Operator splitting method for numerical solving the atmospheric pollutant dispersion problem

N Ravshanov, F Muradov, D Akhmedov

Tashkent University of Information Technologies named after Muhammad al-Khwarizmi, Amir Temur street, 108, 100200, Tashkent, Uzbekistan

E-mail: ravshanzade-09@mail.ru

Annotation. The paper discusses the numerical modeling of transport and diffusion of air pollutants in the atmospheric boundary layer. There was developed a mathematical model of industrial emissions spread in the atmosphere taking into account the deposition velocity of fine particles. The model is described by multidimensional partial differential equations with appropriate initial and boundary conditions. The basic laws of hydrothermodynamics were used in deriving the model. In order to obtain the numerical solution of the problem, we used one of the splitting methods according to physical processes involved (transport, diffusion and absorption), as well as a second-order implicit finite-difference scheme in time. Analysis of numerical results showed that the developed computational algorithm provides sufficient accuracy of the problem solution compared with field measurement data and it has a certain advantage over other numerical methods. In the course of computational experiments, there was determined the degree of influence of such parameters as wind speed and direction, absorption coefficient and physicomechanical properties of particles on the process of atmospheric air pollutants dispersion.

Keywords: *mathematical model, numerical algorithm, approximation, transport and diffusion, atmosphere, air pollutants, particles deposition velocity*

1. Introduction

Growing urgency of environmental issues has emerged considerable amount of theoretical and experimental studies on the process of atmospheric air pollutants dispersion over the last decades. It is well-known that the air quality is influenced by many factors that require consideration in analyzing and forecasting its conditions. Accordingly, such a requirement necessitates the use of methods mathematical modeling and state-of-art machine-computing techniques which in many cases are preferable by economic and environmental criteria.

Aerosols deposition is of particular interest in solving the problems of monitoring and forecasting the contaminants concentration in the atmospheric boundary layer (ABL). The removal of pollutants from ABL mainly occurs due to wet or dry deposition. Wet deposition is the transport (fall-out) of a certain number of particles from the atmosphere to the underlying surface along with precipitation. Dry deposition is a continuous process that largely depends on the physicomechanical properties of the particles and characteristics of turbulent flows. Dry deposition is mainly 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 gravity, represented in terms of the deposition rate.

Most studies dealing with atmospheric dispersion models emphasize the need for a more thorough description of the features of particles deposition process when calculating concentration fields of pollutants at different heights of the atmospheric boundary layer and directly on the underlying surface.

2. Literature Review

Tirabassi and Moreira, using an analytical solution of the advection-diffusion equation [1]

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

showed that the deposition rate changes the particle concentration along the entire length of the ABL. The modeling results showed that gravitational deposition could greatly affect the final concentration of harmful particles in the air and the maximum concentration near the ground. The authors considered particles sizes from 10 to 100 μm at varying heights of emission sources and under different conditions of atmospheric stability. The deposition rate was calculated according to the Stokes law, and the height of the ABL was taken to be 1000 m. The authors also showed the effect of particle sizes on the concentration spread near the ground depending on the conditions of atmospheric stability. Obtained numerical results claim that under conditions of unstable atmosphere for particles of a diameter less than 10 μm the gravitational component of the deposition rate can be neglected. The authors applied a stepwise approximation to the problem by discretization the height h into sub-layers. 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's algorithm.

Chandra, Jaipal and Katiyar developed a mathematical model for the aerosols transfer emitted from a point-like source on the ground, taking into account the particle deposition rate [2]. 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 applying the method of generalized Laplace integral transform. The solution region was limited to the atmospheric surface layer, also the authors took into account the changes in wind velocity and vertical eddy diffusion. The results obtained by the authors demonstrate the influence of the gravitational mode and dry deposition on the spread of pollutants concentration at ground level. They are generally consistent with the results obtained by other researchers.

