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A conjugated equation of transport and diffusion of aerosol particles in the atmosphere considering the capture of particles by vegetation elements

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Abstract. A mathematical model and a numerical algorithm to study the process of transfer and diffusion of harmful substances are discussed in this article. The proposed model considers the capture of particles by plant elements, which plays a significant role in the dynamics of the process under study. The proposed mathematical model monitors and forecasts the environmental conditions of industrial areas, and helps take measures to protect them from the negative impact of anthropogenous factor. To solve the problem posed, a numerical algorithm based on an implicit finite-difference scheme was developed with a high-order accuracy; it makes it possible to conduct computational experiments on a computer.

1 Introduction

The most significant issue, which has drawn much attention recently, is the movement and spread of dangerous substances in the atmosphere. These substances, which may include pollutants, chemicals, and other harmful compounds, can have serious impacts on human health, the environment, and ecosystems. To better understand the behavior and effects of these substances, scientists and researchers have developed several mathematical models, including adjoint equations.

Adjoint equations are a type of mathematical equations used to model the behavior of complex systems such as the TDHS in the atmosphere. These equations are designed to work in conjunction with other mathematical models, such as partial differential equations, commonly used to describe fluid dynamics and transport phenomena.

Researchers and scientists can attempt to create better ways to manage and minimize the effects of pollution and other dangerous substances on human health and the environment by using these equations and to better understand how these compounds behave in the environment.

There are many studies devoted to modeling the process of TDHS in the atmosphere, in which the capture of particles by vegetation elements is considered. One of such works is the study given in article[1], where the modeling of the atmospheric flow and particle transport in city streets was conducted, considering the presence of plantings. The

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simulation results showed that vegetation could significantly reduce the concentration of airborne particles by trapping particles on vegetation elements.

The authors' study [2] discusses the importance and effectiveness of using barriers to reduce air pollution near roads. In the article, the authors examined various types of roadside barriers, including solid ones (e.g. noise screens or walls) and vegetation (e.g. rows of trees or bushes), and investigated their ability to reduce roadside air pollutant concentrations. The research methodology includes site selection and installation of monitoring stations to collect air quality data. The work may have used various analytical methods, simulations, or field experiments to assess the effect of barriers on air quality. The results of the study provide an analysis of the change in the concentration of pollutants near the roadside barriers. The data may be compared with sites without barriers or with different types of barriers to evaluate their effectiveness in reducing air pollution.

The findings from these [3],4 numerical experiments provide insights into how the wind speed field is influenced by the presence of non-homogeneous vegetation cover, such as the effects of forest belts and forest clear-cuts. The use of implicit difference schemes to solve the model equations suggests the researchers were dealing with complex systems that required more robust numerical integration methods.

The authors of article [5] explored the potential of roadside coniferous vegetation to mitigate air pollution. Over the course of a year, the study took air quality readings at four locations in Cincinnati, Ohio, comparing readings at places with and without roadside conifers. The findings demonstrated that roadside conifers significantly reduced air pollution, particularly nitrogen dioxide (NO_2) and particulate matter (PM). Coniferous trees have been observed to lower NO_2 and PM concentrations by up to 30% and 60%, respectively. The ability of roadside conifers to absorb pollutants through their leaves and trap particles on the needles is what the authors credit for their ability to reduce air pollution. The study, according to the authors, emphasizes the value of green infrastructure, such as vegetation along roadsides, in lowering air pollution and enhancing public health.

The authors of article [6] investigate the behaviour of scalar quantity concentrations and fluxes (such as heat, moisture, and pollution) in the area behind forest trails. To examine this phenomenon, the scientists used modeling based on large-scale turbulence simulation (LES). They matched simulated results to experimental data from a German database. The article demonstrates that the wind is non-uniform in the forest zone, and there is an area where the concentrations and fluxes of scalar quantities increase relative to their values in open space. This impact occurs because the forest decreases vertical turbulence and generates more stable conditions, resulting in an increase in scalar concentrations and fluxes in the area behind the forest patches. The article is important for understanding the role of forests in the global cycle of matter and energy and can be useful for developing strategies for managing forest ecosystems to reduce the impact of pollution on the environment. However, it is worth considering that the data in the article are based on simulations and additional field studies are required to confirm the results.

