ESTIMATE OF THE CONCENTRATION VARIANCE OF AN ATMOSPHERIC ADMIXTURE

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The model of atmospheric turbulence is considered which takes into account the single-point distribution laws as applied to pulsations of wind velocity and passive admixture concentration components. The relations between pulsations of wind velocity and concentration components are determined by the Reynolds stress tensor and the turbulent admixture flows. Based on these assumptions and using the simulation methods for pulsations of wind velocity and admixture concentration, the expression has been derived enabling estimation of the admixture concentration variance without solving the corresponding semiempirical equation. The obtained results are compared with the variance values found by traditional methods. The estimates of the application area of the proposed method are obtained.

When simulating the aerosol particle spread in the atmosphere, sometimes it is essential to determine a series of additional characteristics apart from the fields of mathematical expectation of admixture concentration $C(x, y, z, t)$. One of such characteristics is, for example, the concentration variance $\sigma^2(x, y, z, t)$. When the simulation is made using the semiempirical equation of turbulent diffusion, then upon solution of the appropriate equation for the admixture concentration the variance can be found by solving the similar equation.[1,2] In some cases, the concentration variance can be estimated without solving this equation, for example, by means of the algebraic model.[1] However, applicability of such an approach is not quite clear.

This paper describes the method allowing estimation of the concentration variance without invoking the procedure of solution of the appropriate semiempirical equation, as well as discusses the obtained results.

Let us consider the model of the process of turbulent transfer of an admixture in the atmosphere taking into account the following factors: the single-point distribution laws of pulsations of the wind velocity components, which are taken to be normal[3]; the single-point distribution law of pulsations of the concentration[4]; and the correlation between pulsations of the wind velocity components and the admixture concentration. The correlation between pulsations of the wind velocity components is determined by the Reynolds stress tensor, and the turbulent flows of an admixture determine the correlation between pulsations of the admixture concentration and the wind velocity components.[2]

The statistical ensemble representing pulsations of the wind velocity components is given by the following expressions:

$$\hat{U}_x = \sigma_x \alpha_1,\ \hat{U}_y = \sigma_y(a_{21}\alpha_1 + a_{22}\alpha_2),$$

$$\hat{U}_x = \sigma_z(a_{31}\alpha_1 + a_{32}\alpha_2 + a_{33}\alpha_3), \qquad (1)$$

where $\hat{U}_x$, $\hat{U}_y$, $\hat{U}_z$ are pulsations of the wind velocity components; σ_x, σ_y, σ_z are the standard deviations of pulsations; α_m are the normally distributed random successions with the characteristics $\overline{\alpha_m\alpha_n}\ a\,\delta_{mn}$; $\overline{\alpha_m} = 0$, where δ_{mn} is the Kronecker symbol (m, n = 1, 2, 3). The over-bar denotes the procedure of averaging over the statistical ensemble. The coefficients a_{21}, a_{22}, …, a_{33} can be easily found from the relations given by the Reynolds stress tensor and are of the form

$$a_{21} = r_{xy},\ a_{22} = (1 - a_{21}^2)^{0.5},\ a_{31} = r_{xz},$$

$$a_{32} = (r_{yz} - a_{21}a_{31})(1 - a_{21}^2)^{-0.5},$$

$$a_{33} = (1 - a_{31}^2 - a_{32}^2)^{0.5},$$

where r_{xy}, r_{xz}, and r_{yz} are the correlation coefficients of pulsations of the corresponding wind velocity components.

Let $\alpha_0 = \xi_1\alpha_1 + \xi_2\alpha_2 + \xi_3\alpha_3$, where ξ_m are constants. The parameter α_0 is the linear combination of normally distributed variables, and hence it is also normally distributed. Then we give the variance of the parameter α_0

$$\sigma_\alpha^2 = \xi_1^2 + \xi_2^2 + \xi_3^2 = 1. \qquad (2)$$

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The random succession α_0 is connected with the parameter r_0 homogeneously distributed from 0 to 1 by the normal law. Assuming that the values of the distribution function $F(\hat{C})$ are equal to r_0, the solution of the given equation gives the unknown statistical ensemble of the concentration pulsations $(\hat{C})$. According to the definition,[2] the turbulent admixture flows φ_x, φ_y, and φ_z can be written as

