Application of Marchuk method to solving "inverse" problems on the atmospheric admixture transport by use of a statistical calculation technique

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We consider in this paper a method for solution of "inverse" problems of atmospheric admixture dispersal. It is based on solution of the adjoint semispherical equation of turbulent diffusion, as well as on dual representation of the functional of the admixture concentration. It is shown that this classical method can be generalized to the class of problems involving calculation of statistical characteristics of the admixture concentration. As an example, we consider the problem of how a plant with known pollution emission rate can be placed optimally, i.e., in such a way that the admixture concentration at a given location does not exceed the preset threshold within the preset probability limits.

The aerosol and gas pollutant transport in the atmosphere is usually treated in the context of two classes of problems. In the first, "direct" ones, the admixture concentration field is determined from known characteristics of emission sources; while in the second, "inverse" ones, the source types, coordinates, and intensity must be determined from known admixture concentrations at a number of reference points. Within the Euler approach to turbulent diffusion, one can efficiently use the semiempirical equation that follows from the law of mass conservation[1]:

$$\frac{\partial C}{\partial t} + \frac{\partial \overline{U}_i C}{\partial x_i} = Q, \qquad (1)$$

where C are the instantaneous values of the admixture concentration; U_i are the instantaneous values of the velocity components of the medium; t is time; x_i are the spatial coordinates, $i = \overline{1, 3}$; and Q is the term accounting for the pollution sources and sinks. Here, the subscript indicates summation. In equation (1), we represent instantaneous values by the sum of ensemble averages (overbarred) and deviations (primed), $C = \overline{C} + C'$ and $U_i = \overline{U}_i + U'_i$, and average the result over the ensemble. The closure of this expression with the use of gradient hypothesis

$$\overline{U'_i C'} = -K_{ij} \frac{\partial \overline{C}}{\partial x_j}$$

yields[2]:

$$\frac{\partial \overline{C}}{\partial t} + \frac{\partial \overline{U}_i \overline{C}}{\partial x_j} - \frac{\partial}{\partial x_i} K_{ij} \frac{\partial \overline{C}}{\partial x_j} = \overline{Q}, \qquad (2)$$

where K_{ij} are the components of the tensor of turbulent diffusion coefficients.

Let now $K_{ij} = 0$ for $i \neq j$. Generally, equation (2) must account for the particle sedimentation rate V_s, and not only $\overline{U}_z$ (i.e., $\overline{U}_z - V_s$ should be used instead $\overline{U}_z$). The "direct" problem will be solved in the cylindrical domain G, defined by the surface S consisting of cylinder side Σ, base Σ_0 (at $z = 0$), and top Σ_H (at $z = H$) faces. To solve the problem, we complete the equation (2) with the initial and boundary conditions given by

$$\overline{C}(x, y, z, 0) = 0; \quad \overline{C} = 0 \text{ on } \Sigma, \Sigma_H;$$

$$-V_s\overline{C} - K_{zz}\frac{\partial \overline{C}}{\partial z} + V_g\overline{C} = 0 \text{ on } \Sigma_0, \qquad (3)$$

where V_g is the parameter of interaction between particles and boundary Σ_0 ($V_g \geq 0$), on which wind velocity components are all assumed to be zero.

The Marchuk method[3] involves construction of an adjoint problem as formulated by Eq. (2). We multiply Eq. (2) by some function $\overline{C}_*$ and integrate over entire solution domain, to finally obtain, with the account of the condition (3) and nondivergent character of the medium's velocity field, that

$$-\frac{\partial \overline{C}_*}{\partial t} + \frac{\partial \overline{U}_i \overline{C}_*}{\partial x_j} - \frac{\partial}{\partial x_i} K_{ij} \frac{\partial \overline{C}_*}{\partial x_j} = \overline{P}, \qquad (4)$$

with the system of the initial and boundary conditions

$$\overline{C}_*(x, y, z, T) = 0; \ \overline{C}_* = 0 \text{ on } \Sigma, \Sigma_H;$$

$$-K_{zz}\frac{\partial \overline{C}_*}{\partial z} + V_g\overline{C}_* = 0 \text{ on } \Sigma_0; \qquad (5)$$

in addition, we obtain the following dual representation of the functional:

$$J_1 = \int_0^T \mathrm{d}t \int_G \overline{P}\, \overline{C}\, \mathrm{d}G = \int_0^T \mathrm{d}t \int_G \overline{C}_*\, \overline{Q}\, \mathrm{d}G. \qquad (6)$$

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Using Eq. (6) and solution of the problem as it is defined by Eqs. (4) and (5), it is possible to solve a wide range of "inverse" problems of admixture transport in the atmosphere without multiple solution of the direct equations (2) and (3).

