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N Ravshanov[1], T R Shafiev[2], Sh Daliev[3]

[1]Tashkent University of Information Technologies, 108, Amir Temur ave., Tashkent, 100200, Uzbekistan
[2]Bukhara State University, 11, M Ikbol Str., Bukhara, 200114, Uzbekistan
[3]Samarkand State University, 15, University Boulevard, Samarkand, 140104, Uzbekistan

E-mail: tursunshafiyev@gmail.com

Abstract. To conduct a comprehensive study of the significant factors affecting the transfer and diffusion process of aerosol particles in the atmosphere, a mathematical model, numerical and software tools are developed in the paper. Taking into account the physicomechanical properties of harmful substances discarded from industrial production facilities and the characteristics of soil surface, air velocity, and the substance extinction coefficients. When predicting the concentration of harmful substances in the atmosphere, a key factor that affects the transfer and diffusion of aerosol particles in the atmosphere is the velocity of substance transfer in three directions x, y, z , respectively. The problem posed in the paper is solved by the finite-difference method and the results of numerical calculations on a computer are presented in the form of graphs. It was established that the transfer and diffusion processes of aerosol particles in the atmosphere that play an important role are the rate of air mass formation in the surface layer of the atmosphere; the density and linear size of the aerosol particles emitted into the atmosphere; the terrain, which generates the velocity of air propagation in the atmosphere. It was established by computational experiments that the lower the density and mass of a harmful substance particle, the higher its horizontal velocity and the lower its vertical velocity.

1. Introduction

An intensive growth of economic activity, ignoring the nature potential and the laws of its development, has led to the need to solve one of the pressing problems on a global scale. This problem is associated with the tasks of protection and conservation of the environment from negative anthropogenic impact.

Violations of the existing ecological balance in regions with high anthropogenic pressure, and, first of all, persistent air pollution, cause a lot of problems - the growth of oncological, allergic, asthmatic and other diseases among the population, the deterioration of the agricultural land fertility, the state of flora and fauna.

That is why the issues of conducting comprehensive research, monitoring, forecasting and analyzing the process of harmful contamination distribution in the atmosphere are among the most pressing tasks of the environment protection problem.

One of the effective tool for conducting a comprehensive study, monitoring, forecasting managerial decision making on the above mentioned task is the mathematical modeling of the process as a whole.

In recent years, scientists have obtained theoretical and applied results aimed at solving the above-mentioned problems based on a mathematical model, a numerical algorithm and software to conduct computer experiments.

Such prominent scientists as E.P. Mednikov, G.I. Marchuk, M.E. Berland, A.E. Aloyan, V.I. Naats, I.E. Naats, P. B. Mashikhina, P. Zannetti, Youngdeok Hwang, D. Xiao, Adel A. Abdel-Rahman, W.J. Layton and others have been engaged in the mathematical modeling of atmospheric pollution from natural and man-made sources. A school created under the leadership of F. B. Abutaliev, which is now supervised by N. Ravshanov and others, is actively working in our country.

The studies in [1] provide an overview of the current capabilities of regional and mesoscale meteorological modeling related to air pollution survey. The shortcomings of the existing forecasting and monitoring models are discussed and several examples are presented that demonstrate the capabilities of new tools for assessing the ecological state of the region under consideration. The authors emphasize that today computer capacity and memory, especially with regard to graphic supercomplexes, are sufficiently advanced to predict ecological state of the atmosphere on the basis of meteorological models of this scale in combination with Euler models of advection-diffusion or the models of Lagrangian particle dispersion. The air pollution and emergency response can be regularly assessed with this software package.

In [2], a qualitative analysis of classical models for the spread of harmful substances in the atmosphere is made. Particular emphasis is placed on air pollution from automobile exhaust gases. The authors investigated the trajectory of particles for two physical processes, i.e. for transfer and diffusion. A comparative analysis shows that the particle size has a significant affect in its presence in atmospheric air. To obtain the results, computational excrement was conducted based on the Gaussian model.

In article [3] investigated the problems of predicting the spread of harmful substances in the atmosphere. A mathematical model was proposed which takes into account the main weather and climatic factors. Based on the researched results, the authors reveal that the main factors, such as wind speed, soil moisture, soil composition, significantly affect the spread of harmful substances in the atmosphere.

