Известия Саратовского университета. Новая серия. Серия: Математика. Механика. Информатика. 2025. Т. 25, вып. 4. С. 589–599
Izvestiya of Saratov University. Mathematics. Mechanics. Informatics, 2025, vol. 25, iss. 4, pp. 589–599
https://mmi.sgu.ru DOI: https://doi.org/10.18500/1816-9791-2025-25-4-589-599
EDN: https://elibrary.ru/WFWDIR

Article

Simulation modeling of atmospheric pollutant dispersion considering dry deposition and the influence of liquid atmospheric precipitation

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Abstract. The article presents the results of developing a mathematical model for computer simulation of atmospheric pollutant dispersion, taking into account dry deposition and the effects of liquid atmospheric precipitation. This development is based on well-known Gaussian and Ermak mathematical models. In our model, to account for these factors under observed atmospheric precipitation, the plume dispersion equation includes a new multiplier. This multiplier is a concentration increase coefficient, proportional to the increase in pollutant plume mass under the influence of liquid precipitation, derived from the Kelvin equation and Raoult's law. The developed model is implemented as a software package that uses data on known emission sources, meteorological conditions, and monitoring results of pollutant concentrations at specific points within an industrial area. Calculations and a comparative assessment of the model's accuracy have been conducted. It is shown that considering dry deposition and precipitation effects allows for more accurate modeling of pollutant dispersion dynamics in the studied data.

Keywords: ecology, pollutants, Gaussian plume, Ermak model, pollutant deposition, simulation modeling
For citation: Shnaider I. A., Kushnikov V. A., Bogomolov A. S. Simulation modeling of atmospheric pollutant dispersion considering dry deposition and the influence of liquid atmospheric precipitation. *Izvestiya of Saratov University. Mathematics. Mechanics. Informatics*, 2025, vol. 25, iss. 4, pp. 589–599. DOI: https://doi.org/10.18500/1816-9791-2025-25-4-589-599, EDN: WFWDIR

Научная статья
УДК 519.876.5

Имитационное моделирование распространения атмосферного загрязнителя с учетом сухого осаждения и влияния жидких осадков

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Аннотация. В статье представлены результаты разработки математической модели для компьютерного моделирования распространения атмосферных загрязнителей с учетом сухого осаждения и влияния жидких атмосферных осадков. Разработка базируется на известных математических моделях Гаусса и Эрмака. В нашей модели для учета обозначенных факторов в случае наблюдаемых атмосферных осадков уравнение распространения шлейфа получает новый множитель. Это коэффициент увеличения концентрации, пропорционального увеличению массы шлейфа загрязнителя под воздействием жидких осадков, определяемый из уравнения Кельвина и закона Рауля. Разработанная модель реализована в виде программного комплекса, использующего данные об известных источниках выбросов, метеорологические условия и результаты мониторинга концентраций загрязняющих веществ в определенных точках промышленной территории. Проведены расчеты и сравнительная оценка точности предлагаемой модели. Показано, что учет сухого осаждения и влияния осадков позволяет более точно моделировать динамику распространения поллютантов на рассматриваемых данных.

Ключевые слова: экология, поллютанты, Гауссов шлейф, модель Эрмака, осаждение загрязнителя, имитационное моделирование
Для цитирования: *Shnaider I. A., Kushnikov V. A., Bogomolov A. S.* Simulation modeling of atmospheric pollutant dispersion considering dry deposition and the influence of liquid atmospheric precipitation [*Шнайдер И. А., Кушников В. А., Богомолов А. С.* Имитационное моделирование распространения атмосферного загрязнителя с учетом сухого осаждения и влияния жидких осадков] // Известия Саратовского университета. Новая серия. Серия: Математика. Механика. Информатика. 2025. Т. 25, вып. 4. С. 589–599. DOI: https://doi.org/10.18500/1816-9791-2025-25-4-589-599, EDN: WFWDIR

Introduction

The influence of many different factors on pollutant dispersion makes the task of calculating it quite complex and necessitates the imposition of certain restrictions on the initial conditions.

