DISTRIBUTION FUNCTION FOR TIME DURING WHICH THE INTEGRAL CONCENTRATION OF AN ADMIXTURE BEING DISPERSED IN THE ATMOSPHERE REACHES A THRESHOLD VALUE

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We consider the statistics of time during which the integral concentration of an atmospheric admixture reaches some preset threshold value. The distribution functions for that time have been obtained for continuous and discrete processes of the admixture concentration variation. We discuss a possibility of approximating the distribution function for the discrete process by its analog obtained for the case when concentration is a continuous function. Practical significance of the account for statistical nature of the admixture formation to the state when its integral concentration reaches some preset threshold value has been demonstrated by way of a simple example.

The study of the dispersal of an atmospheric admixture is a very important task within the entire scope of the problems on meteorological aspects of the atmospheric pollution. Specific features in the admixture distribution in time and space are also an important part of such studies. Among the characteristics that are widely used to quantify the level of atmospheric contamination is the concentration of a contaminating species. Normally, it is compared with the relevant value of the maximum permissible concentration (MPC) that is being established by state regulations. The latter are based on empirical data and refer to a certain time interval of observations over the concentration variation.[1] Most often one uses MPCs that are connected with short-time effect of admixtures (from minutes to hours) and long-time effects (24 hours and longer). In some cases, the so-called «secondary standards» are introduced. These standards contain concrete limitations on the duration of effects of the contaminating species. An example of such characteristics[1] is given in Table I.

TABLE I. Some secondary standards of air quality in the USA (according to Ref. 1).

Substance	Secondary standard, mg/m^3	Duration of the action, h
Dust (solid particles)	0.15	24
Sulfur dioxide	1.3	3
Carbon monoxide	40.0	1

Thus, when completing some ecological tasks one ought, in the general case, to consider the product of an admixture concentration by time of its effect, instead of the MPC. So, equally strong damage from a concrete contaminating species is reached either with its high concentration and short time of the effect, or with low concentration and relatively long time of action. The above-stated can be quantitatively described by the integral concentration of an admixture

$$D = \int_0^T C(t)\, \mathrm{d}t = T\, \frac{1}{T} \int_0^T C(t)\, \mathrm{d}t = T\, C_T,$$

where $C(t)$ is the instant admixture concentration at a given point; T is duration of its action; C_T is the concentration averaged over time T. Since $C(t)$ is a random value, the integral concentration D and C_T are also random functions of time. If the process of variation of the admixture concentration is ergodic, we have $q_T = \overline{C}$, where $\overline{C}$ is the concentration value averaged over an ensemble.

The aim of this study is to derive the distribution function for time intervals in which the integral concentration of an admixture reaches some preset threshold value.

Below we assume, without any loss of generality, that $C(t)$ is the number concentration of particles. In the case of an admixture being emitted into the atmosphere from a short-lived source there is a time moment when the continuous function $C(t)$, at each point of the space, (defined as a limit of the ratio of particles' number $n(t)$ to volume V as the latter tends to zero) becomes an incorrect characteristic. This is connected with the fact that, if the number of particles $n(t)$ is finite, its ratio to volume V, tending to zero, becomes an indefinite value. In this case one have to consider an integer number of particles $n(t)$ contained in a given finite volume V, instead of $C(t)$. Therefore we consider, in what follows, two cases. In one of

them, the particles' concentration $C(t)$ is a continuous function of time. In the other one, the concentration is defined as $q(t) = n(t)/V$, where $n(t)$ is an integer-valued function.

Let $F(D, t)$ be the distribution function for the integral concentration of the admixture. The value $F(D_0, T)$ can be interpreted as the probability that the integral concentration of the admixture D does not exceed the threshold value D_0: $D < D_0$. Let us denote it by $W\{D < D_0\}$. Let $G(t, D_0)$ be the distribution function of time intervals in which the quantity D reaches D_0 value. The value $G(T, D_0)$ is the probability that for $t \geq T$ the integral concentration D exceeds D_0: $D \geq D_0$. Let us denote it by $W\{t \geq T\}$. Since D is a monotonic function of time, the events $\{t \geq T\}$ and $\{D \geq D_0\}$ are equivalent and their occurrence probabilities are equal. From that it follows that $W\{t \geq T\} = W\{D \geq D_0\} = 1 - W\{D < D_0\}$, and the unknown distribution function for time intervals is $G(T, D_0) = 1 - F(D_0, T)$. The probability density of the time interval in which the integral concentration D reaches the value D_0 is, evidently, as follows

$$g(T, D_0) = -\frac{\partial F(D_0, T)}{\partial T} .$$

The distribution function for the value of integral concentration (according to Ref. 2) has the form

