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D. A. Karshiev
Tashkent Pediatric Medical Institute
associate professor,
Republic of Uzbekistan, Tashkent

F. A. Muradov
Samarkand branch of Tashkent University of Information Technologies named after Muhammad Al Khorezm
associate professor,
Republic of Uzbekistan, Tashkent

V.N. Shirinov
Samarkand branch of Tashkent University of Information Technologies named after Muhammad Al Khorezm
Master student
Republic of Uzbekistan, Samarkand
tel.: +(99897) 927-05-65,
farrux2003@yahoo.com

NUMERICAL SOLUTION OF THE PROBLEM OF HARMFUL EMISSIONS SPREAD IN THE ATMOSPHERE BY THE METHOD OF SPLITTING INTO PHYSICAL PROCESSES

Abstract: *The aim of this paper is to simulate the process of harmful impurities spread in the surface layer of the atmosphere. A model of industrial emissions spread in the atmosphere was developed taking into account the rate of deposition of fine particles, described using a multidimensional partial differential equation with appropriate initial and boundary conditions. The basic laws of hydrothermodynamics were used in deriving the model. To numerically solve the problem, the method of splitting into physical processes (transfer, diffusion, and absorption of harmful particles) was used, as well as an implicit finite-difference scheme in time of the second order of accuracy. Analysis of the results of computational experiments shows that the developed computational algorithm provides sufficient accuracy of the solution compared with field measurement data and has a certain advantage over other numerical methods. In the course of computational experiments, the degree of influence of such parameters as wind velocity (speed) and direction on the process of aerosol particles spread in the atmosphere was established; as well as absorption coefficient and physicomechanical properties of particles.*

Key words: *mathematical model, numerical algorithm, approximation, transfer and diffusion, atmosphere, harmful aerosols, rate of particles deposition.*

Language: *English*

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Introduction

In response to the actualization of the problems of ecological condition of the atmosphere in recent years, a considerable amount of theoretical and experimental research has been conducted on the spread process of pollutants of technogenic and natural origin in the air.

It is known that the quality of atmospheric air is influenced by many factors that require consideration in a detailed analysis of its state and the realization of prognostic estimates. Therefore, to date, one of the main approaches to the study of the harmful emissions spread in the atmosphere, the most acceptable by economic and environmental criteria, is a mathematical modeling that can provide sufficient accuracy in describing and predicting the changes.

The question of aerosols deposition is of particular interest in solving problems of monitoring and predicting the air pollution. The removal of pollutants from the atmosphere mainly occurs through wet or dry deposition. Wet deposition is the transfer (fall-out) of a certain number of particles from the atmosphere to the underlying surface, possible only in the presence of precipitation. Dry deposition is a continuous process, largely dependent on the physicomechanical properties of the particles and the nature of turbulent flows. In the general case, dry deposition is modeled using a single parameter, the deposition rate, which is indicated empirically or determined from the corresponding theoretical relationships. When particles are sufficiently dense and large, then the deposition occurs under the action of gravitational force, represented in terms of a deposition rate.

A number of studies dealing with atmospheric dispersion models emphasize the need for a more thorough description of the features of the aerosol particles deposition when calculating the concentration fields in different layers of the atmosphere and directly on the underlying surface.

2. **Literature Review**

In [1], the authors, using an analytical solution of the advection-diffusion equation

$$u_n \frac{\partial c_n}{\partial x} = K_n \frac{\partial^2 c_n}{\partial z^2} + w_s \frac{\partial c_n}{\partial z} \qquad z_n \le z \le z_{n+1}, \quad n = 1:N,$$

showed that the deposition rate changes the particle concentration along the entire length of the atmospheric boundary layer. The modeling has shown that gravitational deposition can strongly influence the final concentration of harmful particles spread in the air and the maximum concentration near the ground. The authors considered the particles of a diameter from10 to 100 μm at different heights of emission sources and under conditions of atmospheric stability and instability. The deposition rate was calculated according to the Stokes law, and the height of the atmospheric boundary layer was taken to be 1000 m. The authors also showed the effect of particle diameters on the concentration distribution at ground level depending on the conditions of atmospheric stability. The results obtained by the authors show that under conditions of an unstable atmosphere for particles of a diameter less than 10 μm, the gravitational component of the deposition rate can be neglected. It should be noted that the authors applied a stepwise approximation to the problem by discretization the height h on the sublayers. The solution of the problem was obtained using the Laplace transform, but due to the complexity of the integrand, the integration was performed numerically using the Talbot algorithm.

The authors in [2] developed a mathematical model for the aerosols transfer emitted from a point-like source on the ground, taking into account the particle deposition rate. Two-dimensional stationary mass transfer equation

$$u(z)\frac{\partial c}{\partial x} - w_s \frac{\partial c}{\partial z} = \frac{\partial}{\partial z}\left(k_z \frac{\partial c}{\partial z}\right)$$

with appropriate boundary conditions was solved by the authors by applying the method of generalized Laplace integral transform. The solution area was limited to the surface layer of the atmosphere, and changes in wind velocity (speed) and vertical eddy diffusion were taken into account. The results obtained by the authors demonstrate the influence of the gravitational mode and dry deposition of particles on the distribution of their concentration at ground level, and are generally consistent with the results of other researchers.

In [3], the authors conducted a wide review of recent advances in mathematical modeling of the processes of transfer and diffusion of pollutants in the atmosphere. The authors discuss the advantages and disadvantages of the most popular approaches and strategies for model development, namely Gaussian, Lagrangian, Eulerian models, as well as the models of computational fluid dynamics (CFD). A special attention is paid to the issues of parametrization of turbulent mixing in the boundary layer of the atmosphere and the particles deposition; the influence of these processes on the distribution of pollution concentrations is analyzed. The authors also highlight the main methods for numerical solution of problems based on the finite-difference approximation of derivatives, including the method of splitting the original problem into physical processes. Due to the fact that the class of problems under consideration has a large computational capacity, the authors pay attention to the trends in the use of parallel computing technologies using graphic modules or adaptive grid refinement.

