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MATHEMATICAL MODELS AND PROGRAM PACKAGES FOR CALCULATING POLLUTANT TRANSPORT IN THE ATMOSPHERE

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Three mathematical models and program packages for modeling pollution of the atmosphere and the ground surface with pollutants from a source of technogenic dusting are presented. Experimental data are used to verify the programs.

Introduction. Conservation and restoration of the environment is an important scientific and engineering problem. By virtue of this, the emission of radionuclides into the atmosphere due to the disaster at the Chernobyl Nuclear Power Station posed a number of problems connected with predicting subsequent behavior of radionuclides in various ecological systems, including radionuclides deposited on the ground surface. Radionuclides in the upper layers of the ground can spread due to wind transport by turbulent flows in the atmosphere. This results in a change in the radioactive properties of the atmosphere and in global disturbances of ecological systems. Therefore, prediction and estimation of pollutant propagation in the atmosphere is an important problem. Information about mathematical simulation of pollutant transport in the atmosphere can be found in [1-11].

The present paper studies the problem of pollution of the atmosphere and the ground surface with pollutants from a source of technogenic dusting. Three models and the program packages NIKAT, DUST-1, and DUST-2 for implementation of the models have been developed. To verify the programs we used experimental data on the volumetric activity of dusted air with a technogenic source of dusting that were obtained within the framework of the cooperative program KES in 1990-1995. The experiments were conducted in regions of Belarus (Zapol'e village) where pollution of the ground surface layer (1–2 cm) amounted to 8.5–12 Bq/g. Based on a solution of the inverse problem, the parameters (intensity) of the source of dusting were also recovered.

Brief Description of Experimental Measurements. A source of technogenic dusting (a tractor moving in both directions at a velocity of 40 km/h over an experimental course of length 250 m and constantly generating dust for 1.5 h) is considered. The wind direction remained constant during the entire measurement period and was nearly perpendicular to the path of tractor motion. The wind speed was 4 m/sec. The distribution of the concentration of radionuclides in a dust torch was measured at a distance of 10 m from the source center at heights of 1, 2, 3, and 4 m above the ground surface and at distances of 20, 80, and 120 m from the source center at a height of 1 m above the ground surface.

Mathematical Models. At present there were different approaches to the solution of the problem of atmospheric transport of pollutants on in regional and transboundary scales. In principle, all models are divided into two classes – Lagrange and Euler models. The difference consists in the use of moving (Lagrange) and fixed (Euler) coordinate systems.

In the first case spreading and transport of pollutants are calculated along their trajectories in the atmosphere, and in the second case they are calculated with respect to a fixed geoplane-table. Lagrange models are simpler in structure and implementation than Euler ones and have acquired wider application in world practice. However, certain difficulties arise in parametrization of these models. Euler models are more complex in essence

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and require some experience in implementation. In this case the difficulties are mainly associated with modeling the advective term in the diffusion equation.

Gauss Model with Allowance for Torch Depletion. In the majority of industrially developed countries study of atmospheric transport of pollutants (chemical and radioactive) involves utilization of statistical models based on the Taylor theory of turbulent diffusion [12]. This approach is stipulated by the sufficient mathematical simplicity of the formulation of the problem and the operative character of utilization of programs implementing this method.

For a single point source the basic equation for a homogeneous medium can be written as [7]

$$C(x, y, z, t) = \frac{M}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left[-\frac{(x-ut)^2}{2\sigma_x^2}-\frac{y^2}{2\sigma_y^2}-\frac{z^2}{2\sigma_z^2}\right]. \tag{1}$$

This formula corresponds exactly to Fick's diffusion equation

$$\frac{dC}{dt} = \frac{\partial}{\partial x}\left(k_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_z\frac{\partial C}{\partial z}\right), \tag{2}$$

the solution of which in the steady case with the boundary conditions

$$C \to 0 \ \text{ for } \ t \to 0,\ r \to 0;\ C \to 0 \ \text{ for } \ t \to 0,$$

can be represented as

$$C(x, y, z, t) = M(4\pi t)^{-3/2}(k_x k_y k_z)^{-1/2}\exp\left[-\frac{1}{4t}\left(\frac{x^2}{k_x}+\frac{y^2}{k_y}+\frac{z^2}{k_z}\right)\right]. \tag{3}$$

Formula (1) corresponds exactly to Fick's equation (3) provided that the standard deviation or dispersion σ_i and the coefficients of eddy diffusion k_i are related as $\sigma_i = 2k_i t$. For the steady case under the condition of continuous emission from a source at a height H the expression for the instantaneous value of the concentration at the point (x, y, z) with allowance for reflection from the ground has the form

$$C(x, y, z, t) = \frac{M_s}{2\pi u\sigma_y\sigma_z}\exp\left(-\frac{y^2}{2\sigma_y^2}\right)\left\{\exp\left[-\frac{(z-H)^2}{2\sigma_z^2}\right] + R_g\exp\left[-\frac{(z+H)^2}{2\sigma_z^2}\right]\right\}, \tag{4}$$

where R_g accounts for the portion of the cloud reflected from the ground surface.

