TASHKENT UNIVERSITY OF INFORMATION TECHNOLOGIES
NAMED AFTER MUHAMMAD AL-KHWARIZMI

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PREFACE

The 2023 IEEE and IFIP International Conference on Information Science and Communications Technologies ICISCT 2023 invites high-quality recent research results in the areas of Home and Health networking, Electronic commerce, Mobility and Mobile Payment, Broadband access, satellite services, 5G in rural communications, cloud computing, Smart grids, Big data analysis, Cyber security, Internet-of-Things IOT, Mobile and Wireless Communications, optical communications and networking, architectures, protocols, planning and design, management and operation, simulation and performance modeling.

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The main goal of the conference is to bring together scientists and engineers who work and teach in these specialized fields to submit papers and come together in this geographical location. ICISCT 2023 is sponsored and organized by IEEE Uzbekistan Regional Chapter and Tashkent University of Information Technologies TUIT and Technically Sponsored by IEEE Photonics Society https://www.photonicssociety.org

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Model and numerical algorithm for investigation of the transfer and diffusion of aerosol particles in the atmosphere taking into account the capture of particles by vegetation elements*

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***Abstract*—In this paper, a mathematical model and a numerical algorithm are developed for the process of transfer and diffusion of harmful substances, which take into account the wind speed in three directions and the rate of deposition of aerosol particles on the underlying surface, as well as the capture of particles by vegetation elements, which plays a significant role in the dynamics of the object of study. To integrate the task, an implicit finite-difference scheme and an algorithm with the second order of approximation have been developed in time and space variables, with the help of which can be used to carry out numerical calculations on a computer system, on the basis of which it is possible to investigate and predict the ecological state of the industrial region under consideration.**

***Index Terms*—approximation, transport and diffusion, atmosphere, harmful aerosols, numerical algorithm**

I. Introduction

At present, the problems of environmental pollution with hazardous chemicals in the industrialized regions of the globe have become sharply aggravated. By the 21st century, human's technogenic impact on the biosphere and individual geocomponents (atmosphere, hydrosphere, lithosphere and communities of living organisms) has reached enormous proportions. Anthropogenic emissions and discharges are increasing from year to year. They also contain new components that are even more toxic which lead to a violation of the stability of the biosphere, to its destruction. The ecological state of the Earth's biosphere is assessed as a global crisis. The intensive growth of human economic activity, while ignoring the possibilities of nature and the laws of its development, has led to the need to solve one of the pressing problems on a global scale. This problem is related to the tasks of protecting the environment, water resources and underground resources from technogenic factors and negative anthropogenic impacts that directly affect the ecological state of the surface layer of the atmosphere and atmospheric air quality. Conducting comprehensive research, monitoring, forecasting and analysis of the process of the spread of impurities in the atmosphere, in soil and groundwater are among the most urgent tasks in the problem of environmental protection. The solution of these problems is associated with taking into consiferation many factors that affect the dispersion of impurities in the atmosphere, soil and groundwater. These include anthropogenic and meteorological conditions, type of source, properties of impurities, etc. The problems of modeling the transfer and diffusion of harmful substances are studied in scientific schools created under the guidance of foreign scientists J.W. Deardorff, M. Germano, U. Piomelli, L.C. Berselli, G.S. Winckelmans, W.C. Reynolds, T. Iversen., T.E. Nordeng, R. Lange, M. Pekar, G.I. Marchuk, V.V. Penenko, A.E. Aloyan, L.T. Matveeva, V.P. Dimnikova, I.E Naatsa, I.A. Kibelya, L.N. Gutman and others.

In the work [1], for monitoring, forecasting and making managerial decisions to protect the environment of industrial regions, a mathematical model was developed that describes the process of propagation of active aerosol particles emitted from production facilities, which involves weather and climatic factors, forward and reverse reaction rates and the reaction rate decomposition of the mixture by a chemical reaction.

A model, a numerical algorithm, and a software tool was developed by the authors of the work [2] for research, forecasting, and monitoring, as well as for assessing the ecological state of the atmosphere and the underlying surface of the region under consideration by passive and active impurities, which take into account the main parameters and disturbances that affect the object as a whole. A system of nonlinear differential equations in partial derivatives was obtained to determine the speed of movement of aerosol particles under the action of an air flow, which estimate the main physical and mechanical properties of aerosol particles, which play an important role in the process under consideration.

