American Journal of Social and Humanitarian Research
Vol. 7 Issue 4 | **pp.** 147-153 | **ISSN:** 2690-9626
Available online @ https://globalresearchnetwork.us/index.php/ajshr
GLOBAL RESEARCH NETWORK
ONLINE RESEARCH HUB

Article

Mathematical Modeling of Harmful Pollutant Dispersion in The Atmosphere

Nabieva I. S.[1], Boborakhimov B.I.[2], Turkmenova R.[3]

1, 3. Digital Technologies and Artificial Intelligence Development Research Institute Tashkent, Samarkand branch of the Tashkent University of Information Technologies named after Muhammad al-Khwarizmi Samarkand
2. Digital Technologies and Artificial Intelligence Development Research Institute, Tashkent
* Correspondence: irodamubina777@gmail.com

Abstract: This work proposes a mathematical model describing the process of spreading harmful pollutants in the atmosphere, their physical and mechanical properties, and the dynamic calculation of gravitational precipitation rates. The explicit scheme of the finite-difference method is utilized when solving this mathematical model. And in the software representing the distribution of harmful substances in the atmosphere over time some results are presented.

Keywords: harmful substances, diffusion process, wind speed, finite difference method.

Citation: Nabieva I. S., Boborakhimov B. I., Turkmenova R. Mathematical Modeling of Harmful Pollutant Dispersion in The Atmosphere. American Journal of Social and Humanitarian Research 2026, 7(4), 147-153

Received: 10th Dec 2025
Revised: 21th Jan 2026
Accepted: 14th Feb 2026
Published: 29th Mar 2026

1. Introduction

Globally, in the context of rapid urbanization, the increase in the number of industrial facilities, and the increase in transport flows, the problem of mathematical modeling of aerosol mixture transport in the atmosphere is acquiring global significance. The development of effective mathematical models, numerical algorithms, and software tools is the key to forecasting pollutant concentrations and assessing their impact on public health and the ecology of cities and countries. In researching the distribution of pollutants in the atmospheric air, the use of digital technologies and modern mathematical models, including complex numerical methods and algorithms for analyzing diffusion processes, is required.

Excessive air pollution directly affects public health, increasing the risk of chronic respiratory, cardiovascular, and oncological diseases. Furthermore, the accumulation of aerosol mixtures in the terrestrial layer of the atmosphere negatively affects climatic indicators, reduces air transparency, causes smoke formation, and worsens the quality of life.

When modeling the spread of harmful substances in the atmosphere, Eyler, Gauss, and Lagrange approaches are most frequently used. Although they describe the same physical process, they differ in how the substance appears in the air.

In Eyler's approach, the pollutant is viewed as a concentration field at every point in the atmospheric space. In modern air quality models, specifically in systems such as CMAQ and CAMx, this approach is implemented by calculating advection, diffusion, emission, precipitation, and other physicochemical processes in a three-dimensional mesh environment; as a result, concentration values over time are obtained for each mesh cell [1-4]. It has the following form:

$$\frac{\partial C}{\partial t}+\nabla\cdot\left(\mathbf{u}C\right)=\nabla\cdot\left(K\nabla C\right)+S-R;$$

where C - is the concentration, y is the wind speed vector, K - is the diffusion coefficient, S - is the source, and R - is the loss or reaction term. This record is a standardized version of the preservation/diffusion equation for track views presented in the CMAQ documents.

The main advantage of this model is that it provides a full spatial field of concentration across large territories, at city and regional scales, and accounts for several sources and many processes together. However, this approach is complex from a computational perspective: the grid size, time step selection, and numerical algorithms for advection-diffusion significantly influence the model's outcome.

The Gaussian model describes the emission of a substance into the atmosphere as a steady-state flow. EPA documents state that for models such as ISC3 and AERMOD, this approach is applicable to a continuous rise source and averaged meteorological conditions over a certain period of time [5-7]. Recorded as:

$$C\left(x,y,z\right)=\frac{Q}{2\pi u\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{\left(zH\right)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{\left(z+H\right)^2}{2\sigma_z^2}\right)\right];$$

where: Q - is the emission capacity, u - is the wind speed, σ_y,σ_z - are the parameters of transverse and vertical distribution, H - is the effective source height.

