Nonlinear mathematical model for monitoring and predicting the process of transfer and diffusion of fine-dispersed aerosol particles in the atmosphere

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Abstract. Mathematical model for predicting, monitoring and assessing the ecological state of the atmosphere and underlying surface with passive and active impurities is developed in this article; it takes into account the varying rate of particle displacements in the atmosphere. To determine the rate of displacements of fine-dispersed particles in the atmosphere, a system of nonlinear equations has been obtained, which took into account such important factors as: the basic physical-mechanical properties of the particles and the rate of air mass in the atmosphere.

1. Introduction

Prediction, monitoring and assessment of the ecological state of the atmosphere and underlying surface with passive and active impurities, location of industrial enterprises in compliance with the sanitary regional standards of pollution are relevant to the problem of environmental protection.

Today, analysis of environmental data shows that the intensive growth of industry has a great influence on the ecological imbalance of the atmosphere in industrial regions. Most of these environmental problems are noticeable in highly developed industrial countries, such as China, USA, India, Japan, Korea, Russia, France, etc.

Excessive air pollution affects the health of people and living systems, as various chemical elements are absorbed most intensively during breathing. Thus, the relevance of mathematical modeling of the process of harmful aerosol particles propagation is obvious.

Many foreign and domestic authors are engaged in the analysis and modeling of atmospheric pollution in industrial regions.

In recent years, the number of research papers on the development of mathematical modeling of the process of transfer and diffusion of harmful substances in the atmosphere has been growing. The aim of these studies is monitoring and forecasting the state of the atmosphere in industrial regions.

Mathematical modeling of the process of transfer and diffusion of harmful substances into the atmosphere is the problem under consideration in scientific schools created under the guidance of G.I. Marchuk, V.V. Penenko, A.E. Aloyan, L.T. Dymnikov I.E. Naats, I.A. Kibel, L.N. Gutman, F.B. Abutaliev, as well as foreign scientists W.J. Layton, J.H. Ferziger, J.W. Deardorff, M. Germano, U. Piomelli, L.C. Berselli, G.S. Winckelmans, W.C. Reynolds, H. Zidisk, K.A. Welds, K.I. Nappo, J. Gotaas, M. Mullioland, S. Trap, M. Maties, V. Edelman, and others.
In [1], a numerical algorithm has been proposed for solving the equations of propagation of impurities in the atmosphere. As an example of nonlinear difference schemes for solving the transfer equation, a monotonic scheme is used, which approximates the initial differential equation with a second order of accuracy in spatial variables and in time. The author also considers a special hydrodynamic model of meso-scale atmospheric processes, including the process of transfer and diffusion of gas impurities and the optimization models for controlling the capacity of sources using a linear and non-linear programming apparatus.

In [2, 3], achievements in the field of mathematical and numerical modeling of non-stationary transfer of pollutants in the atmospheric boundary layer are described. The authors have developed computational models and corresponding efficient algorithms for the problems of forecasting transfer and diffusion of aerosols, using operational information of a meteorological nature. They have also investigated the qualitative models of the transport theory on the basis of the semi-empirical equation of turbulent diffusion.

In [4], based on the solution of the non-stationary equation of turbulent diffusion with given values of the components of the wind speed \(u, v, w\), diffusion coefficient \(\mu\) and the turbulent mixing coefficient \(\kappa\), a new formula is obtained for calculating the fields of air pollution concentrations.

An analysis of long-term environmental forecasting is made in [5] using available factual information on long-term climate dynamics. On the basis of direct and inverse modeling and methods of the theory of sensitivity, a technique for quantitative risk/vulnerability assessment is described.

A detailed analysis of scientific papers related to the problem of mathematical modeling of the process of transfer and diffusion of aerosol particles in the atmosphere has shown that in mathematical modeling and the study of the process of distribution of harmful substances in the atmosphere, firstly, the rate of displacements of aerosol particles in the atmosphere is not considered depending on the rate of air flow changing with time; secondly, in all the mathematical models of the process, the absorption coefficient of aerosol particles is taken as a constant; thirdly, it was assumed that the distribution of harmful substances emitted from the sources does not reach the considered boundaries of the problem solution area and there is no inflow and outflow of harmful substances through them.

Based on the above, the aim of this paper is to develop a nonlinear mathematical model for monitoring and forecasting the process of transfer and diffusion of harmful substances in the atmosphere in industrial regions; this mathematical model should take into account the possibility of calculating atmospheric pollution by sources, wind speed and direction, precipitation of impurities and weather-climatic factors.