In [3], the authors conducted a capacious review of recent advances in mathematical modeling of the processes of transport and diffusion of air pollutants. The authors discussed the advantages and disadvantages of the most popular approaches and strategies for model development, namely Gaussian, Lagrangian, Eulerian models, as well as the CDF models. Special attention was paid to the issues of parametrization of turbulent mixing in the ABL and the particles deposition. The influence of these processes on the spread of pollution concentrations was analyzed. The authors also highlighted the main methods for numerical solution of problems based on the finite-difference approximation, including the method of splitting the original problem into physical processes. Due to the fact that the class of considered problems has a large computational capacity, the authors pay attention to the trends in parallel computing technologies using GPU or adaptive grid refinement.

Menshov M.V. presented a modified mathematical model of the motion and deposition of a polydisperse aerosol cloud of liquid fertilizers sprayed by an agricultural aircraft [4]. In order to describe the impurity cloud migration process, the author considered the equation of the semi-empirical theory of transport and turbulent diffusion and a set of initial-boundary conditions. Menshov performed a vertical averaging of the main equation assuming that the vertical structure of the concentration is close to the Gaussian plume. The problem solving method is based on the discretization of the source systems in the grid area. The spatial approximation of differential operators is based on monotone schemes and schemes with non-increasing total variation. The algebraic systems of finite-difference equations are solved iteratively using the methods of incomplete factorization, and for time integration the implicit splitting methods are used. Comparisons of calculated results with field data showed that the proposed mathematical model has 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. Thereafter, in another paper, Menshov presented results of applying the developed model to the problem of aerosol formation transport in conditions of rugged terrain. These results showed that the presence of even low flat hills cause significant changes in the nature of the aerosols spread and deposition.

A number of studies on the problem of transport of heavy inhomogeneous impurities in the atmosphere was carried out by Raputa V.F. and his colleagues [5]. The authors proposed a model for reconstructing the fields of deposition of impurity particles emitted from a high-altitude source. Raputa notes that, in contrast to the situation with low-lying emission sources, in modeling the transport of aerosols emitted from high-altitude sources, there are considerable difficulties associated with the uncertainties of source height and power, initial particles distribution in the cloud and meteorological conditions. This explains the relevance of reconstruction models. In order to describe the impurity propagation process, the authors used a semi-kinematic approximation, i.e. it is assumed that turbulent scattering occurs only in horizontal directions, and the vertical movement of particles occurs at a constant Stokes velocity. The authors considered the influence of wind rotation effects on the formation of fields of long-term aerosol impurity fallout. The developed model was tested in a numerical analysis of concentration of Benzo(a)pyrene laid-down on the snow in the vicinity of one of the thermal power plants in Barnaul city (Russia). Analysis of the obtained results showed quite satisfactory agreement between the measured and calculated concentrations of the pollutant at the measurement points.

The process of motion and deposition of particles in turbulent atmospheric flows over heat-generating sources was theoretically investigated by Smirnov N.N. and his colleagues [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 the turbulent flow was obtained by Favre averaging, and it includes the mass balance in the gas phase, the mass balance of the k component, the balance of momentum and energy. In addition to the gravity, resistance and the Archimedes forces, the equations of particles motion take into account random turbulent pulsations in the gas flow. Characteristics of these pulsations are determined using the solution obtained in the framework of the $k-\varepsilon$ model. The results of numerical experiments allowed determining the effect of heat sources on the nature of particles dispersion and deposition.

In [7], there was made an attempt to study the atmospheric dispersion taking into account the particles settling velocity and considering the particle shape as an input parameter of developed model. The authors used a semi-empirical formula for non-spherical particles to determine the sensitivity of the volcanic ash cloud transport process to the particle shape. The process was modeled using the Lagrangian model of atmospheric dispersion. It was found that there is no noticeable difference in the vertical trajectories of spherical and non-spherical particles 1 μm in size. Vertical movement of particles 10 μm is more sensitive to their shape, but the similar pattern of movement of spherical and non-spherical particles is preserved, while the deposition rate is always positive the particles move both down and up, which indicates the predominance of advection and turbulent diffusion. Sensitivity to the shape increases dramatically with increasing particle size, so that non-spherical particles about 100 μm in size settle much slower and can move along the axis of the plume 44% farther from the source than spherical ones. The proposed approach allows to more accurately predicting the concentration of fly ash in the atmosphere and the distance of its movement.