Based on these considerations, in this paper, we consider modeling the process of TDHS in the atmosphere, considering the capture of particles by vegetation elements. This makes it possible to consider the influence of vegetation on the processes of TDHS since plants can capture particles from the air.

2 Formulation of the problem

The crushed conjugate equation of TDHS in the atmosphere has the following form:

$$-\frac{\partial \varsigma^*}{\partial t}+\varsigma^*(\gamma+\varphi)=\frac{\partial}{\partial z}\left(\lambda\frac{\partial \varsigma^*}{\partial z}\right)+\eta\left[\frac{\partial^2\varsigma^*}{\partial x^2}+\frac{\partial^2\varsigma^*}{\partial y^2}\right]+I;$$

If we replace the independent variable $\tau=T-t$, then in place of the adjoint equation of transfer and diffusion we get:

$$\frac{\partial \varsigma}{\partial \tau}=\frac{\partial}{\partial z}\left(\lambda\frac{\partial \varsigma}{\partial z}\right)+\eta\left[\frac{\partial^2\varsigma}{\partial x^2}+\frac{\partial^2\varsigma}{\partial y^2}\right]-\varsigma(\gamma+\varphi)+I; \qquad (1)$$

Corresponding boundary conditions:

$$\varsigma\big|_{t=0}=\varsigma^0; \qquad (2)$$

$$-\eta\frac{\partial\varsigma}{\partial x}\bigg|_{x=0}=\xi\left(\varsigma_E-\varsigma\right); \qquad \eta\frac{\partial\varsigma}{\partial x}\bigg|_{x=l_x}=\xi\left(\varsigma_E-\varsigma\right); \qquad (3)$$

$$-\eta\frac{\partial\varsigma}{\partial y}\bigg|_{y=0}=\xi\left(\varsigma_E-\varsigma\right); \qquad \eta\frac{\partial\varsigma}{\partial y}\bigg|_{y=l_y}=\xi\left(\varsigma_E-\varsigma\right); \qquad (4)$$

$$-\lambda\frac{\partial\varsigma}{\partial z}\bigg|_{z=0}=\left(\beta\varsigma-C_0\right); \qquad \lambda\frac{\partial\varsigma}{\partial z}\bigg|_{z=h_z}=\xi\left(\varsigma_E-\varsigma\right). \qquad (5)$$

Where ς^* – concentration in the atmosphere; ς_E – concentration entering through the boundaries of the considered area; x, y, z – coordinate system; γ – coefficient of absorption of harmful substances in the atmosphere; φ - coefficient characterizing the capture of particles by vegetation elements; $\eta,\ \lambda$ – diffusion and turbulence coefficients; I – source power; ξ – coefficient of mass transfer across the boundaries of the calculation; β – coefficient of interaction of particles with the underlying surface.

3 Solution method

A numerical algorithm was developed to solve this problem. To facilitate the calculation, we consider problems (1)-(5) in a rectangular area $d=\left(0\le x\le l_x, 0\le y\le l_y, 0\le z\le h_z\right)$, and the source of pollution is considered to be located on the surface. Problem (2)-(5) considering boundary conditions is covered by the grid area [7-8].

