NUMERICAL SIMULATION OF AEROSOL SPREADING IN THE ATMOSPHERIC BOUNDARY LAYER

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The numerical model of pollutants transfer under conditions of complicated relief is developed. The experimental results characterizing distribution and distance of aerosol spreading in the region of South Baykal for typical meteorological situations are presented.

Atmospheric aerosol spreading depends on meteorological conditions, orographic nonuniformities of relief, transformation of substances because of chemical and photochemical conversions as well as on interactions of pollutants with the Earth's surface.

In numerical simulating of pollutants transfer in mesoscale boundary layer there appears a problem of recovery of the meteorological fields caused by absence of regular observations over water surface and mountain regions difficult of access. For describing the mesometeorological processes occurring above the thermal and orographic nonuniformities of an underlying surface we propose to use a nonhydrostatic model without simplification of the theory of free convection.[1]

This model makes it possible to study a wide range of mesoscale phenomena, namely, breeze and mountain–valley circulations with outward wind, foehns, orographic waves, mesoscale structure of the meteorological fronts, convection caused by natural or anthropogenic factors and so on.

Motion velocities and turbulent characteristics obtained on the basis of hydrothermodynamic model are used for calculation of the gaseous and aerosol pollutants transfer taking chemical reactions into account. The description of transformation of the substances is realized with different particularization which depends on the initial conditions, rates of the chemical reactions and characteristics of computer systems available.[2,3] Below we present the results of numerical simulation of spreading solid suspensions from industrial enterprises in the region of South Baykal.

As an initial equation of the transfer and turbulent diffusion of the pollutants we take the following differential equation in partial derivatives:

$$\frac{\partial S}{\partial t} + \mathrm{div}(\mathbf{V}\, S) - w_g \frac{\partial S}{\partial z} = \frac{\partial}{\partial x} k_x \frac{\partial S}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial S}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial S}{\partial z} - \alpha S + F, \qquad (1)$$

where t is the time; x, y, and z are the axes of the Cartesian coordinate system, with x and y are the horizontal, while z is the vertical axis; S is the substance concentration; $\mathbf{V}$ is the wind velocity with the components u, v, and w; k_x, k_y, and k_z are the coefficients of the turbulent exchange along horizontal and vertical directions; α is the coefficient of the pollutant nonconservatizm; $F(x, y, z, t)$ is the function describing the distribution and capacity of sources of the substance under consideration; and, w_g is the rate of gravitational sedimentation of aerosols determined by the Stokes formula[4]

$$w_g = (2\rho_n\, g\, r^2)/(9\, \rho\nu),$$

where ρ_n and r are the density and radius of the aerosol particle; g is the acceleration due to gravity; ρ and ν are the density and viscosity of air.

Bearing in mind the solution to the problem on pollutant spreading above the local region, it is natural to assume that the background pollutant spreading is known. Because of absence of detail observation data we take the initial conditions as follows: S is equal to the background distribution and $S = 0$ if there is no background distribution.

The following conditions are considered as boundary ones: $\partial S/\partial x = 0$ at $x = 0,\ X$; $\partial S/\partial y = 0$ at $y = 0,\ Y$; $\partial S/\partial z = 0$ at $z = Z$, where $x = 0$, $x = X$, $y = 0$, $y = Y$, $z = Z$ are the boundaries of the area under calculation.

At the level of underlying surface the boundary condition is formulated taking into account reflection and absorption of impurities as functions of characteristics of an underlying surface.

Since the antisymmetric form of the transfer operator is the most preferable for developing the finite–difference approximations balanced out over energy then, using the equation of continuity for an incompressible atmosphere, we reduce Eq. (1) to the following form:

$$\frac{\partial S}{\partial t} = \frac{1}{2}\mathbf{V}\,\mathrm{grad}\, S + \frac{1}{2}\mathrm{div}(\, S\,\mathbf{V}) - w_g \frac{\partial S}{\partial z} = \frac{\partial}{\partial x} k_x \frac{\partial S}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial S}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial S}{\partial z} - \alpha S + F\,. \qquad (2)$$

The numerical integration of Eq. (2) was carried out in the Cartesian coordinate system using the method of virtual areas.[5] Introducing such areas makes it possible to perform the calculations with an arbitrary function describing the relief, that makes the model more universal.

