contain toxic substances such as carbon monoxide (CO), hydrocarbons and heavy metals. The production of electricity from coal, oil and gas power plants leads to the emission of greenhouse gases and toxic substances. The use of fertilizers, the disposal of animal waste and the burning of crop residues lead to the emission of methane (CH_4), ammonia (NH_3) and other harmful substances. The burning of waste, especially plastic waste, leads to the emission of carcinogenic substances such as dioxins and furans.

Hydrogen, carbon dioxide, and inert gases such as helium, neon, krypton, and xenon make up the remaining constituents. The atmosphere also contains very trace amounts of nitrogen oxide, carbon monoxide, methane, and other industrial and natural gases, but at varying concentrations

Because of the constant evaporation from land and water surfaces, water vapor is also prevalent in the atmosphere. Because it absorbs the majority of the harmful radiation from the Sun that would be harmful to life, the ozone layer is responsible for the existence of life on Earth.

Aerosols (up to 10%) and gases (up to 90%) emitted from human sources are the main causes of atmospheric pollution. It has been discovered that the aerosol composition of the gases released into the environment includes around 160 dangerous chemicals. Transportation, industry, power plants, residential areas, military operations, and nuclear detonations for testing are the main human-caused sources of air pollution.

In this study [1, 2] an effort has been made to use machine learning techniques to mimic the levels of PM2.5, PM10, and NO_2 at two locations in Stuttgart (Marienplatz and Am Neckartor). At these sites, monitoring stations assist in measuring these contaminants. Based on the findings, it has been determined that the pollution data from the neighboring stations significantly influences the pollutant concentration predictions. Additionally, it has been examined whether a comparable approach can be used to estimate pollutant concentrations at other sites. The theory of prediction, influencing elements, and improvement measures were all covered in the systematic description of machine learning (ML) applications in the prediction of atmospheric pollution (mostly particulate particles). By incorporating the physical characteristics of pollutants, matching and enhancing machine learning models, and taking into account the geographical factors of the study area, researchers can increase the prediction model's accuracy.

As mentioned in the introduction, extensive research focused on advancing and refining mathematical models, computational methods, and software systems for addressing issues of atmospheric pollution monitoring and forecasting is actively pursued in numerous prestigious research institutions and universities worldwide. Noteworthy contributions to the development of mathematical modeling methodologies in this area have been made by leading international and domestic scholars, including W.C. Reynolds, G.I. Marchuk, M.E. Berlyand, V.V. Penenko, F.B. Abutaliev, K.S. Karimberdieva, M.L. Arushanov, N. Ravshanov and others.

In the work [3] an accurate numerical method is presented for a class of scalar strongly degenerate convection-diffusion equations. The method is based on the splitting of the convective and diffusive terms. The nonlinear convective part is solved using front tracking and dimensional splitting, while the nonlinear diffusive part is handled with a semi-implicit finite difference scheme. The proposed method incorporates a built-in mechanism to detect and correct non-physical entropy loss, which may occur when large time steps are used. The authors demonstrate that the splitting method accurately resolves sharp gradients, allows for large time steps, and achieves first-order convergence. Despite some minor mass balance errors, the method proves to be highly efficient.

Pollution sources are divided into point and diffuse sources. Point sources emit pollutants from a specific source. Typically, such sources include industrial waste, smoke stacks, and wastewater treatment facilities. Diffuse sources have a diffuse character, making it difficult to link them to a specific location. Examples include agricultural runoff, urban stormwater, and atmospheric deposition.

In this work [4], the standard wind terminology based on the direction from which the winds originate is presented. Since most of the Earth's surface near the equator consists of oceans, it is expressed that these winds absorb heat and moisture as they move toward the equator, as shown in Figure 1.