To ensure as well as the stability of the calculation process, we use an IFDS for equation (1) in the Ox direction:

$$\frac{1}{2}\frac{\varsigma_{i,j,k}^{n+1/3}-\varsigma_{i,j,k}^{n}}{\Delta\tau/3}+\frac{1}{2}\frac{\varsigma_{i+1,j,k}^{n+1/3}-\varsigma_{i+1,j,k}^{n}}{\Delta\tau/3}+\gamma\varsigma_{i,j,k}^{n+1/3}+\varphi\varsigma_{i,j,k}^{n+1/3}=$$

$$=\frac{\eta}{\Delta x^2}\left(\varsigma_{i+1,j,k}^{n+1/3}-2\varsigma_{i,j,k}^{n+1/3}+\varsigma_{i-1,j,k}^{n+1/3}\right)+\frac{\eta}{\Delta y^2}\left(\varsigma_{i,j+1,k}^{n}-2\varsigma_{i,j,k}^{n}+\varsigma_{i,j-1,k}^{n}\right)+$$

$$+\frac{1}{\Delta z^2}\left(\lambda_{k+0,5}\varsigma_{i,j,k+1}^{n}-\left(\lambda_{k+0,5}+\lambda_{k-0,5}\right)\varsigma_{i,j,k}^{n}+\lambda_{k-0,5}\varsigma_{i,j,k-1}^{n}\right)+\frac{1}{3}I.$$

Let's open the brackets and, grouping the equations, we get:

$$A_{i,j,k}\varsigma_{i-1,j,k}^{n+1/3}-B_{i,j,k}\varsigma_{i,j,k}^{n+1/3}+C_{i,j,k}\varsigma_{i+1,j,k}^{n+1/3}=-D_{i,j,k}.$$

Where:

$$A_{i,j,j}=\frac{\eta}{\Delta x^2};\quad B_{i,j,j}=\frac{2\eta}{\Delta x^2}+\frac{3}{2\Delta\tau}+\gamma+\varphi;\quad C_{i,j,j}=\frac{\eta}{\Delta x^2}-\frac{3}{2\Delta\tau};$$

$$d_{i,j,j}=\left(\frac{3}{2\Delta\tau}-\frac{2\eta}{\Delta y^2}-\frac{\lambda_{k+0,5}+\lambda_{k-0,5}}{\Delta z^2}\right)\varsigma_{i,j,k}^{n}+\frac{3}{2\Delta\tau}\varsigma_{i+1,j,k}^{n}+$$

$$+\frac{\eta}{\Delta y^2}\varsigma_{i,j-1,k}^{n}+\frac{\eta}{\Delta y^2}\varsigma_{i,j+1,k}^{n}+\frac{\lambda_{k-0,5}}{\Delta z^2}\varsigma_{i,j,k-1}^{n}+\frac{\lambda_{k+0,5}}{\Delta z^2}\varsigma_{i,j,k+1}^{n}+\frac{1}{3}I.$$

In the boundary condition (3), we use the approximation of the second order of accuracy and have

$$-\eta\frac{-3\varsigma_{0,j,k}^{n+1/3}+4\varsigma_{1,j,k}^{n+1/3}-\varsigma_{2,j,k}^{n+1/3}}{2\Delta x}=\xi\varsigma_E-\xi\varsigma_{0,j,k}^{n+1/3}$$

Or

$$3\eta\varsigma_{0,j,k}^{n+1/3}-4\eta\varsigma_{1,j,k}^{n+1/3}+\eta\varsigma_{2,j,k}^{n+1/3}=2\Delta x\xi\varsigma_E-2\Delta x\xi\varsigma_{0,j,k}^{n+1/3}.$$

$$A_{1,j,k}\varsigma_{0,j,k}^{n+1/3}-B_{1,j,k}\varsigma_{1,j,k}^{n+1/3}+C_{1,j,k}\varsigma_{2,j,k}^{n+1/3}=-D_{1,j,k} \tag{6}$$

Find $\varsigma_{2,j,k}^{n+1/3}$ as follows:

$$\varsigma_{2,j,k}^{n+1/3}=-\frac{A_{1,j,k}}{C_{1,j,k}}\varsigma_{0,j,k}^{n+1/3}+\frac{B_{1,j,k}}{C_{1,j,k}}\varsigma_{1,j,k}^{n+1/3}-\frac{D_{1,j,k}}{C_{1,j,k}}. \tag{7}$$

