Function of concentration distribution for atmospheric polydisperse admixtures

A.I. Borodulin, B.M. Desyatkov, N.A. Lapteva, and A.A. Yarygin

Scientific-Research Institute of Aerobiology, State Scientific Center of Virology and Biotechnology "Vector", Kol'tsovo, Novosibirsk region

Received November 27, 2005

When modeling the spread of atmospheric contaminants, the determination of statistical characteristics of the admixture concentration is of importance. In this paper, the determination of distribution function of atmospheric polydisperse admixtures is considered.

Propagation of atmospheric admixtures is usually simulated by means of semi-empiric equation of the turbulent diffusion[1]:

$$\frac{\partial \overline{C}}{\partial t}+\overline{U}_i\frac{\partial\ \overline{C}}{\partial\, x_i}-V_s\frac{\partial\ \overline{C}}{\partial\, x_z}-\frac{\partial}{\partial x_i}K_{ij}\frac{\partial\ \overline{C}}{\partial\, x_j}=\overline{Q};\ (i,j=\overline{1,3}),\quad (1)$$

where $\overline{C}$ and $\overline{U}_i$ are the mathematical expectations of the admixture concentration and the wind velocity components, V_s is the velocity of gravitational sedimentation of particles, K_{ij} are the components of the tensor of coefficients of turbulent diffusion, $\overline{Q}$ is the term describing the sources and sinks of admixtures, $x_3 = z$ corresponds to the vertical coordinate. The bar over symbol means averaging over the statistical ensemble. Summation over repeated indices is meant. Equation (1) describes propagation of monodisperse fraction of admixtures with aerodynamic diameter D of particles. Therefore, $V_s = V_s(D)$ and $\overline{Q}=\overline{Q}(D)$ are functions of the particle diameter. When determining the concentration of polydisperse systems, the considered range of particle diameter $D_{min} \le D \le D_{max}$ is usually divided into the intervals ΔD, in which V_s and $\overline{Q}$ are assumed to not depend on particle diameter, and the concentration of fractions is determined by Eq. (1); then the concentrations of the found monodisperse fractions are summarized.

Propagation of atmospheric admixtures occurs in the turbulent medium, therefore, determination of some statistical characteristics of concentration fields is of practical importance. In particular, the concentration variance σ^2 can be determined through solving the equation[2]:

$$\frac{\partial\sigma^2}{\partial t}+\overline{U}_i\frac{\partial\sigma^2}{\partial x_i}-V_s\frac{\partial\sigma^2}{\partial x_z}-\frac{\partial}{\partial x_i}K_{ij}\frac{\partial\sigma^2}{\partial x_j}=K_{ij}\frac{\partial\overline{C}}{\partial x_i}\frac{\partial\overline{C}}{\partial x_j}.\quad (2)$$

However, finding the mathematical expectation and the concentration variance is insufficient for determining such characteristics as, for example, the probability of exceeding MPS by the admixture concentration, etc. In this paper we consider the determination of distribution of atmospheric polydisperse admixture concentrations, which allows solving such problems.

Let C_m be the density of the instant value of the concentration of the monodisperse fraction at the axis of the particle diameters. Its mathematical expectation corresponds to the solution of Eq. (1) with the preset density of distribution of the term describing sources of admixture $\overline{Q}_m$ at the axis of the particle diameters. Accordingly, the instant value and the mathematical expectation of the concentration of polydisperse admixture are represented by the formulas

$$C_p=\int_{D_{min}}^{D_{max}} C_m\,dD,\quad \overline{C}_p=\int_{D_{min}}^{D_{max}} \overline{C}_m\,dD.\qquad (3)$$

Equation (2) for the density of the concentration variance of the monodisperse fraction σ_m^2, in which $\overline{C}$ should be replaced by $\overline{C}_m$, corresponds to Eq. (1) written for $\overline{C}_m$.

Since the concentration of polydisperse system is the integral parameter, its distribution function $F(C_p)$ has the form[3]:

$$F(C_p)=1+\frac{1}{2}\left[\mathrm{erf}\left(\frac{C_p-\overline{C}_p}{\beta}\right)-\mathrm{erf}\left(\frac{C_p+\overline{C}_p}{\beta}\right)\right],\quad (4)$$

where erf is the integral of probability, $\overline{C}_p$ is the mathematical expectation of the polydisperse admixture concentration (see Eq. (3)), β is the second parameter of the distribution function. The relationship[3]:

$$\frac{\sigma_p^2}{\overline{C}_p^2}=\mathrm{erf}\left(\frac{\overline{C}_p}{\beta}\right)\left(1+\frac{\beta^2}{2\overline{C}_p^2}\right)-1+\frac{\beta}{\sqrt{\pi}\,\overline{C}_p}\exp\left(-\frac{\overline{C}_p^2}{\beta^2}\right),\quad (5)$$

where σ_p^2 is the concentration variance of the polydisperse admixture, relates β to $\overline{C}_p$ and σ_p^2. The distribution function (4) is the exact analytical

0235-6880/07/03 248-02 $02.00

solution of the Fokker–Plank–Kolmogorov equation and was obtained in the framework of the same assumptions as for deriving Eqs. (1) and (2). The form of $F(C_p)$ is justified by the cycle of experiments carried out in the aerodynamic tube and corresponds to the classic properties of asymptotics of the theory of turbulent combustion.[3] Note that $F(0)$ is the probability of observation of zero values of the concentration of polydisperse admixtures, that is the consequence of the concentration alternation effect.[3]