2. Statement of the problem
To study the process of transfer and diffusion of aerosol particles in the atmosphere, with account of essential parameters \(u, v, w\) of the components of the wind speed in directions \(x, y, z\) and the deposition rate of fine-dispersed particles \(w_s\), respectively, consider a mathematical model based on the law of hydromechanics, using the multidimensional partial differential equation

\[
\frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} + \left( w - w_s \right) \frac{\partial \theta}{\partial z} + \sigma \theta = 
\]
\[
= \mu \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} \right) + \kappa \frac{\partial^2 \theta}{\partial z^2} + \delta Q;
\]

\[
m \frac{du}{dt} = c_f \frac{\pi r^2 \rho_s (u - U)^2};
\]
\[
m \frac{dv}{dt} = c_f \frac{\pi r^2 \rho_s (v - U)^2};
\]
\[
\frac{dw_n}{dt} = -\frac{4}{3} \pi r^3 (\rho_n - \rho_s) g - k_f \mu_n \pi r v + F_n
\]  
\[\text{(4)}\]

and corresponding initial and boundary conditions:

\[
\theta(x, y, z, 0) = \theta_0(x, y, z); \quad \bar{u} = u(0);
\]

\[
\bar{v} = v(0); \quad \bar{w}_g = w_g(0); \quad \text{at } t = 0;
\]

\[
-\mu \frac{\partial \theta}{\partial x} = \xi(\theta_b - \theta) \text{ at } x = 0, \quad \mu \frac{\partial \theta}{\partial x} = \xi(\theta_b - \theta) \text{ at } x = L_x;
\]

\[\text{(6)}\]

\[
-\mu \frac{\partial \theta}{\partial y} = \xi(\theta_b - \theta) \text{ at } y = 0, \quad \mu \frac{\partial \theta}{\partial y} = \xi(\theta_b - \theta) \text{ at } y = L_y;
\]

\[\text{(7)}\]

\[
-\kappa \frac{\partial \theta}{\partial z} = (\beta \theta - F_0) \text{ at } z = 0, \quad \kappa \frac{\partial \theta}{\partial z} = \xi(\theta_b - \theta) \text{ at } z = H_z,
\]

\[\text{(8)}\]

where \( U = \sqrt{u^2 + v^2 + w^2} \).

Here \( m \) is the mass of the particle; \( r \) is the radius of the particle; \( \theta \) is the amount of propagating substance; \( \theta_0 \) is the primary concentration of harmful substances in the atmosphere; \( \sigma \) is the coefficient of absorption of harmful substances in the atmosphere; \( \delta \) is the Dirac function; \( g \) is the acceleration of free fall; \( c_f \) is the drag coefficient of the particles; \( k_f \) is the body shape factor for resistance force; \( F_p \) is the lifting force of the air flow; \( \rho_n \) is the particle density; \( \rho_a \) is the air density; \( \mu_n \) is the air viscosity; \( t \) is time; \( x, y, z \) are the coordinates; \( \mu \) is the diffusion coefficient; \( \beta \) is the coefficient of interaction with the underlying surface; \( Q \) is the source capacity; \( F_0 \) is the number of aerosol particles detached from the roughness of the earth’s surface, \( \kappa \) is the coefficient of turbulence, \( \xi \) is the coefficient to reduce the boundary condition to the dimensional form, \( \theta_b \) is the concentration of suspended substances in adjacent areas of the problems to be solved.

### 3. Method of solution

As the problem (1) - (8) is described by a multidimensional nonlinear partial differential equation with the corresponding initial and boundary conditions, it is difficult to obtain its solution in analytical form. To solve the problem, an implicit finite-difference scheme in time is used with the second order of accuracy in \( x, y, z \), respectively, and a system of algebraic equations is obtained relative to \( \theta \) [6,7]:

\[
\theta_{0,j,k}^{n+\frac{1}{2}} = \frac{b_{i,j,k} \mu - 4 \mu c_{i,j,k}}{a_{i,j,k} \mu - 2\Delta x \xi c_{i,j,k} - 3 \mu c_{i,j,k}} \theta_{i,j,k}^{n+\frac{1}{2}} + \frac{-2\Delta x \xi \theta_{i,j,k} c_{i,j,k} - d_{i,j,k} \mu}{a_{i,j,k} \mu - 2\Delta x \xi c_{i,j,k} - 3 \mu c_{i,j,k}};
\]