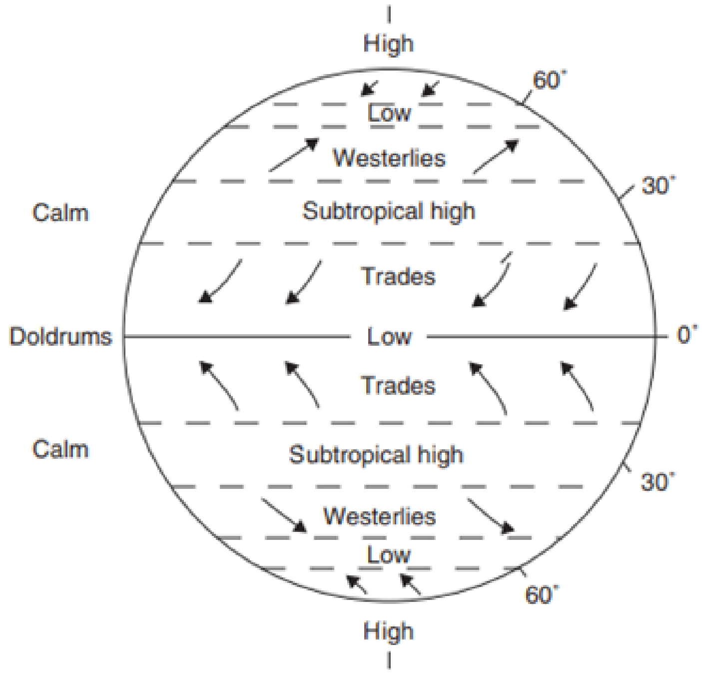

Figure 1 Winds close to the surface across different latitude zones

In the study [5] conducted by Allen and colleagues, the dispersion of volatile organic compounds was examined using a wind tunnel under various wind speed conditions. The results of the study showed that as wind speed increased, the rate of diffusion significantly rose.

In the research [6] by Sahlgren et al., it was determined that urban environments exert a notable influence on the dispersion of pollutants, largely due to wind patterns and local terrain. The study underscores the critical role of geographic dynamics in diffusion processes, emphasizing that accurate assessments of pollutant distribution must account for the complexities introduced by urban settings.

In the article [7] a mathematical model algorithm based on the pollution dispersion equation in a turbulent environment is presented. This approach simultaneously takes into account wind speed, atmospheric turbulence, pollution parameters, and wind direction and strength, which is crucial for determining the volume of dispersion zones. A unique aspect of the study is the use of a coordinate-separated equation for the dispersion of pollutants in a turbulent environment, followed by normalization and parameterization of the conditions.

In the article [8] the movement and diffusion processes of harmful substances in the atmosphere were examined, taking into account various weather conditions and external changes. The research analyzed the migration of pollutants from their sources, their movement due to average air flow (advection), the influence of atmospheric turbulence on their dispersion, and the processes of mass diffusion.

In the articles [9] and [10] the issues of transport and diffusion of harmful aerosol particles in the atmosphere are examined within a two-dimensional framework. This approach considers the inflow and outflow of substances through the boundaries of the region under study. Additionally, the conditions of stable, neutral, and unstable stratification of the air mass in the atmosphere are taken into account.

The accuracy of predicting the diffusion of organic substances in IOA (Insoluble Organic Aqueous) particles using the Stokes-Einstein equation has not been quantitatively assessed, leading to uncertainties in determining diffusion rates based on viscosity measurements. Primarily, under the initiative of the food industry, several tests have been conducted using the Stokes-Einstein equation to predict the diffusion rates of organic substances in organic water matrices, such as saccharid-water. These matrices are utilized in modeling diffusion processes as they represent simple, two-component systems, allowing for the examination of how organic substances move in an aqueous environment in articles [11, 12]. In such cases, the matrices consist of only two different substances, which significantly differs from IOA matrices that contain thousands of various substances [13].

The article [14–17] considers the problems of calculating the concentration of compounds emitted from polluting sources and various aspects of modeling the distribution of harmful substances in the atmosphere.

Many scientists worldwide are currently actively investigating the problems of mathematical modeling of the transport and diffusion processes of hazardous substances in the atmosphere's boundary layer in response to the growing importance of issues pertaining to the ecological state of the atmosphere. Numerous applied and fundamental research have already been conducted and are currently underway using computer modeling methods for the transport and diffusion of dangerous chemicals in the atmospheric boundary layer [17].

In this article [18], a coupled mathematical model of the research object has been developed to monitor and forecast the ecological state of the air in industrial areas, as well as to optimize the placement of industrial facilities. The numerical method was calculated using the finite difference method.

The articles [19–21] consider a mathematical model for studying and forecasting the process of dispersion of harmful aerosol substances in the atmosphere. When obtaining a mathematical model of the object, the main weather and climate factors influencing the transfer and dispersion of harmful substances, and the location of the source were taken into account.