Thus, the solution of the problem of torch evolution in space described by Eq. (4) is reduced, apart from purely computer implementation, to determination of the diffusion parameters σ_i, which, in the general case, are functions of the state of the atmosphere.

In the present paper use is made of the approach to determination of the dispersion σ_i modified by Pasquil and Gifford, according to which σ_y and σ_z are found from the power-law relation (or Pasquil–Gifford tables)

$$\sigma_i(x) = ax^b + c, \tag{5}$$

where x is the distance in meters and a and c depend on the category of the atmosphere stability [2]. Practical calculations by the model were performed on the basis of the computer program NIKAT, which includes a block of graphical programs for postprocessing of computational information.

Model Based on Analytical Solution of the Equation of Turbulent Diffusion with an Extended Source of Dusting. In formalizing the problem based on a direct solution of the differential equation of diffusion the source of technogenic dusting was considered to be linear since the velocity of motion of the dusting source substantially exceeded the wind speed. The coordinate system in the horizontal plane was selected so that the x axis was directed from the center of the source and perpendicular to it in the direction of the wind and the source itself was located on the y axis in the range from $-L/2$ to $L/2$, where L is the length of the linear source. The z axis is directed upward perpendicular to the ground surface. If diffusion processes in the wind direction are disregarded, which is quite justified, and only advective transfer is considered, then in the usual notation the equation of atmospheric diffusion can be written as

$$u \frac{\partial C}{\partial x} - w \frac{\partial C}{\partial z} = \frac{\partial}{\partial z} k_z \frac{\partial C}{\partial z} + \frac{\partial}{\partial y} k_y \frac{\partial C}{\partial y}. \tag{6}$$

The general concept of the solution of this equation was as follows: the equation was solved analytically for the presence of a point source with the coordinates $x = 0$, $y = 0$, $z = H$, and the boundary condition was taken to be

$$uC = M\delta(y)\,\delta(z - H) \quad \text{at} \quad x = 0, \tag{7}$$

where M is the emission of substances from the source per unit time, and $\delta(z - H)$ is the Dirac delta function. Then the solution thus obtained was integrated along the source length.

The boundary conditions at an infinite distance from the source are taken assuming that the concentration vanishes:

$$C \to 0 \quad \text{for} \quad |y| \to \infty, \quad C \to 0 \quad \text{for} \quad |z| \to \infty. \tag{8}$$

On the ground surface

$$k_z \frac{\partial C}{\partial z} - wC = 0 \quad \text{at} \quad z = 0. \tag{9}$$

The relation suggested in [5] for the coefficient of turbulent transfer k_y: $k_y = k_0 u$ makes it possible to simplify integration of Eq. (6) and, when u and k_z are specified by power-law functions of z, i.e., $u = u_1 z^n$, $k_z = k_1 z$, to obtain an analytical solution of Eq. (6) for the ground-level concentration from a point source of height H in the form [13]

$$C_{\text{fl}} = \frac{M H^{\omega(1+n)} u_1^{\omega}}{2(1+n)^{1+2\omega}\,\Gamma(1+\omega)\,(k_1 x)^{1+\omega}\sqrt{\pi k_0 x}} \exp\left[-\frac{u_1 H^{1+n}}{(1+n)^2 k_1 x} - \frac{y^2}{4k_0 x}\right], \tag{10}$$

where $\omega = w/k_1(1 + n)$, w is the rate of precipitation of particles on the ground, which, in turn, depends on the density and size of the aerosol particles and is found by the Stokes formula

$$w = 1.3 \cdot 10^{-2} \rho_d r_d^2. \tag{11}$$

Introducing a new coordinate system $x' = x$, $y' = y - \eta$ and integrating Eq. (7) over the source length, we obtain a formula for the ground-level concentration from a linear source:

$$C_d(x, y) = \int_{-L/2}^{L/2} C_{\text{fl}}(x, y - \eta)\, d\eta$$

or

$$C_d = \frac{M H^{\omega(1+n)} u_1^{\omega}}{2(1+n)^{1+2\omega}\,\Gamma(1+\omega)\,(k_1 x)^{1+\omega}} \exp\left[\frac{u_1 H^{1+n}}{(1+n)^2 k_1 x}\right] \times$$

$$\times \left[\operatorname{erf}\left(\frac{y + L/2}{\sqrt{2}\,\varphi_0 x}\right) - \operatorname{erf}\left(\frac{y - L/2}{\sqrt{2}\,\varphi_0 x}\right)\right], \tag{12}$$

where $\operatorname{erf}(t) = (2/\sqrt{\pi}) \int_0^t \exp(-\xi^2) d\xi$ is the probability integral; $2k_0(x) = \varphi_0^2 x$.

The calculations by this model were based on the computer program DUST-1.

Model Based on Solution of the Equation of Turbulent Diffusion by the Method of Finite Elements. For a linear source of technogenic dusting we also found the distribution of pollutant concentration in the x, z plane by solving the equation of turbulent diffusion (6) for a linear source, which has the form

$$u \frac{\partial C}{\partial x} - w \frac{\partial C}{\partial z} = \frac{\partial}{\partial z} k_z \frac{\partial C}{\partial z} . \tag{13}$$

The boundary conditions for this equation are formulated as follows:

$$C \to 0 \quad \text{for} \quad z \to \infty ;$$

on the ground surface:

$$k_z \frac{\partial C}{\partial z} + (w - v_s) C = 0 ; \tag{14}$$

on the boundary $x = 0$:

$$uC = M\delta (z - H) .$$

The velocity in Eq. (13) changes by the logarithmic law

$$u = u_1 \frac{\ln (z/z_0)}{\ln (z_1/z_0)} , \tag{15}$$

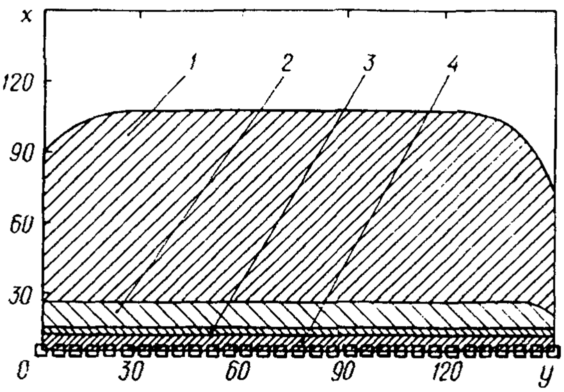
and the coefficient of turbulent transfer changes by the linear law

$$k_z = \begin{cases} \nu + k_1 z/z_1 , & z \le h , \\ \nu + k_1 h/z_1 , & z \ge h . \end{cases} \tag{16}$$

Equation (13) with boundary conditions (14) and parameters (15), (16) was solved by the method of finite elements, the main idea of which is that any continuous quantity, such as pollutant concentration, can be approximated by a discrete model constructed on the basis of a set of piecewise-continuous functions, in the given case on the basis of a set of quadratic functions determined on a finite number of subregions. For this purpose, the region of determination of the continuous quantity is divided into a finite number of subregions called elements. In our case nine-point Lagrange rectangular elements are used. The continuous quantity is approximated on each element by a quadratic polynomial determined by the nodal values of this quantity. The interpolation polynomial for pullutant concentration on an arbitrary element has the form

$$C^{(e)} = [N] \{C\} = [N_i^{(e)}, N_j^{(e)}, N_k^{(e)}, \ldots, N_r^{(e)}] \begin{Bmatrix} C_i \\ C_j \\ C_k \\ \cdot \\ \cdot \\ \cdot \\ C_r \end{Bmatrix} , \tag{17}$$

where r is the number of nodes of an element; the superscript (e) denotes an arbitrary element; N_i are functions of the element form; C_i, C_j, ..., C_r are nodal values of C. An important aspect of the method of finite elements is the possibility of distinguishing a typical element from the set of elements in determining the element function.