\[
\text{where } a_{i,j,k} \theta_{i,j,k}^{n+\frac{1}{2}} - b_{i,j,k} \theta_{i+\frac{1}{2},j,k}^{n+\frac{1}{2}} + c_{i,j,k} \theta_{i-\frac{1}{2},j,k}^{n+\frac{1}{2}} = -d_{i,j,k};
\]

\[
\theta_{N,j,k}^{n+\frac{1}{2}} = \frac{2\Delta x \xi \theta_{0,n-2,j,k} - \beta_{N-2,j,k} \mu - \alpha_{N-2,j,k} \beta_{N-1,j,k} \mu + 4 \beta_{N-1,j,k} \mu}{\alpha_{N-2,j,k} \mu - 4 \alpha_{N-1,j,k} \mu + 2\Delta x \xi + 3 \mu},
\]

where \( \alpha_{0,j,k} \) and \( \beta_{0,j,k} \) are determined by the following way:
$$\alpha_{i,j,k} = \frac{b_{i,j,k} \mu - 4 \mu c_i}{a_{i,j,k} \mu - 2 \Delta x \xi c_{i,j,k} - 3 \mu c_{i,j,k}};$$

$$\beta_{i,j,k} = \frac{-2 \Delta x \xi \theta_{i,j,k} - d_{i,j,k} \mu}{a_{i,j,k} \mu - 2 \Delta x \xi c_{i,j,k} - 3 \mu c_{i,j,k}}$$

and the elements of a transfer matrix — by:

$$a_{i,j,k} = \frac{\mu}{\Delta x};$$

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

$$c_{i,j,k} = \frac{\mu}{\Delta x^2} + \frac{w^{n-1}}{\Delta x};$$

$$d_{i,j,k} = \left( \frac{3}{\Delta t} + \frac{v^{n-1}}{\Delta y} \right) \theta_{i,j,k+1} + \frac{\mu}{\Delta y^2} \theta_{i,j,k} + \frac{\mu}{\Delta y} \theta_{i,j,k-1} + \frac{\kappa_{i,j,k-0.5} + \kappa_{i,j,k+0.5}}{\Delta z^2} \left( \frac{w^{n-1} - w_{i,j,k}}{\Delta z} \right) \theta_{i,j,k+1} + \frac{1}{3} \delta_{i,j,k} Q.$$ 

The values of the concentration sequence $\theta_{i,j,k+1}$, $\theta_{i,j,k+2}$, ..., $\theta_{i,j,k+n}$ are determined by the inverse sweep method.

Similarly, using the above technology on $O_y$ coordinate, we get:

$$\theta_{i,j,k}^{n-1} = \frac{\overline{b}_{i,j,k} \mu - 4 \mu \overline{c}_{i,j,k}}{\overline{a}_{i,j,k} \mu - 2 \Delta y \overline{\xi} c_{i,j,k} - 3 \mu \overline{c}_{i,j,k}} \theta_{i,j,k} - \frac{2 \Delta y \overline{\xi} \theta_{i,j,k} - \overline{d}_{i,j,k} \mu}{\overline{a}_{i,j,k} \mu - 2 \Delta y \overline{\xi} c_{i,j,k} - 3 \mu \overline{c}_{i,j,k}};$$

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

$$\theta_{i,j,k}^{n-1} = \frac{2 \Delta y \xi \theta_{i,j,k} - \overline{\beta}_{i,j,k} \mu - \overline{\alpha}_{i,j,k} \overline{\beta}_{i,j,k} \mu + 4 \overline{\beta}_{i,j,k} \mu}{\overline{\alpha}_{i,j,k} \mu - 2 \Delta y \xi c_{i,j,k} - 3 \mu \overline{c}_{i,j,k}};$$

where, $\overline{\alpha}_{i,j,k}$ and $\overline{\beta}_{i,j,k}$ are determined by the following way:

$$\overline{\alpha}_{i,j,k} = \frac{\overline{b}_{i,j,k} \mu - 4 \mu \overline{c}_{i,j,k}}{\overline{a}_{i,j,k} \mu - 2 \Delta y \overline{\xi} c_{i,j,k} - 3 \mu \overline{c}_{i,j,k}};$$

$$\overline{\beta}_{i,j,k} = \frac{\overline{d}_{i,j,k} \mu - 2 \Delta y \overline{\xi} c_{i,j,k} - 3 \mu \overline{c}_{i,j,k}}{\overline{a}_{i,j,k} \mu};$$