In work [4], proposed a methodology for modeling and optimal control of the hazard of atmospheric pollution in nuclear and in chemical disasters. To predict atmospheric pollution during nuclear and chemical disasters, atmospheric dispersion models and explosion hazard assessment models were used, and with the help of these models, a computational algorithm and an application for monitoring of gas dispersion were developed. The meteorological data were got from the mesoscale weather forecasting model MESO, and the concentration distribution was developed using the CDM model [5].

In [6], investigated air pollution on the ground layer in the drained part of the Aral Sea. Developed mathematical models and numerical algorithms, a computational experiment was carried out on a computer, on the basis of which it was established that the dispersion of aerosol particles in the atmosphere is influenced by the velocity of the air mass of the atmosphere in the surface layer and the turbulence coefficient plays an important role in the deposition rate of aerosol particles. Investigating changes in wind speed, it was found that the dynamics of changes in wind speed in the lower layers of the earth's surface is significantly affected by the roughness coefficient.

A methodology for analyzing scenarios of street pollution modeling with a large flow of vehicles was considered in [7] to predict pollution levels in the city of Riga. Using the Operational Street Pollution Model (OSPM), the authors simulated the concentration levels of pollutants in real situation and in five different situations. According to the data obtained, the authors proposed to respond in time to emergency situations in the region under consideration.

In [8], a numerical solution was developed for some problems of air pollution. The authors of the paper constructed and analyzed (discrete) transparent boundary conditions for the implicit difference scheme. The concepts of positivity and monotonicity of difference schemes were discussed and the properties of difference schemes were briefly considered to solve the advection-diffusion equations arising in the problems of air (and water) pollution.

Analysis of fundamental scientific publications related to the process of harmful substances transfer and diffusion in the atmosphere indicates its wide range. Which is included aerosol particles emission, rise and deposition, diffusion, and transfer by wind, etc. The process of emission of harmful particles into the atmosphere from pollution sources has the ranges comparable to particle sizes from $\sim 10^{-7}$ to 10^3m, while transfer and diffusion, depending on their size and wind velocity, can be realized at distances from several centimeters to thousands of kilometers. Such circumstances greatly complicate the construction of a universal mathematical model for the transfer and diffusion of harmful substances in the atmosphere. So, scientists are forced to develop mathematical models to solve only specific ecological problems. Models of the global transfer based on the research of processes of local mass transfer of harmful substances in the air which is generalized with experimental data [9–12] are widely applied to the task of monitoring and predicting the ecological state of the atmosphere. As the analysis of scientific works related to atmospheric physics shows, these models can be attributed to models studied in the framework of the mechanics of multiphase media.

The analysis of the studies showed that in order to develop an adequate mathematical model of the transfer and diffusion processes of aerosol particles and harmful gases in the atmosphere, it is necessary to take into account the key factors acting on the object as a whole, with the results of computer experiments.

2. Statement of problem. Studying the effect of the above parameters on the process of transfer and diffusion of harmful substances in the atmosphere, accounting for their physical and mechanical properties, is reduced to choosing the range of phenomenon description, which is of the highest priority. In view of [13], an analysis and some assumptions related to the mechanics of multiphase media are given in detail.

It should be noted that the density and viscosity of the air significantly affect the transfer and diffusion of aerosol particles in the atmosphere, and they vary depending on the temperature of the ambient [14].

Numerical computer calculations [13] showed that the concentration of air pollutants is a function of a number of variables, including the emission rate, the distance from the receiver to the source, and weather-climate factors of the region under consideration. A numerical study of the process showed that the most important atmospheric conditions are wind velocity and direction, particle deposition rate, and absorption coefficient of the local atmosphere. It should be noted that if the ambient temperature decreases faster than the wind velocity, unstable equilibrium conditions are intensified in the atmosphere, which lead to an increase in the velocity of particles moving vertically and, consequently, to the expansion of the region of pollutant concentration in the atmosphere.

Introducing the theory of global transfer of harmful aerosol particles in the atmosphere and on the bases of the above assumptions, the problem of transporting a spherical body of radius r_i, density ρ_p can be reduced to a gravitational field under the action of wind forces. Based on the above conditions, to study the components of particles velocity u_p, v_p, w_p in projections x, y, z, respectively, consider the equation:

$$m\frac{du_p}{dt} = c_f \pi r^2 \rho_a (u_p - U)^2; \tag{1}$$

$$m\frac{dv_p}{dt} = c_f \pi r^2 \rho_a (v_p - U)^2; \tag{2}$$

$$m\frac{dw_p}{dt} = -\frac{}{3}\pi r^3(\rho_p - \rho_a)g - k_f \mu_a \pi r w_p + F_n \qquad (3)$$

and corresponding initial conditions:

$$\hat{u}_p = u_p(0), \ \ \hat{v}_p = v_p(0), \ \ \hat{w}_p = w_p(0), \ \ \text{at } t = 0; \qquad (4)$$

where $U = \sqrt{\hat{u} \quad \hat{v} \ + \hat{w}^2}$.