$$\varphi_x = \sigma_x \overline{\alpha_1 \hat{C}}\ ,\ \varphi_y = \sigma_y (a_{21} \overline{\alpha_1 \hat{C}} + a_{22} \overline{\alpha_2 \hat{C}}\ ),$$

$$\varphi_z = \sigma_z (a_{31} \overline{\alpha_1 \hat{C}} + a_{32} \overline{\alpha_2 \hat{C}} + a_{33} \overline{\alpha_3 \hat{C}}\ ).$$

Having expressed the correlations $\overline{\alpha_m \hat{C}}$ in the explicit form and combined them with the weight factors ξ_m, we obtain

$$\frac{\varphi_x}{\sigma_z} \xi_1 + \left(\frac{b_1 \varphi_x}{\sigma_x} + \frac{b_2\, \varphi_y}{\sigma_y} \right) \xi_2 + \\ + \left(\frac{b_3\, \varphi_x}{\sigma_x} + \frac{b_4\, \varphi_y}{\sigma_y} + \frac{b_5\, \varphi_z}{\sigma_z} \right) \xi_3 - \overline{\alpha_0 \hat{C}} = 0. \qquad (3)$$

The constants b_1, b_2, ... b_5 are easily expressed through the parameters a_{21}, a_{22}, ... a_{33}.

Equality (3) in coordinates of ξ_m is the equation of a plane. If the distance from the coordinate origin to this plane is more than unity, then the plane does not touch the sphere (2) and, evidently, it is impossible to determine the constants ξ_m. If this distance is less than unity, the infinite set of ξ_m triplets is determined by coordinates of the points located at the circumference being the intersection line of the sphere and the plane. Thus, the uniquely determinable triplet ξ_m can be found only if the plane is tangent to the sphere, namely,

$$1/\mu = [r_{xc}^2 + (b_1\, r_{xc} + b_2\, r_{yc})^2 + \\ + (b_3\, r_{xc} + b_4\, r_{yc} + b_5\, r_{zc})^2\,]^{0.5} = r_{\alpha c}, \qquad (4)$$

where $r_{\alpha c}$ is the correlation coefficient of the parameters α_0 and $\hat{C}$; r_{xc}, r_{yc}, and r_{zc} are the correlation coefficients of pulsations of the concentration and the wind velocity components. The latter coefficients are determined by the relations: $r_{xc} = \varphi_x/\sigma_x\sigma_c$; $r_{yc} = \varphi_y/\sigma_y\sigma_c$ and $r_{zc} = \varphi_z/\sigma_z\sigma_c$, where σ_c is the standard deviation of concentration pulsations.

It is evident that the correlation coefficient $r_{\alpha c}$ does not depend on the constants ξ_m and at a given distribution law $F(\hat{C})$ (Ref. 4) is the universal function of the intensity of concentration pulsations $I_c = \sigma_c/\overline{C}$. The I_c dependence of $r_{\alpha c}$ is given in Fig. 1 (curve *1*).

From Eq. (4) it might be assumed that the dependence of the product of I_c and $r_{\alpha c}$ as a function of I_c uniquely expresses the dependence of the concentration variance on its mathematical expectation and the turbulent flows of an admixture. Actually, at the given $\overline{C}$, φ_x, φ_y, and φ_z, Eq. (4) multiplied by I_c does not depend explicitly on σ_c. Therefore, by the value of $I_c r_{\alpha c}$ we can uniquely determine the value of I_c, and then the concentration variance. Thus, the proposed model allows us to find the concentration variance without solving of the corresponding equation.[1]

Evidently, the product $I_c r_{\alpha c}$ is also the universal function of I_c. The I_c dependence of the product $I_c r_{\alpha c}$ is given in Fig. 1 (curve *2*). The curve reaches its maximum at $I_c = 3.8$ with the value 1.86. We see that the function reciprocal to $I_c r_{\alpha c}$ also has two values. Its first branch is defined at $0 \le I_c \le 3.8$, and the second branch is defined at $3.8 < I_c$. Assume that $\overline{C}$ = const. It follows from the definition of the turbulent flows that the increase of these flows results in the increasing scale of concentration pulsations and the growth of I_c. The first branch of the reciprocal function describes adequately this case. The I_c behavior at the second branch contradicts to the physical sense, and therefore it should be rejected.