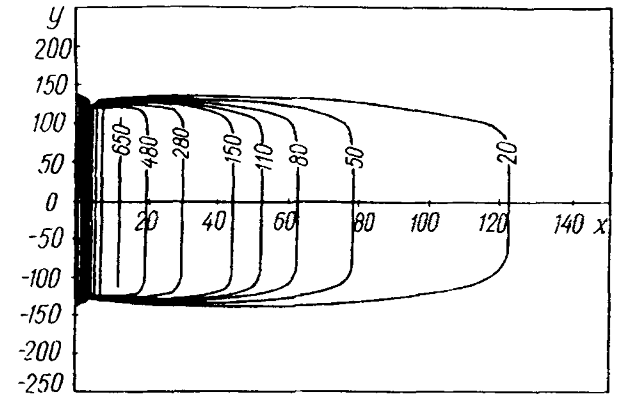


Fig. 1. Isobands of the ground-level concentration at a height 1 m: 1) $0.1 \cdot 10^{-11}$ Ci/m^3; 2) $0.5 \cdot 10^{-11}$; 3) $0.12 \cdot 10^{-10}$; 4) $0.15 \cdot 10^{-10}$. Initial parameters: intensity of the source $M = 5 \cdot 10^{-10}$ Bq/sec, $H = 2.0$ m, $v_s = 0.36$ m/sec. Calculations by the program NIKAT. x, y, m.

Fig. 2. Isolines of the ground-level concentration for a model with a linear source of dusting for the following values of the initial parameters: $u = 4$ m/sec; $H = 0.56$ m; $\varphi_0 = 0.17$. Calculations by the program DUST-1.

This allows one to obtain the element function independently of the element position in the related overall model and of other functions of elements.

Having written the initial differential equation (13) in the form $LC = 0$ (L is the differential operator), we apply the Galerkin method to it, i.e., minimize the calculation error $\varepsilon = L\overline{C}$, where $\overline{C} = \sum N_i C_i$ is the approximate solution to Eq. (13). This requires the validity of the equality

$$\int_R N_i \varepsilon \, dR = 0$$

for each basis function N_i. Mathematically, this equality means that the basis functions should be orthogonal to the error in the region R.

The combination of the Galerkin method and the method of finate elements yields the equations

$$\int_R N_\beta L(C) \, dR = 0 \,, \quad \beta = i, j, k, \ldots$$

Substituting the implicit form of the differential operator L into these equations, transforming the integrands with account for the boundary conditions, and combining the matrices for each element into one matrix for all the elements, we obtain the system of algebraic equations

$$\left[K\right] \left\{C\right\} = \left\{F\right\}, \tag{18}$$

where $[K]$ is the global matrix of rigidity; $\{F\}$ is the global vector of loading; $\{C\}$ is the solution vector.

The matrices $[K^{(e)}]$ and $\{F^{(e)}\}$ for each element have the form

$$\left[K^{(e)}\right] = \frac{\Delta z}{2} \int_{-1}^{1} \int_{-1}^{1} \left\{N\right\} \left[N\right] \left\{u\right\} \left[\frac{\partial N}{\partial \xi}\right] d\xi d\eta - \frac{\Delta x}{2} \int_{-1}^{1} \int_{-1}^{1} \left\{N\right\} \left[N\right] \left\{w\right\} \left[\frac{\partial N}{\partial \eta}\right] d\xi d\eta +$$

$$+ \frac{\Delta x}{\Delta z} \int_{-1}^{1} \int_{-1}^{1} \left\{\frac{\partial N}{\partial \eta}\right\} \left[N\right] \left\{k_z\right\} \left[\frac{\partial N}{\partial \eta}\right] d\xi d\eta - \frac{\Delta x}{2} \int_{-1}^{1} \left\{N\right\} \left[N\right] \left\{v_s\right\} \left[N\right] d\xi + \frac{\Delta x}{2} \int_{-1}^{1} \left\{N\right\} \left[N\right] \left\{w\right\} \left[N\right] d\xi \,,$$

$$\left\{F^{(e)}\right\} = \frac{M \frac{\Delta z}{2}}{\left[N\right]_H \left\{u\right\}} \left[\left\{\frac{\partial N}{\partial \eta}\right\} \left[N\right] + \left\{N\right\} \left[\frac{\partial N}{\partial \eta}\right] \right]_H \left\{k_z\right\} ,$$

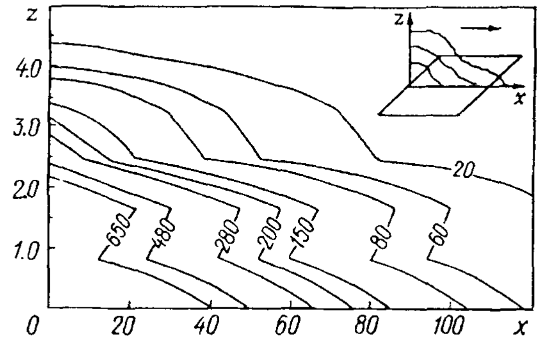


Fig. 3. Isolines of the vertical distribution of the concentration in a dust cloud using the method of finite elements for the following values of the initial parameters: $u = 4$ m/sec; $H = 2.0$ m; $v_s = 0.38$. Calculations by the program DUST-2. z, m.