We substitute the equation (7) instead of $\varsigma_{2,j,k}^{n+1/3}$ into (6) and get $\varsigma_{0,j,k}^{n+1/3}$ the following:

$$3\eta\varsigma_{0,j,k}^{n+1/3} - 4\eta\varsigma_{1,j,k}^{n+1/3} - \frac{A_{1,j,k}}{C_{1,j,k}}\eta\varsigma_{0,j,k}^{n+1/3} + \frac{B_{1,j,k}}{C_{1,j,k}}\eta\varsigma_{1,j,k}^{n+1/3} - \frac{D_{1,j,k}}{C_{1,j,k}}\mu =$$
$$= 2\Delta x\xi\varsigma_E - 2\Delta\,\mathrm{x}\,\xi\varsigma_{0,j,k}^{n+1/3};$$
$$\varsigma_{0,j,k}^{n+1/3} = \frac{4\eta C_{1,j,k} - B_{1,j,k}\eta}{3\eta C_{1,j,k} - A_{1,j,k}\eta + 2\Delta x\xi}\varsigma_{1,j,k}^{n+1/3} + \frac{D_{1,j,k} + 2\Delta x\xi c_{1,j,k}\varsigma_E}{3\eta C_{1,j,k} - A_{1,j,k}\eta + 2\Delta x\xi}. \quad (8)$$

Using the above formulas (8), we find the values of the sweep coefficients $\alpha_{0,j,k}$ and $\beta_{0,j,k}$:

$$\alpha_{0,j,k} = \frac{4\eta C_{1,j,k} - B_{1,j,k}\eta}{3\eta C_{1,j,k} - A_{1,j,k}\eta + 2\Delta x\xi};\;\; \beta_{0,j,k} = \frac{D_{1,j,k} + 2\Delta x\xi c_{1,j,k}e_1\varsigma_E}{3\eta C_{1,j,k} - A_{1,j,k}\eta + 2\Delta x\xi}. \quad (9)$$

Using the above actions in the boundary condition (3), we obtain

$$\eta\frac{\varsigma_{N-2,j,k}^{n+1/3} - 4\varsigma_{N-1,j,k}^{n+1/3} + 3\varsigma_{N,j,k}^{n+1/3}}{2\Delta x} = \xi\varsigma_E - \xi\varsigma_{N,j,k}^{n+1/3}$$

Or

$$\eta\varsigma_{N-2,j,k}^{n+1/3} - 4\eta\varsigma_{N-1,j,k}^{n+1/3} + 3\eta\varsigma_{N,j,k}^{n+1/3} = 2\Delta x\xi\varsigma_E - 2\Delta x\xi\varsigma_{N,j,k}^{n+1/3}. \quad (10)$$

By successively applying the sweep method to N-1 и N-2, we get $\varsigma_{N-1,j,k}^{n+1/3}$ and $\varsigma_{N-2,j,k}^{n+1/3}$:

$$\varsigma_{N-1,j,k}^{n+1/3} = \alpha_{N-1,j,k}\varsigma_{N,j,k}^{n+1/3} + \beta_{N-1,j,k}; \quad (11)$$

$$\varsigma_{N-2,j,k}^{n+1/3} = \alpha_{N-2,j,k}\varsigma_{N-1,j,k}^{n+1/3} + \beta_{N-2,j,k} =$$
$$= \alpha_{N-2,j,k}\left(\alpha_{N-1,j,k}\varsigma_{N,j,k}^{n+1/3} + \beta_{N-1,j,k}\right) + \beta_{N-2,j,k} = \quad (12)$$
$$= \alpha_{N-2,j,k}\alpha_{N-1,j,k}\varsigma_{N,j,k}^{n+1/3} + \alpha_{N-2,j,k}\beta_{N-1,j,k} + \beta_{N-2,j,k}.$$