Since instant values of the concentrations of monodisperse fractions of different diameters are statistically independent, formula for the concentration variance has the form (see analogous formula in Ref. 4)

$$\sigma_p^2 = \int_{D_{min}}^{D_{max}}\int \overline{[C_m(D_1) - \overline{C}_m(D_1)][C_m(D_2) - \overline{C}_m(D_2)]}\,dD_1 dD_2 =$$

$$= 2\int_{D_{min}}^{D_{max}} (D_{max} - D)\,\sigma_m^2(D)\,dD. \qquad (6)$$

To determine $F(C_p)$, it is necessary and sufficient to solve equations (1) and (2) for $\overline{C}_m$, σ_m^2, and to determine $\overline{C}_p$ and β from Eqs. (3), (6), and (5).

Consider the example, in which a stationary point source with the coordinates $x_0 = 5$ km, $y_0 = 10$ km, $z_0 = 50$ km is situated in the left-coast part of the Novosibirsk city (see Fig. 1).

Two types of stationary point sources of polydisperse admixture with the same power but different dispersion composition of particles were set for the range $0 \le D \le 50$ μm:

$$\overline{Q}_{m1} = Q_0 \frac{D_{max} - D}{D_{max} - D_{min}} \delta(x - x_0)\,\delta(y - y_0)\,\delta(z - z_0),$$

$$\overline{Q}_{m2} = Q_0 \frac{D - D_{min}}{D_{max} - D_{min}} \delta(x - x_0)\,\delta(y - y_0)\,\delta(z - z_0),$$

$$Q_0 = 10^{10} \text{ arbitrary units},$$

where δ is delta-function. The source emits mainly fine particles in the first variant, and coarse ones in the second one. The meteorological conditions were taken typical for July in the region. The velocity at the weather-vane level at the left boundary of the area of calculations was set equal to 3 m/s. The results of calculation of $\overline{C}_p$ and σ_p at four points on the line $x > x_0$, $y = 10$ km, $z = 10$ m (see Fig. 1) are presented in the Table.

It is seen in the Table that the calculated values of mathematical expectation of concentrations of two considered polydisperse systems differ insignificantly. At the same time, the values of the standard deviation of the polydisperse admixture concentrations essentially depend on the shape of the initial particle size distribution.

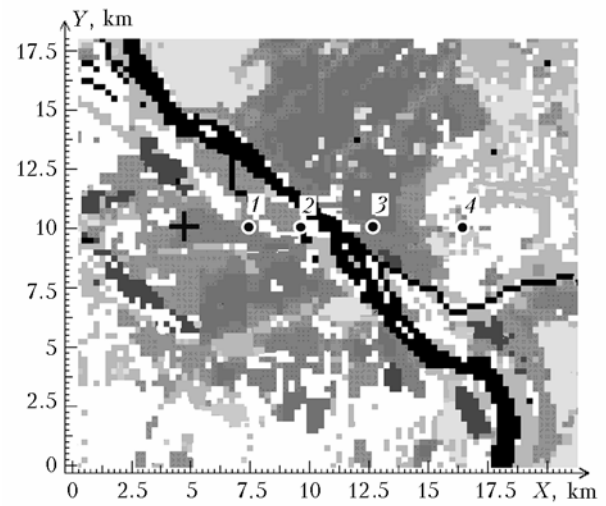

Fig. 1. Schematic image of the area of calculations. The source is marked by cross; the points, at which the mathematical expectations and the standard deviation of the concentration were calculated, are numbered.

Table. Calculated values of $\overline{C}_p$ and σ_p, arbitrary units

Parameter	Distance from the source, km			
	7.5	9.5	12.5	15.5
	variant $\overline{Q}_{m1}$			
$\overline{C}_p$	$1.99 \cdot 10^5$	$2.74 \cdot 10^4$	$3.95 \cdot 10^3$	$6.87 \cdot 10^2$
σ_p	$8.44 \cdot 10^3$	$2.62 \cdot 10^3$	$5.13 \cdot 10^2$	$1.16 \cdot 10^2$
	variant $\overline{Q}_{m2}$			
$\overline{C}_p$	$1.95 \cdot 10^5$	$2.62 \cdot 10^4$	$3.71 \cdot 10^3$	$6.13 \cdot 10^2$
σ_p	$4.72 \cdot 10^3$	$1.41 \cdot 10^3$	$2.71 \cdot 10^2$	$5.77 \cdot 10^1$

References

1. A.S. Monin and A.M. Yaglom, *Statistical Hydromechanics. Mechanics of Turbulence* (Nauka, Moscow, 1965), Part 1, 720 pp.
2. V. Rody, in: *Methods for Calculation of Turbulent Flows* (Mir, Moscow, 1984), pp. 227–321.
3. A.I. Borodulin, G.A. Maistrenko, and B.M. Chaldin, *Statistical Description of the Process of Turbulent Diffusions of Aerosols in the Atmosphere. Method and Applications* (Novosibirsk State University, Novosibirsk, 1992), 124 pp.
4. V.I. Tikhonov, Statistical Radioengineering (Radio i Svyaz', Moscow, 1982), 624 pp.