Determination of the boundary of a spreading cloud of atmospheric admixtures

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The semiempirical turbulent diffusion equation is widely used in simulating the spread of atmospheric admixtures. However, the determination of concentrations of the admixtures at long distances from sources by use of the semiempirical equation is incorrect. Earlier, it was shown that the semiempirical equation could be used for describing the finite-rate diffusion at mobile boundaries, determined by the maximum values of the medium velocity pulsations, under certain limitation on the time of the admixture spread. The three-dimensional problem of determining the boundary of the region, within which the atmospheric admixtures spread is considered.

The semiempirical turbulent diffusion equation[1] is widely used for simulating the spread of atmospheric admixtures. Because of the first derivative with respect to time, it is referred to parabolic equations. As a result, its solutions have the property of "unlimited" spread rate. In other words, small but finite values of the mathematical expectation of the admixture concentration appear in equation solutions in an arbitrary short time after source initiation at arbitrary long distances from the source. This evidently contradicts finiteness of the speed of the admixture particles motion. Therefore, determination of concentrations of atmospheric admixtures by use of the semiempirical equation is incorrect at long distances from sources.

Attempts to overcome this limitation by changing a parabolic equation for a hyperbolic one are known. Such a model of the diffusion for one-dimensional case is described, e.g., in Ref. 1. Nevertheless, these results are impossible to be generalized to the case of an admixture diffusion in the three-dimensional space. This fact has been analyzed in detail in Ref. 2 based on the fundamental properties of the hyperbolic equations.

The one-dimensional boundary problem with the property of finite spread rate of admixtures was formulated and solved in Ref. 3 using natural assumption of finite extrema of the wind speed pulsations as well as the apparatus of the theory of Markovian processes. It was shown that if the spread time T is much longer than the time scale $\tau_0 \approx 18K/U^2$, where K and U are typical values of the coefficient of turbulent diffusion and wind speed, the standard semiempirical turbulent diffusion equation can be used to describe the process of turbulent diffusion of atmospheric admixtures with a finite spread rate. In this case, the boundary condition is to be set at the mobile boundaries defined by the extremum values of the wind speed pulsations.

The above-indicated time limitation yields the estimation $\tau_0 \approx 2$ s at the values $K \approx 5$ m^2/s and $U \approx 7$ m/s, typical for the ground layer. This estimate corresponds to the applicability condition of the semiempirical turbulent diffusion equation, according to which the spread time of atmospheric admixtures is to be much longer than the Lagrangian time scale of wind speed pulsations τ, since in the ground layer the Lagrangian scale reaches the magnitude of tens of seconds. In alternative case, the approach described in Ref. 4 can be used to describe the spread of atmospheric admixtures at short spread times.

According to Ref. 3, one-dimensional case requires the boundary condition for a homogeneous problem and a source, located at the point x_0 and fully emitting an admixture at the time t_0, to be set at the moving boundary defined by the equations

$$\chi_1(x,t) = \int_{t_0}^{t} (\overline{U} + \min \hat{U})\, dt;$$

$$\chi_2(x,t) = \int_{t_0}^{t} (\overline{U} + \max \hat{U})\, dt,$$

where χ_1 and χ_2 are the left-hand and right-hand boundary of the diffusion region, respectively, $\overline{U}$ is the average wind speed, $\hat{U}$ is the instantaneous wind speed pulsation.

In this paper we consider the three-dimensional problem of determining the boundary of the region, within which atmospheric admixtures spread. The solution of this problem allows one to solve the semiempirical equation of turbulent diffusion with finite spread rate using the approach described in Ref. 3.

In deriving the semiempirical equation the averaging of the law of conservation of the amount of matter in moving medium over the period much longer than the Lagrangian scale of the medium speed pulsations[1] is used. Hence, the semiempirical equation describes the motion of an ensemble of "liquid" particles with independent increments of coordinates in nonoverlapping time intervals.[5] Using this feature, define the boundary of a spreading admixture cloud by the method of statistical modeling.

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The increments of coordinates of a liquid particle in a short time $\mathrm{d}t$ are defined by the equations

$$\mathrm{d}x_i = (\overline{U}_i + \hat{U}_i)\,\mathrm{d}t;\ x_i = x, y, z,$$

where $\overline{U}_i$ and $\hat{U}_i$ are the components of the medium velocity averaged over the statistical ensemble and the instantaneous velocity pulsations, respectively. The increment of a coordinate of a liquid particle in the finite-time step Δt is as follows:

$$\Delta x_i = \overline{U}_i \Delta t + \int_t^{t+\Delta t} \hat{U}_i\,\mathrm{d}t.$$