The papers [3]–[5] solved the problem related to monitoring and forecasting the ecological state of the air basin of industrial regions, where there is often a violation of the balance of the sanitary norm of the environment, due to a large amount of emissions of harmful substances into the atmosphere. The authors of the article, when developing a mathematical model of the transfer and diffusion process, calculated existing factors such as soil erosion, which, with unstable air mass stratification, is essential: - Change the concentration of harmful substances in the atmosphere; - Change the speed of movement of the air mass of the atmosphere in three directions over time; - Change the diffusion coefficient and the vertical turbulent mixing coefficient for stable and unstable stratification; - Change the direction of the wind with time per day, depending on the orography of the area; - Change the coefficient of interaction, which depends on the characteristics of the underlying surface of the earth and the orography of the area. Numerical calculations were carried out in a computer system, the results of which are presented in the form of graphical objects. A model of the process of distribution of industrial emissions in the atmosphere was developed in the article [6]–[8], taking into consideration the deposition rate of fine particles, which is described using a multidimensional differential equation in partial derivatives with appropriate initial and boundary conditions. For the numerical solution of the problem, the method of splitting by physical processes was used: transport, diffusion and absorption of harmful particles, as well as an implicit finite-difference scheme in time with the second order of accuracy. Although the above works have obtained significant results of a fundamental and applied nature, they do not consider the spread of harmful substances, considering the heterogeneity and roughness of the earth's surface: vegetation cover, forest belt, high-rise residential and industrial facilities.

II. Formulation of the Problem

With considering the above, we figure on a mathematical model that describes based on the law of hydromechanics in order to study the process of transfer and diffusion of aerosol particles in the atmosphere, including the essential parameters u, ν, ω - the components of the wind speed in directions, x, y, z, respectively, as well as the orography of the area under consideration:

$$\begin{aligned}\frac{\partial \theta}{\partial t} + u\frac{\partial \theta}{\partial x} + v\frac{\partial \theta}{\partial y} + (w - w_g)\frac{\partial \theta}{\partial z} + \sigma\theta + \alpha\theta = \\ = \mu\frac{\partial^2 \theta}{\partial x^2} + \mu\frac{\partial^2 \theta}{\partial y^2} + \frac{\partial}{\partial z}\left(\kappa\frac{\partial \theta}{\partial z}\right) + \delta Q\end{aligned} \quad (1)$$

with the corresponding initial and boundary conditions:

$$\theta|_{t=0} = \theta^0; \quad (2)$$

$$-\mu\frac{\partial \theta}{\partial x}\bigg|_{x=0} = \xi(\theta_E - \theta);\ \mu\frac{\partial \theta}{\partial x}\bigg|_{x=Lx} = \xi(\theta_E - \theta); \quad (3)$$

$$-\mu\frac{\partial \theta}{\partial y}\bigg|_{y=0} = \xi(\theta_E - \theta);\ \mu\frac{\partial \theta}{\partial y}\bigg|_{y=L_y} = \xi(\theta_E - \theta); \quad (4)$$

$$-\kappa\frac{\partial \theta}{\partial z}\bigg|_{z=0} = (\beta\theta - f_0);\ \kappa\frac{\partial \theta}{\partial z}\bigg|_{z=H_z} = \xi(\theta_E - \theta); \quad (5)$$

Where there is θ - the concentration of harmful substances in the atmosphere; t is time; θ^0 – primary concentration of harmful substances in the atmosphere; θ_E - is the concentration entering through the boundaries of the area under consideration; $x,\ y,\ z$ - coordinate system; u, ν, ω - wind speed in three directions; w_g- is the particle settling rate; σ - coefficient of absorption of harmful substances in the atmosphere; $\alpha(z)$ - coefficient characterizing the capture of particles by vegetation elements; $\mu,\ \kappa$ are the diffusion and turbulence coefficients; Q - is the power of the source; δ - is the Dirac function; ξ - is the mass transfer coefficient across the calculation boundaries; β - is the coefficient of particle interaction with the underlying surface.