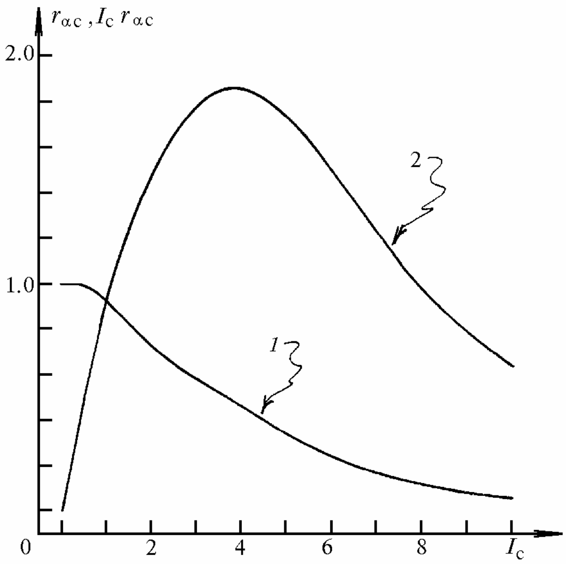

FIG. 1. Dependences of $r_{\alpha c}$ and $I_c r_{\alpha c}$ on the intensity I_c of concentration pulsations.

However, there are more significant restrictions on the intensity I_c of pulsations. These restrictions are associated with the applicability conditions of the distribution law we use for the concentration.[4] The experimental investigations and the data of a series of independent studies show that the distribution function of concentration pulsations $F(\hat{C})$ from Ref. 4 is applicable only for $I_c < 3$. Therefore, we will take into account just this limitation.

An expression is also proposed for determining the constants ξ_m, which, by definition, are the direction cosines of the vector connecting the origin and the point of tangency of the sphere and the plane

$$\xi_1 = \mu\, r_{xc},\ \xi_2 = \mu(b_1\, r_{xc} + b_2\, r_{yc}),$$

$$\xi_3 = \mu(b_3\, r_{xc} + b_4\, r_{yc} + b_5\, r_{zc}).$$

As a practical example we consider the process of spread of a weightless admixture in the half-space $x \ge 0$. Let us assume that the vector of a mean value of the wind velocity $\overline{U_x}$ = const is directed along the x axis. The coefficients of turbulent diffusion may be given as $K_x = 0$; $K_y = K_z = K$ = const. Assume that the stationary point source of particles is located at the origin of the coordinates and emits Q grams of particles per second. The semiempirical equations for determining the admixture concentration and the variance are reduced to the dimensionless form by introducing the scales of time, length, and concentration $T = K(\overline{U_x})^{-2}$, $X = K(\overline{U_x})^{-1}$, and $C = QU_xK^{-2}$. In this case they are of the following form[1,2]:

$$\frac{\partial \overline{C}}{\partial x} - \frac{\partial^2 \overline{C}}{\partial y^2} - \frac{\partial^2 \overline{C}}{\partial z^2} = 0, \tag{5}$$

$$\frac{\partial \sigma_c^2}{\partial x} - \frac{\partial^2 \sigma_c^2}{\partial y^2} - \frac{\partial^2 \sigma_c^2}{\partial z^2} = 2\left(\frac{\partial \overline{C}}{\partial y}\right)^2 + 2\left(\frac{\partial \overline{C}}{\partial z}\right)^2 - 0.16 I_u^2\, \sigma_c^2\,,$$

where I_u is the pulsation intensity of the wind velocity components. The second equation in the system (5) is written with the use of a hypothesis of proportionality of the turbulent diffusion coefficients to the corresponding components of the Reynolds viscous stress tensor,[1,4] what has determined the form of the last-named term describing the dissipation of the concentration variance and the constant value in this term.