M.V. Menshov in [4] proposed a modified mathematical model of transfer and deposition of polydisperse aerosol clouds formed at spraying of liquid fertilizers by agricultural aviation. To describe the migration process of impurity cloud the equation of the semi-empirical theory of transfer and turbulent diffusion and a set of initial-boundary conditions were considered. The author performed a vertical averaging of the basic equation under the assumption that the vertical structure of the concentration was close to the Gaussian plume. The method of solving the problem was based on the discretization of the initial systems in the grid area. The spatial approximation of differential operators was based on monotone schemes and schemes with non-increasing total variation, and algebraic systems of finite-difference equations were solved iteratively using the methods of incomplete factorization, implicit splitting methods were used for time integration. The results obtained by the author have a modeling error not exceeding 12–18%, which can be considered quite acceptable for field experiments due to the natural possibility of the appearance of anomalous wind profiles. In another paper M.V. Menshov, based on the developed model, presented the results of modeling the aerosols transfer in conditions of rugged terrain. The author concluded that the presence of even low flat hills introduced significant changes in the nature of the distribution and deposition of aerosols.

Research carried out by V.F. Raputa and his colleagues is devoted to the problem of transfer of heavy inhomogeneous impurities in the atmosphere [5]. The authors proposed a model for reconstructing the deposition fields of impurity particles from a high-altitude source. The authors noted that, unlike the situation with low-lying emission sources, in modeling the aerosols transfer in the atmosphere from high-altitude sources there were considerable difficulties associated with the uncertainties of the height and source intensity, initial spread of aerosol particles in the cloud, meteorological conditions. This explains the need to create the models of reconstruction. To describe the process of impurity propagation, the authors use the semi-kinematic approximation; it is assumed that turbulent scattering occurs only in horizontal directions, and the vertical motion of particles occurs at a constant Stokes velocity. The authors considered the effects of wind direction change in the atmospheric boundary layer on the formation of a field of long-term aerosol impurity fallout. The developed model was tested in a numerical analysis of snow pollution by benzyperen in the vicinity of one of the thermoelectric power plants in Barnaul. Analysis of the simulation results showed quite satisfactory agreement between the measured and calculated concentrations of pollutants at the measurement points.

The process of motion and deposition of particles in turbulent atmospheric flows over heat-dissipating sources has been theoretically studied by N. N. Smirnov and his colleagues in [6]. The mathematical model developed by the authors takes into account the effects of the two-way interaction of the “gas-particle” system and combines deterministic and stochastic approaches. To describe the behavior of the gas phase, a modified $k-\varepsilon$ model of turbulent flow was used. The system of equations describing turbulent flow was obtained using Favre averaging, and includes the mass balance in the gas phase, the mass balance of the *k*-th component, the balance of momentum and energy.

The equations of motion of particles, besides the forces of gravity, resistance and the Archimedes force, take into account random turbulent pulsations in the gas flow; the characteristics of these pulsations are determined using the solution obtained with the $k-\varepsilon$ model. The results of numerical experiments allowed the authors to determine the effect of heat-dissipating sources on the dispersion and nature of the particles deposition.

In [7], the authors made an attempt to study the atmospheric dispersion taking into account the particle deposition rate, when the shape of the particles served as an input parameter of the model. The authors used a semi-empirical formula for non-spherical particles to determine the sensitivity of the process of volcanic ash cloud transfer to the shape of the particles. The process was modeled using a Lagrange model. It was found that there was no noticeable difference in the vertical trajectories of spherical and non-spherical particles of a size of 1 μm. The vertical motion of particles of 10 μm was more sensitive to shape, but the similar pattern of spherical and non-spherical particles motion was preserved, despite the fact that the deposition rate was always positive and the particles moved downward and upward, indicating the predominance of advection and turbulent diffusion. Sensitivity to the form increased dramatically with size, so non-spherical particles of 100 μm deposed much slower and could move along the axis of the emission plume 44% farther from the source than the spherical ones. The proposed approach allows more accurate predicting the concentration of fly ash in the atmosphere and the distance of its spread.

Naslund E. and Thaning L. presented a solution to the problem of determining the rate of particles deposition at an unstable stratification of the atmosphere [8]. In the equation of motion for solid spherical particles, an overall drag coefficient (resistance coefficient; drag coefficient) was used. Time constants, stopping times, and deposition rates at stable stratification of the atmosphere were calculated for a wide range of Reynolds numbers. The obtained deposition time was compared with the time calculated for the case when the deposition occurred during atmospheric convection. It was found that in this case, solid spherical particles will depose for much longer, which leads to an increase in the drag coefficient caused by an increase in relative velocity between the particles and the air mass flow.

Such an intensification is present both for the horizontal wind field, due to the connection between particles motion in different directions, and for the vertical field. The effect is most pronounced in the region of intermediate Reynolds numbers, slightly above the Stokes range, where an increase in deposition time may be more than 10% for certain frequencies and amplitudes of turbulent fluctuations.

From the analysis of the mentioned above and many other publications, it follows that the deposition rate of aerosol fine particles is often assumed to be constant and is determined on the basis of empirical data for specific types of pollutants. The aim of this work is to create a mathematical model that adequately describes the process of transfer and diffusion of harmful aerosol particles in the atmosphere, taking into account changes in the deposition rate of particles over time and the effect of physical and mechanical properties of the particles. Solid fine particles of spherical shape emitted from stationary ground sources are considered in the paper. The number of physicomechanical properties, which affect the rate of the deposition, includes mass, diameter, and particle density.

3. Statement of the problem

To study the transfer and diffusion of aerosol particles in the atmosphere, taking into account the rate of deposition of fine particles, consider a mathematical model described using a multidimensional partial differential equation

$$\frac{\partial\theta(x,y,z,t)}{\partial t}+u\frac{\partial\theta(x,y,z,t)}{\partial x}+v\frac{\partial\theta(x,y,z,t)}{\partial y}+(w-w_g)\frac{\partial\theta(x,y,z,t)}{\partial z}+\sigma\theta(x,y,z,t)=$$
$$=\mu\left(\frac{\partial^2\theta(x,y,z,t)}{\partial x^2}+\frac{\partial^2\theta(x,y,z,t)}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(\kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\right)+\delta(x,y,z)Q; \qquad (1)$$
$$\frac{dw_g}{dt}=\frac{mg-6\pi krw_g-0,5c\rho sw_g^2}{m}$$

with appropriate initial

$$\theta(x,y,z,t)\big|_{t=0}=\theta_0(x,y,z);$$
$$w_g(0)\big|_{t=0}=w_{g,0}(0) \qquad (2)$$