$$F(D, T) = 1 + \frac{1}{2}\left[\mathrm{erf}\left(\frac{D - \bar{D}}{\beta}\right) - \mathrm{erf}\left(\frac{D + \bar{D}}{\beta}\right)\right],$$

where $\bar{D}$ is the mathematical expectation of the integral concentration of the admixture; β is the second parameter of the distribution function; erf is the probability integral.[3] The parameters are given by the following relations[2]:

$$\bar{D} = \int\limits_0^T \bar{C}(t)\, \mathrm{d}t; \quad \beta^2 = C_0\, \tau \int\limits_0^T \sigma_c^2(t)\, \mathrm{d}t,$$

where σ_c^2 is the variance of the admixture concentration; τ is the characteristic time scale of the concentration pulsations; $q_0 = 1.59$.

The distribution function $F(D, T)$ is an exact analytical solution to the Kolmogorov equation. Its applicability has been verified in several experiments performed in a wind tunnel.[2]

In addition, let us present the expression for the mth moment of the time interval. It follows from the above reasoning that

$$\overline{T^m} = m \int\limits_0^\infty T^{m-1}\,\text{»}F(D, T) - F(D, \infty)]\, \mathrm{d}t$$

$(m = 1, 2, \ldots).$

In the general case, the distribution function $G(T, D_0)$ for time intervals is equal to unity as T tends to infinity. This is caused by the fact that the condition $D \geq D_0$ does not hold for some statistical ensembles of time intervals considered. So, the probability density $g(T, D_0)$ is not normalized to unity in the general case.

Thus, the mathematical simulations of the dispersal of a contaminating admixture, enables one, based on the above reasoning and expressions derived, to determine the statistical characteristics of time moment at which its integral concentration reaches a preset threshold value.

Now let us consider the second case. Let concentration be determined as $q(t) = n(t)/V$. Then the value $D_k = (k\,T)/V$, where k is the mean number of particles observed in a volume V during time T (k is an integer value), is an analog of integral concentration D. Let W_0 be the probability that a particle emitted from a source falls within the volume V during time T. If the source emits q similar particles simultaneously, the probability that k particles fall within the volume V during the time T is, evidently,

$$C_q^k\, W_0^k\, (1 - W_0)^{q-k},$$

where C_q^k is the binomial coefficient. If q tends to infinity, we obtain the probability that k particles are observed in the volume V during time T in the form of the nonuniform Poisson law[3]:

$$P(k) = \sum_{i=0}^{k} \frac{1}{i!}\, (\bar{k})^i \exp(-\bar{k}), \quad (k = 0, 1, 2, \ldots),$$

where $\bar{k}$ is mathematical expectation of the value k that, in the general case, depends on time. The connection between the mathematical expectation $\bar{k}$ and the variance σ_k^2 is described by the formula

$$\bar{k} = \sigma_k^2 = \int\limits_0^T \nu(t)\, \mathrm{d}t,$$

where ν is the number of particles falling into the volume V per unit time.

Let $Q(t, k_0)$ be the distribution function for time intervals in which the number of particles k reaches a preset threshold value k_0 in a given volume V. Let the changes in k occur at the moments t_k. Then the value $Q(T, k_0)$ is the probability that k does not exceed k_0 at the moment $T > t_k$. Let us denote it by $W\{T > t_k\}$. Since the integral concentration D_k is a monotonic function of time, the events $\{T > t_k\}$ and $\{k > k_0 - 1\}$ are statistically equivalent. From that it follows that $W\{T > t_k\} = W\{k > k_0 - 1\}$. Then

$$W\{t_k > T\} = 1 - W\{k \leq k_0 - 1\}$$

and

$$Q(T, k) = 1 - \sum_{i=0}^{k-1} \frac{1}{i!} \, (\bar{k})^i \exp(-\bar{k})$$

$(k = 1, 2, \ldots)$.

The probability density corresponding to function $Q(T, k)$ has the form

$$q(T, k) = \frac{(\bar{k})^{k-1}}{(k-1)!} \exp(-\bar{k}) \frac{\partial \bar{k}}{\partial t}.$$

In the case when $\bar{C}$, σ_c, and ν are constant, we obtain

$$G(\xi, D_0) = \frac{1}{2} \left[\mathrm{erf}\left(\frac{a_1 + \xi}{a_2 \, \xi^{0.5}} \right) - \mathrm{erf}\left(\frac{a_1 - \xi}{a_2 \, \xi^{0.5}} \right) \right];$$

$$Q(\xi, k_0) = 1 - \sum_{i=0}^{k_0-1} \frac{1}{i!} (\nu \, \tau \, \xi)^i \exp(-\nu \, \tau \, \xi);$$

$a_1 = D_0 / (\bar{C} \, \tau)^{-1}$, $a_2 = (C_0 \, \sigma_c) / \bar{C}$, $\xi = t / \tau$.