III. Solving Method

Further, for the numerical integration of problem (1)-(5), we introduce the notation.

$$\bar{w} = w - w_g; \theta = e^{\frac{ux+vy}{2\mu} + \frac{\bar{w}z}{2\kappa}}\tilde{\theta} \quad (6)$$

and substituting relation (6) into equation (1) and simplifying like terms, we end up with the following:

$$\frac{\partial \tilde{\theta}}{\partial t} + \sigma_1\tilde{\theta} = \mu\frac{\partial^2 \tilde{\theta}}{\partial x^2} + \mu\frac{\partial^2 \tilde{\theta}}{\partial y^2} + \frac{\partial}{\partial z}\left(\kappa\frac{\partial \tilde{\theta}}{\partial z}\right) + e_1\delta Q \quad (7)$$

Here $\sigma_1 = \frac{\kappa u^2 + \kappa v^2 + \mu\bar{w}^2 + 4\sigma\mu\kappa + 4\alpha\mu\kappa}{4\mu\kappa}$; $e_1 = e^{-\left(\frac{ux+vy}{2\mu} + \frac{\bar{w}z}{2\kappa}\right)}$;

The initial and boundary conditions for (7), respectively, are as follows:

$$\tilde{\theta}\Big|_{t=0} = \tilde{\theta}^0; \quad (8)$$

$$-\mu\frac{\partial \tilde{\theta}}{\partial x}\bigg|_{x=0} = \xi\left(e_1\theta_E - \tilde{\theta}\right);\ \mu\frac{\partial \tilde{\theta}}{\partial x}\bigg|_{x=L_x} = \xi\left(e_1\theta_E - \tilde{\theta}\right); \quad (9)$$

$$-\mu\frac{\partial \tilde{\theta}}{\partial y}\bigg|_{y=0} = \xi\left(e_1\theta_E - \tilde{\theta}\right);\ \mu\frac{\partial \tilde{\theta}}{\partial y}\bigg|_{y=L_y} = \xi\left(e_1\theta_E - \tilde{\theta}\right); \quad (10)$$

$$-\kappa\frac{\partial \tilde{\theta}}{\partial z}\bigg|_{z=0} = \left(\beta\tilde{\theta} - e_1 f_0\right);\ \kappa\frac{\partial \tilde{\theta}}{\partial z}\bigg|_{z=H_z} = \xi\left(e_1\theta_E - \tilde{\theta}\right). \quad (11)$$

To simplify the solution, we consider equations (7)-(11) in a rectangular $D = (0 \le x \le L_x,\ 0 \le y \le L_y,\ 0 \le z \le H_z)$ area and assume that the source of pollution is in the surface layer of the earth. For the numerical solution of problem (7)-(11), we cover the change field with an unknown grid corresponding to the steps, taking into consideration the boundary conditions:

$\Omega_{xyzt} = \{(x_i = i\Delta x,\ y_j = j\Delta y, z_k = k\Delta z,\ \tau_n = n\ \Delta t);$
$i = \overline{1, N_x};\ j = \overline{1, M_y},\ k = \overline{1, L_z},\ n = \overline{0, N_t},\ \Delta t = \frac{1}{N_t}\Big\}.$

We use an implicit difference scheme to ensure a high order of approximation in terms of time and space variables, as well as the stability of the calculation process, we obtain a finite difference scheme: In the direction of the Ox:

$$\frac{\tilde{\theta}^{n+1/3}_{i,j,k}-\tilde{\theta}^{n}_{i,j,k}}{\Delta t/3}+\sigma_1\tilde{\theta}^{n+1/3}_{i,j,k}=$$
$$=\frac{\mu}{\Delta x^2}\left(\tilde{\theta}^{n+1/3}_{i+1,j,k}-2\tilde{\theta}^{n+1/3}_{i,j,k}+\tilde{\theta}^{n+1/3}_{i-1,j,k}\right)+$$
$$+\frac{\mu}{\Delta y^2}\left(\tilde{\theta}^{n}_{i,j+1,k}-2\tilde{\theta}^{n}_{i,j,k}+\tilde{\theta}^{n}_{i,j-1,k}\right)+$$
$$+\frac{1}{\Delta z^2}\left(\begin{array}{c} l\kappa_{k+0,5}\tilde{\theta}^{n}_{i,j,k+1}- \\ -\left(\kappa_{k-0,5}+\kappa_{k+0,5}\right)\tilde{\theta}^{n}_{i,j,k}+ \\ +\kappa_{k-0,5}\tilde{\theta}^{n}_{i,j,k-1}\end{array}\right)+$$
$$+\frac{1}{3}e_1\delta_{i,j,k}Q.$$

