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NONLINEAR MATHEMATICAL MODEL FOR MONITORING AND FORECASTING THE PROCESS OF DISTRIBUTING AEROSOL PARTICLES IN THE ATMOSPHERE

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Abstract. In this article there was developed a mathematical model for predicting, monitoring and assessing the ecological state of the atmosphere and underlying surface by passive and active impurities, where the varying velocity of particles in the atmosphere are considered. The successful solution of the tasks of monitoring and predicting the level of atmospheric pollution by harmful substances released from production facilities into the environment is based on the use of mathematical models that take into account the physical characteristics of the propagation of impurities, the relationship between the concentrations of impurities and environmental parameters: change in wind speed and direction over time, harmful absorption coefficient substances into the atmosphere, the rate of deposition of fine particles, soil properties, etc.

To determine the speed of movement of fine particles in the atmosphere, a system of nonlinear equations has obtained, where the basic physic mechanical properties of the particles and the velocity of the air mass in the atmosphere were considered, which play an important role. A qualitative analysis of the solution has been carried out and a numerical algorithm has been compiled for conducting a computational experiment on a computer.

Since the developed nonlinear mathematical model is described by a multidimensional nonlinear partial differential equation with the corresponding initial and boundary conditions, a numerical algorithm using an implicit finite-difference scheme is developed to solve it.

Keywords: mathematical model, transfer and diffusion of harmful substances, climatic factor, numerical algorithm.

Introduction

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

Today, analysis of environmental data shows that the intensive growth of industrial volume 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 the USA, Russia, France, India, Japan, Korea and others. Of course, the growth rate of production development has a negative effect on the ecological status of industrial regions. The deterioration of ecology in the atmosphere of industrial zones arises due to an increase in the concentration of harmful substances and gas pollution of the atmosphere.

Hazardous air pollution affects people's health, as various chemical elements are absorbed most intensively by the body during breathing. Thus, the relevance of mathematical modelling of the propagation of harmful aerosol particles is obvious.

Mathematical modelling of the transfer process, diffusion and harmful substances (carbon dioxide, fine aerosol passive and active particles) into the atmosphere are engaged in scientific schools created under the guidance of G.I. Marchuk, V.V. Penenko, A.E. Aloyan, L.T. Matveeva, V.P. Dymnikova I.E. Naatsa, E.A. Zakarina, I.A. Kibel, L.N. Gutman, FB 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, Kh. Zidisk, K.A. Welds, K.I. Nappo, J. Gotaas, M. Mullioland, S. Trap, M. Maties, V. Edelman, and others.

The author [1] proposed a numerical algorithm for solving the equations of propagation of impurities in the atmosphere. As an example of nonlinear difference schemes for solving the transport equation, a monotone scheme developed by Van Lear was used and which was based on a non-linear scheme by Fromm that approximates the original differential equation with a second order of accuracy in spatial variables and in time.

In the works [2-5], achievements in the field of mathematical and numerical modelling of unsteady 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 the transfer and scattering of aerosols, using operational information of a meteorological nature.

In the work [6], the types of environmental pollutants were considered from the point of view of the choice of fuel characteristics for thermal power plants. The list of emissions of large industrial zones by type of pollutants and their physic-chemical properties is indicated. In the study, impact assessment was performed using baseline data for the worst-case using Gauss formulas. Based on the software created, an assessment of the quality of atmospheric air in the considered regions of India has been carried out.

In the article [7] a mathematical model was developed for determining the concentration of pollutants in the air as a function of time and frequency averaging. The author demonstrated how the proposed model can be used to correlate air quality criteria with air quality standards and emission standards.

In the work [8], using mathematical modeling, two-dimensional modeling of the wind field and dispersion of pollutants in parallel street arrays was performed, and the results were compared with the available experimental data in a wind tunnel. From the calculations performed, it was demonstrated that rapid chemical reactions with consequences for the concentrations of certain pollutants are of great danger to health.

In the work [9], based on solving a nonstationary turbulent diffusion equation with given values of the components of wind speed u, v, w, diffusion coefficient - μ and turbulent mixing coefficient - k, a new formula was obtained for calculating the fields of air pollution concentrations created by point or other industrial sources where the formula takes into account the interaction of the processes of scattering and transfer of impurities in the direction of the axes of the Cartesian coordinate system.

The author has found computational formulas that allow to obtain concentration fields over surfaces of any complexity, under any meteorological conditions and wind speeds, including when calm.

In the article [10] there was made an analysis of long-term environmental forecasting using mathematical modelling using available information about the long-term climate dynamics. The processes of describing the mathematical model of hydrodynamics in the climate system, models of transfer and transformation of moisture, chemically and optically active pollutants in gas and aerosol states are investigated. The authors developed a set of models used to solve scientific and practical problems, to assess the environmental prospects of industrial regions.

In the article [11], numerical 3D models were proposed for estimating the level of air pollution by motor vehicle emissions. A feature of the proposed numerical models is the ability to predict the level of air pollution in the conditions of development. Motor vehicle emissions are modelled by a series of point sources, which are specified using the Dirac delta function. The proposed models provide an opportunity to quickly obtain information about the level of air pollution in areas where motorways pass.

In the article [12] the problems of modelling the process of atmospheric pollution using ecological and biological models of the logistic type and the Gause type, as well as the refinement and forecasting of the process development using the Prony method are considered. To solve the first problem, two models were built: logistic, which does not consider the cleaning process and the Lotka-Volterra model, in which the cleaning processes are already considered.

In the article [13], a mathematical model for calculating atmospheric pollution was developed based on a "torch" type model. This model considers the possibility of calculating atmospheric pollution by several point sources, the rate of emission of a pollutant, the distance of the measurement point from the source of pollution, the speed and direction of the wind, the stability of the atmosphere, deviations of torch sizes in horizontal and vertical directions.

By the authors of the work [14] there was considered the modelling of the state of atmospheric air quality using various mathematical approaches describing physical and chemical processes that are modelled depending on the type of pollution, emission parameters, meteorological, topographical and other conditions affecting the dispersion of pollutants.

In the article [15] the protection of the air basin, based on compliance with the standards of quality of the atmosphere, including the factor of chemical pollution is considered. It is emphasized by an important link in the scheme of rationing the purity of air is the calculation of the concentrations generated by various sources, for example, pipes of industrial enterprises, vehicles and air transport.