2 Problem Statement

Based on the above, important parameters for studying the transport and diffusion of aerosol particles in the atmosphere include the composition of wind speeds in different directions and the topography of the areas under consideration. We will examine a mathematical model describing these aspects based on the principles of hydromechanics:

$$\begin{gathered}\frac{\partial\theta}{\partial t}+u\frac{\partial\theta}{\partial x}+v\frac{\partial\theta}{\partial y}+(w-w_g)\frac{\partial\theta}{\partial z}+\theta(\sigma+\alpha)= \\ =D_x\left(T,|u|,d_p\right)\frac{\partial^2\theta}{\partial x^2}+D_y\left(T,|v|,d_p\right)\frac{\partial^2\theta}{\partial y^2}+D_z\left(T,|w-w_g|,d_p\right)\frac{\partial^2\theta}{\partial z^2}+Q,\end{gathered} \tag{1}$$

relevant initial and boundary conditions:

$$\theta|_{t=0} = \theta^0, \tag{2}$$

$$\begin{aligned}
&\left.\frac{\partial\theta}{\partial x}\right|_{x=0} = \frac{\theta_{Ex0}(t) - \theta|_{x=0}}{l_x}, \quad \left.\frac{\partial\theta}{\partial x}\right|_{x=L_x} = \frac{\theta_{ExL}(t) - \theta|_{x=L_x}}{l_x},\\
&\left.\frac{\partial\theta}{\partial y}\right|_{y=0} = \frac{\theta_{Ey0}(t) - \theta|_{y=0}}{l_y}, \quad \left.\frac{\partial\theta}{\partial y}\right|_{y=L_y} = \frac{\theta_{EyL}(t) - \theta|_{y=L_y}}{l_y},\\
&\left.\frac{\partial\theta}{\partial z}\right|_{z=0} = \frac{\theta_{Ez0}(t) - \theta|_{z=0}}{l_z}, \quad \left.\frac{\partial\theta}{\partial z}\right|_{z=L_z} = \frac{\theta_{EzL}(t) - \theta|_{z=L_z}}{l_z}.
\end{aligned} \tag{3}$$

Here, θ is the concentration of harmful substances in the atmosphere; t is time; $\theta_{Ex0}(t)$, $\theta_{ExL}(t)$, $\theta_{Ey0}(t)$, $\theta_{EyL}(t)$, $\theta_{Ez0}(t)$, $\theta_{EzL}(t)$ are the concentrations passing through the boundaries of the considered areas; x, y, z are coordinates of the system; u, ν, w are the wind speeds in three directions; w_g is the settling velocity of the particles; σ is the coefficient of absorption of harmful substances in the atmosphere; α is the coefficient that organizes the retention of particles by plant elements; D_x, D_y, D_z are the diffusion coefficients; Q is the source power; δ is the Drak function; d_p is the particle diameter; l_x, l_y, l_z unit length in the corresponding directions.

The following functions are used to calculate the pollutant concentration $\theta_{Ex0}(t)$, $\theta_{ExL}(t)$, $\theta_{Ey0}(t)$, $\theta_{EyL}(t)$, $\theta_{Ez0}(t)$, $\theta_{EzL}(t)$ – carried by the flow at the boundary and the values in the region near the boundary.

$$\begin{aligned}
&\theta_{Ex0}(t) = \begin{cases} Q_a, \ (t_{x0} - t) \wedge (u \geqslant 0), \\ \theta|_{x=0}. \end{cases} \quad \theta_{ExL}(t) = \begin{cases} Q_a, \ (t_{xL} - t) \wedge (u \leqslant 0), \\ \theta|_{x=L_x}. \end{cases}\\
&\theta_{Ey0}(t) = \begin{cases} Q_a, \ (t_{y0} - t) \wedge (v \geqslant 0), \\ \theta|_{y=0}. \end{cases} \quad \theta_{EyL}(t) = \begin{cases} Q_a, \ (t_{yL} - t) \wedge (v \leqslant 0), \\ \theta|_{y=L_y}. \end{cases}\\
&\theta_{Ez0}(t) = \begin{cases} Q_a, \ (t_{z0} - t) \wedge (w \geqslant 0), \\ \theta|_{z=0}. \end{cases} \quad \theta_{EzL}(t) = \begin{cases} Q_a, \ (t_{zL} - t) \wedge (w \leqslant 0). \\ \theta|_{z=L_z}. \end{cases}
\end{aligned} \tag{4}$$

Here, L_x, L_y, L_z are the length, width, and height of the area under consideration.

Initially, we use a grid consisting of a set of discrete points that represent an approximation of the continuous change in the variables we are studying:

$$\Omega_{x,y,z,t} = \Bigg\{ (x_i = i\Delta x, y_j = j\Delta y, z_k = k\Delta z, t_n = n\Delta t)\,,$$
$$i = \overline{1, I}; j = \overline{1, J}; k = \overline{1, K}; \mathrm{n} = \overline{0, N_t}, \Delta t = \frac{t}{N} \Bigg\},$$

Q observed at the boundary is defined as follows:

$$Q = \begin{cases} Q_m, \ \delta(x_i - x_q)(y_j - y_q)(z_k - z_q)(t_n - t_q) = 1, \\ 0. \end{cases} \tag{5}$$

Q_a, Q_m – the power at each point of the source emitting a harmful substance outside the field and inside the field, respectively.

$$\forall (x_q, y_q, z_q) \in \Omega_q, \tag{6}$$

where, x_q, y_q, z_q are the source location point, x_i, y_j, z_k is the calculation point, Ω_q is the source location area.