We tear off the brackets and grouping similar terms of the equation, we get:

$$\begin{array}{c}\frac{\mu}{\Delta x^2}\tilde{\theta}^{n+1/3}_{i-1,j,k}-\left(\frac{3}{\Delta t}+\sigma_1+\frac{2\mu}{\Delta x^2}\right)\tilde{\theta}^{n+1/3}_{i,j,k}+\frac{\mu}{\Delta x^2}\tilde{\theta}^{n+1/3}_{i+1,j,k}= \\ =-\left(\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta y^2}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\right)\tilde{\theta}^{n}_{i,j,k}+\frac{\mu}{\Delta y^2}\tilde{\theta}^{n}_{i,j-1,k}+\right. \\ \left.+\frac{\mu}{\Delta y^2}\tilde{\theta}^{n}_{i,j+1,k}+\frac{\kappa_{k-0,5}}{\Delta z^2}\tilde{\theta}^{n}_{i,j,k-1}+\frac{\kappa_{k+0,5}}{\Delta z^2}\tilde{\theta}^{n}_{i,j,k+1}+\frac{1}{3}e_1\delta_{i,j,k}Q\right).\end{array} \tag{12}$$

To simplify the above equation, we introduce the following notation:
$a_{i,j,k}=\frac{\mu}{\Delta x^2}$; $b_{i,j,k}=\frac{3}{\Delta t}+\sigma_1+\frac{2\mu}{\Delta x^2}$; $c_{i,j,k}=\frac{\mu}{\Delta x^2}$;

$$d_{i,j,k}=\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta y^2}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\right)\tilde{\theta}^{n}_{i,j,k}+$$
$$\frac{\mu}{\Delta y^2}\tilde{\theta}^{n}_{i,j-1,k}+\frac{\mu}{\Delta y^2}\tilde{\theta}^{n}_{i,j+1,k}+\frac{\kappa_{k-0,5}}{\Delta z^2}\tilde{\theta}^{n}_{i,j,k-1}+$$
$$+\frac{\kappa_{k+0,5}}{\Delta z^2}\tilde{\theta}^{n}_{i,j,k+1}+\frac{1}{3}e_1\delta_{i,j,k}Q.$$

We write equation (12) as a system of tridiagonal linear algebraic equations using the above notation:

$$a_{i,j,k}\tilde{\theta}^{n+1/3}_{i-1,j,k}-b_{i,j,k}\tilde{\theta}^{n+1/3}_{i,j,k}+$$
$$+c_{i,j,k}\tilde{\theta}^{n+1/3}_{i+1,j,k}=-d_{i,j,k}.$$

We also approximate the first part of the boundary condition (9) with the second order of accuracy:

$$-\mu\frac{-3\tilde{\theta}^{n+1/3}_{0,j,k}+4\tilde{\theta}^{n+1/3}_{1,j,k}-\tilde{\theta}^{n+1/3}_{2,j,k}}{2\Delta x}=\xi e_1\theta_E-\xi\tilde{\theta}^{n+1/3}_{0,j,k}$$

or

$$\begin{array}{c}3\mu\tilde{\theta}^{n+1/3}_{0,j,k}-4\mu\tilde{\theta}^{n+1/3}_{1,j,k}+\mu\tilde{\theta}^{n+1/3}_{2,j,k}= \\ 2\Delta xe_1\xi\theta_E-2\Delta x\xi\tilde{\theta}^{n+1/3}_{0,j,k}.\end{array} \tag{13}$$

From the resulting tridiagonal system of linear algebraic equations

$$a_{1,j,k}\tilde{\theta}^{n+1/3}_{0,j,k}-b_{1,j,k}\tilde{\theta}^{n+1/3}_{1,j,k}+c_{1,j,k}\tilde{\theta}^{n+1/3}_{2,j,k}=-d_{1,j,k}$$

find $\tilde{\theta}^{n+1/3}_{2,j,k}$ as follows:

$$\tilde{\theta}^{n+1/3}_{2,j,k}=-\frac{a_{1,j,k}}{c_{1,j,k}}\tilde{\theta}^{n+1/3}_{0,j,k}+\frac{b_{1,j,k}}{c_{1,j,k}}\tilde{\theta}^{n+1/3}_{1,j,k}-\frac{d_{1,j,k}}{c_{1,j,k}}. \tag{14}$$