In the article [16], an effective model of direct numerical modelling of dispersion of toxic gases in the atmosphere, considering the terrain relief, was proposed. The calculation of the velocity field of the wind flow is carried out based on the potential flow. The method of marking the design domain used in the model makes it possible to form any geometric shape of the relief.

In the articles [17-20], an actual problem is considered related to solving the problem of monitoring and forecasting the ecological state of the air basin of industrial regions, where there is an imbalance in the sanitary norms of the environment due to the large amount of emissions of harmful substances. To solve this problem, a mathematical model has been developed that describes the process in question using the equations of hydromechanics with the corresponding initial and boundary conditions.

A detailed analysis of scientific papers related to the problem of mathematical modelling of the process of transfer and diffusion of aerosol particles in the atmosphere showed that in mathematical modelling and the study of the spread of harmful substances in the atmosphere, firstly, the change in wind speed in directions, which varies with time and from changes in the speeds of the air flow of air is not considered, secondly, in all the mathematical models of the process, the absorption coefficient of aerosol particles was taken DC, in the third, it was assumed that the spread of harmful substances emitted from sources does not reach the borders of the area under consideration for solving the problem and there is no inflow and outflow of harmful substances through them.

Based on the foregoing, the purpose of this article is to develop a non-linear mathematical model for monitoring and predicting the process of transfer and diffusion of harmful substances in the atmosphere of industrial regions. This model should consider the possibility of calculating atmospheric pollution by sources, wind speed and direction, sedimentation of impurity particles, as well as weather and climatic factors.

Main part

Statement of the problem. To study the process of transport and diffusion of aerosol particles in the atmosphere, considering the essential parameters u, v, w of the components of the wind speed in directions x, y, z and the deposition rate of fine particles w_g, respectively, we consider a mathematical model describing, based on the law of hydromechanics, using the multidimensional partial differential equation.

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

$$m\frac{du}{dt}=c_f\pi r^2\rho_в(u-U)^2; \quad (2)$$

$$m\frac{dv}{dt}=c_f\pi r^2\rho_в(v-U)^2; \quad (3)$$

$$m\frac{dw_g}{dt}=-\frac{4}{3}\pi r^3(\rho_n-\rho_в)g-k_f\mu_в\pi r w_g+F_n \quad (4)$$

and the corresponding initial and boundary conditions:

$$\theta(x,y,z,0)=\theta_0(x,y,z),$$

$$\hat{u}=u(0),\ \ \hat{v}=v(0),\ \ \hat{w}_g=w_g(0),\ \ \text{at } t=0, \quad (5)$$

$$-\mu\frac{\partial\theta}{\partial x}=\xi(\theta_b-\theta)\ \text{at}\ x=0, \quad (6)$$

$$\mu\frac{\partial\theta}{\partial x}=\xi(\theta_b-\theta)\ \text{at}\ x=L_x, \quad (7)$$

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

$$\mu\frac{\partial\theta}{\partial y}=\xi(\theta_b-\theta)\ \text{at}\ y=\mathrm{L_y}, \quad (9)$$

$$-\kappa\frac{\partial\theta}{\partial z}=(\beta\theta-F_0),\ \text{at}\ z=0 \quad (10)$$

$$\kappa\frac{\partial\theta}{\partial z}=\xi\left(\theta_b-\theta\right),\ \text{at}\ z=H_z \quad (11)$$

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

Here m is the particle mass; r is the radius of the particle; θ is the amount of propagating substance; θ_0 is the primary concentration of harmful substances in the atmosphere; σ is the coefficient of absorption of harmful substances in the atmosphere; δ is Dirac function; g is free fall acceleration; c_f isthe coefficient of drag of particles; k_f is the body shape factor for resistance force; F_n is the lifting force of the air flow; ρ_n is the particle density; $\rho_в$ is the air density; $\mu_в$ is air viscosity; t is time; x, y, z are the coordinates; μ is the diffusion coefficient; β is the coefficient of interaction with the underlying surface; Q is the power sources; F_0 is the number of aerosol particles detached from the roughness of the earth's surface; κ is the coefficient of turbulence; ξ is the coefficient for carrying out the boundary condition to the dimensional form; θ_b is the concentration of suspended substances in the neighbouring areas of the tasks.

Solution Method. Since the problem (1) - (11) is described by a multidimensional nonlinear partial (1)differential equation with the corresponding initial and boundary conditions, it is difficult to obtain its solution in analytical form. To solve the problem, we use an (2) implicit finite-difference scheme in time with the second order of accuracy, respectively, in x, y and z:

$$\frac{\theta_{i,j,k}^{n+\frac{1}{3}}-\theta_{i,j,k}^{n}}{\Delta t/3}+u^{n+\frac{1}{3}}\frac{\theta_{i+1,j,k}^{n+\frac{1}{3}}-\theta_{i,j,k}^{n+\frac{1}{3}}}{\Delta x}+v^{n+\frac{1}{3}}\frac{\theta_{i,j+1,k}^{n}-\theta_{i,j,k}^{n}}{\Delta y}+\left(w-w_g^{n+\frac{1}{3}}\right)\frac{\theta_{i,j,k+1}^{n}-\theta_{i,j,k}^{n}}{\Delta z}+$$
$$+\sigma\theta_{i,j,k}^{n+\frac{1}{3}}=\mu\frac{\theta_{i+1,j,k}^{n+\frac{1}{3}}-2\theta_{i,j,k}^{n+\frac{1}{3}}+\theta_{i-1,j,k}^{n+\frac{1}{3}}}{\Delta x^2}+\mu\frac{\theta_{i,j+1,k}^{n}-2\theta_{i,j,k}^{n}+\theta_{i,j-1,k}^{n}}{\Delta y^2}+$$
$$+\frac{\kappa_{k+0,5}\theta_{i,j,k+1}^{n}-\left(\kappa_{k+0,5}+\kappa_{k-0,5}\right)\theta_{i,j,k}^{n}+\kappa_{k-0,5}\theta_{i,j,k-1}^{n}}{\Delta z^2}+\frac{1}{3}\delta_{i,j,k}Q;$$