Research on modeling air pollutant dispersion dates back to the 1930s. Early analytical and approximate solutions to the advection–diffusion equations were developed under various simplifying assumptions. Among these, the Gaussian plume model became the most widely used, offering a solution to the transport equation under assumptions of constant wind speed and direction. The model assumes a normal distribution of pollutant particles along three axes. Dispersion values are determined based on the generalization of experimental data for various meteorological situations.

Subsequently, modifications of the Gaussian plume model were obtained for more stringent initial conditions. The Gaussian plume model also served as the basis for various models and methods for calculating air pollutant concentrations, obtained by combining it with other approaches. A combination with the Lagrangian particle movement model was presented in [1], where a simulation program for volcanic ash dispersion was developed. The latter model is based on the Lagrangian particle dispersion model and allows for more accurate forecasting of emission concentrations and predicting the localization of pollution's potential sources.

Then, various solutions to the transport equation were considered, taking into account addi-

tional factors such as dry deposition or the terrain influence. A model incorporating sedimentation effects was developed by D. L. Ermak [2] and later implemented as a computer simulation model that showed improvements compared to the basic Gaussian plume model [3].

The study by Boulos Alam et al. [4] investigates pollutant dispersion in urban-like environments using CFD simulations under neutral and slightly stable atmospheric conditions. The study compares the performance of first- and second-order turbulence closure models, with validation against the MUST field experiment. Results show that the $k - \epsilon$ model, especially when combined with an algebraic Scalar Gradient Diffusion Hypothesis (SGDH), provides better accuracy, capturing up to 75% of concentration values within a factor of two under slightly stable conditions. Although the Scalar Flux Transport Equation (DFM) model also performs well, its high computational cost may hinder practical use. A consistent underestimation of observed concentrations across models highlights the need for further refinement.

Other recent advancements in pollutant dispersion modeling have focused on enhancing accuracy and computational efficiency through novel approaches and improved turbulence representations. Lin [5] conducted a study on pollutant dispersion using Eulerian RANS simulations, focusing on anisotropic and near-source diffusivity behavior. The research highlighted the importance of considering anisotropic turbulence and near-source effects to improve the accuracy of dispersion models. While specific error metrics were not provided, the study emphasized the enhanced realism achieved by incorporating these factors. Advantages include improved modeling of complex dispersion patterns close to sources, though increased model complexity may lead to higher computational demands.

Fuchs et al. [6] developed the DAD-drift model, a modular approach for estimating spray drift at the landscape scale. The model combines a mechanistic droplet model, micrometeorological data, and a 3D Gaussian diffusion framework. Validated against two field trials, it achieved a high correlation with observed data ($R^2 = 0.931$, $RSR = 0.260$), demonstrating robustness across various environmental conditions and nozzle types. Key advantages include its modular design and adaptability to diverse scenarios, though reliance on detailed input parameters may limit applicability in data-sparse regions.

Chaloupecka et al. [7] focused on physical modeling techniques to simulate gas dispersion for emergency planning in both urban and rural settings. The study emphasized the importance of accurate dispersion modeling to inform emergency response strategies. While specific results and error metrics are not detailed, the research advocates for the integration of physical models into emergency preparedness frameworks. Advantages include the potential for real-time scenario planning, though limitations may arise from the complexity of urban topographies and the need for high-resolution data.

Lumet et al. [8] developed a surrogate modeling approach that combines Proper Orthogonal Decomposition (POD) and Gaussian Process Regression (GPR) to emulate Large-Eddy Simulations (LES) of urban pollutant dispersion. This method significantly reduces computational costs while maintaining accuracy, enabling rapid ensemble predictions. Applied to the MUST field experiment, the surrogate model improved concentration field predictions and accounted for atmospheric internal variability. Advantages include enhanced computational efficiency and uncertainty quantification, but the surrogate's accuracy depends on the quality and representativeness of the training data.