Here, $\theta_{Ex0}(t),\ \theta_{ExL}(t),\ \theta_{Ey0}(t),\ \theta_{EyL}(t),\ \theta_{Ez0}(t),\ \theta_{EzL}(t)$ are defined as functions dependent on time and is used in cases where a harmful substance enters the domain from the external environment in other cases, it is considered as the current value. In the process we are currently analyzing, the harmful substance is treated not as point or linear sources, but as a spatial source within the domain.

To ensure the adequacy of the mathematical model and numerical results, it is essential to correctly select the parameters and coefficients in the model and to choose numerical methods that are appropriate for the process. Therefore, the diffusion coefficient was calculated in relation to all spatial coordinates, depending on the components of velocity, temperature, and the size of the particles, for each time layer.

Considering the wind speed, particle size and D_m calculations, the diffusion coefficient in x, y and z directions is calculated as follows:

$$
\begin{aligned}
D_x &= D_m\left(1+\alpha\frac{|u|}{d_p}\right),\\
D_y &= D_m\left(1+\alpha\frac{|v|}{d_p}\right),\\
D_z &= D_m\left(1+\alpha\frac{|w-w_g|}{d_p}\right).
\end{aligned}
\tag{7}
$$

D_m is calculated as (8) follows:

$$
D_m=\frac{k_B T}{6\pi\eta d_p},
\tag{8}
$$

taking into account wind speed and particle size, functions (7) were obtained. Due to the large influence of temperature on the diffusion process, we add the argument T to η and obtain function (9).

$$
\eta\left(T\right)=\eta_0\left(\frac{T}{T_0}\right)^{3/2}\left(\frac{T_0+S}{T+S}\right),
\tag{9}
$$

we replace the argument η in functions (7) with the argument $\eta(T)$ and get the following result:

$$
\begin{aligned}
D_x(T,\left|u\right|,d_p) &= \frac{k_B T}{6\pi\eta\left(T\right)d_p}\left(1+a\frac{|u|}{d_p}\right),\\
D_y(T,\left|v\right|,d_p) &= \frac{k_B T}{6\pi\eta\left(T\right)d_p}\left(1+a\frac{|v|}{d_p}\right),\\
D_z(T,\left|w-w_g\right|,d_p) &= \frac{k_B T}{6\pi\eta\left(T\right)d_p}\left(1+a\frac{|w-w_g|}{d_p}\right).
\end{aligned}
\tag{10}
$$

Finding the diffusion coefficient using functions (10).
Here, k_B is the Boltzmann constant; η is the dynamic viscosity of the fluid; D_m is the molecular diffusion coefficient; a is the dimensionless coefficient expressing the advective influence; η_0 va T_0 are the viscosity and temperature; S is the constant for the Sutherland relation for gases.

3 Numerical solution

Discretize the model using the finite difference method.

$$\frac{\theta_{i,j,k}^{n+1}-\theta_{i,j,k}^{n}}{\Delta t}=-\left[u_{i,j,k}^{n}\left(\frac{\theta_{i+1,j,k}^{n}-\theta_{i-1,j,k}^{n}}{2\Delta x}\right)+\right.$$
$$\left.+v_{i,j,k}^{n}\left(\frac{\theta_{i,j+1,k}^{n}-\theta_{i,j-1,k}^{n}}{2\Delta y}\right)+(w_{i,j,k}^{n}-w_g)\left(\frac{\theta_{i,j,k+1}^{n}-\theta_{i,j,k-1}^{n}}{2\Delta z}\right)\right]+$$
$$+D_x(T,\left|u_{i,j,k}^{n}\right|,d_p)\left(\frac{\theta_{i-1,j,k}^{n}-2\theta_{i,j,k}^{n}+\theta_{i+1,j,k}^{n}}{\Delta x^2}\right)+$$
$$+D_y(T,\left|v_{i,j,k}^{n}\right|,d_p)\left(\frac{\theta_{i,j-1,k}^{n}-2\theta_{i,j,k}^{n}+\theta_{i,j+1,k}^{n}}{\Delta y^2}\right)+$$
$$+D_z(T,\left|w_{i,j,k}^{n}-w_g\right|,d_p)\left(\frac{\theta_{i,j,k-1}-2\theta_{i,j,k}+\theta_{i,j,k+1}}{\Delta z^2}\right)+\sigma\theta_{i,j,k}^{n}+\alpha\theta_{i,j,k}^{n}+Q_{i,j,k}^{n}.$$