open the brackets, we get the form:

$$\frac{3}{\Delta t}\theta_{i,j,k}^{n+\frac{1}{3}}-\frac{3}{\Delta t}\theta_{i,j,k}^{n}+\frac{u^{n+\frac{1}{3}}}{\Delta x}\theta_{i+1,j,k}^{n+\frac{1}{3}}-\frac{u^{n+\frac{1}{3}}}{\Delta x}\theta_{i,j,k}^{n+\frac{1}{3}}+$$
$$+\frac{v^{n+\frac{1}{3}}}{\Delta y}\theta_{i,j+1,k}^{n}-\frac{v^{n+\frac{1}{3}}}{\Delta y}\theta_{i,j,k}^{n}+\frac{w-w_g^{n+\frac{1}{3}}}{\Delta z}\theta_{i,j,k+1}^{n}-$$
$$-\frac{w-w_g^{n+\frac{1}{3}}}{\Delta z}\theta_{i,j,k}^{n}+\sigma\theta_{i,j,k}^{n+\frac{1}{3}}=\frac{\mu}{\Delta x^2}\theta_{i+1,j,k}^{n+\frac{1}{3}}-\frac{2\mu}{\Delta x^2}\theta_{i,j,k}^{n+\frac{1}{3}}+$$
$$+\frac{\mu}{\Delta x^2}\theta_{i-1,j,k}^{n+\frac{1}{3}}+\frac{\mu}{\Delta y^2}\theta_{i,j+1,k}^{n}-\frac{2\mu}{\Delta y^2}\theta_{i,j,k}^{n}+$$
$$+\frac{\mu}{\Delta y^2}\theta_{i,j-1,k}^{n}+\frac{\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k+1}^{n}-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k}^{n}+$$
$$+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta_{i,j,k-1}^{n}+\frac{1}{3}\delta_{i,j,k}Q;$$

Next, we introduce the notation:

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

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

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

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

$$+\left(\frac{\kappa_{k-0,5}}{\Delta z^2}-\frac{w-w_g^{n+\frac{1}{3}}}{\Delta z}\right)\theta^n_{i,j,k+1}+\frac{1}{3}\delta_{i,j,k}Q;$$

as a result, the equation can be reduced to a three-diagonal system of linear algebraic equations:

$$a_{i,j,k}\theta^{n+\frac{1}{3}}_{i-1,j,k}-b_{i,j,k}\theta^{n+\frac{1}{3}}_{i,j,k}+c_{i,j,k}\theta^{n+\frac{1}{3}}_{i+1,j,k}=-d_{i,j,k}\tag{12}$$

Now, by approximating the boundary condition (6), we obtain:

$$-\mu\frac{-3\theta^{n+\frac{1}{3}}_{0,j,k}+4\theta^{n+\frac{1}{3}}_{1,j,k}-\theta^{n+\frac{1}{3}}_{2,j,k}}{2\Delta x}=\xi\left(\theta_b-\theta^{n+\frac{1}{3}}_{0,j,k}\right)$$

or

$$3\mu\theta^{n+\frac{1}{3}}_{0,j,k}-4\mu\theta^{n+\frac{1}{3}}_{1,j,k}+\mu\theta^{n+\frac{1}{3}}_{2,j,k}=$$

$$=2\Delta x\xi\theta_b-2\Delta x\xi\theta^{n+\frac{1}{3}}_{0,j,k}\tag{13}$$

Further, from equation (12) we find $\theta^{n+\frac{1}{3}}_{2,j,k}$:

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

Substituting $\theta^{n+\frac{1}{3}}_{2,j,k}$ from (14) into (13) we find $\theta^{n+\frac{1}{3}}_{0,j,k}$ in the following way:

$$3\mu\theta^{n+\frac{1}{3}}_{0,j,k}-4\mu\theta^{n+\frac{1}{3}}_{1,j,k}-\frac{a_{1,j,k}\mu}{c_{1,j,k}}\theta^{n+\frac{1}{3}}_{0,j,k}+\frac{b_{1,j,k}\mu}{c_{1,j,k}}\theta^{n+\frac{1}{3}}_{1,j,k}-$$

$$-\frac{d_{1,j,k}\mu}{c_{1,j,k}}=2\Delta x\xi\theta_b-2\Delta x\xi\theta^{n+\frac{1}{3}}_{0,j,k};$$

or

$$\left(-\frac{a_{1,j,k}\mu}{c_{1,j,k}}+2\Delta x\xi+3\mu\right)\theta^{n+\frac{1}{3}}_{0,j,k}=$$

$$=\left(-\frac{b_{1,j,k}\mu}{c_{1,j,k}}+4\mu\right)\theta^{n+\frac{1}{3}}_{1,j,k}+\frac{d_{1,j,k}\mu}{c_{1,j,k}}+2\Delta x\xi\theta_b;$$

in the end, we get:

$$\theta^{n+\frac{1}{3}}_{0,j,k}=\frac{b_{1,j,k}\mu-4\mu c_{1,j,k}}{a_{1,j,k}\mu-2\Delta\xi xc_{1,j,k}-3\mu c_{1,j,k}}\theta^{n+\frac{1}{3}}_{1,j,k}+$$

$$+\frac{-2\Delta x\xi\theta_b c_{1,j,k}-d_{1,j,k}\mu}{a_{1,j,k}\mu-2\Delta x\xi c_{1,j,k}-3\mu c_{1,j,k}}$$

where $\alpha_{0,j,k}$ and $\beta_{0,j,k}$ are defined in the following way:

$$\alpha_{0,j,k}=\frac{b_{1,j,k}\mu-4\mu c_1}{a_{1,j,k}\mu-2\Delta x\xi c_{1,j,k}-3\mu c_{1,j,k}};$$

$$\beta_{0,j,k}=\frac{-2\Delta x\xi\theta_b c_{1,j,k}-d_{1,j,k}\mu}{a_{1,j,k}\mu-2\Delta x\xi c_{1,j,k}-3\mu c_{1,j,k}}.\tag{15}$$

Now, by approximating the boundary condition (7), we obtain:

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

or

$$\mu\theta_{N-2,j,k}-4\mu\theta_{N-1,j,k}+3\mu\theta_{N,j,k}=$$

$$=2\Delta x\xi\theta_b-2\Delta x\xi\theta_{N,j,k}\tag{16}$$

Using the sweep method for the sequence N, N-1 and N-2 we find $\theta^{n+\frac{1}{3}}_{N-1,j,k}$ and $\theta^{n+\frac{1}{3}}_{N-2,j,k}$:

$$\theta^{n+\frac{1}{3}}_{N-1,j,k}=\alpha_{N-1,j,k}\theta^{n+\frac{1}{3}}_{N-1,j,k}+\beta_{N-1,j,k};\tag{17}$$

$$\theta_{N-2,j,k}=\alpha_{N-2,j,k}\theta_{N-1,j,k}+\beta_{N-2,j,k}=$$
$$=\alpha_{N-2,j,k}\left(\alpha_{N-1,j,k}\theta_{N,j,k}+\beta_{N-1,j,k}\right)+$$
$$+\beta_{N-2,j,k}=\alpha_{N-2,j,k}\alpha_{N-1,j,k}\theta_{N,j,k}+$$
$$+\alpha_{N-2,j,k}\beta_{N-1,j,k}+\beta_{N-2,j,k}.\tag{18}$$

Substituting $\theta^{n+\frac{1}{3}}_{N-1,j,k}$ and $\theta^{n+\frac{1}{3}}_{N-2,j,k}$ from (18), (19) into (17) we find $\theta^{n+\frac{1}{3}}_{N,j,k}$:

$$\alpha_{N-2,j,k}\alpha_{N-1,j,k}\mu\theta^{n+\frac{1}{3}}_{N,j,k}+\alpha_{N-2,j,k}\beta_{N-1,j,k}\mu+$$

$$+\beta_{N-2,j,k}\mu-4\alpha_{N-1,j,k}\mu\theta^{n+\frac{1}{3}}_{N,j,k}-$$

$$-4\beta_{N-1,j,k}\mu+3\mu\theta^{n+\frac{1}{3}}_{N,j,k}=$$

$$=2\Delta x\xi\theta_b-2\Delta x\xi\theta^{n+\frac{1}{3}}_{N,j,k};$$

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

$$\theta_{N,j,k}^{n+\frac{1}{3}}=\frac{2\Delta x\xi\theta_b-\beta_{N-2,j,k}\mu-\alpha_{N-2,j,k}\beta_{N-1,j,k}\mu+4\beta_{N-1,j,k}\mu}{\alpha_{N-2,j,k}\alpha_{N-1,j,k}\mu-4\alpha_{N-1,j,k}\mu+2\Delta x\xi+3\mu}; \quad (19)$$

Concentration sequence values $\theta_{N-1,j,k}^{n+\frac{1}{3}}$, $\theta_{N-2,j,k}^{n+\frac{1}{3}}$, ..., $\theta_{1,j,k}^{n+\frac{1}{3}}$ determined by the method of reverse sweep. Similarly, using the above technology on the coordinate OY we get:

$$\frac{\theta_{i,j,k}^{n+\frac{2}{3}}-\theta_{i,j,k}^{n+\frac{1}{3}}}{\Delta t/3}+u^{n+\frac{2}{3}}\frac{\theta_{i+1,j,k}^{n+\frac{1}{3}}-\theta_{i,j,k}^{n+\frac{1}{3}}}{\Delta x}+v^{n+\frac{2}{3}}\frac{\theta_{i,j+1,k}^{n+\frac{2}{3}}-\theta_{i,j,k}^{n+\frac{2}{3}}}{\Delta y}+$$

$$+\left(w-w_g^{n+\frac{2}{3}}\right)\frac{\theta_{i,j,k+1}^{n+\frac{1}{3}}-\theta_{i,j,k}^{n+\frac{1}{3}}}{\Delta z}+\sigma\theta_{i,j,k}^{n+\frac{2}{3}}=$$

$$=\mu\frac{\theta_{i+1,j,k}^{n+\frac{1}{3}}-2\theta_{i,j,k}^{n+\frac{1}{3}}+\theta_{i-1,j,k}^{n+\frac{1}{3}}}{\Delta x^2}+\mu\frac{\theta_{i,j+1,k}^{n+\frac{2}{3}}-2\theta_{i,j,k}^{n+\frac{2}{3}}+\theta_{i,j-1,k}^{n+\frac{2}{3}}}{\Delta y^2}+$$

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

open the brackets, we get the form:

$$\frac{3}{\Delta t}\theta_{i,j,k}^{n+\frac{2}{3}}-\frac{3}{\Delta t}\theta_{i,j,k}^{n+\frac{1}{3}}+\frac{u^{n+\frac{2}{3}}}{\Delta x}\theta_{i+1,j,k}^{n+\frac{1}{3}}-$$

$$-\frac{u^{n+\frac{2}{3}}}{\Delta x}\theta_{i,j,k}^{n+\frac{1}{3}}+\frac{v^{n+\frac{2}{3}}}{\Delta y}\theta_{i,j+1,k}^{n+\frac{2}{3}}-\frac{v^{n+\frac{2}{3}}}{\Delta y}\theta_{i,j,k}^{n+\frac{2}{3}}+$$

$$+\frac{w-w_g^{n+\frac{2}{3}}}{\Delta z}\theta_{i,j,k+1}^{n+\frac{1}{3}}-\frac{w-w_g^{n+\frac{2}{3}}}{\Delta z}\theta_{i,j,k}^{n+\frac{1}{3}}+$$

$$+\sigma\theta_{i,j,k}^{n+\frac{2}{3}}=\frac{\mu}{\Delta x^2}\theta_{i+1,j,k}^{n+\frac{1}{3}}-\frac{2\cdot\mu}{\Delta x^2}\theta_{i,j,k}^{n+\frac{1}{3}}+$$

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

$$+\frac{\mu}{\Delta y^2}\theta_{i,j-1,k}^{n+\frac{2}{3}}+\frac{\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k+1}^{n+\frac{1}{3}}-$$

$$-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k}^{n+\frac{1}{3}}+$$

$$+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta_{i,j,k-1}^{n+\frac{1}{3}}+\frac{1}{3}\delta_{i,j,k}Q;$$