Krassas et al. [9] evaluated various numerical models to predict pollutant dispersion over Tokyo's Polytechnic University campus. The study assessed model performance against observed data, highlighting discrepancies and areas for improvement. While specific error metrics are not provided, the research underscores the challenges of modeling dispersion in complex urban environments. Advantages include the practical application of models to real-world settings, though disadvantages involve potential inaccuracies due to simplified assumptions and the need for high-resolution input data.

Pariyar et al. [10] introduced a time-fractional advection-diffusion model to capture the

anomalous diffusion behavior observed in pollutant dispersion. This approach accounts for memory effects and non-local dynamics, providing a more accurate representation of pollutant transport. The model offers improved flexibility over classical integer-order models, though it requires careful calibration of fractional parameters and may involve increased computational complexity.

Jiao et al. [11] utilized Large Eddy Simulation (LES) to study pollutant dispersion over buildings with stepped roofs, a common architectural feature in urban areas. The research reveals how roof geometry influences airflow patterns and pollutant distribution. LES provides detailed insights into turbulent flow structures, enhancing understanding of dispersion mechanisms. The main advantage is the high-resolution depiction of complex flow fields, though LES is computationally intensive and may not be practical for large-scale or real-time applications.

In Russia, current regulatory practices are based on methodologies approved by Order No. 273 of June 6, 2017, "On the approval of methods for calculating the dispersion of emissions of harmful (pollutant) substances in the ambient air"[1], which for the regulation of environmental impacts. However, these methods do not account for important atmospheric factors such as humidity, precipitation, and dry deposition of pollutant particles. This omission compromises prediction accuracy and limits the reliability of identifying pollution sources under real meteorological conditions.

The primary objective of this work is to develop and implement an enhanced numerical model for pollutant dispersion that accounts for key atmospheric factors neglected in standard regulatory methods, thereby improving the realism and reliability of air quality assessments under variable weather conditions. An improved production model for pollutant dispersion was developed based on the D. Ermak model to enhance prediction accuracy and foster the development of competitive domestic software and mathematical tools for environmental monitoring. The proposed modification incorporates the effects of humidity, precipitation, and other meteorological factors, enabling a more realistic simulation of pollutant behavior in the atmospheric boundary layer.

Thus, the present study integrates into the current scientific discourse on the advancement of numerical models for atmospheric transport and addresses the urgent need for improving dispersion predictions under complex meteorological influences. The results of this research can be applied both in the development of updated regulatory methodologies and as part of real-time environmental monitoring systems.

1. Model derivation

Notation

The influence of atmospheric humidity, precipitation washout of plumes, and the dry deposition of pollutant particles due to gravity leads to an underestimation of the predicted concentrations in areas near the source of pollution, and consequently, an overestimation in more distant areas. [12] We developed a dispersion model that accounts for humidity and gravitational effects to improve the accuracy of pollutant concentration predictions in the study area.

Our production model takes into account the effects of humidity and gravity on plume formation. The Table lists all the variables and symbols used in this model.

The model is based on the plume dispersion model by D. Ermak, which includes the dry deposition of pollutants:

$$C(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \cdot e_1 \cdot \left[e_2 - \sqrt{2\pi}\frac{W_0 \sigma_z}{K_z} \cdot e_3 \cdot \operatorname{erfc}\left(\frac{W_0}{\sqrt{2K_z}} + \frac{z+H}{\sqrt{2}\sigma_z}\right)\right], \quad (1)$$

[1]On the approval of methods for calculating the dispersion of emissions of harmful (pollutant) substances in the ambient air. Order of the Ministry of Natural Resources of the Russian Federation of June 6, 2017, No. 273. *Collection of Laws of the Russian Federation*, 2017, no. 37.