In the theory of method as introduced in Ref. 3, the solution $\overline{C}(x_1, y_1, z_1, T)$ of the "direct" problem defined by Eq. (2) with $\overline{Q} = Q_0\,\delta(x - x_0)\,\delta(y - y_0) \times \delta(z - z_0)\,\delta(t)$, where z_0, y_0, z_0 are the coordinates of the point instantaneous pollution source and Q_0 is the particulate mass released into the atmosphere at the time $t = 0$, and the solution $\overline{C}_*(x_0, y_0, z_0, 0)$ of "inverse" problem defined by Eq. (4) with $\overline{P} = \delta(x - x_1) \times \delta(y - y_1)\,\delta(z - z_1)\,\delta(t - T)$ have fundamental importance. According to Eq. (6), we have in this case

$$\overline{C}(x_1, y_1, z_1, T) = Q_0\,\overline{C}_*(x_0, y_0, z_0, 0). \quad (7)$$

The function $\overline{C}_*$ at the point x_1, y_1, z_1 at time $t = T$ quantifies the contribution to the mathematical expectation of the concentration of an admixture spreading from the source located at the point x_0, y_0, z_0 and activated at $t = 0$. Alternatively, the Green's function $\overline{C}_*(x_0, y_0, z_0, 0)$ is customarily called the sensitivity function.

The applicability of the method is limited by the fact that relation (6) uses solely average concentration. Since atmospheric admixture transport is a random process, this method fails to solve many practically important problems where distribution laws of admixture concentration must be known. The present work generalizes the Marchuk method to the problems dealing with the calculation of statistical characteristics of pollutants spreading in the atmosphere.

Let us consider the solution of Eq. (1) in the domain G, corresponding to $-\infty < x, y, z < +\infty$. Using the method outlined above and the function C_*, we obtain

$$-\frac{\partial C_*}{\partial t} - \frac{\partial U_i C_*}{\partial x_i} = P \quad (8)$$

and, assuming that C and C_* vanish at infinity, the integral identity can be written

$$\int_0^T \mathrm{d}t \int_G PC\,\mathrm{d}G = \int_0^T \mathrm{d}t \int_G C_*\,Q\,\mathrm{d}G. \quad (9)$$

Assuming that $Q = \overline{Q}$ and $P = \overline{P}$ in it, we obtain

$$C(x_1, y_1, z_1, T) = Q_0\,C_*(x_0, y_0, z_0, 0). \quad (10)$$

Raising both sides of expression (10) to an integer power $m > 0$ and averaging over an ensemble yields a set of the initial statistical moments of concentration

$$\overline{C^m}(x_1, y_1, z_1, T) = Q_0^m \overline{C_*^m}(x_0, y_0, z_0, 0). \quad (11)$$

Now, using standard rules of the probability theory,[4] we can construct the characteristic function of admixture concentration and, applying Fourier transform, determine its distribution function $F(C; x, y, z, t)$:

$$F(C; x_1, y_1, z_1, T) = F(Q_0 C_*; x_0, y_0, z_0, 0). \quad (12)$$

The relationship (12) is a generalization of the equation (7) and quantifies the probability with which the admixture concentration produced by the source of a known intensity, but unknown coordinates exceeds some threshold value at a given point.