Naslund and Thaning presented a solution to the problem of determining the particles settling velocity under unstable atmospheric stratification [8]. The common drag coefficient was used in the equation of motion of solid spherical particles. Time constants, stopping times, and settling velocities under sustained atmospheric stratification were calculated for a wide range of Reynolds numbers. The obtained settling time was compared with the time calculated for the case when precipitation occurred during atmospheric convection. It was found that in this case, solid spherical particles will settle for much longer, which leads to rising the value of the drag coefficient because of increasing in the relative velocity between the particles and the air mass flow. Such a gain is present both for the horizontal wind field, due to the connection between the movement of particles in different directions, and for the vertical field. The effect is most pronounced in the area 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.

As it follows from the analysis of mentioned above many other thematic publications, the deposition rate is often assumed to be constant and it is determined on the basis of empirical data for specific types of pollutants. The aim of this work is the development of a mathematical model that adequately describes the particles deposition rate which varies in time and depends on altitude. As particles we consider solid fine-dispersed particles of spherical shape emitted from stationery ground-level industrial sources. As main physico-mechanical properties that affect the particles deposition rate we consider their mass, diameter and atmospheric density.

3. Problem Statement

In order to study the process of transport and diffusion of aerosol particles in the atmosphere taking into account their deposition rate, let us consider the mathematical model described by multidimensional partial differential equations

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

with appropriate initial

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

and boundary conditions

$$-\mu\frac{\partial\theta(x,y,z,t)}{\partial x}\bigg|_{x=0}=\xi\left(\theta_E-\theta(0,y,z,t)\right);\ \mu\frac{\partial\theta(x,y,z,t)}{\partial x}\bigg|_{x=L_x}=\xi\left(\theta_E-\theta(L_x,y,z,t)\right); \quad (3)$$

$$-\mu\frac{\partial\theta(x,y,z,t)}{\partial y}\bigg|_{y=0}=\xi\left(\theta_E-\theta(x,0,z,t)\right);\ \mu\frac{\partial\theta(x,y,z,t)}{\partial y}\bigg|_{y=L_y}=\xi\left(\theta_E-\theta(x,L_y,z,t)\right); \quad (4)$$

$$-\kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\bigg|_{z=0}=\left(\beta\theta(x,y,0,t)-f(x,y)\right);\ \kappa(z)\frac{\partial\theta(x,y,z,t)}{\partial z}\bigg|_{z=H}=\xi\left(\theta_E-\theta(x,y,H,t)\right). \quad (5)$$

Here, θ – concentration of harmful substances in the atmosphere; θ_0 – primary concentration; θ_E – concentration incoming through boundaries of considered area; x, y, z – coordinate system; u, v, w – wind velocity in three directions; w_g – particles deposition rate; σ – atmospheric absorption coefficient; $\mu,\ \kappa(z)$ – respectively, the diffusion and turbulence coefficients; Q – the emitter power; $\delta_{i,j}$ – Dirac function; $f(x, y)$ – entrainment of particles into the atmosphere from the underlying ground surface; β – particle-surface interaction coefficient; c – dimensionless value equal to 0.5; ρ – atmospheric density; r – particle radius; s – particle cross-sectional area; g – acceleration of gravity; ξ – dimensionality reduction parameter; $L_x,\ L_y$ – respectively, the length and the width of considered area; H – the height of the ABL.

Unlike the works of other authors, within this mathematical model, the particles deposition rate is described by the second equation of problem (1). Since, the problem (1) – (5) is described by a multidimensional nonlinear partial differential equations, it is practically impossible to find the 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 transport in the direction of the air mass motion; the second is the substance molecular diffusion in the atmosphere. It is also possible to distinguish the third process – the absorption of the 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 solved sequentially or in parallel 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 solves sharp gradients exactly, it can use large time steps and it has first order convergence. Despite the fact that the method has minor errors in the mass balance, it is nonetheless quite effective.

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

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

The proposed scheme was implemented according to Kurganov and Tadmor’s central difference scheme for accurate modeling of advection-reaction processes. The basic partial differential equation is divided into two sub-problems which are 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 scheme has the splitting error, which differs from the error in traditional schemes. Numerical results demonstrate sufficient reliability of the proposed scheme.