$$\text{where} \quad e_1 = \exp\left(-\frac{W_{\text{set}}(z-H)}{2K_z} - \frac{W_{\text{set}}^2\sigma_z^2}{8K_z^2}\right), \quad e_2 = \exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right),$$
$$e_3 = \exp\left(\frac{W_0(z+H)}{K_z} + \frac{W_0^2\sigma_z^2}{2K_z^2}\right).$$

In Equation (1) $K_z = \sigma_z^2 u/2x$ is the eddy diffusivity coefficient; $W_{\text{set}} = \rho g d^2/18\mu$ is the settling velocity of spherical particles according to Stokes' law, where ρ is the density of the pollutant particle, d is the diameter of the pollutant particle, g is the acceleration due to gravity, μ is the air viscosity; $W_0 = W_{\text{dep}} - 1/2 \cdot W_{\text{set}}$, where $W_{\text{dep}} > 0$ is the dry deposition velocity of pollutant particles, determined experimentally.

Table. Variables used in the pollutant dispersion model derivation

Variable	Description	Units
$C(x, y, z)$	Pollutant concentration at spatial point (x, y, z)	kg/m^3
x, y, z	Spatial coordinates	m
H	Height of the emission source	m
Q	Pollutant emission rate	kg/s
u	Wind speed	m/s
σ_y, σ_z	Gaussian dispersion parameter in the y, z direction	m
K_z	Turbulent diffusion coefficient in the z direction	m^2/s
ρ	Particle density	kg/m^3
d	Particle diameter	m
g	Gravitational acceleration	m/s^2
W_{set}	Sedimentation (settling) velocity by Stokes' law	m/s
W_{dep}	Dry deposition velocity (empirical)	m/s
W_0	Composite parameter related to deposition and sedimentation	m/s
C_1	Increased concentration under precipitation conditions	kg/m^3
C_0	Initial concentration	kg/m^3
m_s	Total droplet mass including water	kg
m_p	Dry pollutant particle mass	kg
M_w	Molar mass of water	kg/mol
M_p	Molar mass of pollutant	kg/mol
ν_p	Amount of substance (pollutant)	mol
ν_w	Amount of substance (water)	mol
RH	Relative humidity	dimensionless (0-1)
ϑ	Hygroscopic growth factor (binding coefficient with water)	dimensionless

D. Ermak's model, despite its advantages over the Gaussian model [3], does not take into account the influence of atmospheric precipitation on pollutant dispersion. We will consider the influence of precipitation on the mass and, therefore, on the speed of pollutant dispersion. To do this, we will use the fact from Koehler's theory [13], which states that the concentration of a pollutant changes proportionally to the change in the mass of the pollutant plume due to precipitation. Using a combination of Kelvin's equation and Raoult's law [14] for droplet mass increase, we can obtain a coefficient for the increase in concentration. Kelvin's Equation describes how the saturation vapor pressure over a droplet surface depends on its curvature (droplet size) and surface tension. Raoult's Law (Solute Effect) describes how dissolved solutes (pollutants) lower the vapor pressure of water. The Koehler equation (combining both effects) predicts the critical droplet size for activation [14]. So, concentration of pollutant after the washout C_1 can be found as

$$C_1 = C_0 \cdot \frac{m_s}{m_p},$$

where $m_p = \frac{1}{6}\pi\rho d^3$ is the dry mass of the pollutant particle.

The mass of a droplet (formed in the cloud of the droplet's plume) with diameter d can be found as [13]:

$$\frac{1}{6}\pi\rho d^3 = M_w\nu_w + M_p\nu_p.$$

The dry mass of the pollutant particle can be found using the formula $m_p = \frac{\pi}{6}\rho_p d_p^3$.

The amount of pollutant substance is given by $\nu_p = \frac{m_p}{M_p}$.

The amount of water substance in the droplet can be found as $\nu_w = \frac{\mathrm{RH}\cdot\vartheta\cdot\nu_p}{1-\mathrm{RH}}$ [14].