The value at the boundary points of the field can be discretized in the following form:

$$\frac{\theta_{0,j,k}^{n+1}-\theta_{1,j,k}^{n+1}}{\Delta x}=-\frac{\theta_{Ex1}^{n+1}-\theta_{0,j,k}^{n+1}}{\Delta x},\quad \frac{\theta_{I,j,k}^{n+1}-\theta_{I-1,j,k}^{n+1}}{\Delta x}=\frac{\theta_{Ex2}^{n+1}-\theta_{I,j,k}^{n+1}}{\Delta x},$$
$$\frac{\theta_{i,0,k}^{n+1}-\theta_{i,1,k}^{n+1}}{\Delta y}=-\frac{\theta_{Ey1}^{n+1}-\theta_{i,0,k}^{n+1}}{\Delta y},\quad \frac{\theta_{i,J,k}^{n+1}-\theta_{i,J-1,k}^{n+1}}{\Delta y}=\frac{\theta_{Ey2}^{n+1}-\theta_{i,J,k}^{n+1}}{\Delta y},$$
$$\frac{\theta_{i,j,0}^{n+1}-\theta_{i,j,1}^{n+1}}{\Delta z}=-\frac{\theta_{Ez1}^{n+1}-\theta_{i,j,0}^{n+1}}{\Delta z},\quad \frac{\theta_{i,j,K}^{n+1}-\theta_{i,j,K-1}^{n+1}}{\Delta z}=\frac{\theta_{Ez2}^{n+1}-\theta_{i,j,K}^{n+1}}{\Delta z}.$$

This numerical method is an advection-diffusion equation, which is a finite-difference discretization of the differention equation. The superscript $n+1$ is used for the new time step, and n is used for the current time step. If we divide the discretized equation by time, then the calculation of the concentration value at time $n+1$ will be as follows:

$$\theta_{i,j,k}^{n+1}=\theta_{i,j,k}^{n}-\Delta t\left[u_{i,j,k}^{n}\left(\frac{\theta_{i+1,j,k}^{n}-\theta_{i-1,j,k}^{n}}{2\Delta x}\right)+\right.$$
$$\left.+v_{i,j,k}^{n}\left(\frac{\theta_{i,j+1,k}^{n}-\theta_{i,j-1,k}^{n}}{2\Delta y}\right)+(w_{i,j,k}^{n}-w_g)\left(\frac{\theta_{i,j,k+1}^{n}-\theta_{i,j,k-1}^{n}}{2\Delta z}\right)\right]+$$
$$+\Delta t\left[D_x(T,\left|u_{i,j,k}^{n}\right|,d_p)\left(\frac{\theta_{i-1,j,k}^{n}-2\theta_{i,j,k}^{n}+\theta_{i+1,j,k}^{n}}{\Delta x^2}\right)+\right.$$
$$+D_y(T,\left|v_{i,j,k}^{n}\right|,d_p)\left(\frac{\theta_{i,j-1,k}^{n}-2\theta_{i,j,k}^{n}+\theta_{i,j+1,k}^{n}}{\Delta y^2}\right)+$$
$$\left.+D_z(T,\left|w_{i,j,k}^{n}-w_g\right|,d_p)\left(\frac{\theta_{i,j,k-1}-2\theta_{i,j,k}+\theta_{i,j,k+1}}{\Delta z^2}\right)+\sigma\theta_{i,j,k}^{n}+\alpha\theta_{i,j,k}^{n}+Q_{i,j,k}^{n}\right].$$

The boundary conditions refer to the time integration in the following form, if we separate the value at the boundary point from the discretized form:

$$\theta_{0,j,k}^{n+1}=\frac{\theta_{Ex1}^{n+1}+\theta_{1,j,k}^{n+1}}{2},$$

$$\theta_{I,j,k}^{n+1} = \frac{\theta_{E_{x2}}^{n+1} + \theta_{I-1,j,k}^{n+1}}{2},$$
$$\theta_{i,0,k}^{n+1} = \frac{\theta_{E_{y1}}^{n+1} + \theta_{i,1,k}^{n+1}}{2},$$
$$\theta_{i,J,k}^{n+1} = \frac{\theta_{E_{y2}}^{n+1} + \theta_{i,J-1,k}^{n+1}}{2},$$
$$\theta_{i,j,0}^{n+1} = \frac{\theta_{E_{z1}}^{n+1} + \theta_{i,j,1}^{n+1}}{2},$$
$$\theta_{i,j,K}^{n+1} = \frac{\theta_{E_{z2}}^{n+1} + \theta_{i,j,K-1}^{n+1}}{2}.$$