The advantage of the Gaussian model lies in its simplicity and efficiency. In the EPA screening models, SCREEN3 and TSCREEN are used specifically for maximum or rapid assessment based on the Gaussian approach. Therefore, it is very convenient for point sources, preliminary engineering assessments, and regulatory screening tasks. But the limitation of this model is also obvious: it relies on the steady-state hypothesis, meaning one average value of meteorological parameters is taken for the model period. The AERMOD document clearly states that this model is a steady-state plume model and uses uniform meteorological values for the model period; The CAP88-PC document notes that it cannot model changes in complex terrain. Therefore, accuracy decreases in areas with rapidly changing wind fields or complex geometry.

In the Lagrange approach, matter is observed as the movement of particles or puffs through the atmosphere. One of the most well-known examples of this approach is the HYSPLIT NOAA system, which can model the trajectory and dispersion of substances in the atmosphere from local to global scales [8-10].

$$x_{t+\Delta t}=x_t+u\Delta t+u'\Delta t;$$

$$y_{t+\Delta t}=y_t+v\Delta t+v'\Delta t;$$

$$z_{t+\Delta t}=z_t+w\Delta t+w'\Delta t;$$

here, u',v',w' represent turbulent random components.

According to the HYSPLIT description, the model calculation method is hybrid in nature: advection and diffusion calculations are performed using the Lagrange method, i.e., in a movable coordinate system, while the concentration is calculated on a three-dimensional rigid grid, as in the Eyler method. The model can use a puff or particle approach. The greatest advantage of this approach is that it is very convenient for describing time-varying wind fields, emergency emissions, smoke transport, volcanic ash, radioactive substances, and other dangerous impurities. The NOAA page states that HYSPLIT is used specifically for wild smoke, volcanic ash, radioactive materials, and various pollutants.

When modeling the spread of harmful substances in the atmosphere, the Gaussian model is convenient for applied engineering calculations due to its simplicity and speed, but it yields a sufficient result only under stable and homogeneous conditions. The Euler model describes physical processes more deeply and spatially, so it is more effective for large areas and pollution systems from many sources. The Lagrange model is the most flexible method for complex atmospheric conditions and extreme emissions, where the wind field changes over time. Consequently, when selecting models, the main criteria are calculation speed, data accessibility, meteorological complexity, and research objective.

This article [11,12] presents authors studying the mathematical modeling of the distribution of aerosol particles in the atmosphere on the surface, focusing on accounting for the influence of Earth's surface heterogeneity, vegetation, relief, as well as industrial and urban objects. Numerical experiments accounted for changes in sedimentation rates and turbulent diffusion in forest massifs. In this study, the process of particle transport and diffusion is modeled by a multidimensional advective-diffusion equation, taking into account the spatial components of wind speed, precipitation rate, and absorption coefficients.

Mathematical models

This model analyzes aspects such as important factors for studying the migration and diffusion process of aerosol particles in the atmosphere, the composition of wind speed in various directions, and forecasting the spread of harmful substances in the areas under consideration.

$$\frac{\partial \theta}{\partial t}+\frac{\partial u\theta}{\partial x}+\frac{\partial v\theta}{\partial y}+\frac{\partial w\theta}{\partial z}-\frac{\partial w_g\theta}{\partial z}+\sigma\theta+\alpha\theta=$$
$$=\frac{\partial^2 D_x\theta}{\partial x^2}+\frac{\partial^2 D_y\theta}{\partial y^2}+\frac{\partial^2 D_z\theta}{\partial z^2}+\delta Q; \tag{1}$$

initial and boundary conditions:

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

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

Here, θ - concentration, t - time, u, v, w - wind speed, w_g - settling speed of particles, D_x, D_y, D_z - diffusion coefficient, Q - source, θ_E - external concentration, σ - absorption, α - plant absorption.