For time discretization the Crank–Nikholson scheme and method of multicomponent splitting[5] were used.

Let us introduce the grid with the main nodal points

$$x_i = i\,\Delta x;\quad y_j = j\,\Delta y;\quad z_k = k\,\Delta z;\quad i = 1 \dots I,\quad j = 1 \dots J,\quad k = 1 \dots K\,;$$

where Δx and Δy are the horizontal steps; Δz is the vertical step. Let us use also the auxiliary points $x_{i+1/2}$, $y_{j+1/2}$, and $z_{k+1/2}$ located in the middle of the main intervals.

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To simplify the further discussion let us designate

$$S_{i,\,j,\,k} = S(x_i,\ y_j,\ z_k,\ t_s),\ t_s = \tau\cdot\Delta t\ (\tau = 0,\ 1,\ \ldots),$$

$$(A_1\,S)_{i,\,j,\,k} = \frac{u_{i+1/2\,,\,j,\,k}\,S_{i+1,\,j,\,k} - u_{i-1/2\,,\,j\,,\,k}\,S_{i-1\,,\,j\,,\,k}}{2\,\Delta x} +$$

$$+\frac{k_{x\ i+1/2,\,j,\,k}(S_{i+1\,,j\,,k}-S_{i\,,j\,,k})}{\Delta x^2}+\frac{k_{x\ i-1/2\,,j\,,k}(S_{i\,,j\,,k}-S_{i-1\,,\,j\,,\,k})}{\Delta x^2},$$

$$(A_2\,S)_{i,\,j,\,k} = \frac{v_{i\,,\,j+1/2\,,\,k}\,S_{i\,,\,j+1\,,\,k} - v_{i\,,\,j-1/2\,,\,k}\,S_{i\,,\,j-1\,,\,k}}{2\,\Delta y} +$$

$$+\frac{k_{y\ i,j+1/2,k}\,(S_{i,j+1,k} - S_{i,j,k})}{\Delta y^2} + \frac{k_{y\ i,j-1/2,k}\,(S_{i,j,k} - S_{i,j-1,\,k})}{\Delta y^2},$$

$$(A_3\,S)_{i,\,j,\,k}=\frac{(w_{i,j,k+1/2} - w_g)S_{i,j,k+1} - (w_{i,j,k-1/2} - w_g)\,S_{i,j,k-1}}{2\,\Delta z} +$$

$$+\frac{k_{z\ i,j,k+1/2}\,(S_{i,j,k+1} - S_{i,j,k})}{\Delta z^2} + \frac{k_{z\ i,j,k-1/2}\,(S_{i,j,k} - S_{i\,,j,k-1})}{\Delta z^2},$$

where Δt is the time step.

In this case the finite–difference analogs of Eq. (2) can be written down in the form

$$(E + \frac{\Delta t}{2}\,A^{\tau}_{\xi})\ S^{\,\tau+\xi/4-1} = (E - \frac{\Delta t}{2}\,A^{\tau}_{\xi})\ S^{\,\tau+(\xi-1)/4-1},\ \xi = 1,\ 2,\ 3;$$

$$S^{\,\tau+1/4} = S^{\,\tau-1/4} + 2\ \Delta t\ F^{\,\tau};$$

$$(E + \frac{\Delta t}{2}\,A^{\tau}_{5-\xi})\ S^{\,\tau+\xi/4} = (E - \frac{\Delta t}{2}\,A^{\tau}_{5-\xi})\ S^{\,\tau+(\xi-1)/4},\ \xi = 2,\ 3,\ 4;$$

where E is the unit matrix. To realize numerically the finite–difference equations we use the technique of nonmonotonic run.[6]

The numerical solution to Eq. (1) was compared with the analytical solution to the nonstationary equation of the pollutant spreading[7]:

$$S = \frac{M}{(4\pi\ t)^{3/2}\sqrt{k_x\ k_y\ k_z}}\ \exp\left[-\frac{(x - u\ t)^2}{4\ k_x\ t} - \frac{y^2}{4\ k_y\ t}\right]\times$$

$$\times\left\{\exp\left[-\frac{(z - H)^2}{4\ k_z\ t}\right] + \exp\left[-\frac{(z + H)^2}{4\ k_z\ t}\right]\right\},$$

which was obtained at the action of an instantaneous point source with capacity M at the point (0, 0, H) and point in time $t = 0$.