Checking convergence and continuing iteration,

$$R_\theta = \left| \frac{\theta^{n+1} - \theta^n}{\theta^{n+1}} \right|.$$

If the residual values R_θ are less than a given value, the iteration process stops. If the residual values are greater than the specified value, then we continue the iterative process.

4 Results

In these [23–25] articles, the process of harmful substance dispersion in the atmosphere has been analyzed using different speeds and various time intervals in computer simulations, and the results have been presented.

Several results have been obtained using software tools to model the diffusion process of harmful substances in the atmosphere based on the following indicators. In this case, $u = 1m/s$, $v = 1m/s$, $w = 0.2m/s, T = 30°\text{C}$, $k_B = 1.38\text{e}^{-23}$ J/K, $\eta_0 = 1.81\text{e}^{-5}$, $T_0 = 306.15°$ C, $\alpha = 0.01, S = 110.4m^3$ based on the given values, the computational results have been obtained, and the diffusion process, as well as the time-dependent dispersion of particles with a quantity of $d_p = 1e^{-7}m$, has been observed.

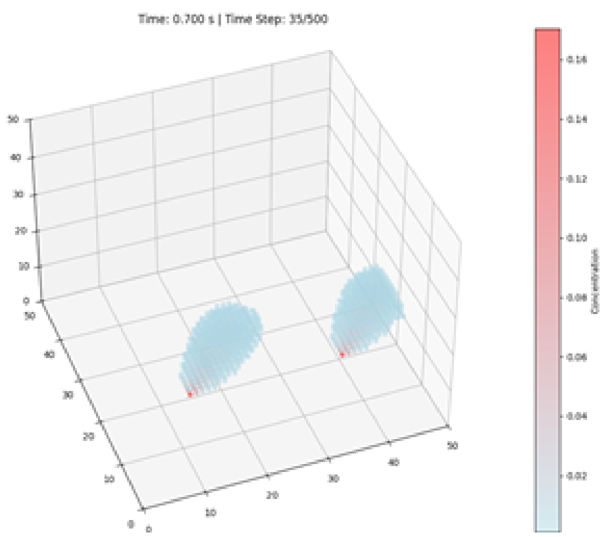

Figure 2 The examined time conditions $t = 0.7h$

In the next obtained results, the particle size $d_p = 1e^{-8}m$ was considered at different times.