and the elements of transfer matrix on $O_y$ — by:
\[ \tilde{\alpha}_{i,j,k} = \frac{\mu}{\Delta y^2}; \]

\[ \tilde{\eta}_{i,j,k} = \frac{3}{\Delta t} + \frac{2\mu}{\Delta y^2} - \frac{v^2}{\Delta y} + \sigma; \]

\[ \tilde{\xi}_{i,j,k} = \frac{\mu}{\Delta y^2} + \frac{v^2}{\Delta y}; \]

\[ \tilde{a}_{i,j,k} = \left( \frac{3}{\Delta t} + \frac{2\mu}{\Delta x} + \frac{w^2}{\Delta z} - \frac{2\mu}{\Delta x^2} \right) \theta_{i,j,k} + \left( \frac{\mu}{\Delta x} - \frac{u^2}{\Delta x} \right) \theta_{i,j,k}; \]

\[ + \frac{\kappa_{k+0.5}}{\Delta x^2} \theta_{i,j,k-1} + \left( \frac{\kappa_{k+0.5}}{\Delta x^2} - \frac{w^2}{\Delta z} \right) \theta_{i,j,k} + \frac{w}{\Delta z} \theta_{i,j,k+1} + 1 \frac{3}{3} \delta_{i,j,k} Q. \]

The values of the concentration sequence \[ \theta_{i,M-1,k}, \theta_{i,M-2,k}, \ldots, \theta_{i,1,k} \] are determined by the inverse sweep method.

Similarly, using the above technology on \[ Oz \] coordinate and get:

\[ \theta_{i,j,0}^{n+1} = \frac{4\kappa_c}{3\kappa_c - \tilde{a}_{i,j,1} \kappa} - \frac{2\Delta \beta}{\Delta \beta} \theta_{i,j,1}^{n+1} + \frac{\tilde{m}_{i,j,1} \kappa + 2F_0 \Delta z \tilde{c}_{i,j,1}}{3\kappa_c - \tilde{a}_{i,j,1} \kappa - 2\Delta \beta}; \]

\[ \tilde{a}_{i,j,k}^{n+1} - \tilde{b}_{i,j,k} \theta_{i,j,k} + \tilde{c}_{i,j,k} \theta_{i,j,k} = -\tilde{\eta}_{i,j,k}, \]

\[ \theta_{i,j,0}^{n+1} = \frac{4\tilde{\alpha}_{i,j,1} - \tilde{\alpha}_{i,j,1} \kappa - \tilde{\beta}_{i,j,1} \kappa - \tilde{\beta}_{i,j,1} \kappa}{\tilde{a}_{i,j,1} - 4\tilde{a}_{i,j,1} + 3} = \frac{4 - \tilde{a}_{i,j,1} - \tilde{\beta}_{i,j,1} \kappa - \tilde{\beta}_{i,j,1} \kappa}{\tilde{a}_{i,j,1} - 4\tilde{a}_{i,j,1} + 3}, \]

where \[ \tilde{a}_{i,j,0} \] and \[ \tilde{b}_{i,j,0} \] are determined by the following way:

\[ \tilde{a}_{i,j,0} = \frac{4\kappa \tilde{c}_{i,j,1} - \tilde{p}_{i,j,1} \kappa}{3\kappa \tilde{c}_{i,j,1} - \tilde{a}_{i,j,1} \kappa - 2\Delta \beta}; \]

\[ \tilde{b}_{i,j,0} = \frac{\tilde{d}_{i,j,1} \kappa + 2\Delta \beta \tilde{c}_{i,j,1} F_0}{3\kappa \tilde{c}_{i,j,1} - \tilde{a}_{i,j,1} \kappa - 2\Delta \beta} \]

and the elements of the transfer matrix on \[ Oz \] by:

\[ \tilde{a}_{i,j,k} = \frac{\kappa_{k+0.5}}{\Delta z^2}; \]

\[ \tilde{b}_{i,j,k} = \frac{3}{\Delta t} + \frac{\kappa_{k+0.5} + \kappa_{k+0.5}}{\Delta z^2} - \frac{w - w^{n+1}}{\Delta z} + \sigma; \]
\[ \omega_{i,j,k} = \frac{\kappa_{x=0.5}}{\Delta z^2} + \frac{w - w^{(n+1)}}{\Delta z}; \]

\[ \overline{t}_{i,j,k} = \frac{3}{\Delta t} + \frac{u^{(n+1)}}{\Delta x} + \frac{v^{(n+1)}}{\Delta y} - \frac{2\mu}{\Delta x^2} \theta_{i,j,k}^{(n+1)} + \frac{2\mu}{\Delta y^2} \theta_{i,j-1,k}^{(n+1)} + \left( \frac{\mu}{\Delta x^2} - \frac{u^{(n+1)}}{\Delta x} \right) \theta_{i+1,j,k}^{(n+1)} + \left( \frac{\mu}{\Delta y^2} - \frac{v^{(n+1)}}{\Delta y} \right) \theta_{i,j+1,k}^{(n+1)} + \frac{1}{3} \delta_{i,j,k} Q. \]