Here m is the mass of the particle; r is the particle radius; g is the acceleration of free fall; c_f is the drag coefficient of particles; k_f is the body shape coefficient for resistance force; F_n is the lifting force of the air flow; ρ_p is the particle density; ρ_a is the air density; μ_a is the air viscosity; t is time.

Accounting for the flow rate of particles in the atmosphere, with relations (1) - (4), a mathematical model of the process of transfer and diffusion of harmful substances in the atmosphere can be written in the following form (based on the laws of hydromechanics):

$$\frac{\partial\theta}{\partial t} + u_p\frac{\partial\theta}{\partial x} + v_p\frac{\partial\theta}{\partial y} + w_p\frac{\partial\theta}{\partial z} + \sigma\theta = \mu\left(\frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2}\right) + \frac{\partial}{\partial z}\left(\kappa\frac{\partial\theta}{\partial z}\right) + \delta\left(x,y,z\right)Q; \qquad (5)$$

and corresponding initial and boundary conditions:

$$\left.\begin{aligned} &\theta(x,y,z,0)\big|_{t=0} = \theta_0(x,y,z);\ u_p(0)\big|_{t=0} = u_{p,0}(0);\\ &v_p(0)\big|_{t=0} = v_{p,0}(0);\ \ w_p(0)\big|_{t=0} = w_{p,0}(0); \end{aligned}\right\} \qquad (6)$$

$$-\mu\frac{\partial\theta}{\partial x} = \xi(\theta_b - \theta) \text{ at x=0, } \ \mu\frac{\partial\theta}{\partial x} = \xi(\theta_b - \theta) \text{ at x=L}_x; \qquad (7)$$

$$-\mu\frac{\partial\theta}{\partial y} = \xi(\theta_b - \theta) \text{ at y=0, } \ \mu\frac{\partial\theta}{\partial y} = \xi(\theta_b - \theta) \text{ at y=L}_y; \qquad (8)$$

$$-\kappa\frac{\partial\theta}{\partial z} = (\beta\theta - F_0), \text{ at z = 0, } \ \kappa\frac{\partial\theta}{\partial z} = \xi\left(\theta_b - \theta\right), \text{ at } \ z = H_z \qquad (9)$$

Here θ is the concentration of emitted substance; θ_0 – the primary concentration of harmful substances in the atmosphere; σ – the coefficient of absorption of harmful substances in the atmosphere; δ – Dirac function; x, y, z – the coordinates; μ – the diffusion coefficient; β – the coefficient of interaction with the underlying surface; Q the sources strength; F_0 – the number of aerosol particles detached from the roughness of ground surface, κ – the turbulence coefficient, ξ – the coefficient to reduce the boundary condition to dimensional form, θ_b – the concentration of suspended substances in neighboring regions of the problems under solution.

From the statement of problem, it follows that to solve the problem of transfer and diffusion of pollutants in the atmosphere (4) – (11), it is necessary to calculate the flow rate of aerosol particles in the atmosphere (1) – (4).

3. Solution method. The method for solving equation (1) – (4) was given in [15,16].

4. **Computational experiment (CE).** Based on the developed numerical algorithm [11], [12], a software tool in C # was compiled and computational experiments were conducted on a computer (Figs. 2 – 4). The interface of the developed program is shown in Fig. 1.