Substituting $\varsigma_{N-1,j,k}^{n+1/3}$ and $\varsigma_{N-2,j,k}^{n+1/3}$ into (11), (12) instead of $\varsigma_{N-1,j,k}^{n+1/3}$ and $\varsigma_{N-2,j,k}^{n+1/3}$ в (10) we get $\varsigma_{N,j,k}^{n+1/3}$:

$$\alpha_{N-2,j,k}\alpha_{N-1,j,k}\eta\varsigma_{N,j,k}^{n+1/3}+\alpha_{N-2,j,k}\beta_{N-1,j,k}\eta+\beta_{N-2,j,k}\eta-4\alpha_{N-1,j,k}\eta\theta_{N,j,k}^{n+1/3}-$$
$$-4\beta_{N-1,j,k}\eta+3\eta\varsigma_{N,j,k}^{n+1/3}=2\Delta x\xi\varsigma_E-2\Delta x\xi\varsigma_{N,j,k}^{n+1/3};$$

$$\varsigma_{N,j,k}^{n+1/3}=\frac{2\Delta x\xi\varsigma_E-\left(\beta_{N-2,j,k}+\alpha_{N-2,j,k}\beta_{N-1,j,k}-4\beta_{N-1,j,k}\right)\eta}{2\Delta x\xi+\left(\alpha_{N-2,j,k}\alpha_{N-1,j,k}-4\alpha_{N-1,j,k}+3\right)\eta}. \tag{13}$$

Concentration values are determined by reverse sweep in order of successively decreasing index i. $\varsigma_{N-1,j,k}^{n+1/3}$, $\varsigma_{N-2,j,k}^{n+1/3}$, ..., $\varsigma_{0,j,k}^{n+1/3}$.

Similarly, for equation (1) in the direction Oy, we obtain a finite difference relation:

$$\bar{a}_{i,j,k}\varsigma_{i,j-1,k}^{n+2/3}-\bar{b}_{i,j,k}\varsigma_{i,j,k}^{n+2/3}+\bar{c}_{i,j,k}\varsigma_{i,j+1,k}^{n+2/3}=-\bar{d}_{i,j,k}.$$

Where

$$\bar{a}_{i,j,j}=\frac{\eta}{\Delta y^2};\quad \bar{b}_{i,j,j}=\frac{2\eta}{\Delta y^2}+\frac{3}{2\Delta\tau}+\gamma+\varphi;\quad \bar{c}_{i,j,j}=\frac{\eta}{\Delta y^2}-\frac{3}{2\Delta\tau};$$
$$\bar{d}_{i,j,j}=\left(\frac{3}{2\Delta\tau}-\frac{2\eta}{\Delta x^2}-\frac{\lambda_{k+0,5}+\lambda_{k-0,5}}{\Delta z^2}\right)\varsigma_{i,j,k}^{n+1/3}+\frac{\eta}{\Delta x^2}\varsigma_{i-1,j,k}^{n+1/3}+$$
$$+\frac{\eta}{\Delta x^2}\varsigma_{i+1,j,k}^{n+1/3}+\frac{3}{2\Delta\tau}\varsigma_{i,j+1,k}^{n+1/3}+\frac{\lambda_{k-0,5}}{\Delta z^2}\varsigma_{i,j,k-1}^{n+1/3}+\frac{\lambda_{k+0,5}}{\Delta z^2}\varsigma_{i,j,k+1}^{n+1/3}+\frac{1}{3}I.$$

$$\bar{\alpha}_{i,0,k}=\frac{4\eta\bar{c}_{i,1,k}-\bar{b}_{i,1,k}\eta}{3\eta\bar{c}_{i,1,k}-\bar{a}_{i,1,k}\eta+2\Delta y\xi};\quad \bar{\beta}_{i,0,k}=\frac{\bar{d}_{i,1,k}+2\Delta y\xi\bar{c}_{i,1,k}\varsigma_E}{3\eta\bar{c}_{i,1,k}-\bar{a}_{i,1,k}\eta+2\Delta y\xi}.$$

$$\varsigma_{i,M,k}^{n+2/3}=\frac{2\Delta y\xi\varsigma_E-\left(\bar{\beta}_{i,M-2,k}+\bar{\alpha}_{i,M-2,k}\bar{\beta}_{i,M-1,k}-4\bar{\beta}_{i,M-1,k}\right)\eta}{2\Delta y\xi+\left(\bar{\alpha}_{i,M-2,k}\bar{\alpha}_{i,M-1,k}-4\bar{\alpha}_{i,M-1,k}+3\right)\eta}.$$