So, the mass of bounded water is

$$m_w = \nu_w \cdot M_w = \frac{\mathrm{RH}\cdot\vartheta\cdot\nu_p\cdot M_w}{1-\mathrm{RH}}.$$

From here, the total mass of the droplet can be found as

$$m_s = m_p + m_w = \nu_p M_p + \frac{\mathrm{RH}\cdot\vartheta\cdot\nu_p\cdot M_w}{1-\mathrm{RH}}.$$

So, the concentration increase coefficient can be found as

$$K_{RH} = \frac{m_s}{m_p} = \frac{6}{\pi\rho_p d_p^3}\left(\frac{\mathrm{RH}\cdot\vartheta\cdot\nu_p\cdot M_w}{1-\mathrm{RH}} + \nu_p M_p\right).$$

Then, the pollutant concentration at a point in the study area for cases with and without precipitation can be expressed as

$$C(x,y,z) = \begin{cases} \frac{Q}{2\pi u\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\cdot e_1\cdot\left[e_2 - \sqrt{2\pi}\frac{W_0\sigma_z}{K_z}\cdot e_3\cdot\operatorname{erfc}\left(\frac{W_0}{\sqrt{2K_z}} + \frac{z+H}{\sqrt{2}\sigma_z}\right)\right], \\ \qquad \text{without precipitation}, \\ \frac{Q}{2\pi u\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\cdot e_1\cdot\left[e_2 - \sqrt{2\pi}\frac{W_0\sigma_z}{K_z}\cdot e_3\cdot\operatorname{erfc}\left(\frac{W_0}{\sqrt{2K_z}} + \frac{z+H}{\sqrt{2}\sigma_z}\right)\right]\cdot K_{RH}, \\ \qquad \text{with precipitation}. \end{cases}$$

2. Developed software

To implement the proposed approach, we developed, calibrated, and tested a stationary production model for calculating pollutant dispersion using the high-level programming language Python. The program interface is shown in Fig. 1.

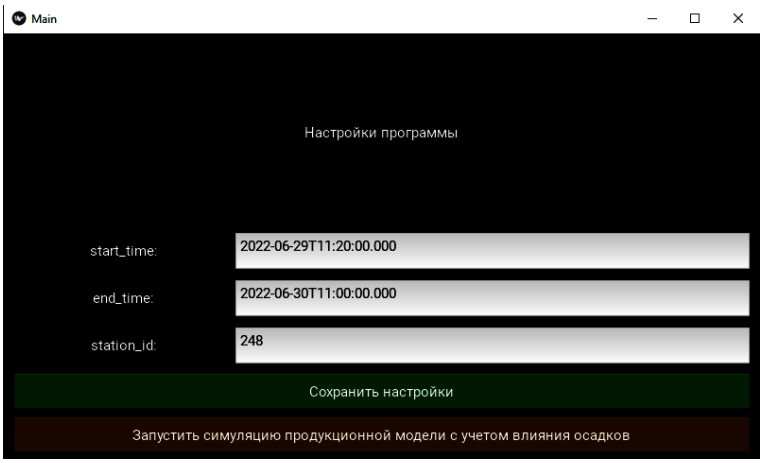


Fig. 1. The developed software's interface (color online)

We configured the program to accept as input the start and end of the time interval for which the atmospheric pollutant dispersion is to be simulated, along with the sensor code whose data (wind speed and direction, air humidity) are used in the modeling process.

Additional parameters, such as the number of emission sources, their spatial coordinates, source heights, and emission intensities, grid size and resolution, particle density and diameter, molar mass, and pollutant hygroscopicity coefficient, were specified in the configuration file located in the root directory of the project.

During the study, we used a Microsoft SQL Server database containing environmental and meteorological data collected at 20-minute intervals over the past three years.

The study area is an industrial zone measuring 5 km by 5 km near a populated area, with predominantly flat terrain (Fig. 2).