The diffusion coefficient given in the mathematical model is calculated dynamically, taking into account the influence of wind speed, particle diameter, and temperature. And this process is presented in these works [13-15].

2. Materials and Method

Numerical solution

First, we replace the region of continuous change of the sought variables with a computational network consisting of a set of discrete points where the solution can be predicted, i.e., the region of change in the concentration of harmful substances is covered by a mesh step region. The representation of the equation in discrete form is as follows:

$$\theta^{n+1}_{i,j,k}=\theta^{n}_{i,j,k}-$$

$$-\Delta t\left[\begin{array}{l}\begin{cases} u^{n}_{i-1/2,j,k}\left(\dfrac{\theta^{n}_{i,j,k}-\theta^{n}_{i-1,j,k}}{2\Delta x}\right)+u^{n}_{i+1/2,j,k}\left(2\dfrac{\theta^{n}_{i+1,j,k}-\theta^{n}_{i,j,k}}{\Delta x}\right) & agar\ u^{n}_{i,j,k}<0; \\ u^{n}_{i-1/2,j,k}\left(\dfrac{\theta^{n}_{i-1,j,k}-\theta^{n}_{i,j,k}}{2\Delta x}\right)+u^{n}_{i+1/2,j,k}\left(\dfrac{\theta^{n}_{i,j,k}-\theta^{n}_{i+1,j,k}}{2\Delta x}\right) & agar\ u^{n}_{i,j,k}\geq 0. \end{cases} + \\ +\begin{cases} v^{n}_{i,j-1/2,k}\left(\dfrac{\theta^{n}_{i,j,k}-\theta^{n}_{i,j-1,k}}{2\Delta y}\right)+v^{n}_{i,j+1/2,k}\left(\dfrac{\theta^{n}_{i,j+1,k}-\theta^{n}_{i,j,k}}{2\Delta y}\right) & agar\ v^{n}_{i,j,k}<0; \\ v^{n}_{i,j-1/2,k}\left(\dfrac{\theta^{n}_{i,j-1,k}-\theta^{n}_{i,j,k}}{2\Delta y}\right)+v^{n}_{i,j+1/2,k}\left(\dfrac{\theta^{n}_{i,j,k}-\theta^{n}_{i,j+1,k}}{2\Delta y}\right) & agar\ v^{n}_{i,j,k}\geq 0. \end{cases} + \\ +\begin{cases} w^{n}_{i,j,k-1/2}\left(\dfrac{\theta^{n}_{i,j,k}-\theta^{n}_{i,j,k-1}}{2\Delta z}\right)+w^{n}_{i,j,k+1/2}\left(\dfrac{\theta^{n}_{i,j,k+1}-\theta^{n}_{i,j,k}}{2\Delta z}\right) & agar\ \ w^{n}_{i,j,k}<0; \\ w^{n}_{i,j,k-1/2}\left(\dfrac{\theta^{n}_{i,j,k-1}-\theta^{n}_{i,j,k}}{2\Delta z}\right)+w^{n}_{i,j,k+1/2}\left(\dfrac{\theta^{n}_{i,j,k}-\theta^{n}_{i,j,k+1}}{2\Delta z}\right) & agar\ \ w^{n}_{i,j,k}\geq 0. \end{cases} - \\ -w^{\ \ n}_{g i,j,k-1/2}\left(\dfrac{\theta^{n}_{i,j,k}-\theta^{n}_{i,j,k-1}}{\Delta x}\right)-w^{\ \ n}_{g i,j,k+1/2}\left(\dfrac{\theta^{n}_{i,j,k+1}-\theta^{n}_{i,j,k}}{\Delta x}\right)\end{array}\right]+$$