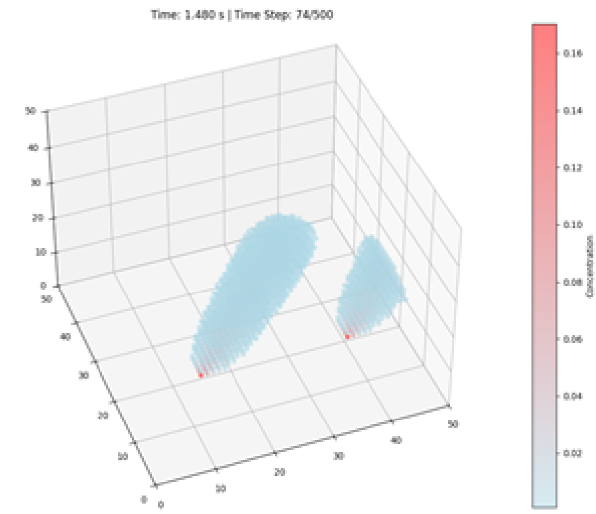

Figure 3 The examined time conditions $t = 1.4h$

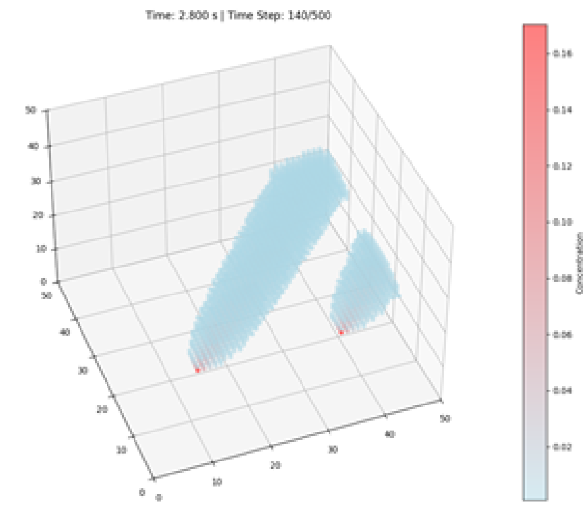

Figure 4 The examined time conditions $t = 2.4h$

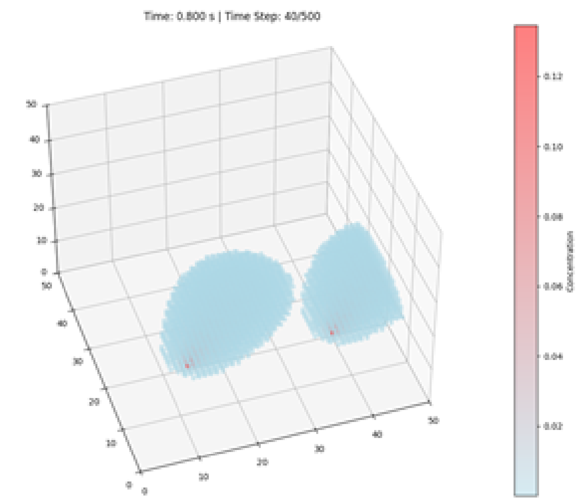

Figure 5 The examined time conditions $t = 0.8h$

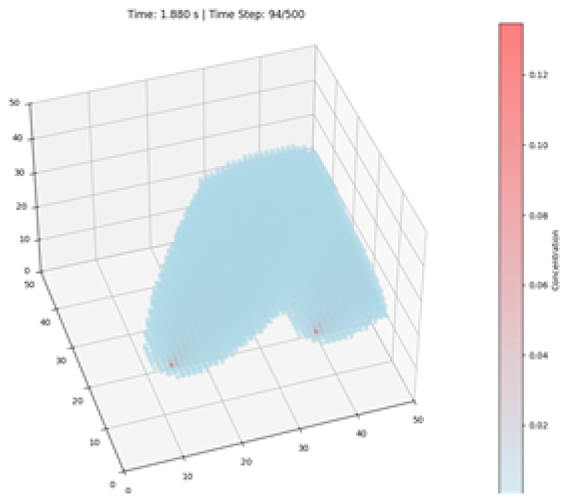

Figure 6 The examined time conditions $t = 1.88h$

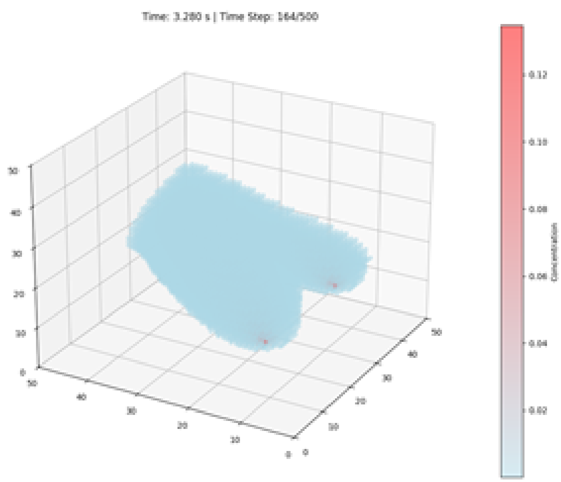

Figure 7 The examined time conditions $t = 3.2h$

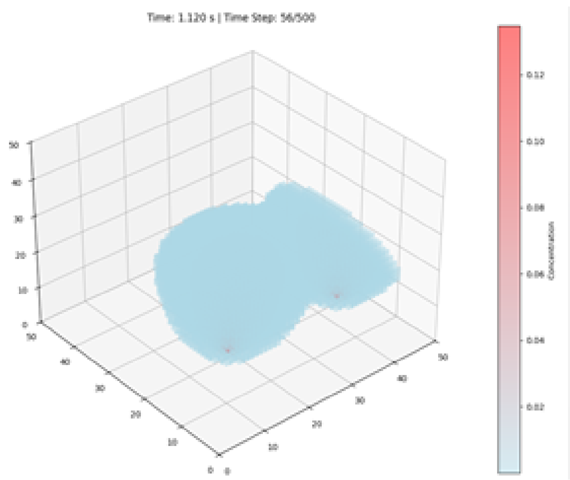

Figure 8 The examined time conditions $t = 1.3h$

In the next obtained results, the particle size $d_p = 1e^{-9}$ m was considered at different times.