If the time step Δt is much longer than the Lagrangian time scale τ, the variance of the coordinate increment is defined by the equation[6]

$$\sigma_i^2 = 2K_i\Delta t,$$

where K_i are the components of the tensor of diffusion coefficients used in solving the semiempirical turbulent diffusion equation. Values of K_i are defined by the corresponding variances of pulsations of the wind velocity components.[6] It is known, that the distribution function of pulsations of the wind velocity components can be approximated by normal law.[7] Therefore, the final expression for the coordinate increment of a liquid particle in the time Δt has the form

$$\Delta x_i = \overline{U}_i \Delta t + \alpha_i\sigma_i,$$

where α_i are the random normally distributed numbers with zero mean and unit variance. Let us limit the span of pulsations of the wind velocity components by three standard deviations. To simulate α_i, we shall use the truncated normal law:

$$F(\alpha_i) =$$

$$= \begin{cases} 0;\ \alpha_i \le -3 \\ \dfrac{1}{2\operatorname{erf}(3/\sqrt{2})}\left[\operatorname{erf}\left(\alpha_i/\sqrt{2}\right) + \operatorname{erf}\left(3/\sqrt{2}\right)\right];\ -3 < \alpha_i < 3, \\ 1;\ \alpha_i \ge 3, \end{cases}$$

where $F(\alpha_i)$ is the α_i distribution function, erf is the probability integral.

Thus obtained relations for coordinate increments of liquid particles in the time Δt provide for the statistical simulation of an admixture cloud boundary. In this case, extrema of the pulsations of wind velocity components agree with the input parameters of the semiempirical equation, i.e., turbulent diffusion coefficients.

To obtain the trajectory of a liquid particle, it is necessary and sufficient to have statistically independent sequences of three random numbers r_i equidistributed over the range from 0 to 1. By solving the equation $r_i = F(\alpha_i)$, one can find α_i values. The coordinates of all liquid particles from the ensemble calculated by the above-described technique at the time t define the boundary of the admixture cloud, which corresponds to the solution of the semiempirical equation of turbulent diffusion with a finite spread rate.

In the case of the admixture diffusion from an instant point source in the absence of admixture transfer by the averaged wind field, $\overline{U}_i = 0$, and $K_i = \text{const}$, the surfaces of equal concentrations in the solution of the semiempirical turbulent diffusion equation are to be a family of ellipsoids

$$\frac{x^2}{A_x} + \frac{y^2}{A_y} + \frac{z^2}{A_z} = 1$$

with the axes A_i. Because of the symmetry properties of the problem and the above arguments, the boundaries of the cloud of a spreading admixture in this case also have the ellipsoid shape with the axes $A_i = 3\sqrt{2K_i\Delta t}$.

Consider the problem of admixture diffusion under condition of nonuniform landscape. Let a source be located in the left-bank part of Novosibirsk at the point $x = 5$ km, $y = 11$ km, $z = 100$ m (Fig. 1), and emits to the atmosphere $N = 10^{10}$ particles of a nonsettling admixture at the time $t_0 = 0$.

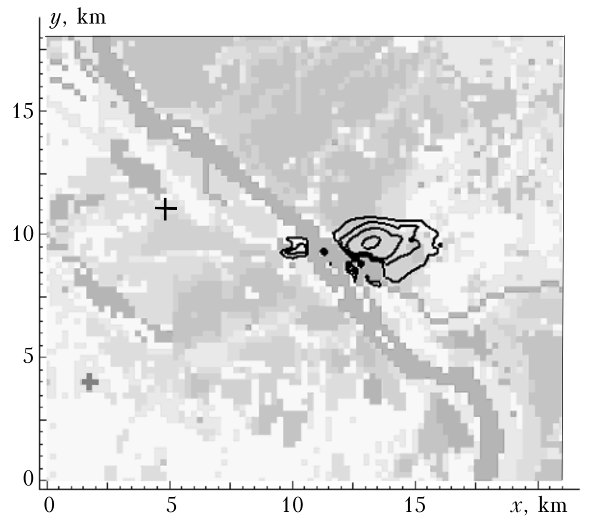

Fig. 1. Calculation area and concentration isolines. The source is marked by the cross.

Different scales of gray correspond to various types of the landscape, i.e., buildings with different number of storeys, forestry, steppe, Ob river, etc. The x-axis is directed horizontally eastward, y-axis is perpendicular to it directed northward in the horizontal-plane while z-axis comes upright. The calculation area is covered by a uniform rectangular grid of 84×72 cells with the 250-m horizontal step and 30 cells with the 50-m vertical step.

The weather conditions were preset typical for 15:00 of local time of a July day with the westerly wind of 5 m/s at the height of the weather vane mounted at the weather site in Ogurtsovo village on the left bank of Ob river. Fields of average values of wind velocity components and temperature were determined with a digital-analytical model.[8] The components of the tensor of turbulent diffusion coefficients were obtained using an algebraic model similar to that in Ref. 9. In this model, the components are expressed in terms of universal functions of the dimensionless stability criterion, i.e., the gradient Richardson number defined by the fields of average wind speed and temperature.