$$+\Delta t D_x(T,\left|u^{n}_{i,j,k}\right|,d_p)\left(\frac{\theta^{n}_{i-1,j,k}-2\theta^{n}_{i,j,k}+\theta^{n}_{i+1,j,k}}{\Delta x^2}\right)+\Delta t D_y(T,\left|v^{n}_{i,j,k}\right|,d_p)\left(\frac{\theta^{n}_{i,j-1,k}-2\theta^{n}_{i,j,k}+\theta^{n}_{i,j+1,k}}{\Delta y^2}\right)+$$

$$+\Delta t D_z(T,\left|w^{n}_{i,j,k}\right|,d_p)\left(\frac{\theta^{n}_{i,j,k-1}-2\theta^{n}_{i,j,k}+\theta^{n}_{i,j,k+1}}{\Delta z^2}\right)-\Delta t D_z(T,\left|w^{\ \ n}_{g i,j,k}\right|,d_p)\left(\frac{\theta^{n}_{i,j,k-1}-2\theta^{n}_{i,j,k}+\theta^{n}_{i,j,k+1}}{\Delta z^2}\right)-$$

$$-\Delta t\sigma\theta^{n}_{i,j,k}-\Delta t\alpha\theta^{n}_{i,j,k}+\Delta t Q^{n}_{i,j,k}.$$

The mathematical model presented above was solved using the explicit scheme of the finite difference method. To ensure the stability of numerical solutions, the choice of steps in time and space, convergence conditions, and iterative processes have been substantiated.

3. Result and Discussion

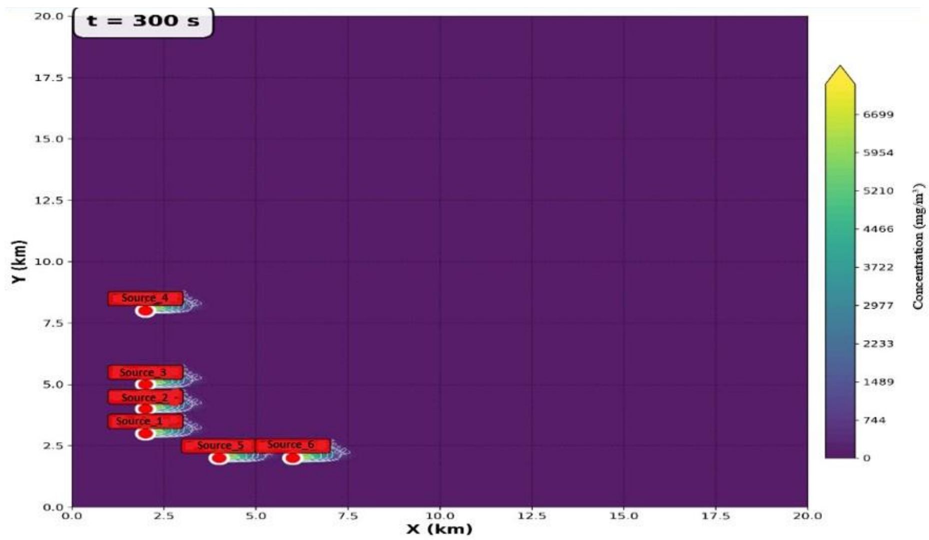

Figure 1. Concentration area at time t=300 s

Figure 1 shows the pollution clouds of six sources that are completely separated from each other. Even the nearest sources, Source-1 and Source-2, are located at a distance of 1 km from each other, and their clouds have not yet merged. This fact shows that the model works physically correctly: the advection-diffusion process does not unite the spheres of influence of neighboring sources until sufficient time has passed.