Fig. 2. The industrial area under study and the objects located on it (color online)

Five stationary environmental monitoring stations, designated as R_1, R_2, R_3, R_4, R_5 and marked with green markers on the map are installed in this area. These stations measure the concentrations of pollutants in the air and collect meteorological data, including wind speed and direction, air temperature and humidity, and atmospheric pressure. In addition, registered emission sources S_1, S_2, S_3, such as oil refineries, wastewater treatment plants, and chemical storage facilities, are located in the area.

The following declared characteristics of these objects are known: location, altitude above sea level, operating hours, and emission intensity of pollutants into the atmosphere. It is also known that other industrial facilities in this area could be potential sources of pollution. Environmental monitoring data for the study area were obtained from a commercial organization responsible for conducting environmental assessments in the region and adjacent settlements. However, some meteorological parameters, such as insolation and precipitation, necessary for the simulations, were not available from this source. To supplement these missing data, we dynamically acquired relevant meteorological information via API calls to the OpenMeteo.com service at each simulation time step.

The output data are provided in an Excel file containing concentration values for each selected time step at the specified point of interest. Additionally, the simulation results include a heatmap of pollutant concentrations and a graphical visualization of the dispersion over a mapped area.

3. Simulation results

The experiments were conducted on a desktop computer with the following specifications: AMD Ryzen 7 5700X processor (8 cores, 16 threads, 3.4 GHz base clock), 32GB DDR4 RAM running Windows 10 64-bit. Each iteration corresponds to a simulation of air pollutant dispersion over a 20-minute time period. To ensure the interpretability of results, we simulate a full 24-hour day, which consists of 72 iterations. The entire daily simulation takes approximately 20 seconds. After all iterations have completed, the average pollutant concentration for the day is calculated and used for mapping. The simulation results are displayed as a map showing the pollutant distribution and a heat map of concentrations.

Let's take a look at some of the results. Figure 2 shows the simulation outcomes for hydrogen sulfide dispersion using the D. Ermak model, without considering pollutant removal by precipitation. According to meteorological observations, precipitation in the form of rain was observed throughout the day, and the atmosphere was predominantly highly unstable (classes A–B).

Figure 3 shows the simulation results for hydrogen sulfide dispersion using our production model, and how pollutant washout by precipitation affects dispersion on the same date. Considering pollutant washout helps to reduce the overestimated values typical of all exponential models in areas far from the pollution source. As seen in Fig. 3, there are more areas close to the source with elevated pollutant concentrations, which is confirmed by environmental monitoring data for the studied area.