and boundary conditions

$$-\mu\frac{\partial\theta(x,y,z,t)}{\partial x}\bigg|_{x=0}=\xi\big(\theta_E-\theta(0,y,z,t)\big);$$
$$\mu\frac{\partial\theta(x,y,z,t)}{\partial x}\bigg|_{x=L_x}=\xi\big(\theta_E-\theta(L_x,y,z,t)\big); \qquad (3)$$
$$-\mu\frac{\partial\theta(x,y,z,t)}{\partial y}\bigg|_{y=0}=\xi\big(\theta_E-\theta(x,0,z,t)\big);$$
$$\mu\frac{\partial\theta(x,y,z,t)}{\partial y}\bigg|_{y=L_y}=\xi\big(\theta_E-\theta(x,L_y,z,t)\big); \qquad (4)$$
$$-\kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\bigg|_{z=0}=\big(\beta\theta(x,y,0,t)-f(x,y)\big);$$
$$\kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\bigg|_{z=H}=\xi\big(\theta_E-\theta(x,y,H,t)\big). \qquad (5)$$

Here θ is the concentration of harmful substances in the atmosphere; θ_0 is the primary concentration; θ_E is the concentration flowing across the boundaries of the area under consideration; x, y, z is the coordinate system; u, v, w is the wind velocity in three directions; w_g is the particle deposition rate; σ is the coefficient of the absorbing capacity of the atmosphere; $\mu, \kappa(z)$ are the coefficients of diffusion and turbulence, respectively; Q is the power of the point stationary source of emission; $\delta_{i,j}$ is the Dirac function; $f(x,y)$ is the emission of harmful substances into the atmosphere from the underlying surface of the ground; β is the coefficient of particles interaction with the underlying surface; c is the dimensionless value equal to 0.5; ρ is the density of the atmosphere; r is the particle radius; s is the cross-sectional area of the particles; g is the acceleration of gravity; ξ is the parameter of reduction to a single dimension; L_x, L_y are the length and the width of the area under consideration; H is the height of the atmospheric layer.

Unlike the studies of other authors, here the deposition rate is described by the second equation in (1). Since, the problem (1) - (5) is described by a multidimensional nonlinear partial differential equation with the appropriate initial and boundary conditions, it is practically impossible to find its exact solution in analytical form. Therefore, the main approach to solving the problem is a numerical method.

In the first equation (1), two physical processes are clearly distinguished: the first is the substance transfer in the direction of motion of the air mass of the atmosphere; the second is the molecular diffusion of a substance in the atmosphere. It is also possible to distinguish the third process — the absorption of a substance by the air mass of the atmosphere, mainly due to the increased moisture-content. In this case, it would be reasonable to use the method of splitting into physical processes at each time layer.

4. Solution method

The idea of the splitting method is to reduce the original multidimensional problem to problems of a simpler structure, which are then sequentially or in parallel solved by known numerical methods. This can be achieved in a variety of ways, therefore, by now a large number of different additive difference schemes have been created.

For example, the exact numerical method for the class of scalar strongly degenerate convection-diffusion equations is presented in [9]. The method is based on the splitting of convective and diffusion terms.

The nonlinear, convective part is solved using front tracking and size splitting, while the nonlinear diffusion part is solved by a semi-implicit finite-difference scheme. The method proposed by the authors has a built-in mechanism for detecting and correcting the non-physical loss of entropy, which can occur if the time step is large. In the paper the authors demonstrate that the splitting method exactly allows sharp gradients, can use large time steps, has first order convergence. Despite the fact that the method has small errors in the mass balance, it is nonetheless quite effective.

Simpson M., Landmana K., and Clement P. proposed an unconventional operator splitting scheme for solving the advection-diffusion-reaction equation of the following type [10]

$$\frac{\partial c}{\partial t}=D\frac{\partial^2 c}{\partial x^2}-v\frac{\partial c}{\partial x}+f\left(c\right).$$

The above scheme was implemented according to the A. Kurganov and E. Tadmor central difference scheme for accurate modeling of advection-reaction processes. The basic partial differential equation is divided into two subproblems, solved sequentially during each time step. Unlike traditional methods, the scheme proposed by the authors provides a very effective method for solving the advection-diffusion-reaction equation for any value of the Peclet number. The analysis of mass balance errors shows that the unconventional scheme proposed by the authors has a splitting error, which differs from the error in traditional schemes. Numerical results demonstrate sufficient reliability of the proposed scheme.

Geiser J. and Kravvaritis Ch. presented a new approach to the construction of a method of domain decomposition based on an iterative splitting method [11]. The proposed two-stage iterative splitting scheme for solving a linear evolution equation is based on the separation in space and time. The authors studied the convergence properties of the method. The effectiveness of the proposed method is shown by comparing the numerical results with the additive method of Schwarz wave relaxation.

The use of the method of physical splitting for modeling the process of harmful substances spread in the atmosphere is discussed in [12] by Havasi A. and Farago I. To illustrate the method of physical splitting, the authors use the Euler's Danish model. The basic equation for the pollutants transfer over long distances

$$\frac{\partial c}{\partial t}+\nabla\cdot\left(\underline{u}c\right)=\nabla\cdot\left(\underline{K}\nabla c\right)+R\left(\underline{x},c\right)+E+gc$$

with the appropriate initial and boundary conditions is reduced to several subsystems describing physical processes: horizontal transfer, horizontal diffusion, chemical reactions with emission, deposition and vertical exchange. The authors pay special attention to the question of error occurrence as a result of the separation procedure. The authors cite several cases where this error disappears, but emphasize that in practice this rarely happens, so it is important to analyze and carefully select the applied schemes and keep the error as small as possible.

In general, the analysis of scientific publications on the problems of solving complex non-stationary problems for partial differential equations shows a great attention of researchers paid to the construction of additive schemes. In the studies, the advantages of the splitting method by physical processes compared to other grid methods are noted. At the same time, the issue of improvement remains open due to the fact that further optimization and various modifications of this method can provide an increase in the rate of obtaining solutions with a given accuracy.

In the present study, to numerically solve the problem (1) - (5), it is assumed that a smooth function in all spaces is the sought for solution. Using the additivity of fundamentally different physical processes of mass transfer and diffusion in the atmosphere in a time interval $t_n \le t \le t_{n+1}$, consider each process as a separate task.