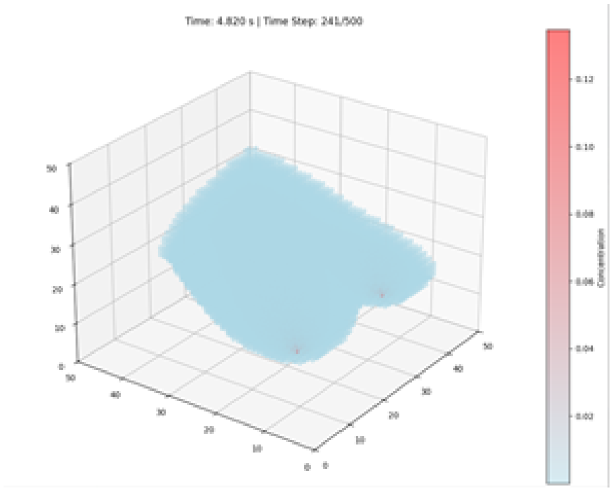

Figure 9 The examined time conditions $t = 4.8h$

Harmful substances in the atmosphere corresponding to particle sizes $d_p = 1e^{-7}$, $d_p = 1e^{-9}$, $d_p = 1e^{-9}$ are shown in the following table.

Particle Size	**Primary Pollutants**	**Secondary Pollutants**
100 nm ($1e^{-7}$ m)	Black carbon (BC), soot, organic carbon (OC), metal oxides (Pb, Cd, Ni, As), viruses (SARS-CoV-2, influenza)	Secondary organic aerosols (SOA), ammonium sulfate, ammonium nitrate, sulfuric acid aerosols
10 nm ($1e^{-8}$ m)	Diesel exhaust particles (DEP), metal oxide nanoparticles (TiO_2, ZnO, SiO_2), ultrafine soot	Nucleation-mode sulfate and nitrate particles, condensed hydrocarbons
1 nm ($1e^{-9}$ m)	Metal clusters (Fe, Cu, Ag), carbon nanoclusters (C_{60}, PAHs)	Sulfuric acid clusters, ammonia and amines, radical species ($OH\cdot$, $NO_3\cdot$)

These nanoscale pollutants play a critical role in air quality, climate change, and human health, as ultrafine particles can penetrate deep into the lungs and bloodstream, causing adverse effects.

5 Conclusion

The calculation results showed that for modeling the transfer of pollutants in the lower layers of the atmosphere, near the Earth's surface, a mathematical model was developed that takes into account the wind speed in three directions and the orography of the studied area, and the numerical method was solved using the finite difference method in explicit form. In addition, different wind speeds were taken into account in each result. When the speed of air masses in the atmosphere exceeds the critical value, the dispersion of the substance can be considered only taking into account the effect of atmospheric convection. If the wind speed approaches zero, the dispersion of pollutants in the lower layers of the atmosphere is carried out mainly by diffusion. The use of this technique reduces the calculation time and reduces the number of iteration steps.

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ПЕРЕНОСА И ДИФФУЗИИ ЗАГРЯЗНЯЮЩИХ ЧАСТИЦ С УЧЕТОМ ХАРАКТЕРИСТИК ВОЗДУШНОГО ПОТОКА И ТЕМПЕРАТУРЫ

Набиева И.С.

irodamubina777@gmail.com

Научно-исследовательский институт развития цифровых технологий и искусственного интеллекта,

100125, Узбекистан, г. Ташкент, Мирзо-Улугбекский р-он, м-в Буз-2, д. 17А.

В статье рассматриваются результаты экспериментальных и численных исследований процессов загрязнения атмосферы в промышленных зонах. Предложенная математическая модель помогает решать задачи, связанные с мониторингом и прогнозированием состояния окружающей среды в промышленных зонах, а также с принятием решений по защите от негативного воздействия антропогенных факторов. Изучаются физико-химические свойства веществ, участвующих в процессе дисперсии в атмосфере. В процессе диффузии учитываются диаметр частиц, температура и скорость ветра. Для проверки адекватности разработанной математической модели были проведены вычислительные эксперименты на компьютере. Анализ вычислительных экспериментов показал, что с увеличением скорости ветра концентрация загрязнителей вокруг источника не наблюдается, а площадь их распределения со временем расширяется. Когда скорость воздушных масс в атмосфере превышает критическое значение, диффузия вещества происходит только за счет эффекта перехода в атмосферу. Также отмечаются изменения концентрации загрязнителей в слоях атмосферы во времени в зависимости от фактической скорости ветра.

Ключевые слова: математическая модель, метод конечных разностей, экология, диаметр частиц, скорость ветра, процесс диффузии.

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