For the given example, the expression for determining σ_c, according to the above-derived relation (4), is the following:

$$I_c\, r_{\alpha c} = \frac{1}{I_u\, \overline{C}}\left[\left(\frac{\partial \overline{C}}{\partial y}\right)^2 + \left(\frac{\partial \overline{C}}{\partial z}\right)^2\right]^{0.5}. \tag{6}$$

The right-hand side of Eq. (6) can be found using the numerical methods for the solution of the first equation of the system (5) (see Ref. 5). Then, as follows from curve *2* in Fig. 1, we can determine the pulsation intensity I_c and then calculate the admixture concentration variance using the given values of $\overline{C}$.

Figure 2 gives the example of the comparison of the calculated results on the concentration pulsation intensity I_c obtained using the numerical methods for solution of the set of equations (5) (abscissa) with the pulsation intensity obtained using the relation (6) without solving the set of equations (5) (ordinate). The points in the figure correspond to the points of the calculation pattern and are given for $50 \le x \le 10^4$ and $0 \le (y^2 + z^2)^{1/2} \le 10^4$. The dashed line is drawn at a 45° angle to the axes. In calculation, it was believed that $I_u = 0.10$. The agreement obtained at $I_c < 0.8$ is wholly satisfactory because the results are within the errors of the numerical methods used in calculations. In this case, the determination error of the pulsation intensity of the admixture concentration does not exceed 5%.

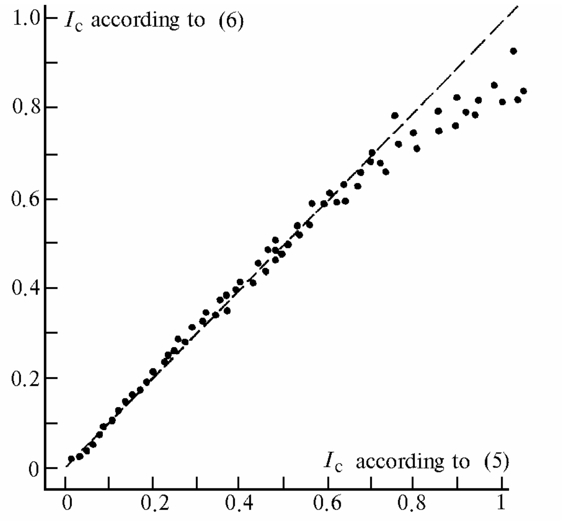

FIG. 2.

It is clear from the data given in Fig. 1, that at $I_c < 0.8$, the I_c dependence of $I_c r_{\alpha c}$ is practically linear with an accuracy no less than 5%. Therefore, for $I_c < 0.8$ Eq. (6) is greatly simplified

$$I_c = \frac{1}{I_u\, \overline{C}}\left[\left(\frac{\partial \overline{C}}{\partial y}\right)^2 + \left(\frac{\partial \overline{C}}{\partial z}\right)^2\right]^{0.5}. \tag{7}$$

This comment refers also to the general form of the given equation (4) at $I_c < 0.8$.

In conclusion, we dwell on the comparison of this given approach with the above-mentioned algebraic method. The essence of the algebraic method consists in the assumption of the balance of generation and the dissipation of the variance (see the two terms in the right-hand side of the second equation of the set of equations (5)). According to the above-said, for this example we have the following expression for the intensity of concentration pulsations:

$$I_c = \frac{3.54}{I_u\, \overline{C}}\left[\left(\frac{\partial \overline{C}}{\partial y}\right)^2 + \left(\frac{\partial \overline{C}}{\partial z}\right)^2\right]^{0.5}. \tag{8}$$

Hence it follows that at least in the above-mentioned specific case the algebraic approach to the determination of the concentration variance gives the variance estimates, which are unsuitable for practical use.

Thus, we are able to verify that the use of the sufficiently simple but physically substantial model enables us to estimate the variance of the admixture concentration without solving the corresponding equation. It is evident that the considered approach is not based on a specific type of the distribution laws of the wind velocity and concentration. Therefore, it can be improved by setting more accurate distribution functions with a wider range of applicability. This approach is also suitable for practical implementation because when simulating the admixture spread using traditional methods it does not involve additional unknown values.

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