The process of substance transfer with its preservation along the trajectory is considered as task A:

$$\frac{\partial\theta_1(x,y,z,t)}{\partial t}+u\frac{\partial\theta_1(x,y,z,t)}{\partial x}+v\frac{\partial\theta_1(x,y,z,t)}{\partial y}+\left(w-w_g\right)\frac{\partial\theta_1(x,y,z,t)}{\partial z}+ +\frac{1}{2}\sigma\theta_1(x,y,z,t)=\frac{1}{2}\delta(x,y,z)Q \tag{1A}$$

with initial

$$\theta_1(x,y,z,0)=\theta_2^n(x,y,z) \text{ at } t=t_n;$$
$$w_g(0)\Big|_{t=t_n}=w_{g,0}(0)$$

and boundary conditions

$$-\mu\frac{\partial\theta_1(x,y,z,t)}{\partial x}\bigg|_{x=0}=\xi\left(\theta_E-\theta_1(0,y,z,t)\right);$$
$$\mu\frac{\partial\theta_1(x,y,z,t)}{\partial x}\bigg|_{x=L_x}=\xi\left(\theta_E-\theta_1(L_x,y,z,t)\right); \tag{6}$$

$$-\mu\frac{\partial\theta_1(x,y,z,t)}{\partial y}\bigg|_{y=0}=\xi\left(\theta_E-\theta_1(x,0,z,t)\right);$$
$$\mu\frac{\partial\theta_1(x,y,z,t)}{\partial y}\bigg|_{y=L_y}=\xi\left(\theta_E-\theta_1(x,L_y,z,t)\right); \tag{7}$$

$$-\kappa(z)\frac{\partial\theta_1(x,y,z,t)}{\partial z}\bigg|_{z=0}=\left(\beta\theta_1(x,y,0,t)-f(x,y)\right);$$
$$\kappa(z)\frac{\partial\theta_1}{\partial z}\bigg|_{z=H}=\xi\left(\theta_E-\theta_1(x,y,H,t)\right). \tag{8}$$

The process of substance diffusion in the atmosphere, taking into account the absorption of particles in the air mass is considered as task B:

$$\frac{\partial\theta_2(x,y,z,t)}{\partial t}+\frac{1}{2}\sigma\theta_2(x,y,z,t)=\mu\left(\frac{\partial^2\theta_2(x,y,z,t)}{\partial x^2}+\frac{\partial^2\theta_2(x,y,z,t)}{\partial y^2}\right)+ +\frac{\partial}{\partial z}\left(\kappa(z)\frac{\partial\theta_2(x,y,z,t)}{\partial z}\right)+\frac{1}{2}\delta(x,y,z)Q \tag{1Б}$$

with initial

$$\theta_2(x,y,z,t_l)=\theta_1^{l+1}(x,y,z,t_{l+1})$$

and boundary conditions

$$-\mu\frac{\partial\theta_2(x,y,z,t)}{\partial x}\bigg|_{x=0}=\xi\left(\theta_E-\theta_2(0,y,z,t)\right);$$
$$\mu\frac{\partial\theta_2(x,y,z,t)}{\partial x}\bigg|_{x=L_x}=\xi\left(\theta_E-\theta_2(L_x,y,z,t)\right); \tag{9}$$

$$-\mu \frac{\partial \theta_2(x,y,z,t)}{\partial y}\bigg|_{y=0} = \xi\left(\theta_E - \theta_2(x,0,z,t)\right);$$
$$\mu \frac{\partial \theta_2(x,y,z,t)}{\partial y}\bigg|_{y=L_y} = \xi\left(\theta_E - \theta_2(x,L_y,z,t)\right); \tag{10}$$

$$-\kappa(z) \frac{\partial \theta_2(x,y,z,t)}{\partial z}\bigg|_{z=0} = \left(\beta\theta_2(x,y,0,t) - f(x,y)\right);$$
$$\kappa(z) \frac{\partial \theta_2(x,y,z,t)}{\partial z}\bigg|_{z=H} = \xi\left(\theta_E - \theta_2(x,y,H,t)\right). \tag{11}$$

To solve these equations, an implicit second-order finite-difference scheme for approximation in time is used [13].

Equation (1A) is approximated by a finite difference scheme in x direction, and after some transformations a three-diagonal system of linear algebraic equations (SLAE) is obtained

$$a_{1,i,j,k}\theta_{1,i-1,j,k}^{n+\frac{1}{3}} - b_{1,i,j,k}\theta_{1,i,j,k}^{n+\frac{1}{3}} + c_{1,i,j,k}\theta_{1,i+1,j,k}^{n+\frac{1}{3}} = -d_{1,i,j,k},$$

where

$$a_{1,i,j,k} = \frac{|u|+u}{2\Delta x};\quad b_{1,i,j,k} = \frac{3}{\Delta t} + \frac{u}{\Delta x} + \frac{1}{2}\sigma;\quad c_{1,i,j,k} = -\frac{|u|-u}{2\Delta x};$$

$$d_{1,i,j,k} = \frac{|v|+v}{2\Delta y}\theta_{1,i,j-1,k}^{n} + \left(\frac{3}{\Delta t} - \frac{v}{\Delta y} - \frac{w-w_g}{\Delta z}\right)\theta_{1,i,j,k}^{n} - \frac{|v|-v}{2\Delta y}\theta_{1,i,j+1,k}^{n} +$$
$$+\frac{|w-w_g|+(w-w_g)}{2\Delta z}\theta_{1,i,j,k-1}^{n} - \frac{|w-w_g|-(w-w_g)}{2\Delta z}\theta_{1,i,j,k+1}^{n} + \frac{1}{6}\delta_{i,j,k}Q.$$

Boundary condition (6) is approximated by x, grouping similar terms, and using the sweep method; the sweep coefficients are found

$$\alpha_{1,0,j,k} = \frac{4\mu c_{1,1,j,k} - b_{1,1,j,k}\mu}{3\mu c_{1,1,j,k} - a_{1,1,j,k}\mu + 2\Delta x\xi};\quad \beta_{1,0,j,k} = \frac{d_{1,1,j,k} + 2\Delta x\xi c_{1,1,j,k}\theta_E}{3\mu c_{1,1,j,k} - a_{1,1,j,k}\mu + 2\Delta x\xi}.$$