$\theta^{n+2/3}_{i,2,k}$ in equation (14) we substitute in (13) and get the following:

$$3\mu\tilde{\theta}^{n+1/3}_{0,j,k}-4\mu\tilde{\theta}^{n+1/3}_{1,j,k}-\frac{a_{1,j,k}}{c_{1,j,k}}\mu\tilde{\theta}^{n+1/3}_{0,j,k}+$$
$$+\frac{b_{1,j,k}}{c_{1,j,k}}\mu\tilde{\theta}^{n+1/3}_{1,j,k}-\frac{d_{1,j,k}}{c_{1,j,k}}\mu=$$
$$=2\Delta xe_1\xi\theta_E-2\Delta x\xi\tilde{\theta}^{n+1/3}_{0,j,k};$$

or

$$\begin{array}{c}\left(3\mu+\frac{a_{1,j,k}}{c_{1,j,k}}\mu+2\Delta x\xi\right)\tilde{\theta}^{n+1/3}_{0,j,k}= \\ =\left(4\mu-\frac{b_{1,j,k}}{c_{1,j,k}}\mu\right)\tilde{\theta}^{n+1/3}_{1,j,k}+ \\ +\frac{d_{1,j,k}}{c_{1,j,k}}\mu+2\Delta xe_1\xi\theta_E;\end{array} \tag{15}$$

As a result, we find $\tilde{\theta}^{n+1/3}_{0,j,k}$ from equation (15):

$$\begin{array}{c}\tilde{\theta}^{n+1/3}_{0,j,k}=\frac{4\mu c_{1,j,k}-b_{1,j,k}\mu}{3\mu c_{1,j,k}-a_{1,j,k}\mu+2\Delta x\xi}\tilde{\theta}^{n+1/3}_{1,j,k}+ \\ +\frac{d_{1,j,k}+2\Delta x\xi c_{1,j,k}e_1\theta_E}{3\mu c_{1,j,k}-a_{1,j,k}\mu+2\Delta x\xi}.\end{array} \tag{16}$$

Using the given formulas (16), we find the values of the sweep coefficients $\alpha_{0,j,k}$ and $\beta_{0,j,k}$:

$$\begin{array}{c}\alpha_{0,j,k}=\frac{4\mu c_{1,j,k}-b_{1,j,k}\mu}{3\mu c_{1,j,k}-a_{1,j,k}\mu+2\Delta x\xi}; \\ \beta_{0,j,k}=\frac{d_{1,j,k}+2\Delta x\xi c_{1,j,k}e_1\theta_E}{3\mu c_{1,j,k}-a_{1,j,k}\mu+2\Delta x\xi}.\end{array} \tag{17}$$

We also approximate the second part of the boundary condition (9):

$$\mu\frac{\tilde{\theta}^{n+1/3}_{N-2,j,k}-4\tilde{\theta}^{n+1/3}_{N-1,j,k}+3\tilde{\theta}^{n+1/3}_{N,j,k}}{2\Delta x}=$$
$$=\xi e_1\theta_E-\xi\tilde{\theta}^{n+1/3}_{N,j,k}$$

or

$$\begin{array}{c}\mu\tilde{\theta}^{n+1/3}_{N-2,j,k}-4\mu\tilde{\theta}^{n+1/3}_{N-1,j,k}+3\mu\tilde{\theta}^{n+1/3}_{N,j,k}= \\ =2\Delta xe_1\xi\theta_E-2\Delta x\xi\tilde{\theta}^{n+1/3}_{N,j,k}.\end{array} \tag{18}$$

Sequentially applying the sweep method for N, N-1 and N-2 , we find $\tilde{\theta}^{n+1/3}_{N-1,j,k}$ and $\tilde{\theta}^{n+1/3}_{N-2,j,k}$

$$\tilde{\theta}^{n+1/3}_{N-1,j,k}=\alpha_{N-1,j,k}\tilde{\theta}^{n+1/3}_{N,j,k}+\beta_{N-1,j,k}; \tag{19}$$

$$\begin{array}{c}\tilde{\theta}^{n+1/3}_{N-2,j,k}=\alpha_{N-2,j,k}\tilde{\theta}^{n+1/3}_{N-1,j,k}+\beta_{N-2,j,k}= \\ =\alpha_{N-2,j,k}\left(\alpha_{N-1,j,k}\tilde{\theta}^{n+1/3}_{N,j,k}+\beta_{N-1,j,k}\right)+ \\ +\beta_{N-2,j,k}=\alpha_{N-2,j,k}\alpha_{N-1,j,k}\tilde{\theta}^{n+1/3}_{N,j,k}+ \\ +\alpha_{N-2,j,k}\beta_{N-1,j,k}+\beta_{N-2,j,k}.\end{array} \tag{20}$$