We introduce the following notation:

$$\overline{a}_{i,j,k}=\frac{\mu}{\Delta y^2};\qquad \overline{b}_{i,j,k}=\frac{3}{\Delta t}+\frac{2\mu}{\Delta y^2}-\frac{v^{n+\frac{2}{3}}}{\Delta y}+\sigma;$$

$$\overline{c}_{i,j,k}=\frac{\mu}{\Delta y^2}+\frac{v^{n+\frac{2}{3}}}{\Delta y};$$

-

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

$$+\frac{\mu}{\Delta x^2}\theta_{i-1,j,k}^{n+\frac{1}{3}}+\left(\frac{\mu}{\Delta x^2}-\frac{u^{n+\frac{2}{3}}}{\Delta x}\right)\theta_{i+1,j,k}^{n+\frac{1}{3}}+$$

$$+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta_{i,j,k-1}^{n+\frac{1}{3}}+\left(\frac{\kappa_{k-0,5}}{\Delta z^2}-\frac{w-w_g^{n+\frac{2}{3}}}{\Delta z}\right)\theta_{i,j,k+1}^{n+\frac{1}{3}}+\frac{1}{3}\delta_{i,j,k}Q;$$

as a result, the equation can be reduced to a three-diagonal system of linear algebraic equations:

$$\overline{a}_{i,j,k}\theta_{i,j-1,k}^{n+\frac{2}{3}}-\overline{b}_{i,j,k}\theta_{i,j,k}^{n+\frac{2}{3}}+\overline{c}_{i,j,k}\theta_{i,j+1,k}^{n+\frac{2}{3}}=-\overline{d}_{i,j,k} \quad (20)$$

Now, by approximating the boundary condition (8), we obtain:

$$-\mu\frac{-3\theta_{i,0,k}^{n+\frac{2}{3}}+4\theta_{i,1,k}^{n+\frac{2}{3}}-\theta_{i,2,k}^{n+\frac{2}{3}}}{2\Delta y}=\xi\left(\theta_b-\theta_{i,0,k}^{n+\frac{2}{3}}\right)$$

or

$$3\mu\theta_{i,0,k}^{n+\frac{2}{3}}-4\mu\theta_{i,1,k}^{n+\frac{2}{3}}+\mu\theta_{i,2,k}^{n+\frac{2}{3}}=$$

$$=2\Delta y\xi\theta_b-2\Delta y\xi\theta_{i,0,k}^{n+\frac{2}{3}} \quad (21)$$

Further, from equation (20) we find $\theta_{i,2,k}^{n+\frac{2}{3}}$:

$$\theta_{i,2,k}^{n+\frac{2}{3}}=-\frac{\overline{a}_{i,1,k}}{\overline{c}_{i,1,k}}\theta_{i,0,k}^{n+\frac{2}{3}}+$$

$$+\frac{\overline{b}_{i,1,k}}{\overline{c}_{i,1,k}}\theta_{i,1,k}^{n+\frac{2}{3}}-\frac{\overline{d}_{i,1,k}}{\overline{c}_{i,1,k}}. \quad (22)$$

Substituting $\theta_{i,2,k}^{n+\frac{2}{3}}$ from (22) into (21) we find $\theta_{i,0,k}^{n+\frac{2}{3}}$:

$$3\mu\theta_{i,0,k}^{n+\frac{2}{3}}-4\mu\theta_{i,1,k}^{n+\frac{2}{3}}-\frac{\overline{a}_{i,1,k}}{\overline{c}_{i,1,k}}\theta_{i,0,k}^{n+\frac{2}{3}}+\frac{\overline{b}_{i,1,k}\mu}{\overline{c}_{i,1,k}}\theta_{i,1,k}^{n+\frac{2}{3}}-$$

$$-\frac{\overline{d}_{i,1,k}\mu}{\overline{c}_{i,1,k}}=2\Delta y\xi\theta_b-2\Delta y\xi\theta_{i,0,k}^{n+\frac{2}{3}};$$

or

$$\left(-\frac{\bar{a}_{i,1,k}\mu}{\bar{c}_{i,1,k}}+2\Delta y\xi+3\right)\theta_{i,0,k}^{n+\frac{2}{3}}=$$

$$=\left(-\frac{\bar{b}_{i,1,k}\mu}{\bar{c}_{i,1,k}}+4\mu\right)\theta_{i,1,k}^{n+\frac{2}{3}}+\frac{\bar{d}_{i,1,k}\mu}{\bar{c}_{i,1,k}}+2\Delta y\xi\theta_b;$$

in the end, we get:

$$\theta_{i,0,k}^{n+\frac{2}{3}}=\frac{\bar{b}_{i,1,k}\mu-4\mu\bar{c}_{i,1,k}}{\bar{a}_{i,1,k}\mu-2\Delta y\xi\bar{c}_{i,1,k}-3\mu\bar{c}_{i,1,k}}\theta_{i,1,k}^{n+\frac{2}{3}}+$$

$$+\frac{-2\Delta y\bar{c}_{i,1,k}\xi\theta_b-\bar{d}_{i,1,k}\mu}{\bar{a}_{i,1,k}\mu-2\Delta y\bar{c}_{i,1,k}-3\mu\bar{c}_{i,1,k}};$$

where, $\bar{\alpha}_{i,0,k}$ $\bar{\beta}_{i,0,k}$ and are defined in the following way:

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

$$\bar{\beta}_{i,0,k}=\frac{-2\Delta y\xi\theta_b\bar{c}_{i,1,k}-\bar{d}_{i,1,k}\mu}{\bar{a}_{i,1,k}\mu-2\Delta y\xi\bar{c}_{i,1,k}-3\mu\bar{c}_{i,1,k}}; \qquad (23)$$