From the second boundary condition (6) the concentration values at the $0x$ axis boundary are found

$$\theta_{1,N,j,k}^{n+\frac{1}{3}} = \frac{2\Delta x\xi\theta_E - \left(\beta_{1,N-2,j,k} + \alpha_{1,N-2,j,k}\beta_{1,N-1,j,k} - 4\beta_{1,N-1,j,k}\right)\mu}{2\Delta x\xi + \left(\alpha_{1,N-2,j,k}\alpha_{1,N-1,j,k} - 4\alpha_{1,N-1,j,k} + 3\right)\mu}.$$

The values of the concentration sequence, in this case $\theta_{N-1,j,k}^{n+\frac{1}{3}}$, $\theta_{N-2,j,k}^{n+\frac{1}{3}}$,..., $\theta_{1,j,k}^{n+\frac{1}{3}}$ are determined by the method of reverse sweep

$$\theta_{i,j,k}^{n+\frac{1}{3}} = \alpha_{i,j,k}\theta_{i+1,j,k}^{n+\frac{1}{3}} + \beta_{i,j,k};\ i=\overline{N-1,1},\ j=\overline{0,M},\ k=\overline{0,L}.$$

Next, perform similar actions in the direction of $0y$ coordinate:

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

Here

$$\bar{a}_{1,i,j,k} = \frac{|v|+v}{2\Delta y}; \quad \bar{b}_{1,i,j,k} = \frac{3}{\Delta t} + \frac{v}{\Delta y} + \frac{1}{2}\sigma; \quad \bar{c}_{1,i,j,k} = -\frac{|v|-v}{2\Delta y};$$

$$\bar{d}_{1,i,j,k} = \frac{|u|+u}{2\Delta x}\theta_{1,i-1,j,k}^{n+\frac{1}{3}} + \left(\frac{3}{\Delta t} - \frac{u}{\Delta x} - \frac{w-w_g}{\Delta z}\right)\theta_{1,i,j,k}^{n+\frac{1}{3}} - \frac{|u|-u}{2\Delta x}\theta_{1,i+1,j,k}^{n+\frac{1}{3}} +$$

$$+\frac{|w-w_g|+(w-w_g)}{2\Delta z}\theta_{1,i,j,k-1}^{n+\frac{1}{3}} - \frac{|w-w_g|-(w-w_g)}{2\Delta z}\theta_{1,i,j,k+1}^{n+\frac{1}{3}} + \frac{1}{6}\delta_{i,j,k}Q.$$

Boundary condition (7) is approximated by y and (7) sweep coefficients $\bar{\alpha}_{i,0,k}$ and $\bar{\beta}_{i,0,k}$ are found

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

and, accordingly, the concentration values at $0y$ axis boundary are

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

Similarly, in the z direction we get SLAE

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

Here

$$\bar{\bar{a}}_{1,i,j,k} = \frac{|w-w_g|+(w-w_g)}{2\Delta z}; \quad \bar{\bar{b}}_{1,i,j,k} = \frac{3}{\Delta t} + \frac{w-w_g}{\Delta z} + \frac{1}{2}\sigma; \quad \bar{\bar{c}}_{1,i,j,k} = -\frac{|w-w_g|-(w-w_g)}{2\Delta z};$$

$$\bar{\bar{d}}_{1,i,j,k} = \frac{|u|+u}{2\Delta x}\theta_{1,i-1,j,k}^{n+\frac{2}{3}} + \left(\frac{3}{\Delta t} - \frac{u}{\Delta x} - \frac{v}{\Delta y}\right)\theta_{1,i,j,k}^{n+\frac{2}{3}} - \frac{|u|-u}{2\Delta x}\theta_{1,i+1,j,k}^{n+\frac{2}{3}} +$$

$$+\frac{|v|+v}{2\Delta y}\theta_{1,i,j-1,k}^{n+\frac{2}{3}} - \frac{|v|-v}{2\Delta y}\theta_{1,i,j+1,k}^{n+\frac{2}{3}} + \frac{1}{6}\delta_{i,j,k}Q.$$

Boundary condition (8) is approximated by z and the recurrence relations to determine the sweep coefficients are obtained:

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

and then the concentration values on the $0z$ axis boundary are found

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

Solutions of problem (1A) - (8) and the second equation in (1) serve as initial conditions for problem (1B) - (11).

Equation (1B) is approximated in x direction, and after the necessary transformations, it is reduced to SLAE

$$a_{2,i,j,k}\theta_{2,i-1,j,k}^{n+\frac{1}{3}} - b_{2,i,j,k}\theta_{2,i,j,k}^{n+\frac{1}{3}} + c_{2,i,j,k}\theta_{2,i+1,j,k}^{n+\frac{1}{3}} = -d_{2,i,j,k}.$$

Here

$$a_{2,i,j,k} = \frac{\mu}{\Delta x^2}; \quad b_{2,i,j,k} = \frac{3}{\Delta t} + \frac{2\mu}{\Delta x^2} + \frac{1}{2}\sigma; \quad c_{2,i,j,k} = \frac{\mu}{\Delta x^2};$$

$$d_{2,i,j,k}=\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta y^2}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\right)\theta^n_{i,j,k}+\frac{\mu}{\Delta y^2}\theta^n_{i,j-1,k}+\frac{\mu}{\Delta y^2}\theta^n_{i,j+1,k}+$$

$$+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta^n_{i,j,k-1}+\frac{\kappa_{k+0,5}}{\Delta z^2}\theta^n_{i,j,k+1}+\frac{1}{6}\delta_{i,j,k}Q.$$

Similar to the problem (1A), for the boundary condition (9), the recurrence relations to calculate the sweep coefficients with respect to x are obtained

$$\alpha_{2,0,j,k}=\frac{4\mu c_{2,1,j,k}-b_{2,1,j,k}\mu}{3\mu c_{2,1,j,k}-a_{2,1,j,k}\mu+2\Delta x\xi};\quad \beta_{2,0,j,k}=\frac{d_{2,1,j,k}+2\Delta x\xi c_{2,1,j,k}\theta_E}{3\mu c_{2,1,j,k}-a_{2,1,j,k}\mu+2\Delta x\xi}$$

and the recurrence relation to calculate the concentration of suspended particles at the boundary of the problem solution region