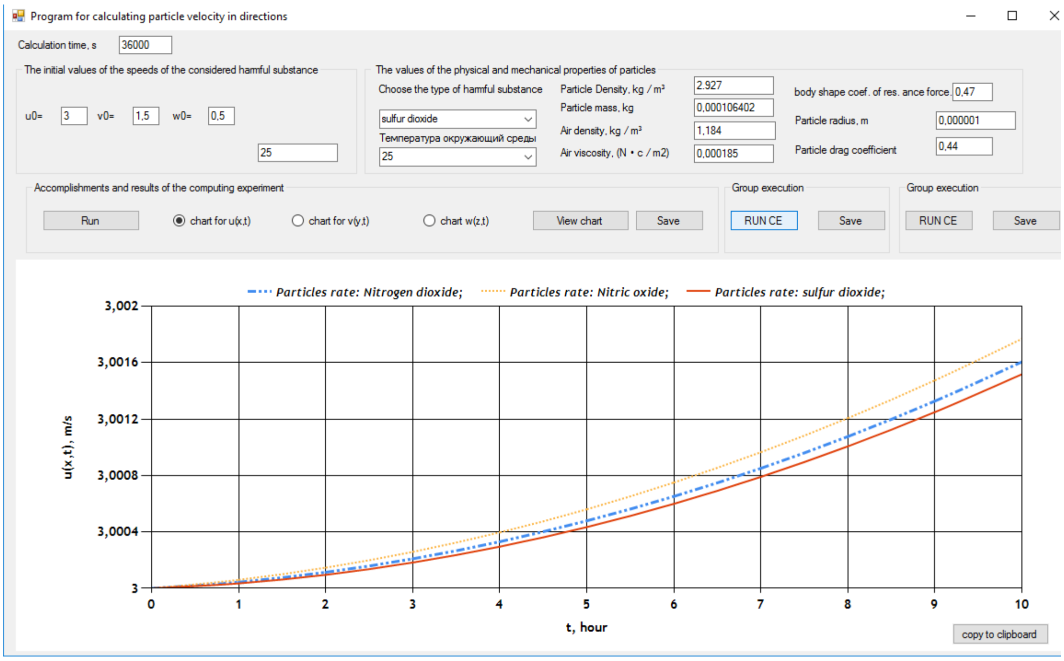

Figure 1. Primary window of the software for conducting CE

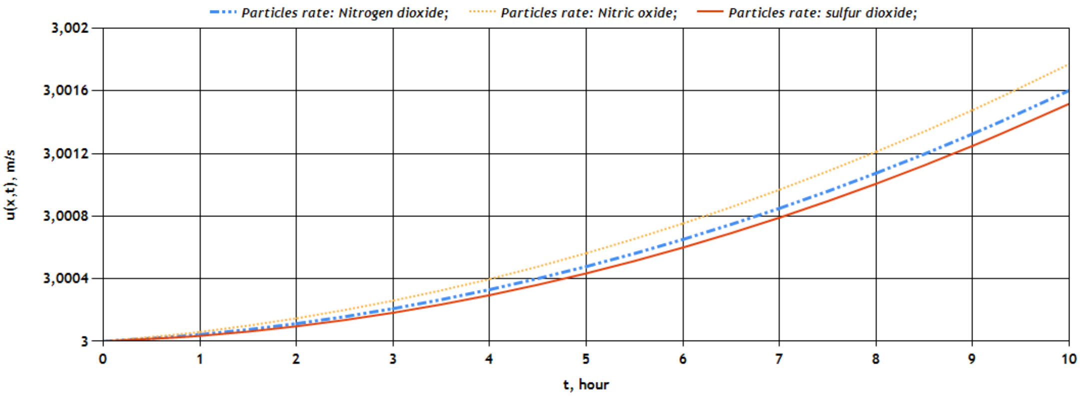

Figure 2. Changes in particles rate of harmful substances along the coordinate OX depending on time at $u = 3\,\text{m/s}$.

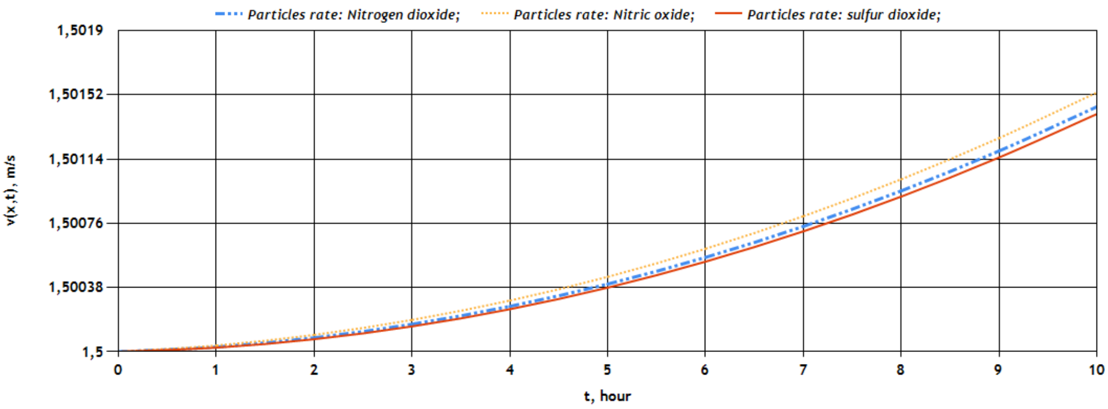

Figure 3. Changes in particles rate of harmful substances along the coordinate OY depending on time at $v_0 = 1{,}5\,\text{m/s}$.