The values of the concentration sequence \( \theta_{i,j,k}^{(n+1)}, \theta_{i,j-1,k}^{(n+1)}, \ldots, \theta_{i,j+1,k}^{(n+1)} \) are determined by the inverse sweep method.

To solve equation (2), an implicit scheme is used:

\[ \frac{u^{(n+1)} - u^n}{\Delta t/3} = \frac{c_f \pi r^2 \rho_e \left( 2u^{(n+1) - \bar{u}^2} - 2u^{(n+1)} U + U^2 \right)}{m}; \]

\[ \frac{u^{(n+1)} - u^{(n-1)}}{\Delta t/3} = \frac{c_f \pi r^2 \rho_e \left( 2u^{(n+1) - \bar{u}^2} - 2u^{(n+1)} U + U^2 \right)}{m}; \]

\[ \frac{u^{(n+1)} - u^n}{\Delta t/3} = \frac{c_f \pi r^2 \rho_e \left( 2u^{(n+1) - \bar{u}^2} - 2u^{(n+1)} U + U^2 \right)}{m}. \]

To solve equation (3), an implicit scheme is used:

\[ \frac{v^{(n+1)} - v^n}{\Delta t/3} = \frac{c_f \pi r^2 \rho_e \left( 2\bar{v}^{(n+1) - \bar{v}^2} - 2v^{(n+1)} U + U^2 \right)}{m}; \]

\[ \frac{v^{(n+1)} - v^{(n-1)}}{\Delta t/3} = \frac{c_f \pi r^2 \rho_e \left( 2\bar{v}^{(n+1) - \bar{v}^2} - 2v^{(n+1)} U + U^2 \right)}{m}; \]

\[ \frac{v^{(n+1)} - v^n}{\Delta t/3} = \frac{c_f \pi r^2 \rho_e \left( 2v^{(n+1) - \bar{v}^2} - 2v^{(n+1)} U + U^2 \right)}{m}. \]

Similarly, to solve equation (4), an implicit scheme is used:

\[ \frac{w^{(n+1)} - w^n}{\Delta t/3} = \frac{-4\pi r^3 \left( \rho_n - \rho_e \right) g - 3k_f \mu_e \pi r w^{(n+1)} + 3F_n}{3m}; \]

\[ \frac{w^{(n+1)} - w^{(n-1)}}{\Delta t/3} = \frac{-4\pi r^3 \left( \rho_n - \rho_e \right) g - 3k_f \mu_e \pi r w^{(n+1)} + 3F_n}{3m}; \]

\[ \frac{w^{(n+1)} - w^n}{\Delta t/3} = \frac{-4\pi r^3 \left( \rho_n - \rho_e \right) g - 3k_f \mu_e \pi r w^{(n+1)} + 3F_n}{3m}. \]
The convergence of the iterative process is verified using the following conditions:

\[ \left| s^{(s+1)} - s^{(s)} \right| < \epsilon; \left| v^{(s+1)} - v^{(s)} \right| < \epsilon; \left| w^{(s+1)} - w^{(s)} \right| < \epsilon. \]

Here \( \epsilon \) is the required accuracy of the solution; \( S \) is the number of iterations, the initial iterative value is chosen equal to the solution at the previous time layer.

4. Conclusions
To predict, monitor and assess the ecological state of the atmosphere and underlying surface with passive and active impurities, a mathematical model has been developed that takes into account the varying rate of displacements of particles in the atmosphere.

To determine the rate of displacements of fine-dispersed particles in the atmosphere, a system of nonlinear equations is obtained, which takes into account the basic physicomechanical properties of the particles and the rate of displacements of the atmospheric air mass, which play an important role.

As the developed nonlinear mathematical model for monitoring and predicting the propagation of aerosol particles in the atmosphere is described by a multidimensional nonlinear partial differential equation with corresponding initial and boundary conditions, a numerical algorithm using an implicit finite difference scheme is developed.

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