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

Further, similar actions in y direction are performed

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

Here

$$\bar{a}_{2,i,j,k}=\frac{\mu}{\Delta y^2};\quad \bar{b}_{2,i,j,k}=\frac{3}{\Delta t}+\frac{2\mu}{\Delta y^2}+\frac{1}{2}\sigma;\quad \bar{c}_{2,i,j,k}=\frac{\mu}{\Delta y^2};$$

$$\bar{d}_{2,i,j,k}=\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta x^2}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\right)\theta^{n+\frac{1}{3}}_{i,j,k}+\frac{\mu}{\Delta x^2}\theta^{n+\frac{1}{3}}_{i-1,j,k}+\frac{\mu}{\Delta x^2}\theta^{n+\frac{1}{3}}_{i+1,j,k}+$$

$$+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta^{n+\frac{1}{3}}_{i,j,k-1}+\frac{\kappa_{k+0,5}}{\Delta z^2}\theta^{n+\frac{1}{3}}_{i,j,k+1}+\frac{1}{6}\delta_{i,j,k}Q.$$

For boundary condition (10), the second order approximation is applied and the sweep coefficients are found

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

to determine the concentration of aerosol particles at the end of the boundary of the problem solution region, the following ratio is obtained

$$\theta^{n+\frac{2}{3}}_{2,i,M,k}=\frac{2\Delta y\xi\theta_n-\left(\bar{\beta}_{2,i,M-2,k}+\bar{\alpha}_{2,i,M-2,k}\bar{\beta}_{2,i,M-1,k}-4\bar{\beta}_{2,i,M-1,k}\right)\mu}{2\Delta y\xi+\left(\bar{\alpha}_{2,i,M-2,k}\bar{\alpha}_{2,i,M-1,k}-4\bar{\alpha}_{2,i,M-1,k}+3\right)\mu}$$

in the direction of y coordinate.

Similarly, in z direction we get SLAE

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

where

$$\bar{\bar{a}}_{2,i,j,k}=\frac{\kappa_{k-0,5}}{\Delta z^2};\quad \bar{\bar{b}}_{2,i,j,k}=\frac{3}{\Delta t}+\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}+\frac{1}{2}\sigma;\quad \bar{\bar{c}}_{2,i,j,k}=\frac{\kappa_{k+0,5}}{\Delta z^2};$$

$$\bar{\bar{d}}_{2,i,j,k} = \left(\frac{3}{\Delta t} - \frac{2\mu}{\Delta x^2} - \frac{2\mu}{\Delta y^2}\right)\theta_{i,j,k}^{n+\frac{2}{3}} + \frac{\mu}{\Delta x^2}\theta_{i-1,j,k}^{n+\frac{2}{3}} + \frac{\mu}{\Delta x^2}\theta_{i+1,j,k}^{n+\frac{2}{3}} +$$

$$+\frac{\mu}{\Delta y^2}\theta_{i,j-1,k}^{n+\frac{2}{3}} + \frac{\mu}{\Delta y^2}\theta_{i,j+1,k}^{n+\frac{2}{3}} + \frac{1}{6}\delta_{i,j,k}Q.$$

Approximate the boundary condition (11) and obtain relationships to find the values of the sweep coefficients $\bar{\bar{\alpha}}_{i,j,0}$ and $\bar{\bar{\beta}}_{i,j,0}$

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

From the second equation of the boundary condition (11) the concentration values in $0z$ direction at $z = L_z$ are obtained

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

As for the second equation of the original problem (1), to solve it, an implicit finite-difference scheme of the second order approximation in time is used:

by x

$$\frac{w_g^{n+\frac{1}{3}} - w_g^n}{\Delta t/3} = \frac{mg - 6\pi\kappa(z)rw_g^{n+\frac{1}{3}} - 0{,}5c\rho s\left(2\tilde{w}_g w_g^{n+\frac{1}{3}} - \tilde{w}_g^2\right)}{m};$$

$$3mw_g^{n+\frac{1}{3}} - 3mw_g^n = mg\Delta t - 6\pi\kappa(z)r\Delta tw_g^{n+\frac{1}{3}} - c\rho s\Delta t\tilde{w}_g w_g^{n+\frac{1}{3}} + 0{,}5c\rho s\Delta t\tilde{w}_g^2;$$

$$\left(3m + 6\pi\kappa(z)r\Delta t + c\rho s\Delta t\tilde{w}_g\right)w_g^{n+\frac{1}{3}} = 3mw_g^n + mg\Delta t + 0{,}5c\rho s\Delta t\tilde{w}_g^2;$$

$$w_g^{n+\frac{1}{3}} = \frac{3m}{3m + 6\pi\kappa(z)r\Delta t + c\rho s\Delta t\tilde{w}_g}w_g^n + \frac{mg\Delta t + 0{,}5c\rho s\Delta t\tilde{w}_g^2}{3m + 6\pi\kappa(z)r\Delta t + c\rho s\Delta t\tilde{w}_g};$$

by y

$$\frac{w_g^{n+\frac{2}{3}} - w_g^{n+\frac{1}{3}}}{\Delta t/3} = \frac{mg - 6\pi\kappa(z)rw_g^{n+\frac{2}{3}} - 0{,}5c\rho s\left(2\tilde{w}_g w_g^{n+\frac{2}{3}} - \tilde{w}_g^2\right)}{m};$$

$$3mw_g^{n+\frac{2}{3}} - 3mw_g^{n+\frac{1}{3}} = mg\Delta t - 6\pi\kappa(z)r\Delta tw_g^{n+\frac{2}{3}} - c\rho s\Delta t\tilde{w}_g w_g^{n+\frac{2}{3}} + 0{,}5c\rho s\Delta t\tilde{w}_g^2;$$

$$\left(3m + 6\pi\kappa(z)r\Delta t + c\rho s\Delta t\tilde{w}_g\right)w_g^{n+\frac{2}{3}} = 3mw_g^{n+\frac{1}{3}} + mg\Delta t + 0{,}5c\rho s\Delta t\tilde{w}_g^2;$$

$$w_g^{n+\frac{2}{3}} = \frac{3m}{3m + 6\pi\kappa(z)r\Delta t + c\rho s\Delta t\tilde{w}_g}w_g^{n+\frac{1}{3}} + \frac{mg\Delta t + 0{,}5c\rho s\Delta t\tilde{w}_g^2}{3m + 6\pi\kappa(z)r\Delta t + c\rho s\Delta t\tilde{w}_g};$$