Similarly, in equation (1), replacing differential operators with finite-difference operators in the direction of the Oz axis, we obtain:

$$\bar{\bar{a}}_{i,j,k}\varsigma_{i,j,k-1}^{n+1}-\bar{\bar{b}}_{i,j,k}\varsigma_{i,j,k}^{n+1}+\bar{\bar{c}}_{i,j,k}\varsigma_{i,j,k-1}^{n+1}=-\bar{\bar{d}}_{i,j,k}$$

Where

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$$\bar{\bar{a}}_{i,j,j} = \frac{\lambda_{k-0,5}}{\Delta z^2}; \quad \bar{\bar{b}}_{i,j,j} = \frac{\lambda_{k+0,5}+\lambda_{k-0,5}}{\Delta z^2} + \frac{3}{2\Delta\tau} + \gamma + \varphi; \quad \bar{\bar{c}}_{i,j,j} = \frac{\lambda_{k+0,5}}{\Delta z^2} - \frac{3}{2\Delta\tau};$$

$$\bar{\bar{d}}_{i,j,j} = \left(\frac{3}{2\Delta\tau} - \frac{2\eta}{\Delta x^2} - \frac{2\eta}{\Delta y^2}\right)\varsigma_{i,j,k}^{n+2/3} + \frac{\eta}{\Delta x^2}\varsigma_{i+1,j,k}^{n+2/3} + \frac{\eta}{\Delta x^2}\varsigma_{i-1,j,k}^{n+2/3} +$$

$$+\frac{\eta}{\Delta y^2}\varsigma_{i,j+1,k}^{n+2/3} + \frac{\eta}{\Delta y^2}\varsigma_{i,j-1,k}^{n+2/3} + \frac{3}{2\Delta\tau}\varsigma_{i,j,k+1}^{n+2/3} + \frac{1}{3}I.$$

$$\bar{\bar{\alpha}}_{i,j,0} = \frac{4\lambda_1\bar{\bar{c}}_{i,j,1} - \bar{\bar{b}}_{i,j,1}\lambda_1}{3\lambda_1\bar{\bar{c}}_{i,j,1} - \bar{\bar{a}}_{i,j,1}\lambda_1 - 2\Delta z\beta}; \quad \bar{\bar{\beta}}_{i,j,0} = \frac{\bar{\bar{d}}_{i,j,1}\lambda_1 + 2\Delta z\bar{\bar{c}}_{i,j,1}C_0}{3\lambda_1\bar{\bar{c}}_{i,j,1} - \bar{\bar{a}}_{i,j,1}\lambda_1 - 2\Delta z\beta}.$$

$$\varsigma_{i,j,l}^{n+1} = \frac{2\Delta z\xi\varsigma_E - \left(\bar{\bar{\beta}}_{i,j,l-2} + \bar{\bar{\alpha}}_{i,j,l-2}\bar{\bar{\beta}}_{i,j,l-1} - 4\bar{\bar{\beta}}_{i,j,l-1}\right)\lambda_l}{2\Delta z\xi + \left(\bar{\bar{\alpha}}_{i,j,l-2}\bar{\bar{\alpha}}_{i,j,l-1} - 4\bar{\bar{\alpha}}_{i,j,l-1} + 3\right)\lambda_l}.$$

4 Experimental results

The concentration of pollutants changes over time under the influence of various factors, such as interaction with the environment, natural decomposition or increase / decrease in the power of pollution sources, etc.