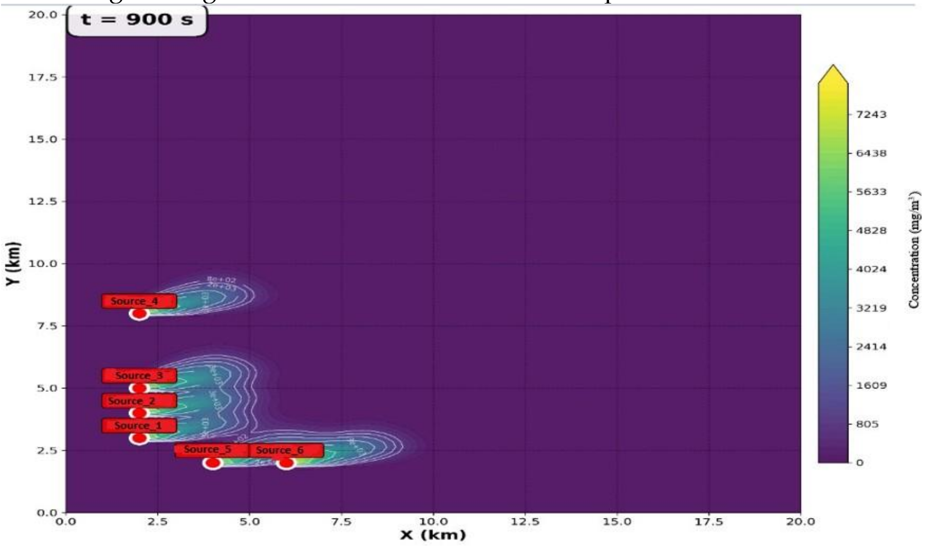

Figure 2. Concentration area at time t=900 s

Figure 2 shows that the length of the Source-4 cloud in the east-northeast direction extends over a distance of 9–10 km. This indicates the key role of advection: in 900 seconds, the wind carries the substance to a distance of 3.0 * 900 = 2700 m.

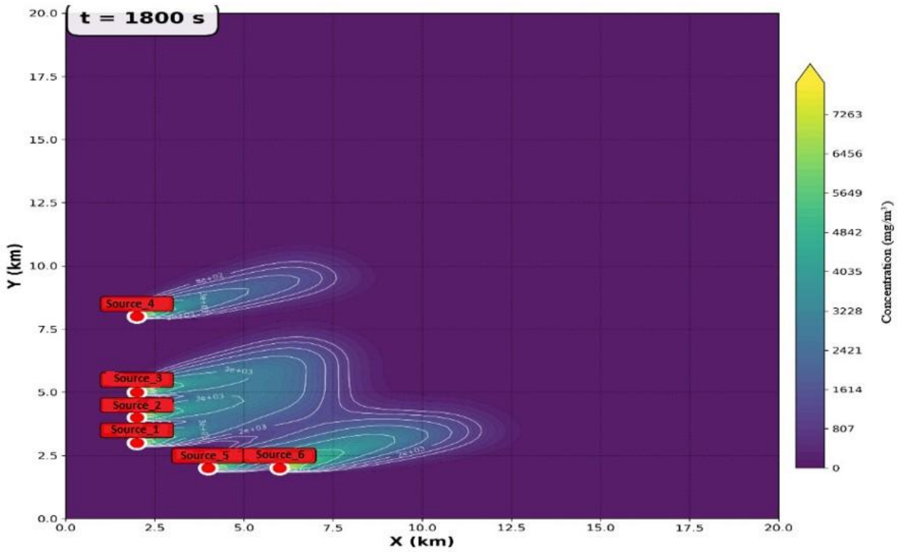

Figure 3. Concentration area at time t=1800 s

If we consider the entire concentration field as a whole, in the eastern half of the computational region, the influence of all sources is felt together. In the northeastern region, i.e., in the km and km zones, background pollution with low concentrations (below 800 mg/m^3) has formed, which is a superposition of the diffusion lengths of all six sources.