Substituting $\tilde{\theta}^{n+1/3}_{N-1,j,k}$ and $\tilde{\theta}^{n+1/3}_{N-2,j,k}$ from (19) and (20) in equation (18) we find $\tilde{\theta}^{n+1/3}_{N,j,k}$:

$$\begin{gathered}\alpha_{N-2,j,k}\alpha_{N-1,j,k}\mu\tilde{\theta}^{n+1/3}_{N,j,k}+\alpha_{N-2,j,k}\beta_{N-1,j,k}\mu+\\+\beta_{N-2,j,k}\mu-4\alpha_{N-1,j,k}\mu\tilde{\theta}^{n+1/3}_{N,j,k}-\\-4\beta_{N-1,j,k}\mu+3\mu\tilde{\theta}^{n+1/3}_{N,j,k}=\\=2\Delta xe_1\xi\theta_E-2\Delta x\xi\tilde{\theta}^{n+1/3}_{N,j,k};\end{gathered}$$

$$\tilde{\theta}^{n+1/3}_{N,j,k}=\frac{2\Delta xe_1\xi\theta_E}{2\Delta x\xi+(\alpha_{N-2,j,k}\alpha_{N-1,j,k}-4\alpha_{N-1,j,k}+3)\mu}-\\-\frac{(\beta_{N-2,j,k}+\alpha_{N-2,j,k}\beta_{N-1,j,k}-4\beta_{N-1,j,k})\mu}{2\Delta x\xi+(\alpha_{N-2,j,k}\alpha_{N-1,j,k}-4\alpha_{N-1,j,k}+3)\mu}. \tag{21}$$

In the reverse course of the sweep in succession, the values of the concentrations are determined $\tilde{\theta}^{n+1/3}_{N-1,j,k}, \tilde{\theta}^{n+1/3}_{N-2,j,k},\dots,$ $\tilde{\theta}^{n+1/3}_{0,j,k}$ are in the following form:
$\tilde{\theta}^{n+1/3}_{i,j,k}=\alpha_{i,j,k}\tilde{\theta}^{n+1/3}_{i+1,j,k}+\beta_{i,j,k};$
$i=\overline{N-1,0},\ j=\overline{1,M-1},\ k=\overline{1,L-1}.$
Applying the above procedures in the direction Oy and we have the following:

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

Here

$$\bar{a}_{i,j,k}=\frac{\mu}{\Delta y^2};\quad \bar{b}_{i,j,k}=\frac{3}{\Delta t}+\sigma_1+\frac{2\mu}{\Delta y^2};\quad \bar{c}_{i,j,k}=\frac{\mu}{\Delta y^2};$$

$$\begin{gathered}\bar{d}_{i,j,k}=\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta x^2}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\right)\tilde{\theta}^{n+1/3}_{i,j,k}+\\ \frac{\mu}{\Delta x^2}\tilde{\theta}^{n+1/3}_{i-1,j,k}+\frac{\mu}{\Delta x^2}\tilde{\theta}^{n+1/3}_{i+1,j,k}+\\+\frac{\kappa_{k-0,5}}{\Delta z^2}\tilde{\theta}^{n+1/3}_{i,j,k-1}+\frac{\kappa_{k+0,5}}{\Delta z^2}\tilde{\theta}^{n+1/3}_{i,j,k+1}+\\+\frac{1}{3}e_1\delta_{i,j,k}Q.\end{gathered}$$

$$\bar{\alpha}_{i,0,k}=\frac{4\mu\bar{c}_{i,1,k}-\bar{b}_{i,1,k}\mu}{3\mu\bar{c}_{i,1,k}-\bar{a}_{i,1,k}\mu+2\Delta y\xi};\quad \bar{\beta}_{i,0,k}=\frac{\bar{d}_{i,1,k}+2\Delta ye_1\bar{c}_{i,1,k}\xi\theta_E}{3\mu\bar{c}_{i,1,k}-\bar{a}_{i,1,k}\mu+2\Delta y\xi}. \tag{22}$$