As an example, we will consider the problem of placing a plant at a certain point x_0, y_0, z_0, which is assumed to emit the mass Q_0 of material at time $t = 0$. We impose the condition that the probability W_0 of finding the admixture at some point x_1, y_1, z_1 at time $t = T$ with the instantaneous concentration C less than some (e.g., maximum permissible) threshold C_0 equals $F(C_0)$. We assume that the distribution function of the admixture concentration has the form[5]

$$F(C) = 1 + \frac{1}{2}\left[\mathrm{erf}\left(\frac{C - \overline{C}}{\beta}\right) - \mathrm{erf}\left(\frac{C + \overline{C}}{\beta}\right)\right], \quad (13)$$

where erf(...) is the error function; β is the second parameter of the distribution law, related to the variance σ^2 of the concentration by the following formula:

$$\frac{\sigma^2}{\overline{C}^2} = \mathrm{erf}(\beta_0)\left(1 + \frac{1}{2\beta_0^2}\right) - 1 + \frac{1}{\sqrt{\pi}\beta_0}\exp(-\beta_0^2),$$

$$\beta_0 = \overline{C}/\beta. \quad (14)$$

The validity of formula (13), expressing the distribution function, was confirmed experimentally under conditions of turbulent boundary layer realized in a wind tunnel[5]; it is an exact analytical solution of Kolmogorov equation,[6] while its asymptotic behavior closely matches that of the classic asymptotes of the distribution law for the admixture concentration in the theory of turbulent combustion.[5]

Solution of the adjoint problem as it is formulated by Eqs. (4) and (5) yields the field $\overline{C}_*(x, y, z, 0)$. Now let us determine the variance σ^2 of the concentration[7]

$$\frac{\partial \sigma^2}{\partial t} + \frac{\partial U_i \sigma^2}{\partial x_i} - \frac{\partial}{\partial x_i} K_{ij} \frac{\partial \sigma^2}{\partial x_j} = 2K_{ij}\frac{\partial \overline{C}}{\partial x_i}\frac{\partial \overline{C}}{\partial x_j} - \alpha\,\sigma^2, \quad (15)$$

$$\sigma^2(x, y, z, 0) = 0; \quad \sigma^2 = 0 \text{ on } \Sigma, \Sigma_H;$$

$$-2V_s\sigma^2 - K_{zz}\frac{\partial \sigma^2}{\partial z} + 2V_g\sigma^2 = 0 \text{ on } \Sigma_0. \quad (16)$$

The adjoint problem, Eqs. (15) and (16), has the form[8]

$$-\frac{\partial \sigma_*^2}{\partial t} - \frac{\partial U_i \sigma_*^2}{\partial x_i} - \frac{\partial}{\partial x_i} K_{ij}\frac{\partial \sigma_*^2}{\partial x_j} = -\alpha\sigma_*^2 + \overline{R}, \quad (17)$$

$$\sigma_*^2(x, y, z, T) = 0; \quad \sigma_*^2 = 0 \text{ on } \Sigma, \Sigma_H;$$

$$-V_s\sigma_*^2 - K_{zz}\frac{\partial \sigma_*^2}{\partial z} + 2V_g\sigma_*^2 = 0 \text{ on } \Sigma_0. \qquad (18)$$

Now, solving Eqs. (17) and (18) for

$$\overline{R} = 2K_{ij}\frac{\partial \overline{C}_*}{\partial x_i}\frac{\partial \overline{C}_*}{\partial x_j}, \qquad (19)$$

yields the field $\sigma_*^2(x, y, z, 0) = 0$. From the problem formulation,

$$W_0 = F(C_0; x_1, y_1, z_1, T). \qquad (20)$$

Also, with the account of Eq. (11), we have

$$\begin{aligned} &\overline{C}(x_1, y_1, z_1, T) = Q_0\overline{C}_*(x_0, y_0, z_0, 0); \\ &\sigma^2(x_1, y_1, z_1, T) = Q_0^2\sigma_*^2(x_0, y_0, z_0, 0). \end{aligned} \qquad (21)$$

Now, from the equation (14) we can determine the second parameter, β, of the distribution law. Thus, W_0 is prescribed in the problem formulation, while the parameters in Eq. (20) are defined as the functions of coordinates x_0, y_0, z_0 of the pollution source. Thus, depending on the form of F, the equation (20) defines the surface on which the conditions imposed on the problem are satisfied.