Consider the algorithm for particle trajectory simulation. For each trajectory of the particle ensemble, emitted by the source, coordinate increments were determined at the $n + 1$ Δt-time step. In so doing the values $\overline{U}_i^n$ and K_i^n were determined at each step by means of the linear interpolation over 8 nodes of the computational grid, which surround the current coordinate of a particle. Sequences of independent pseudorandom numbers equidistributed over the range from 0 to 1 were generated by the residue method[10]:

$$r_{k+1} = \{Mr_k\},\ r_0 = 2^{-m},$$

where M is sufficiently large integer; m is the number of bits in the mantissa of memory cells. The period of such sequences equals to 2^{m-2}. It is about 10^9 for standard 32-bit processors. The subprogram DRAND[11] from the function library of the Compaq Visual FORTRAN package, version 6.5 was used to generate random numbers. Average values and variances of random sequences satisfied the condition of standard uniform distribution for random numbers within the range from 0 to 1: $\overline{r_i} = 0.5$ and $\sigma_{ri}^2 = 1/12$ accurate to better than 10^{-5}. Correlation coefficients of pairs of the random sequences used differed from zero by less than 10^{-6}.

If z-coordinate at the $n + 1$ time step was below the level of underlying surface, the passage to the next ensemble trajectory simulation was performed and the particle was considered absorbed by the underlying surface. The procedure was the same in the case when the coordinates obtained at the $n + 1$ time step exceeded the side and top boundaries of the preset rectangular area. After determining the set of coordinates of the whole particle ensemble at the time t, cells of the calculation rectangular area, which contains at least one particle, were defined. Such cells were marked by unity. Empty cells were marked by zero. Thus, a domain determining the boundary of the cloud of a spreading admixture was distinguished inside the calculation rectangular area.

The program for calculating the cloud boundary was tested with an example of admixture diffusion in the uniform field of wind velocity and at constant turbulent diffusion coefficients $\overline{U}_i$ = const and K_i = const. The calculations gave the cloud boundary in the form of an ellipsoid, the axes of which coincided with the theoretical values $A_i = 3\sqrt{2K_i\Delta t}$ accurate to one step of the calculation chart.

Figure 2 shows an example of the cloud boundary obtained for $t = 800$ s in the horizontal cross section $z = 50$ m for admixture diffusion over Novosibirsk. The considered ensemble consisted of $8 \cdot 10^4$ particles.

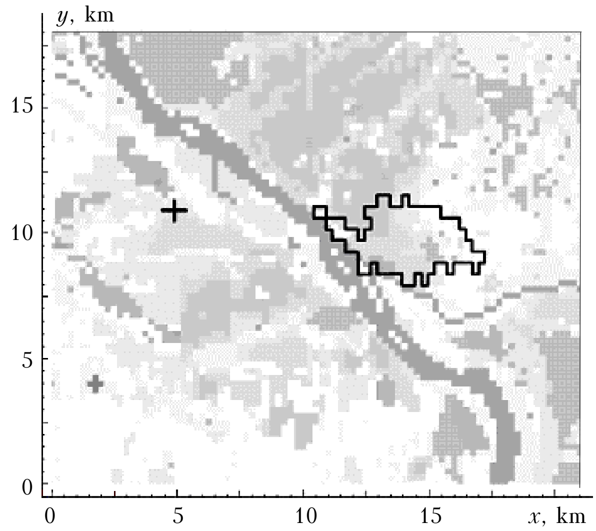

Fig. 2. Cloud boundary in $z = 50$ m cross section at $t = 800$ s (bold line); the cross denotes the source.

Calculations have shown that the double and greater increase of the number of ensemble particles for this example does not result in any significant change of the air admixture cloud boundary. Concentration isolines for this example have been obtained by the numerical solution of the turbulent diffusion equation (see Fig. 1). Concentration values of the given isolines correspond to 2.5, 2.0, 1.5, and 1.0 m^{-3} and decrease toward the boundary of the calculated domain. The set of admixture concentration isolines shown coincides in its characteristic sizes with the boundary obtained by the method of statistical modeling.

Thus, general view of the cloud boundary and concentration isolines are not totally similar while an admixture diffusing in nonuniform medium in contrast to the case of diffusion in a uniform field of wind velocity and at constant values of turbulent diffusion coefficients. Probably, reasons for this are the thermal inhomogeneity of the underlying surface and a complicated nonuniform landscape. Note, that out of the obtained cloud boundary there is large amount of the admixture in the solutions of the semiempirical equation, which cannot be reliable due to finite spread rate of particles. In particular, according to the solution of the semiempirical equation, more than 50% of the admixture is out of the cloud boundary, determined by the method of statistical modeling, at the time $t = 800$ s. Also note, that less than 3% of the admixture is out of the cloud boundary in the case of admixture diffusion in the uniform field of wind velocity and at constant values of the turbulent diffusion coefficients.

The considered approach is relevant in simulating the spread of air admixtures to short distances from a source when describing variations of concentration fields of air admixtures, including cases of complicated nonuniform landscape.

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