$$\tilde{\theta}^{n+2/3}_{i,M,k}=\frac{2\Delta ye_1\xi\theta_E}{2\Delta y\xi+(\bar{\alpha}_{i,M-2,k}\bar{\alpha}_{i,M-1,k}-4\bar{\alpha}_{i,M-1,k}+3)\mu}-\\-\frac{\left(\bar{\beta}_{i,M-2,k}+\bar{\alpha}_{i,M-2,k}\bar{\beta}_{i,M-1,k}-4\bar{\beta}_{i,M-1,k}\right)\mu}{2\Delta y\xi+(\bar{\alpha}_{i,M-2,k}\bar{\alpha}_{i,M-1,k}-4\bar{\alpha}_{i,M-1,k}+3)\mu}. \tag{23}$$

Similarly, applying the above procedures in the direction of Oz, we get the following:

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

Here

$$\bar{\bar{a}}_{i,j,k}=\frac{\kappa_{k-0,5}}{\Delta z^2};\quad \bar{\bar{b}}_{i,j,k}=\frac{3}{\Delta t}+\sigma_1+\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2};\quad \bar{\bar{c}}_{i,j,k}=\frac{\kappa_{k+0,5}}{\Delta z^2};$$

$$\begin{gathered}\bar{\bar{d}}_{i,j,k}=\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta x^2}-\frac{2\mu}{\Delta y^2}\right)\tilde{\theta}^{n+2/3}_{i,j,k}+\frac{\mu}{\Delta x^2}\tilde{\theta}^{n+2/3}_{i-1,j,k}+\\+\frac{\mu}{\Delta x^2}\tilde{\theta}^{n+2/3}_{i+1,j,k}+\frac{\mu}{\Delta y^2}\tilde{\theta}^{n+2/3}_{i,j-1,k}+\\+\frac{\mu}{\Delta y^2}\tilde{\theta}^{n+2/3}_{i,j+1,k}+\frac{1}{3}e_1\delta_{i,j,k}Q^{n+1},\end{gathered}$$

$$\bar{\bar{\alpha}}_{i,j,0}=\frac{4\kappa_1\bar{\bar{c}}_{i,j,1}-\bar{\bar{b}}_{i,j,1}\kappa_1}{3\kappa_1\bar{\bar{c}}_{i,j,1}-\bar{\bar{a}}_{i,j,1}\kappa_1-2\Delta z\beta};\quad \bar{\bar{\beta}}_{i,j,0}=\frac{\bar{\bar{d}}_{i,j,1}\kappa_1+2e_1\Delta z\bar{\bar{c}}_{i,j,1}f}{3\kappa_1\bar{\bar{c}}_{i,j,1}-\bar{\bar{a}}_{i,j,1}\kappa_1-2\Delta z\beta}. \tag{24}$$

$$\tilde{\theta}^{n+1}_{i,j,L}=\frac{2\Delta ze_1\xi\theta_E}{2\Delta z\xi+(\bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\alpha}}_{i,j,L-1}-4\bar{\bar{\alpha}}_{i,j,L-1}+3)\kappa_L}-\\-\frac{\left(\bar{\bar{\beta}}_{i,j,L-2}+\bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\beta}}_{i,j,L-1}-4\bar{\bar{\beta}}_{i,j,L-1}\right)\kappa_L}{2\Delta z\xi+(\bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\alpha}}_{i,j,L-1}-4\bar{\bar{\alpha}}_{i,j,L-1}+3)\kappa_L}. \tag{25}$$

As a result, a mathematical model and a numerical algorithm were obtained for monitoring and predicting the process of the spread of harmful substances in the atmosphere, considering the heterogeneity and roughness of the earth's surface: vegetation cover, forest belt, high-rise residential and industrial facilities.

IV. Computational Experiment and Discussion of Results

Computational experiments were carried out to study the process of transfer and diffusion of harmful substances in the atmosphere, taking into account the heterogeneity and roughness of the earth's surface: vegetation cover, forest belts, high-rise residential and industrial facilities. As follows from the results of the numerical calculations, the dynamics of changes in the concentration of harmful substances in the atmosphere significantly depends on the wind speed in the surface layer of the atmosphere (Fig. 1). From the dynamics of the transfer of pollutants in the atmosphere, it can be seen (Fig. 2, 3) that, depending on the change in the direction and speed of the wind, the concentration of pollutants in the atmosphere and the area of their transfer change over time.