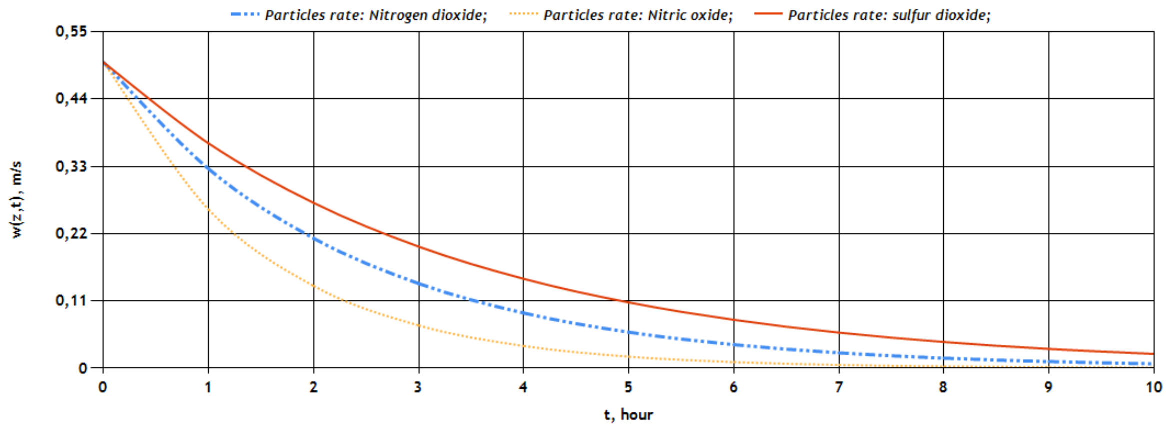

Figure 4. Changes in particles rate of harmful substances along the coordinate OZ depending on time at $w_0 = 0,5$ m/s.

From numerical calculations performed on a computer, it is seen that the physicochemical properties of the particles (size, mass, density and shape) substantially affect the particle rate path and the concentration distribution of harmful substances in the atmosphere. In computational experiments carried out at certain air rates it was stated that the smaller the mass and density of harmful substances particles, the higher the horizontal velocity; the vertical velocity increases slightly over time.

Numerical calculations were carried out to determine the particle rate path of nitrogen dioxide (IV), nitric oxide (II) and sulfur dioxide in vertical direction at an initial velocity of motion $w_0 = 0,5$ m/s; it was stated that with an increase in horizontal velocity of particles motion, their vertical velocity decreases.

A computational experiment was conducted to calculate the particle rate path of nitrogen dioxide (IV), nitric oxide (II) and sulfur dioxide in horizontal direction depending on the air velocity of the atmosphere at $u_0 = 3$ m/s; it was stated that the velocity of particles motion increases over time logarithmically.

Numerical calculations showed that transfer and diffusion substantially depend on the vertical distribution of the turbulence coefficient; it was stated that the wind direction in the region under consideration plays a significant role in the dispersion of harmful substances in the atmosphere in horizontal direction.

Numerical calculation results showed that the dispersion of aerosol particles in the atmosphere is affected by the air velocity in the surface layer and the dynamics of changes in wind velocity in the lower layers of the ground surface are significantly affected by the roughness coefficient of the ground.

CE stated that the turbulence coefficient influences the deposition rate of aerosol particles, it grows in a vertical direction according to the linear law, the air temperature of the atmosphere affects the growth of wind velocity in a vertical direction, and with decreasing air temperature wind velocity in vertical direction increases exponentially.

5. Conclusions.

The results of computational experiments have established that the physicomechanical properties of harmful substance particles play an important role in their motion both in horizontal and vertical directions. An analysis of numerical calculations showed that the smaller the density and mass of the particles the higher their horizontal velocity; in vertical direction they increase slightly.

From the analysis of numerical calculations it follows that the essential role on the dispersion region of aerosol particles in the atmosphere surface layer plays: firstly, the rates of air formation in the surface layer of the atmosphere; secondly, the density and linear size and the shape of aerosol particles emitted into the atmosphere; thirdly, the terrain, which generates the air velocity in the atmosphere and is the key factor acting on the transfer and diffusion of pollutants in the atmosphere.

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