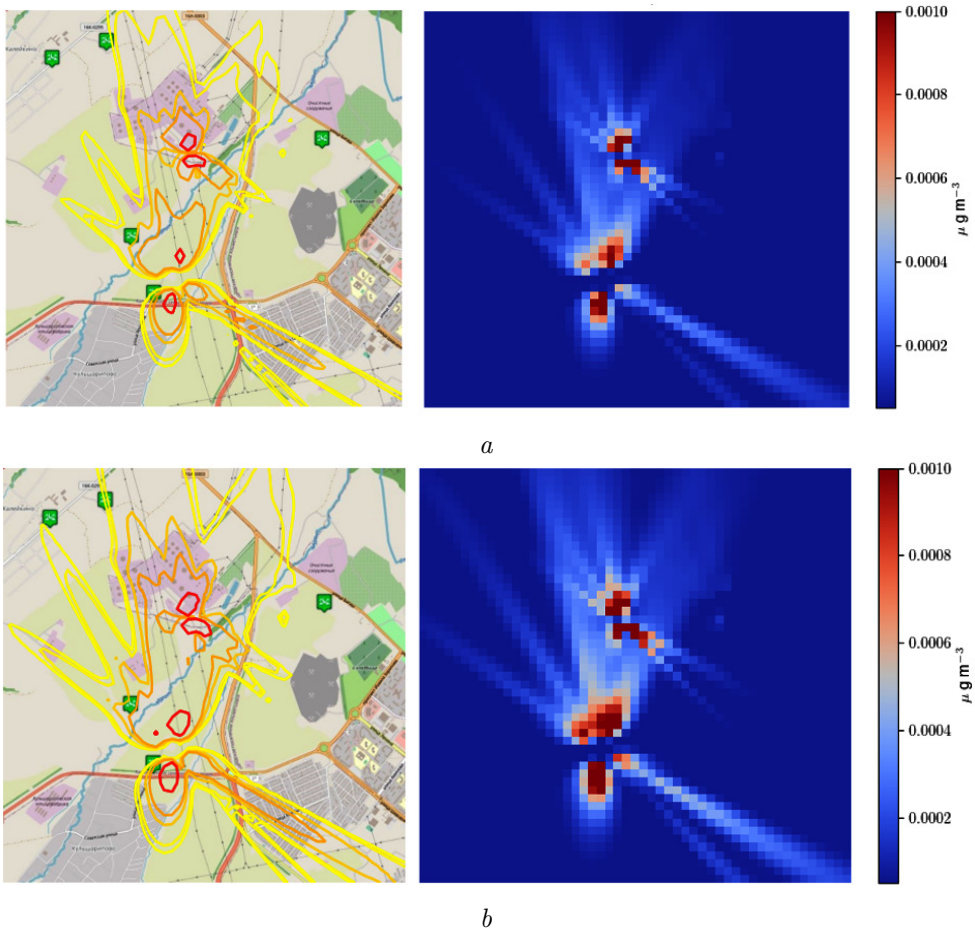
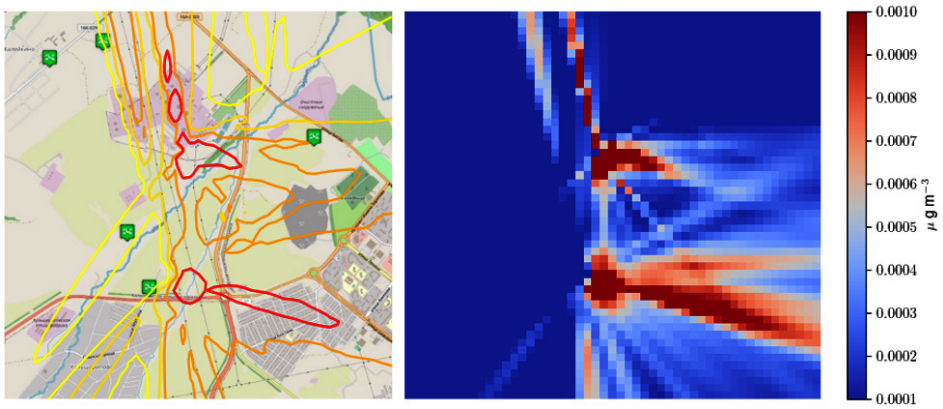


Fig. 3. Hydrogen sulfide dispersion on May 1, 2021: *a* reflects the case without considering plume washout by atmospheric precipitation; *b* reflects the case of considering plume washout by atmospheric precipitation (color online)

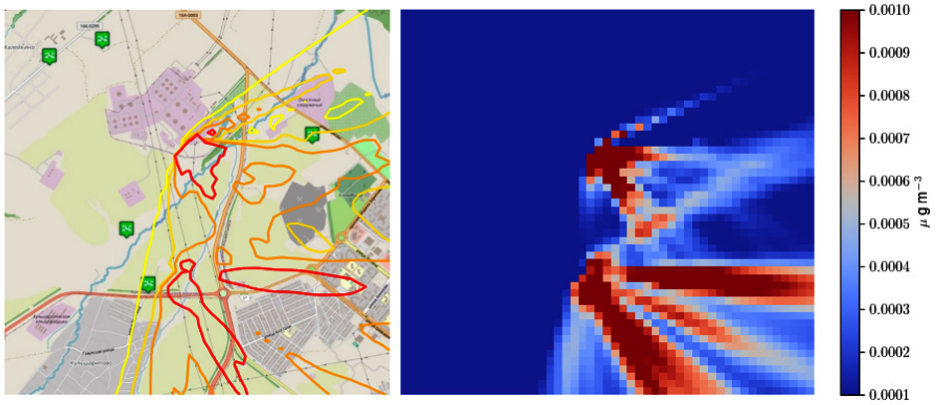
The model incorporating plume washout showed a notable improvement in predictive accuracy, achieving a mean absolute error (MAE) of $MAE = 0.000086$ and a mean absolute percentage error (MAPE) of 41.04%. In comparison, our implementation of the D. Ermak model yielded a higher MAE of 0.000135 and a MAPE of 48.51%, highlighting the superior performance of the proposed approach.