Geiser and Kravvaritis presented a new approach to domain decomposition based on an iterative splitting method [11]. The proposed two-stage iterative scheme for solving linear evolution equation is based on the space-time operator splitting. The authors studied the convergence properties of the method. The effectiveness of the proposed method was 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 was discussed in [12] by Havasi and Farago. To illustrate the method of physical splitting, the authors used the Danish Eulerian model. The basic equation for the pollutants transport 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 was reduced to several subsystems describing such physical processes as: horizontal transport, horizontal diffusion, chemical reactions, deposition and vertical exchange. The authors pay special attention to the issue of error occurrence as a result of the splitting procedure. The authors adduce several cases when this error disappears, but emphasize that in practice this rarely happens, so it is important to analyze and carefully select the applied schemes with a view to keep the error as small as possible.

Overall, the analysis of thematic publications shows a great attention of researchers paid to the construction of additive schemes. Many authors note the advantages of the method of splitting by physical processes compared to other grid methods. At the same time, the issue of improvement remains open due to the fact that further optimization and various modifications of this method can speed up solutions obtaining with given accuracy.

Here, for the numerical solution of the problem (1) – (5) we assume that a smooth function in all spaces is the desired solution. Using the additivity of different physical processes of mass transport and diffusion in the atmosphere in the time interval $t_n \le t \le t_{n+1}$, let us consider each process as separate sub-problem.

The process of transport of substance with its preservation along the trajectory is considered as problem A:

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

with initial

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

and boundary conditions

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

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

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

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

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

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 them, we use an implicit finite-difference scheme of the second-order approximation in time [13].

Equation (1A) is approximated by x, and after some transformations we obtain a three-diagonal system of linear algebraic equations (SLAE)

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

where

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

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

Boundary condition (6) is approximated by x, grouping similar terms and then using the Thomas algorithm we find coefficients

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

The values of concentration at the $0x$ axis boundary can be found from the second boundary condition (6)

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

The concentration values $\theta_{N-1,\,j,k}^{n+\frac{1}{3}}$, $\theta_{N-2,\,j,k}^{n+\frac{1}{3}}$,..., $\theta_{1,\,j,k}^{n+\frac{1}{3}}$ are determined using back substitution

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

Next, we perform similar steps in the direction of $0y$:

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

Here

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

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

Boundary condition (7) is approximated by y and we can find sweep coefficients

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

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

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

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

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

$$\bar{\bar{d}}_{1,i,\,j,k} = \frac{|u|+u}{2\Delta x}\theta_{1,i-1,\,j,k}^{n+\frac{2}{3}} + \left(\frac{3}{\Delta t} - \frac{u}{\Delta x} - \frac{v}{\Delta y}\right)\theta_{1,i,\,j,k}^{n+\frac{2}{3}} - \frac{|u|-u}{2\Delta x}\theta_{1,i+1,\,j,k}^{n+\frac{2}{3}} +$$
$$+\frac{|v|+v}{2\Delta y}\theta_{1,i,\,j-1,k}^{n+\frac{2}{3}} - \frac{|v|-v}{2\Delta y}\theta_{1,i,\,j+1,k}^{n+\frac{2}{3}} + \frac{1}{6}\delta_{i,\,j,k}Q.$$

Boundary condition (8) is approximated by z. The recurrence relations to determine the sweep coefficients are as follows

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

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

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

The obtained 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

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

$$d_{2,i,j,k}=\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta y^2}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\right)\theta_{i,j,k}^{n}+\frac{\mu}{\Delta y^2}\theta_{i,j-1,k}^{n}+\frac{\mu}{\Delta y^2}\theta_{i,j+1,k}^{n}+$$
$$+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta_{i,j,k-1}^{n}+\frac{\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k+1}^{n}+\frac{1}{6}\delta_{i,j,k}Q.$$

For the boundary condition (9), the recurrence relations to determine the sweep coefficients with respect to x are obtained following way