and by z

$$\frac{w_g^{n+1} - w_g^{n+\frac{2}{3}}}{\Delta t/3} = \frac{mg - 6\pi\kappa(z)rw_g^{n+1} - 0{,}5c\rho s\left(2\tilde{w}_g w_g^{n+1} - \tilde{w}_g^2\right)}{m};$$

$$3mw_g^{n+1} - 3mw_g^{n+\frac{2}{3}} = mg\Delta t - 6\pi\kappa(z) r\Delta t w_g^{n+1} - c\rho s\Delta t\tilde{w}_g w_g^{n+1} + 0,5c\rho s\Delta t\tilde{w}_g^2;$$

$$\left(3m + 6\pi\kappa(z) r\Delta t + c\rho s\Delta t\tilde{w}_g\right) w_g^{n+1} = 3mw_g^{n+\frac{2}{3}} + mg\Delta t + 0,5c\rho s\Delta t\tilde{w}_g^2;$$

$$w_g^{n+1} = \frac{3m}{3m + 6\pi\kappa(z) r\Delta t + c\rho s\Delta t\tilde{w}_g} w_g^{n+\frac{2}{3}} + \frac{mg\Delta t + 0,5c\rho s\Delta t\tilde{w}_g^2}{3m + 6\pi\kappa(z) r\Delta t + c\rho s\Delta t\tilde{w}_g}.$$

When solving on each layer, an iterative method is used, the convergence of which is checked using the condition

$$\left|w_g^{(S+1)} - w_g^{(S)}\right| < \varepsilon,$$

where ε is the accuracy of the iteration method.

Thus, for the problems under consideration, using the method of splitting into physical processes, a conservative numerical algorithm was obtained; its implementation on a computer makes possible to investigate and predict the process of harmful substances spread in the atmosphere.

5. Solution method

To carry out computational experiments on a computer, a software tool in the C ++ language was created. In calculations, the following input parameters are taken: the dimensions of the problem solving region are 21x21 km, the emission source is located in the centre of the region; the height of the outfall of the emission pipe is 100 m above the ground; the source power is 100 mg/m^3 per second; the initial value of the deposition rate of particles is 0.00015 m/s; the absorption coefficient is 0.00048 1/s**;** wind velocity (speed) is 5 m/s; wind direction - 130°.

Evaluation of the efficiency of the developed algorithm for solving problem (1) - (5) based on the method of physical splitting was performed by comparing the results of calculations with field measurement data and calculations based on other numerical methods for solving the above-mentioned problem [14-15]. In Figures 1 - 4, the distribution of the fine particles concentration in each case is given for the time $t = 5$ at a height of 200 meters above the ground. The colors indicate concentration values in kg/m^3 per second.

The sizes and shapes of plumes in Figures 1 - 4 visually have minimal differences. Nevertheless, the analysis of numerical results shows quite a tangible advantage of the developed computational algorithm based on the method of splitting into physical processes.

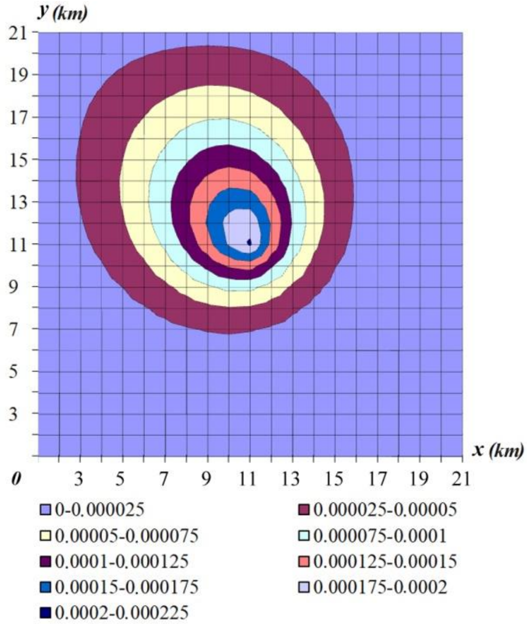

Figure 1. Field measurement data

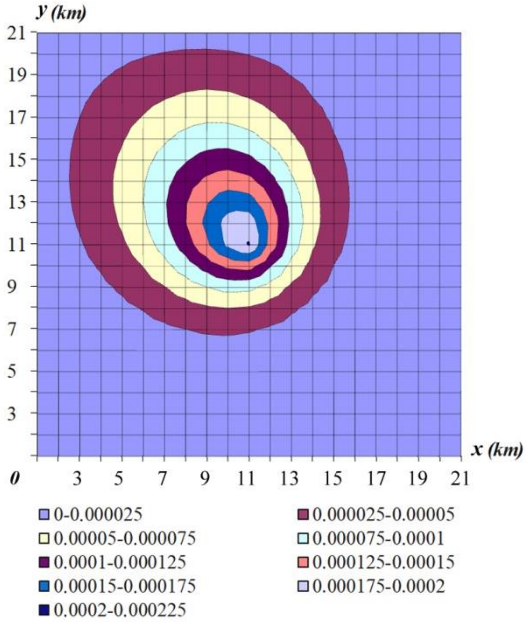

Figure 2. The method of physical splitting.

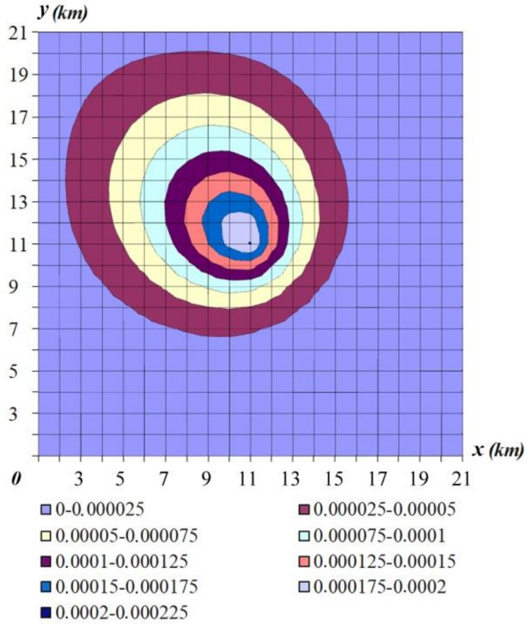

Figure 3. Finite-difference scheme of the 2nd order approximation.