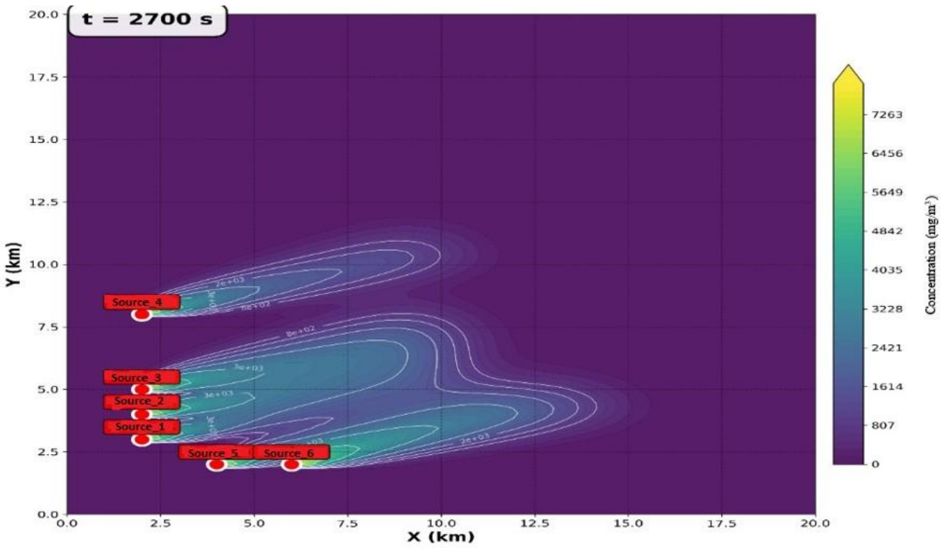

Figure 4. Concentration area at time t=2700 s

Figure 3 shows the interaction between the distribution area of Source 4 and the distribution area of Source 1-3. In the $x \approx 7-9$ km section, the boundary zone between the two distribution areas is eroded. This situation reflects a problem that is frequently encountered in environmental monitoring practice: if there are several pollution sources in the same area, it is difficult to link the measured concentration to a specific source within the monitoring area.

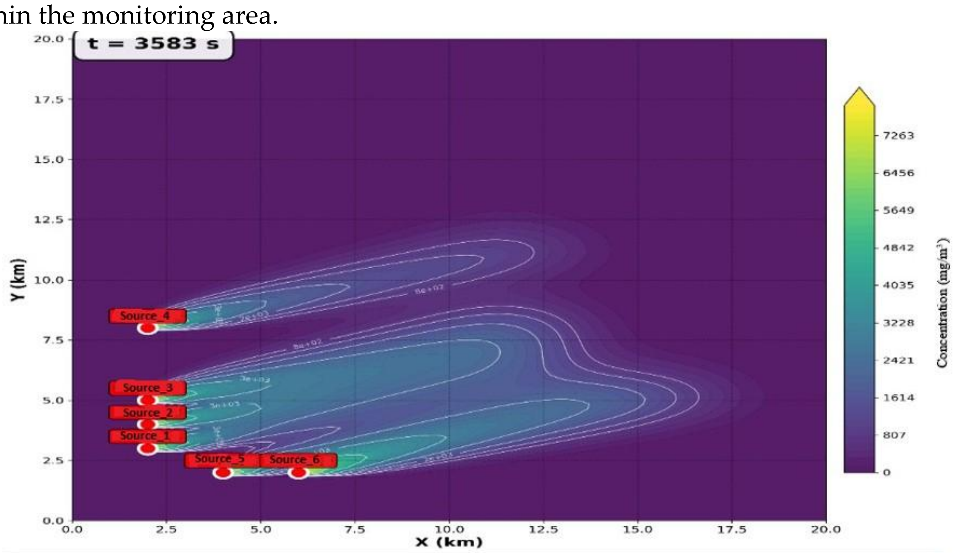

Figure 5. Concentration area at time t=3583 s

In the final 3583 second simulation moment (Fig. 5), the concentration field reached its most developed state.We see that a dust particle emerging from six medium-power sources over an hour spreads over a distance of 15 km under the influence of wind at a speed of 3.16 m/s.