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

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

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

Next, we perform similar actions in y direction

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

Here

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

$$\bar{d}_{2,i,j,k}=\left(\frac{3}{\Delta t}-\frac{2\mu}{\Delta x^2}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\right)\theta_{i,j,k}^{n+\frac{1}{3}}+\frac{\mu}{\Delta x^2}\theta_{i-1,j,k}^{n+\frac{1}{3}}+\frac{\mu}{\Delta x^2}\theta_{i+1,j,k}^{n+\frac{1}{3}}+$$
$$+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta_{i,j,k-1}^{n+\frac{1}{3}}+\frac{\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k+1}^{n+\frac{1}{3}}+\frac{1}{6}\delta_{i,j,k}Q.$$

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

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

in order to determine the concentration of aerosol particles at the boundary of the problem solution region in the direction of y coordinate , we obtain the following recurrence relation

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

Similarly, in z direction we obtain SLAE

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

where

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

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

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

Approximating the boundary condition (11) next we obtain relationships to find the values of the sweep coefficients

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

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

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

As for the second equation of the original problem (1), in order 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

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

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

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

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

As can be seen from the above algorithm description, an iterative method is used on each layer, its convergence is verified by following condition

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

where ε is the accuracy of the iterative method.

Thus, for the considered problem there was developed a conservative numerical algorithm using the method of splitting into physical processes. Its programming implementation makes possible to investigate and forecast the process of harmful substances spread in the atmosphere.

5. Results and Discussion

To carry out computational experiments there was written a software tool in C ++ programming language. In the calculations, the following input parameters were taken: the problem solving area is 21×21 km in size, where the emitter is located right in the center; the height of chimney stack mouth is 100 m above the ground; the emitter power is 100 mg/m^3 per second; the initial value of particles deposition rate is 0.00015 m/s; atmospheric absorption coefficient is to 0.00048 1/second; wind speed is 5 m/s and wind direction is 130° degree.

The evaluation of efficiency of the developed algorithm for solving problem (1) – (5) based on the method of splitting into physical processes was performed by comparing numerical results with field measurement data and calculations based on other numerical methods [14–15]. In figures 1–4, the spread 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.

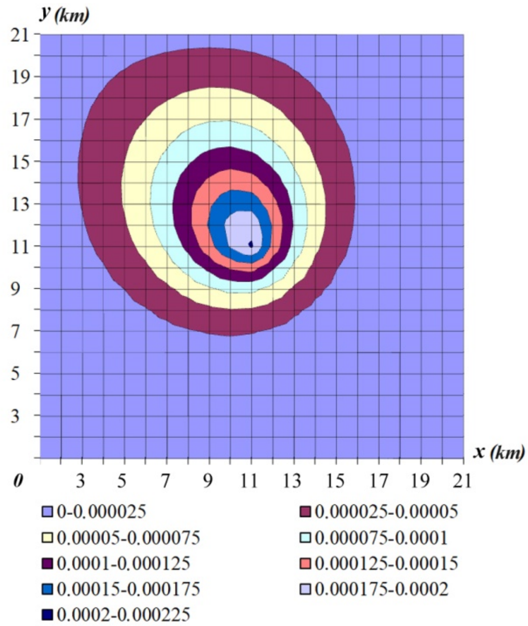

Figure 1. Field measurement data.

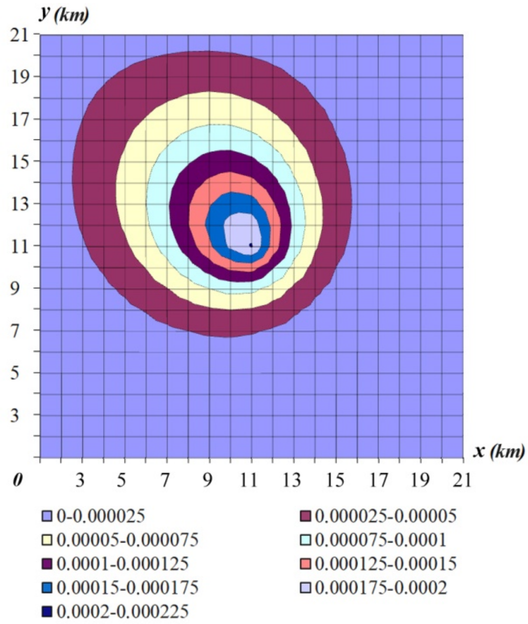

Figure 2. The operator splitting method.