TABLE 1. Experimental and Calculated Values of Ground-Level Concentrations, mBq/m^3

Distance from the source Y, m	Calculation by the programs and experiment	Concentration at a point, mBq/m^3, for the height of the point, m			
		1	2	3	4
10	NIKAT	648	1151	65	50
	DUST-1	650	–	–	–
	DUST 2	650	563	113	41
	Experiment	650	800	110	–
20	NIKAT	292	352	299	–
	DUST-1	480	–	–	–
	DUST-2	510	409	64	34
	Experiment	480	–	–	–
80	NIKAT	48	58	65	–
	DUST-1	50	–	–	–
	DUST-2	72		8.7	5.1
	Experiment	50	–	–	–
120	NIKAT	26	32	36	–
	DUST-1	20	–	–	–
	DUST-2	20	16	2.4	1.4
	Experiment	25	–	–	–

with the one-dimensional integrals in the matrix $[K^{(e)}]$ being calculated only for the elements corresponding to the boundary $z = 0$ and the loading vector being determined for the elements where the source is positioned at a height H. Calculations by this model were performed on the basis of the computer program DUST-2.

Results and Discussion. Using the developed models and packages of programs we processed experimental measurements of the propagation of radionuclides in the atmosphere and recovered parameters of the source of technogenic dusting from the available values of the ground-level concentration at the given points of the experimental site. This scientific problem was solved by three methods and, as the calculations showed, all these methods can be used to solve problems of this class. Figures 1 and 2 show distributions (isobands and isolines) of the ground-level concentration of radionuclides in a dust cloud at a height of 1 m above the ground surface within the experimental site. Figure 3 presents isolines of pollutant concentration in the vertical plane x, z obtained from solution of the equation of eddy diffusion by the method of finite elements. As is seen from the figures and Table

1, the results of the calculations are in good agreement with full-scale measurements. We note that in the Gauss model the source of dusting was represented in the form of a set of point sources located on the boundary, and the solution was found as a superposition of solutions from N point sources that were switched on over time and modeled the motion of the source of technogenic dusting. Moreover, since the model, in the general case, is constructed for a gas or aerosol cloud, the correction was made by parameters of the rate of gravitational sedimentation that were considered within the range of 0.25–0.5 m/sec. The characteristics of a source of dusting of intensity $5 \cdot 10^{-10}$ Ci/sec at a height within 0.5–2 m with a rate of sedimentation $v_s = 0.25$ m/sec can be considered most acceptable.

Table 1 presents calculated and experimental values of ground-level concentrations of radionuclides in a dust cloud. The parameters characterizing the processes of dry and wet removal of pollutants and the coefficients of vertical turbulent diffusion are determined with limited accuracy and undergo substantial fluctuations. As is shown in [6], this also introduces model errors within 5–30% irrespective of the type of model. Moreover, with the existing uncertainties in the errors of the initial and experimental data and the parameters of the models (for any type of model), the errors of modeling may amount to 50% for short times (1 day) intervals and 10–15% for intervals of 1 month or more.

The suggested models and programs, nevertheless, allow prediction of the space-time distribution of radionuclides with account for the actual wind field and atmospheric conditions. The discrepancies between the calculated and experimental data did not exceed 35–40%.

NOTATION

H, height of the source of emission; k_x, k_y, k_z, coefficients of diffusion; u, wind speed; t, time; σ_x, σ_y, σ_z, diffusion parameters (standard deviations); C, pollutant concentration; v_s, rate of dry sedimentation of radionuclides; x, y, z, Cartesian coordinates (in the wind direction, perpendicular to the wind, in the vertical direction); R_g, correction factor to allow for the effect of torch reflection from the ground; w, rate of gravitational sedimentation of particles on the ground; ρ_d, density of the dust particles; r_d, radius of the dust particles; φ_0, root-mean-square deviation of the wind direction; L, source length; Γ, gamma function; k_1, n, parameters of the state of the atmosphere; z_0, roughness of the ground surface; ν, coefficient of molecular diffusion for air.

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