Calculations were carried out at the following values of parameters: $M = 10^6$ mg/s, $H = 120$ m, $u = 4$ m/s, $v = 0$, $k_x = k_y = 500$ m^2/s, $k_z = 5$ m^2/s, $\Delta x = \Delta y = 250$ m, $\Delta z = 30$ m, $\Delta t = 30$ s. Temporal variation of the pollutant concentration is shown in Fig. 1.

The comparison between numerical solutions to Eq. (1) and well–known analytical solutions to nonstationary equations of pollutant spreading also shows that they well agree with the analytical solutions both at the altitude of the source and near the Earth's surface.

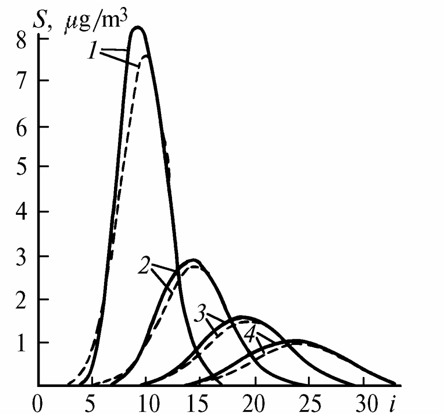

FIG. 1. Variation of pollutant concentration at the altitude of nonstationary point source at the following points in time: 5 *(1),* 10 *(2),* 15 *(3), and* 20 min *(4); solid line shows the numerical solution, dashed line corresponds to analytical one.*

Now let us discuss the numerical experiments characterizing the distribution of solid suspensions from anthropogenic sources in regions of the Angara and South Baykal in typical meteorological situations. The total ejections from industrial enterprises of Irkutsk, Angarsk, Usol'e Sibirskoe, Cheremkhovo, Zima, Shelekhov, Slyudyanka, and Baykal'sk were under consideration.

To simulate this process we selected integration area of 400 by 250 km^2 with the altitude of 2 km above the underlying surface; the steps with respect to time and horizontal directions were 300 s and 5 km, respectively; while the vertical steps were given in the following form:

$$\Delta z = \begin{cases} 50\ \text{m} & \text{for}\quad z \le 150\ \text{m}, \\ 150 & \text{for}\quad 150 < z \le 300, \\ 200 & \text{for}\quad 300 < z \le 500, \\ 500 & \text{for}\quad z > 150. \end{cases}$$

The coefficient of turbulent exchange in vertical direction was obtained from the equations of turbulent energy balance:

$$k_x = \left(k_0 + \sqrt{V^{\,2}/2}\right)\Delta x;\ k_y = \left(k_0 + \sqrt{V^{\,2}/2}\right)\Delta y,$$

where $0 < k_0 \le 1$.

Experiment 1. In the East Siberia there establishes the Asian anticyclone, whose characteristic features are as follows: high atmospheric pressure, the ground and elevated inversions with weak winds. The solid suspension particles fall mainly in the nearest vicinity of their sources. But in the region of South Baykal there exist the winds, caused by the strong temperature gradients between water surface and land, with a pronounced monsoon component providing the transfer of pollutants ejected by the industrial enterprises of Slyudyanka and Baykal'sk. Pollutants are transferred towards Lake Baykal, in this case the areas of superposition of their fields of pollution can take place.

Figure 2 shows the calculated concentrations of the solid suspensions near the ground in fractions of the average daily maximum permissible concentration being equal to 0.15 mg/m^3.