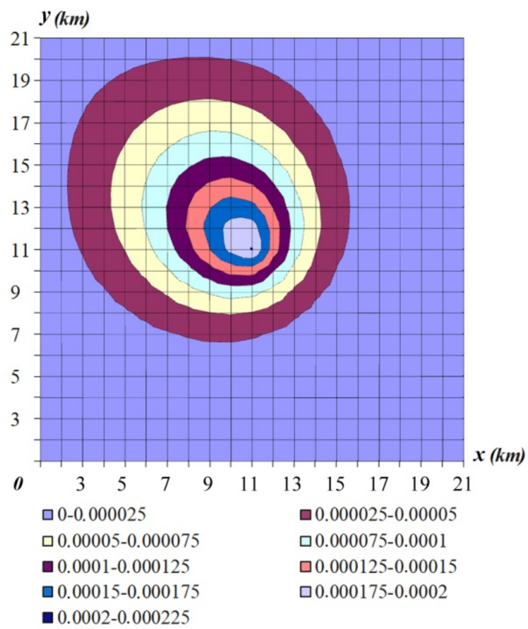

Figure 3. Finite-difference scheme of the second-order approximation.

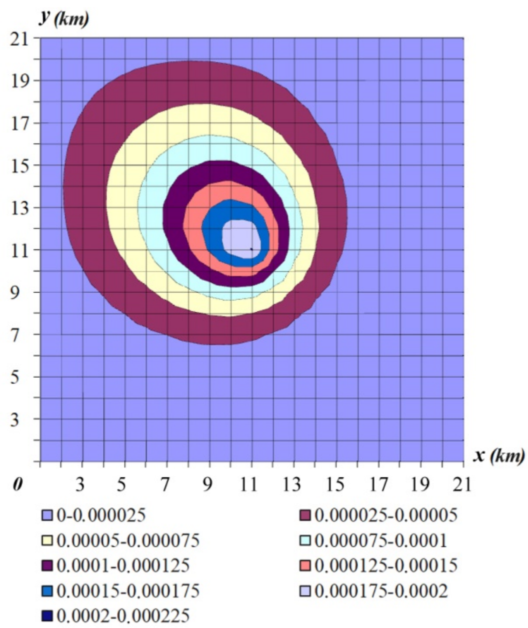

Figure 4. Solution based on variable substitution method.

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 operator splitting method.

The diagram in figure 5 shows the values of harmful particles concentration along the middle line of the problem solving area by x direction, obtained by various methods. In table 1 there are presented the efficiency indices of different developed algorithms.

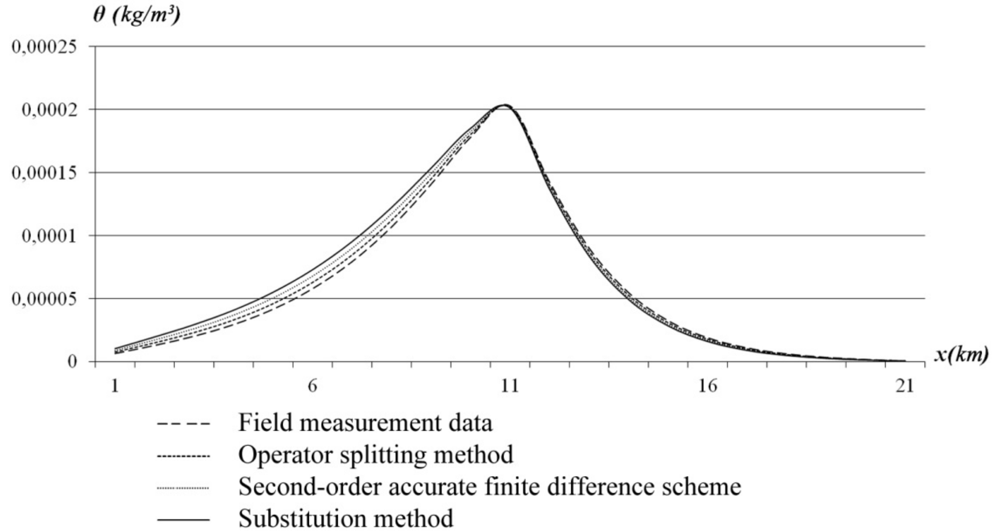

Figure 5. Consistency of various numerical methods of problem solution with real measurement data.