The average percentage error of Ermak's model without considering the influence of precipitation was nearly identical to the error of the previously developed Gaussian plume model implementation, with a MAPE of 48.82% [15]. The obtained deviation values are within the range of errors for exponential plume models, as described by M. R. Beychok [16].

The choice of the sensor used as the primary data source also has some impact on the simulation results. Greater accuracy can be achieved by running simulations for a single time interval multiple times, using data from different sensors. Let's examine the simulation results for October 20, 2022 (Fig. 4).



a



b

Fig. 4. Hydrogen sulfide dispersion on October 20, 2022, considering plume washout by atmospheric precipitation; data sourced: *a* from sensor R_1; *b* from sensor R_5 (color online)

A comparison of the results for the area containing sensor R_1 shows a lower mean absolute error, $\mathrm{MAE}_1 = 0.0001081$, when using data from this sensor, compared to data from sensor R_5, which has a mean absolute error of $\mathrm{MAE}_5 = 0.0001771$. However, this approach requires a significantly larger number of simulations, proportional to the number of points of interest, and consequently, more time for analysis and result interpretation.

Overall, the model demonstrates sufficient accuracy for further use. This model takes into account both dry deposition and the effects of atmospheric precipitation and pollutant washout. However, there are some limitations to the model. For example, it is not suitable for cases with low wind speeds (< 1 m/s), and it does not account for complex terrain or structures that could affect pollutant dispersion. Therefore, it may not be suitable for areas with significant topography. Additionally, the model does not consider possible chemical reactions between pollutants in the plume and other pollutants, which could affect the accuracy of the predictions. Despite these limitations, the model provides a valuable basis for solving inverse problems such as the localization of unknown sources of atmospheric emissions by enabling more accurate modeling of pollutant dispersion patterns [15].

The developed program allows users to simulate the dispersion of air pollutants from multiple sources within the adjustable study area. Users can configure the grid size, study area, number, and characteristics of the sources in the configuration file. The source code implementing the developed model and a sample dataset for simulations are available via the link https://github.com/xtelias/Localisation-of-air-pollution-point-source. For access to the web version of the software, please contact the author via email at es1098@mail.ru.

Conclusion

This study presents a new production-level atmospheric dispersion model that is based on the mathematical framework of D. Ermak's work, but has been extended to include the effects of atmospheric precipitation on pollutant washout. The model is implemented as a computer simulation tool that uses meteorological data and emission source information to simulate the dispersion of pollutants in a defined area.

The system also includes automated graphical visualization of simulation results, which aligns with current standards for environmental monitoring systems. Validation of the model demonstrated a significant improvement in predictive accuracy due to the incorporation of washout processes, achieving a mean absolute percentage error of 41.04% compared to 48.51% for the original D. Ermak model. This indicates enhanced reliability in simulating pollutant behavior under realistic atmospheric conditions, making it a valuable tool for environmental management and planning.

This method is suitable for practical applications in environmental risk assessment, ecological monitoring, and real-time decision support for industrial and governmental stakeholders.

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Поступила в редакцию / Received 13.05.2025
Принята к публикации / Accepted 20.07.2025
Опубликована / Published 28.11.2025