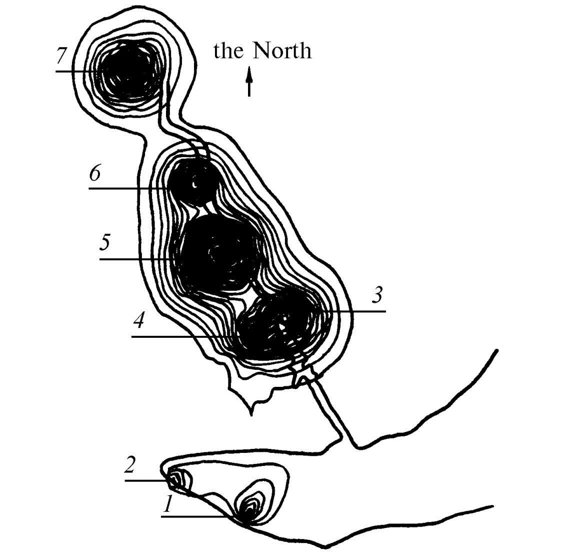

FIG. 2. Isolines of concentrations of the solid suspensions near the underlying surface at the absence of outward flow (step is equal to 15 μg/m^3). Baykal'sk (1), Slyudyanka (2), Irkutsk (3), Shelekhov (4), Angarsk (5), Usol'e Sibirskoe (6), and Cheremkhovo (7).

The principal pollution of the atmosphere above Baykal is due to industrial enterprises of Slyudyanka and Baykal'sk. It should be noted that as input data for calculations we used only data on ejections of industrial elevated sources. Raising the dust from dumps of the heat and power stations and the mining enterprises as well as the ejections from objects of housing and communal services and transport exhaust gas were not taken into consideration in these calculations.

Experiment 2. The wind field was taken as characteristic for the northwest type with frontal division transit and powerful invasions of the cold air masses. The stream of solid suspended particles caught out by the northwest transfer rushes along valley of the Angara with upper boundary speed of 10 m/s towards Baykal (see Fig. 3). In the nearest vicinity of the industrial centres the pollution decreases in comparison with experiment 1.

To study the effect of mountain ridges on the air masses transit above Baykal we carried out the calculations for an orographicly uniform place. Being compared with the above-mentioned calculations, they show that mountain ridges significantly effect on the air transfer and pollutant spreading above the lake. So, for the northwest transfer there appear the areas of accumulation and "reflection" of the pollutants near the orographic nonuniformities on the eastern coast of Lake Baykal (see Fig. 3).

Analysis of results of the numerical calculations for different meteorological conditions shows that Baykal'sk pull and paper mill (BPPM) and the industrial enterprises of Slyudyanka contribute the maximum of pollutants into the atmosphere above South Baykal. This contribution exceeds the maximum permissible concentrations. Because of different altitudes of the pollution sources the pollutants ejected by the BPPM spread over larger areas than from the enterprises of Slyudyanka. By virtue of remoteness and existence of orographic barriers the Irkutsk – Cheremkhovo industrial complex effects on the atmospheric pollution above South Baykal significantly less than BPPM and the enterprises of Slyudyanka, this contribution does not exceed the average daily concentrations adopted for harmful pollutants ejected into the atmosphere.

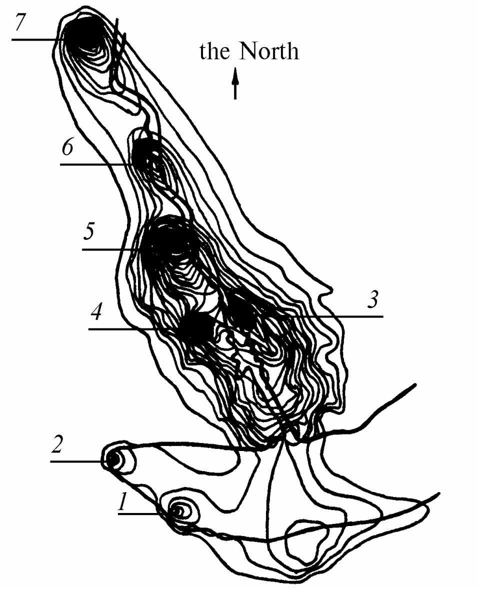

FIG. 3. Isolines of concentrations of the solid suspended particles near underlying surface for the northwest wind (step is equal to 15μg/m^3). Baykal'sk (1), Slyudyanka (2), Irkutsk (3), Shelekhov (4), Angarsk (5), Usol'e Sibirskoe (6), and Cheremkhovo (7).

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