As it could be seen, the results of numerical solution of the problem of harmful emissions spread in the atmosphere obtained by the operator splitting method by physical processes have minimal differences with the measurement data. The considered method has 5-10% higher accuracy minimal computation time.

Table 1. The efficiency of computational algorithms based on different numerical methods.

Indices	The operator splitting method	Finite-difference scheme of the second-order approximation	Variable substitution method
Accuracy (%)	95.07	90.25	85.53
Time (мс)	1.2	1.5	1.9

It was found from carryed computational experiments that when the integration step is reduced in time, the solution of sub-problems (1A) – (8) and (1B) – (11) tends to the solution of the basic problem (1) – (5). Although the operator splitting method gives good results, inaccuracies in the solutions of sub-problems can arise due to changes in parameters u, v, w, w_g, μ, $\kappa(z)$ both in time and space.

According to the results of numerical calculations an increase of the horizontal speed of the air mass leds to increase of the harmful substances concentration in the ABL. This is especially evident when the wind speed is ≥ 2.5 m/s and is clearly observed at h = 200-300 m. It was also found that with increasing intensity of aerosol emitters, the area where the concentration exceeds the permissible sanitary norms increases. In the case of unstable stratification, the concentration spread has a pike-shaped pattern, i.e. it reaches the maximum in a short period of time. In such cases, horizontal flows play a major role in harmful substances spread.

The spread 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 conditions 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 ABL 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 10 – 18 % of aerosol particles 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 particles transport and deposition. Thus, it follows from the calculations that the vertical transport of aerosol particles largely depends on both vertical component of the wind 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 mathematical software can be successfully used for optimal location of newly constructed facilities in industrial regions; for assessing the scale of industrial emissions into the environment; for estimating the concentrations of harmful substances in the atmosphere and on the underlying surface, followed by the decision making to minimize the risks of environmental disruption.

References

[1] Tirabassi T and Moreira D 2017 *Proc. of 18th Int. Conf. on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes* (Bologna)
[2] Chandra P, Jaipal and Katiyar V K 2011 *Int. J. of Math. Sci. and Appl.* **1** 1591
[3] Leelossy A, Molnar F, Izsak F, Havasi A, Lagzi I and Meszaros R 2014 *Centr. Euro. J. of Geosciences* **6** 257
[4] Menshov M V 2007 *J. of Samara State Technical University, Ser. Phys. and Math. Sci.* **15** 176
[5] Raputa V F, Shlychkov V A, Lezhenin A A, Romanov A N and Yaroslavtseva T V 2014 *Atmospheric and Oceanic Optics* **27** 713
[6] Smirnov N N, Nikitin V F, Legros J C and Shevtsova V M 2002 *Aerosol Sci. and Tech.* **36** 101
[7] Saxby J, Beckett F, Cashman K, Rust A and Tennant E 2018 *J. of Volcanology and Geothermal Res.* **362** 32
[8] Naslund E and Thaning L 1991 *Aerosol Sci. and Tech.* **14** 247
[9] Holden H, Hvistendahl K and Lie K 2000 *Computational Geosciences* **4** 287
[10] Simpson M, Landmana K and Clement P 2005 *Math. and Comp. in Simulation* **70** 44
[11] Geiser J and Kravvaritis Ch 2009 *Appl. Num. Math.* **59** 608
[12] Havasi A, Bartholy J and Farago I 2001 *Idojaras* **105** 39
[13] Ravshanov N, Sharipov D K and Toshtemirova N 2013 *Privolzhsky Sci. J.* **12-1** 39
[14] Ravshanov N, Muradov F, Narzullaeva N and Morzitsin I 2017 *Probl. of Comp. and Appl. Math.* **2** 20
[15] Sharipov D K, Muradov F and Ravshanov Z N 2017 *Probl. of Comp. and Appl. Math.* **6** 15