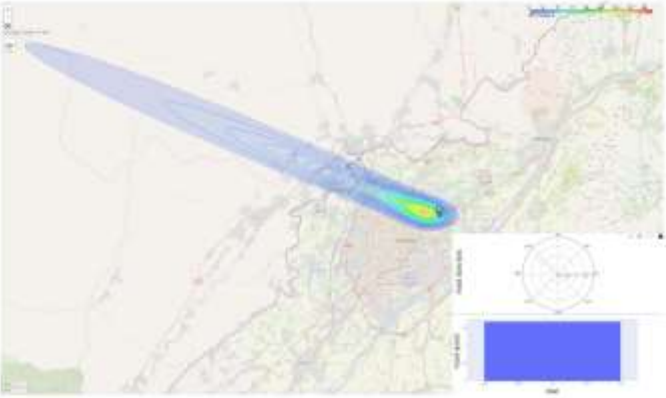

Fig. 1. Dynamics of transfer and diffusion of aerosol particles in the atmosphere at Q = 1000 mg/m3; H=50 m; u=1.5 m/s; t = 1 h.

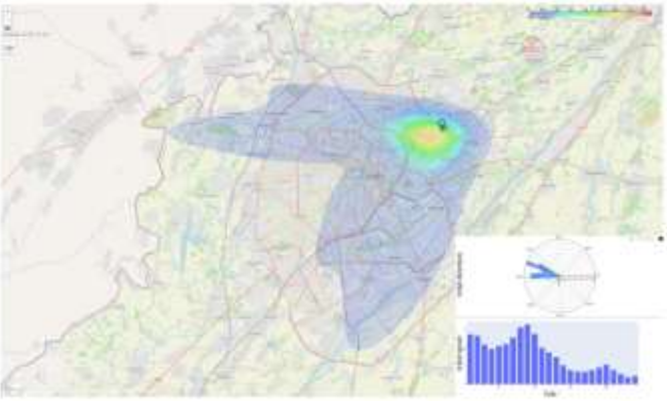

Fig. 2. Dynamics of transfer and diffusion of aerosol particles in the atmosphere at Q = 1000 mg/m3; H=100 m; t = 24 h; u=3.5 m/s.

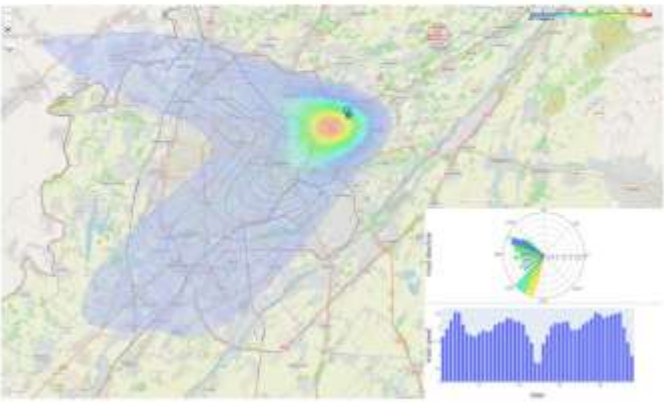

Fig. 3. Dynamics of transfer and diffusion of aerosol particles in the atmosphere at Q = 1000 mg/m3; H=100 m; t = 48 h; u=3 m/s.

V. Conclusions

A mathematical model has been developed to monitor and predict the concentration of pollutants in the atmosphere of the region under consideration, that takes into consideration the wind speed in three directions and the rate of deposition of aerosol particles on the underlying surface, as well as the capture of particles by vegetation elements, which plays a significant role in the dynamics of the process. Thus, in this work, a numerical algorithm has been developed for solving the problem (1)-(5) with the second order of approximation in time and space variables. By software implementation of the developed model and algorithm, it is possible to carry out SE on a computer to study and predict the ecological state of the industrial regions under consideration.

It can be seen from the figures 1,2,3 that the change in the concentration of aerosols in the atmosphere depends significantly on the actual change in wind speed by day, the coefficient characterizing the capture of particles by vegetation elements and the horizontal diffusion coefficient, as well as the vertical turbulence coefficient. The concentration of pollutants in the surface layer of the atmosphere changes over time depending on the actual wind speeds.

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