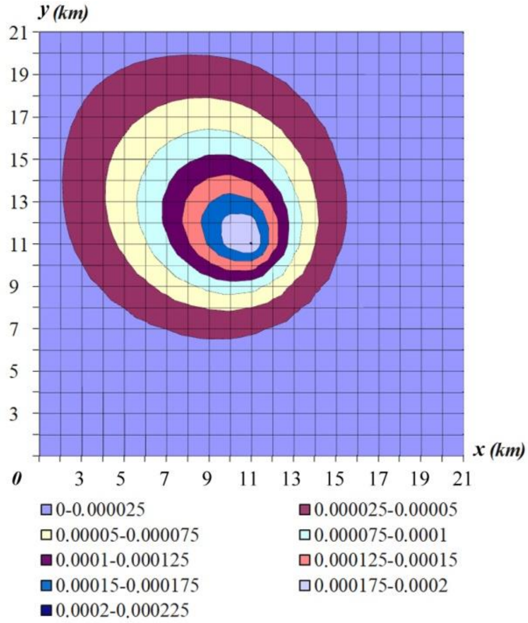

Figure 4. Solution based on variable substitution method

Figure 5 shows a graph of the harmful particles concentration along the middle line of the region of the problem solution on x, obtained by various methods. Table 1 presents the efficiency indices of the algorithms developed on the basis of considered numerical methods.

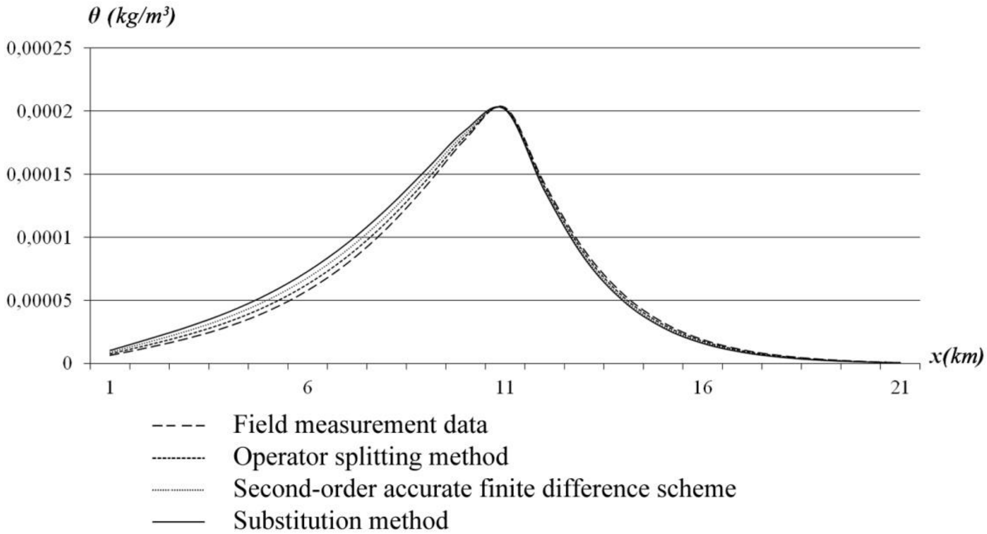

Figure 5. Consistency of various numerical methods of problem solution with real measurement data

As could be seen, the results of numerical solution of the problem of harmful emissions spread in the atmosphere obtained by the method of physical splitting have minimal differences with the measurement data. Accuracy is 5-10% higher while the computation time is the shortest.

Table 1. Indices of the efficiency of computational algorithms

Indices	Physical splitting method	Finite difference scheme of the 2nd order approximation	Variable substitution method
Accuracy (%)	95.07	90.25	85.53
Time (m/s)	1.2	1.5	1.9

Computational experiments have established that when the integration step is reduced in time, the solution of individual problems (1A) - (8) and (1B) - (11) tends to the solution of the basic problem (1) - (5). Although the method of splitting into physical processes gives good results, inaccuracies in the solution of split problems can arise due to a change in parameters $u,\ v,\ w,\ w_g,\ \mu,\ \kappa(z)$ in time and in spatial variables.

According to the results of numerical calculations on a computer with an increase in the horizontal velocity of the air mass of the atmosphere, the concentration of harmful substances in the surface layer increases. This is especially evident when the wind velocity (speed) is ≥ 2.5 m/s and is clearly observed at h = 200-300 m. It is also established that with increasing intensity of aerosol generators, the region where the concentration exceeds the permissible sanitary norms increases. In the case of unstable stratification, the concentration distribution has a pikelike pattern, that is, it reaches the maximum in a short period of time. In such cases, horizontal flows play a major role in harmful substances spread in the atmosphere.

The distribution of the concentration of harmful aerosol particles in the atmosphere is significantly affected by the absorption coefficient σ. The absorption coefficient of harmful particles depends on the state of the air mass (temperature and moisture-content) of the atmosphere, and varies during the day and the time of year. As the value of σ increases, the concentration of harmful substances in the atmospheric surface layer decreases. It has been established by computational experiments that the atmospheric basin of the industrial regions of Uzbekistan is characterized by an average absorption of aerosol particles from 10 to 18 %. Absorption occurs at air moisture-content from 70 to 80%.

Computational experiments were carried out under the condition that aerosol particles of different diameters are emitted into the atmosphere, which plays a significant role in the process of transfer and deposition rate of particles. Thus, it follows from the calculations that the transport of aerosol particles vertically largely depends on both vertical component of the wind velocity (speed) and physicomechanical properties of the particles (radius, mass and cross-sectional area), as well as the atmospheric density and the acceleration of gravity.

6. Conclusion

Comparison of the results of computational experiments with measurement data and the regularities revealed by other authors, showed their satisfactory agreement.

Based on the above, we can conclude that the developed model adequately describes the process of atmospheric dispersion of pollutants and their deposition. The computational algorithm for solving a problem based on the method of splitting into physical processes is quite effective and gives good results.

The aim of creating the considered models and algorithms was to enable analysis, monitoring and predicting the process of harmful industrial emissions spread in the surface layer of the atmosphere.

The results obtained in the form of information, mathematical equations and software can be successfully used, for example, for optimal location of newly constructed facilities in industrial regions; for assessing the scale of industrial emissions into the environment; concentrations of harmful substances in the atmosphere and on the underlying surface, followed by the decision making to minimize the risks of environmental violations.

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