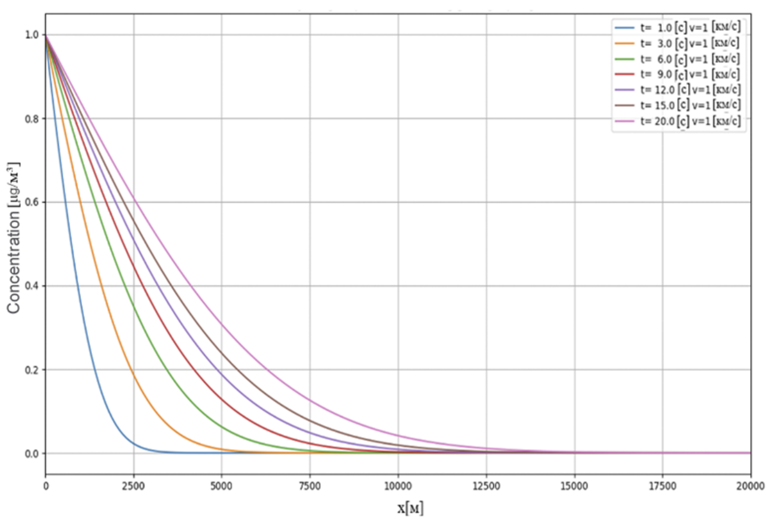

Fig. 1. Concentration of CO_2 (mg/m^3) in the atmospheric air over time t along the plume axis from the leeward side at a height h = 50 m at wind speed ν = 1 m/s, source power (100 meter section of the road with low traffic) Q =1000 mg/m^3 and diffusion coefficient $\eta_x = 0,1$. $\eta_y = 0,1$.

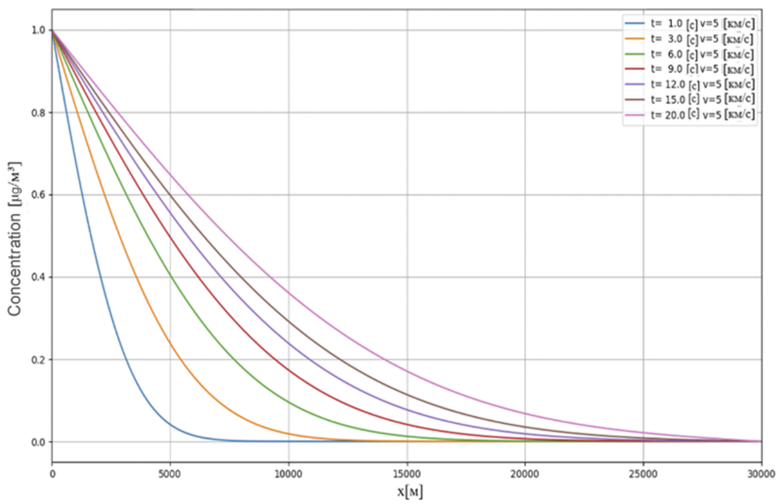

Fig. 2. Change in CO_2 concentration (mg/m^3) in the atmosphere over time at ν =5 m/s. Other input data is shown in Figure 1.

Figures 1- 2 show that wind speed affects the transport of pollutants from the place of release, while with increasing wind speed, the drop in the concentration of pollutants over time becomes close to linear. Higher wind speeds lead to faster movement of pollutants in the environment, which somewhat evens out the distribution of pollutants, reducing the likelihood of the.

5 Conclusions

To solve this problem, an IFDS with a high order of accuracy was used, which makes it possible to conduct computational experiments on a computer. Thus, the results of the study allow us to conclude that the change in pollutant concentrations depending on various points in time and parameters (wind speed, source power, height, and diffusion coefficient) occurs dynamically and depends on the interaction of these factors.

As a result, a mathematical model and a numerical algorithm were developed for research, forecasting, and making managerial decisions to protect the environment and industrial air basins, where particle capture by vegetation elements, which plays a significant role in the process dynamics, is considered. Although research is ongoing to model the transport and diffusion of aerosol particles with respect to particle capture by vegetation elements, they are already showing the potential of using vegetation cover to improve air quality in cities.

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