4. Conclusion

In this work, a mathematical model based on the advective-diffusion equation was developed to model the spread of harmful substances in the atmosphere. The numerical solution was implemented using a finite difference scheme and the Upwind sampling method, and the solution's stability was guaranteed based on the Kurant-Friedrich-Levi (CFL) condition. The calculation experiments included an analysis of harmful emissions from six pollution sources.

REFERENCES

[1] Byun, D., Schere, K.L., 2006. Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. Appl. Mech. Rev. 59, 51–77. https://doi.org/10.1115/1.2128636

[2] Grell, G.A., Peckham, S.E., Schmitz, R., McKeen, S.A., Frost, G., Skamarock, W.C., Eder, B., 2005. Fully coupled "online" chemistry within the WRF model. Atmos. Environ. 39, 6957–6975. https://doi.org/10.1016/j.atmosenv.2005.04.027

[3] Zhang, Y., 2008. Online-coupled meteorology and chemistry models: history, current status, and outlook. Atmospheric Chem. Phys. 8, 2895–2932. https://doi.org/10.5194/acp-8-2895-2008

[4] Jacobson, M.Z., "Development and application of a new air pollution modeling system—Part II: Aerosol module structure and design." Atmospheric Environment, 2001, Vol. 35, Issue 34, pp. 5835–5852. DOI: 10.1016/S1352-2310(01)00393-9.

[5] Hanna, S.R., Briggs, G.A., Hosker, R.P., "Handbook on Atmospheric Diffusion." U.S. Department of Energy, 1982.

[6] Holmes, N.S., Morawska, L., 2006. A review of dispersion modelling and its application to the dispersion of particles: An overview of different dispersion models available. Atmos. Environ. 40, 5902–5928. https://doi.org/10.1016/j.atmosenv.2006.06.003

[7] Turner, D.B., "Workbook of Atmospheric Dispersion Estimates: An Introduction to Dispersion Modeling." CRC Press, 1994.

[8] Haertel P. A Lagrangian ocean model for climate studies // Climate. – 2019. – Vol. 7, №. 41. – P. 1–24.

[9] Anfossi P., Ferrero D., Tinarelli G., Trini Castelli S. A new Lagrangian particle model for the simulation of dense gas dispersion // Atmospheric Environment. –2000. – Vol. 27A, №. 9. – P. 1551–1558.

[10] Barbero D., Tinarelli G., Silibello C., Nanni A., Gariazzo C., Stafoggia M., Viegi G. Reduction of simulation times by application of a kernel method in a high-resolution Lagrangian particle dispersion model // Air Quality, Atmosphere & Health. – 2024. – Vol. 17, №. 10. – P. 2105–2117.

[11] Ravshanov N., Nazarov S., Nazarov E., and Boborahimov B., "Development of a Mathematical Model of Aerosol Particles' Distribution Process in the Surface Layer of the Atmosphere Taking into Account the Earth's Heterogeneous Surface," AIP Conf. Proc. – 2024. – Vol. 3004. – Article 060004.

[12] Ravshanov N., Nazarov S. E., and Boborahimov B., "Modeling the Process of Pollutant Spread in the Atmosphere with Account for the Capture of Particles by Vegetation Elements," Lobachevskii J. Math. – 2024. 45(3), 1213–1226

[13] Nabieva I.S. Numerical modeling of the transport and diffusion of pollutant particles taking into account airflow characteristics and temperature // Problems of Computational and Applied Mathematics. – 2025. – №1(63). – Pp. 27-40.\

[14] Ravshanov N, Nabieva I., Sapaeva D., Hojiev N. Mathematical modeling of the distribution of pollutants in the atmosphere, taking into account their physical and mechanical properties // Proc. of SPIE. – 2025. – Vol. 13662. – Pp.136620K-1–136620K-6. – DOI: 10.1117/12.3072577

[15] Ravshanov N., Nabieva I.S., Boborakhimov B.I. Software for predicting the spread of harmful substances in the atmosphere, taking into account their type and wind speed // Problems of Computational and Applied Mathematics. – 2025. – №2/2(66). – Pp. 54-59.