Figure 1 presents the solution of the "inverse" problem formulated above; the calculations were made for the case of the spread of nitrogen dioxide over Novosibirsk from the stationary source with the intensity equivalent to that of the system of power plants TES–2 and TES–3 operating in the city. The river Ob (shown in dark) crosses the city in the south-north direction. The city is divided by the river into two halves, and its different parts are shown by different gray shaded zones (in the center of the figure). The point where we imposed the condition that $C < C_0$ with a prescribed probability W_0 was chosen to lie at the central square of the city on the right-hand bank of the river at a height of 2 m above the ground surface. In the figure, the contour lines are horizontal sections of the surface defined by formula (20) at the height 50 m above the ground surface. The outermost contour line corresponds to the condition that instantaneous nitrogen dioxide concentration is less than the maximum permissible one with the probability $W_0 = 0.95$, the innermost with the probability $W_0 = 0.05$, and the middle one with the probability $W_0 = 0.5$.

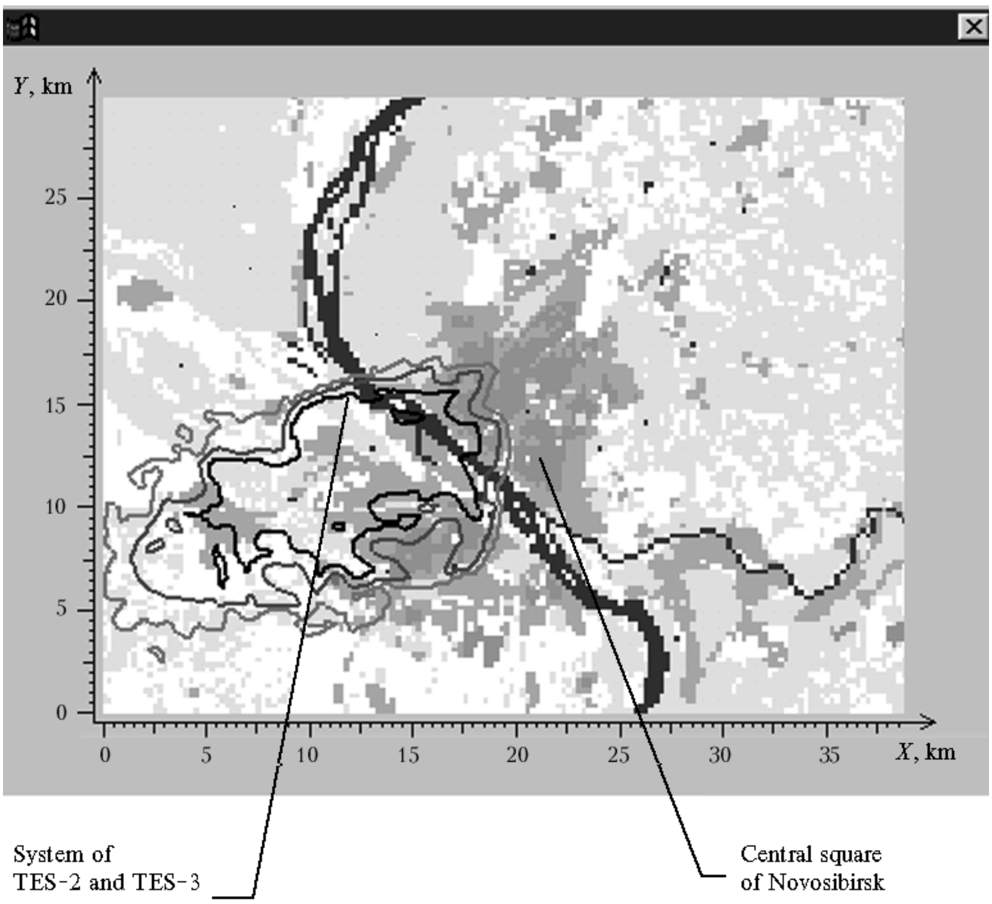

Fig. 1.

The calculations were made for typical, nearly calm, daylight, summertime meteorological conditions. These contour lines give approximate locations of the plants emitting pollutants into the atmosphere under given meteorological conditions where they are safe for the center of the city. In reality, TES–2 and TES–3 are located on the left-hand bank of the river Ob in the region enclosed by the contour line with $W_0 = 0.05$.

In the example considered above, unlike Ref. 3, the criterion of plant placement is based on the probability that concentration of an admixture is below some preset threshold. That kind of the problems cannot be solved by applying only classical interpretation of Marchuk method. In this regard, with formulas derived in this paper, the method introduced in Ref. 3 can be used to solve a wider range of problems including “inverse” problems of the spread of atmospheric pollutants with the help of information on the distribution laws of the admixture concentration.

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