Now, by approximating the boundary condition (9), we obtain:

$$\mu\frac{\theta_{i,M-2,k}^{n+\frac{2}{3}}-4\theta_{i,M-1,k}^{n+\frac{2}{3}}+3\theta_{i,M,k}^{n+\frac{2}{3}}}{2\Delta y}=$$

$$=\xi\left(\theta_b-\theta_{i,M,k}^{n+\frac{2}{3}}\right)$$

or

$$\mu\theta_{i,M-2,k}^{n+\frac{2}{3}}-4\mu\theta_{i,M-1,k}^{n+\frac{2}{3}}+3\mu\theta_{i,M,k}^{n+\frac{2}{3}}=$$

$$=2\Delta y\xi\theta_b-2\Delta y\xi\theta_{i,M,k}^{n+\frac{2}{3}} \qquad (24)$$

Using the sweep method for the sequence M, M-1 and M-2, we find $\theta_{i,M-1,k}^{n+\frac{2}{3}}$ and $\theta_{i,M-2,k}^{n+\frac{2}{3}}$:

$$\theta_{i,M-1,k}^{n+\frac{2}{3}}=\bar{\alpha}_{i,M-1,k}\theta_{i,M,k}^{n+\frac{2}{3}}+\bar{\beta}_{i,M-1,k}; \qquad (25)$$

$$\theta_{i,M-2,k}^{n+\frac{2}{3}}=\bar{\alpha}_{i,M-2,k}\theta_{i,M-1,k}^{n+\frac{2}{3}}+\bar{\beta}_{i,M-2,k}=$$

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

$$+\bar{\beta}_{i,M-2,k}=\bar{\alpha}_{i,M-2,k}\bar{\alpha}_{i,M-1,k}\theta_{i,M,k}^{n+\frac{2}{3}}+ \qquad (26)$$

$$+\bar{\alpha}_{i,M-2,k}\bar{\beta}_{i,M-1,k}+\bar{\beta}_{i,M-2,k}.$$

Substituting $\theta_{i,M-1,k}^{n+\frac{2}{3}}$ and $\theta_{i,M-2,k}^{n+\frac{2}{3}}$ from (25), (26) instead of (24) we find $\theta_{i,M,k}^{n+\frac{2}{3}}$:

$$\bar{\alpha}_{i,M-2,k}\bar{\alpha}_{i,M-1,k}\mu\theta_{i,M,k}^{n+\frac{2}{3}}+$$

$$+\bar{\alpha}_{i,M-2,k}\bar{\beta}_{i,M-1,k}\mu+\bar{\beta}_{i,M-2,k}\mu-$$

$$-4\cdot\bar{\alpha}_{i,M-1,k}\mu\theta_{i,M,k}^{n+\frac{2}{3}}-4\bar{\beta}_{i,M-1,k}\mu+$$

$$+3\mu\theta_{i,M,k}^{n+\frac{2}{3}}=2\Delta y\xi\theta_b-2\Delta y\xi\theta_{i,M,k}^{n+\frac{2}{3}};$$

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

$$=2\Delta y\xi\theta_b-\bar{\beta}_{i,M-2,k}\mu-\bar{\alpha}_{i,M-2,k}\bar{\beta}_{i,M-1,k}\mu+4\bar{\beta}_{i,M-1,k}\mu;$$

$$\theta_{i,M,k}^{n+\frac{2}{3}}=\frac{2\Delta y\xi\theta_b-\bar{\beta}_{i,M-2,k}\mu-\bar{\alpha}_{i,M-2,k}\bar{\beta}_{i,M-1,k}\mu+4\bar{\beta}_{i,M-1,k}\mu}{\bar{\alpha}_{i,M-2,k}\bar{\alpha}_{i,M-1,k}\mu-4\bar{\alpha}_{i,M-1,k}\mu+2\cdot\Delta y\xi+3\mu}; \qquad (27)$$

The values of the concentration sequence $\theta_{i,M-1,k}^{n+\frac{2}{3}}$, $\theta_{i,M-2,k}^{n+\frac{2}{3}}$, ..., $\theta_{i,1,k}^{n+\frac{2}{3}}$ are determined by the inverse sweep method.

Similarly, using the above technology on the coordinate OZ and get:

$$\frac{\theta_{i,j,k}^{n+1}-\theta_{i,j,k}^{n+\frac{2}{3}}}{\Delta t/3}+u^{n+1}\frac{\theta_{i+1,j,k}^{n+\frac{2}{3}}-\theta_{i,j,k}^{n+\frac{2}{3}}}{\Delta x}+v^{n+1}\frac{\theta_{i,j+1,k}^{n+\frac{2}{3}}-\theta_{i,j,k}^{n+\frac{2}{3}}}{\Delta y}+$$

$$+\left(w-w_g^{n+1}\right)\frac{\theta_{i,j,k+1}^{n+1}-\theta_{i,j,k}^{n+1}}{\Delta z}+$$

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

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

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

or

$$\frac{3}{\Delta t}\theta_{i,j,k}^{n+1}-\frac{3}{\Delta t}\theta_{i,j,k}^{n+\frac{2}{3}}+\frac{u^{n+1}}{\Delta x}\theta_{i+1,j,k}^{n+\frac{2}{3}}-$$
$$-\frac{u^{n+1}}{\Delta x}\theta_{i,j,k}^{n+\frac{2}{3}}+\frac{v^{n+1}}{\Delta y}\theta_{i,j+1,k}^{n+\frac{2}{3}}-\frac{v^{n+1}}{\Delta y}\theta_{i,j,k}^{n+\frac{2}{3}}+$$
$$+\frac{w-w_g^{n+1}}{\Delta z}\theta_{i,j,k+1}^{n+1}-\frac{w-w_g^{n+1}}{\Delta z}\theta_{i,j,k}^{n+1}+$$
$$+\sigma\theta_{i,j,k}^{n+1}=\frac{\mu}{\Delta x^2}\theta_{i+1,j,k}^{n+\frac{2}{3}}-\frac{2\mu}{\Delta x^2}\theta_{i,j,k}^{n+\frac{2}{3}}+$$
$$\frac{\mu}{\Delta x^2}\theta_{i-1,j,k}^{n+\frac{2}{3}}+\frac{\mu}{\Delta y^2}\theta_{i,j+1,k}^{n+\frac{2}{3}}-\frac{2\mu}{\Delta y^2}\theta_{i,j,k}^{n+\frac{2}{3}}+$$
$$+\frac{\mu}{\Delta y^2}\theta_{i,j-1,k}^{n+\frac{2}{3}}+\frac{\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k+1}^{n+1}-$$
$$-\frac{\kappa_{k-0,5}+\kappa_{k+0,5}}{\Delta z^2}\theta_{i,j,k}^{n+1}+\frac{\kappa_{k-0,5}}{\Delta z^2}\theta_{i,j,k-1}^{n+1}+\frac{1}{3}\delta_{i,j,k}Q;$$

we introduce the following notation:

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

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

as a result, the equation can be reduced to a three-diagonal system of linear algebraic equations for OZ :

$$\bar{\bar{a}}_{i,j,k}\theta_{i,j,k-1}^{n+1}-\bar{\bar{b}}_{i,j,k}\theta_{i,j,k}^{n+1}+\bar{\bar{c}}_k\theta_{i,j,k+1}^{n+1}=-\bar{\bar{d}}_{i,j,k}\quad(28)$$

Now, approximating the boundary condition (10), we obtain:

$$-\kappa\frac{-3\theta_{i,j,0}^{n+1}+4\theta_{i,j,1}^{n+1}-\theta_{i,j,2}^{n+1}}{2\Delta z}=(\beta\theta_{i,j,0}^{n+1}-F_0);$$

or

$$3\kappa\theta_{i,j,0}^{n+1}-4\kappa\theta_{i,j,1}^{n+1}+\kappa\theta_{i,j,2}^{n+1}=$$
$$=2\Delta z\beta\theta_{i,j,0}^{n+1}-2\Delta zF_0;\quad(29)$$

further, from equation (28) we find $\theta_{i,j,2}^{n+1}$:

$$\theta_{i,j,2}^{n+1}=-\frac{\bar{\bar{a}}_{i,j,1}}{\bar{\bar{c}}_{i,j,1}}\theta_{i,j,0}^{n+1}+\frac{\bar{\bar{b}}_{i,j,1}}{\bar{\bar{c}}_{i,j,1}}\theta_{i,j,1}^{n+1}-\frac{\bar{\bar{d}}_{i,j,1}}{\bar{\bar{c}}_{i,j,1}};\quad(30)$$

Substituting $\theta_{i,j,2}^{n+1}$ from (30) into (29) we find $\theta_{i,j,0}^{n+1}$:

$$3\kappa\theta_{i,j,0}^{n+1}-4\kappa\theta_{i,j,1}^{n+1}-\frac{\bar{\bar{a}}_{i,j,1}\kappa}{\bar{\bar{c}}_{i,j,1}}\theta_{i,j,0}^{n+1}+$$
$$+\frac{\bar{\bar{b}}_{i,j,1}\kappa}{\bar{\bar{c}}_{i,j,1}}\theta_{i,j,1}^{n+1}-\frac{\bar{\bar{d}}_{i,j,1}\kappa}{\bar{\bar{c}}_{i,j,1}}=2\Delta z\beta\theta_{i,j,0}^{n+1}-2\Delta zF_0;$$

or

$$\left(3\kappa-\frac{\bar{\bar{a}}_{i,j,1}\kappa}{\bar{\bar{c}}_{i,j,1}}-2\Delta z\beta\right)\theta_{i,j,0}^{n+1}=$$
$$=\left(4\kappa-\frac{\bar{\bar{b}}_{i,j,1}\kappa}{\bar{\bar{c}}_{i,j,1}}\right)\theta_{i,j,1}^{n+1}+\frac{\bar{\bar{d}}_{i,j,1}\kappa}{\bar{\bar{c}}_{i,j,1}}-2\Delta zF_0;$$

in the end, we get:

$$\theta_{i,j,0}^{n+1}=\frac{4\kappa\bar{\bar{c}}_{i,j,1}-\bar{\bar{b}}_{i,j,1}\kappa}{3\kappa\bar{\bar{c}}_{i,j,1}-\bar{\bar{a}}_{i,j,1}\kappa-2\Delta z\beta}\theta_{i,j,1}^{n+1}+$$
$$+\frac{\bar{\bar{d}}_{i,j,1}\kappa+2F_0\Delta z\bar{\bar{c}}_{i,j,1}}{3\kappa\bar{\bar{c}}_{i,j,1}-\bar{\bar{a}}_{i,j,1}\kappa-2\Delta z\beta};\quad(31)$$

where $\bar{\bar{\alpha}}_{i,j,0}$ and $\bar{\bar{\beta}}_{i,j,0}$ are defined in the following way:

$$\bar{\bar{\alpha}}_{i,j,0}=\frac{4\kappa\bar{\bar{c}}_{i,j,1}-\bar{\bar{b}}_{i,j,1}\kappa}{3\kappa_1\bar{\bar{c}}_{i,j,1}-\bar{\bar{a}}_{i,j,1}\kappa_1-2\Delta z\beta};$$
$$\bar{\bar{\beta}}_{i,j,0}=\frac{\bar{\bar{d}}_{i,j,1}\kappa+2\Delta z\bar{\bar{c}}_{i,j,1}F_0}{3\kappa\bar{\bar{c}}_{i,j,1}-\bar{\bar{a}}_{i,j,1}\kappa-2\Delta z\beta}.\quad(32)$$

Now, approximating the boundary condition (11), we obtain:

$$\kappa\frac{\theta_{i,j,L-2}^{n+1}-4\theta_{i,j,L-1}^{n+1}+3\theta_{i,j,L}^{n+1}}{2\Delta z}=\xi(\theta_b-\theta);\quad(33)$$

Using the sweep method for the sequence L, L-1, and L-2, we find $\theta_{i,j,L-1}^{n+1}$ and $\theta_{i,j,L-2}^{n+1}$:

$$\theta_{i,j,L-2}^{n+1}-4\theta_{i,j,L-1}^{n+1}+3\theta_{i,j,L}^{n+1}=0;$$
$$\theta_{i,j,L-1}^{n+1}=\bar{\bar{\alpha}}_{i,j,L-1}\theta_{i,j,L}^{n+1}+\bar{\bar{\beta}}_{i,j,L-1};\quad(34)$$

$$\theta_{i,j,L-2}^{n+1} = \bar{\bar{\alpha}}_{i,j,L-2}\theta_{i,j,L-1}^{n+1} + \bar{\bar{\beta}}_{i,j,L-2} = = \bar{\bar{\alpha}}_{i,j,L-2}\left(\bar{\bar{\alpha}}_{i,j,L-1}\theta_{i,j,L}^{n+1} + \bar{\bar{\beta}}_{i,j,L-1}\right) + +\bar{\bar{\beta}}_{i,j,L-2} = \bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\alpha}}_{i,j,L-1}\theta_{i,j,L}^{n+1} + +\bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\beta}}_{i,j,L-1} + \bar{\bar{\beta}}_{i,j,L-2}; \quad (35)$$

Substituting $\theta_{i,j,L-1}^{n+1}$ and $\theta_{i,j,L-2}^{n+1}$ from (34), (35) instead of (33) we find $\theta_{i,j,L}^{n+1}$:

$$\bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\alpha}}_{i,j,L-1}\theta_{i,j,L}^{n+1} + \bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\beta}}_{i,j,L-1} + \bar{\bar{\beta}}_{i,j,L-2} - -4\bar{\bar{\alpha}}_{i,j,L-1}\theta_{i,j,L}^{n+1} + \bar{\bar{\beta}}_{i,j,L-1} + 3\theta_{i,j,L}^{n+1} = 0;$$

$$\left(\bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\alpha}}_{i,j,L-1} - 4\bar{\bar{\alpha}}_{i,j,L-1} + 3\right)\theta_{i,j,L}^{n+1} = = 4\bar{\bar{\beta}}_{i,j,L-1} - \bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\beta}}_{i,j,L-1} - \bar{\bar{\beta}}_{i,j,L-2};$$

$$\theta_{i,j,L}^{n+1} = \frac{4\bar{\bar{\beta}}_{i,j,L-1} - \bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\beta}}_{i,j,L-1} - \bar{\bar{\beta}}_{i,j,L-2}}{\bar{\bar{\alpha}}_{i,j,L-2}\bar{\bar{\alpha}}_{i,j,L-1} - 4\bar{\bar{\alpha}}_{i,j,L-1} + 3} = = \frac{\left(4 - \bar{\bar{\alpha}}_{i,j,L-2}\right)\bar{\bar{\beta}}_{i,j,L-1} - \bar{\bar{\beta}}_{i,j,L-2}}{\left(\bar{\bar{\alpha}}_{i,j,L-2} - 4\right)\bar{\bar{\alpha}}_{i,j,L-1} + 3}. \quad (36)$$

Concentration sequence values $\theta_{i,j,L-1}^{n+1}$, $\theta_{i,j,L-2}^{n+1}$,..., $\theta_{i,j,1}^{n+1}$ are determined by the method of reverse sweep.

To solve equation (2), we use an implicit scheme:

$$\frac{u^{n+\frac{1}{3}} - u^n}{\Delta t/3} = \frac{c_f \pi r^2 \rho_в \left(2\tilde{u}u^{n+\frac{1}{3}} - \tilde{u}^2 - 2u^{n+\frac{1}{3}}U + U^2\right)}{m};$$

$$\frac{u^{n+\frac{2}{3}} - u^{n+\frac{1}{3}}}{\Delta t/3} = \frac{c_f \pi r^2 \rho_в \left(2\tilde{u}u^{n+\frac{2}{3}} - \tilde{u}^2 - 2u^{n+\frac{2}{3}}U + U^2\right)}{m};$$

$$\frac{u^{n+1} - u^{n+\frac{2}{3}}}{\Delta t/3} = \frac{c_f \pi r^2 \rho_в \left(2\tilde{u}u^{n+1} - \tilde{u}^2 - 2u^{n+1}U + U^2\right)}{m};$$

Further, to solve equation (3), we use an implicit scheme:

$$\frac{v^{n+\frac{1}{3}} - v^n}{\Delta t/3} = \frac{c_f \pi r^2 \rho_в \left(2\tilde{v}v^{n+\frac{1}{3}} - \tilde{v}^2 - 2v^{n+\frac{1}{3}}U + U^2\right)}{m};$$

$$\frac{v^{n+\frac{2}{3}} - v^{n+\frac{1}{3}}}{\Delta t/3} = \frac{c_f \pi r^2 \rho_в \left(2\tilde{v}v^{n+\frac{2}{3}} - \tilde{v}^2 - 2v^{n+\frac{2}{3}}U + U^2\right)}{m};$$

$$\frac{v^{n+1} - v^{n+\frac{2}{3}}}{\Delta t/3} = \frac{c_f \pi r^2 \rho_в \left(2\tilde{v}v^{n+1} - \tilde{v}^2 - 2v^{n+1}U + U^2\right)}{m};$$

Similarly, to solve equation (4), we use an implicit scheme:

$$\frac{w_g^{n+\frac{1}{3}} - w_g^n}{\Delta t/3} = \frac{-4\pi r^3 (\rho_n - \rho_в) g - 3\kappa_f \mu_в \pi r w_g^{n+\frac{1}{3}} + 3F_n}{3m};$$

$$\frac{w_g^{n+\frac{2}{3}} - w_g^{n+\frac{1}{3}}}{\Delta t/3} = \frac{-4\pi r^3 (\rho_n - \rho_в) g - 3k_f \mu_в \pi r w_g^{n+\frac{2}{3}} + 3F_n}{3m};$$

$$\frac{w_g^{n+1} - w_g^{n+\frac{2}{3}}}{\Delta t/3} = \frac{-4\pi r^3 (\rho_n - \rho_в) g - 3k_f \mu_в \pi r w_g^{n+1} + 3F_n}{3m};$$

The convergence of the iterative process is verified using the conditions:

$$\left|u^{(s+1)} - u^{(s)}\right| < \varepsilon; \left|v^{(s+1)} - v^{(s)}\right| < \varepsilon; \left|w_g^{(s+1)} - w_g^{(s)}\right| < \varepsilon.$$

Here ε is the required accuracy of the solution, S is the number of iterations, and the initial iterative value is chosen equal to the solution at the previous time layer.

Conclusions

To predict, monitor and evaluate the ecological state of the atmosphere and underlying surface with passive and active impurities, a mathematical model has been developed that considers the varying velocity of particles in the atmosphere.

To determine the speed of movement of fine particles in the atmosphere, a system of nonlinear equations was obtained, which considered the basic physic mechanical properties of the particles and the speed of movement of the atmospheric air mass, which play an important role.

Since 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 was developed to solve it.

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