Physical nature of continuous and discrete random processes is different in principle, so we have no a possibility of coming from one distribution type to another with by a passage to a limit. But, then one can use the function $G(\xi, D_0)$ to approximate the function $Q(\xi, D_0)$. Taking

$$D = D_k, \quad D_0 = (k_0 T) / V, \quad \bar{D} = \bar{D}_k = \nu \, T^2 / V,$$

we obtain the approximation function in the form

$$G_0(\xi, k_0) = \frac{1}{2} \,\text{»erf}\,(a + b\xi) - \mathrm{erf}\,(a - b\xi)];$$

$a = k_0 \,\text{»} C_0 (\nu \, \tau)^{0.5}]^{-1}$, $b = C_0^{-1} (\nu \, \tau)^{0.5}$.

The distributions $Q(\xi, k_0)$ and $G_0(\xi, k_0)$ have two initial moments

$$\overline{\xi_k} = k_0 / (\nu \, \tau),$$

$$\bar{\xi} = b^{-1} \,\text{»exp}\,(-a^2) / \pi^{0.5} + \mathrm{erf}\,(a)],$$

$$\overline{\xi_k^2} = \frac{k_0}{(\nu \, \tau)^2} \left(1 + \frac{1}{k_0} \right), \quad \overline{\xi^2} = \frac{1}{b^2} \left(\frac{1}{2} + a^2 \right).$$

The conditions

$$\bar{\xi} \le (1 + \varepsilon) \, \overline{\xi_k}, \quad (1 - \varepsilon)^2 \, \overline{\xi_k^2} \le \overline{\xi^2},$$

where ε is an error, are taken as a criterion of the closeness between $Q(\xi, k_0)$ and $G_0(\xi, k_0)$. The domain of values of k_0 and $(\nu \, \tau)$ corresponding to close distributions $Q(\xi, k_0)$ and $G_0(\xi, k_0)$ for $\varepsilon = 0.01$ is as follows:

$$-0.02 \, k_0^2 + 0.78 \, k_0 \le (\nu \, \tau) \le 0.21 \, k_0^2; \, k_0 \ge 4.$$

The rate of particles' invasion into the volume V is, by definition, as follows:

$$\nu = - \int_S (\varphi \cdot \mathbf{dS}),$$

where φ is the vector of aerosol admixture flux; $\mathbf{dS}$ is a surface element of the volume V. The integral must be taken over surface S of the volume V under condition that the dot product of the vector φ and normal to the surface is negative.

Let us consider the function $G(\xi, D_0)$. It is evident that in the above accepted dimensionless variables the value a_1 estimates the mathematical expectation of the time interval in which the integral concentration reaches a preset boundary value. The parameters of this distribution function are determined by the mathematical expectation of concentration $\bar{C}$, intensity of its pulsation $I_c = \sigma_c / \bar{C}$, and by the threshold value of the integral concentration D_0. The Figure 1 presents an example how the distribution function of time intervals depends on the parameters a_1 and a_2.

Below, in Table II one can see the mathematical expectations of time intervals in which integral concentration reaches a preset threshold value within the standard deviation interval. Those are calculated by the relations presented above as functions of I_c and a_1.

TABLE II. *Mathematical expectation of time, plus minus standard deviation, in which the integral concentration reaches a preset threshold value depending on the intensity of concentration pulsation.*

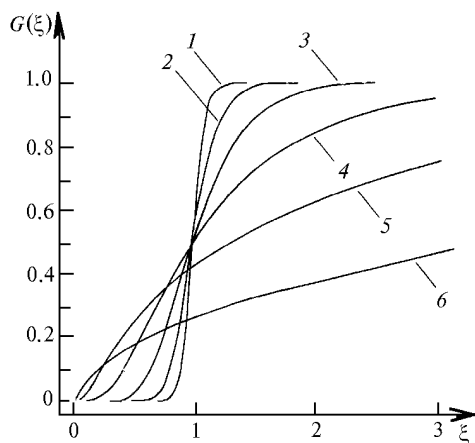| a_1	I_c			
	0.125	0.25	0.5	1.0
0.01	0.02 ± 0.03	0.08 ± 0.11	0.28 ± 0.31	0.56 ± 0.41
0.10	0.11 ± 0.05	0.14 ± 0.13	0.34 ± 0.46	1.26 ± 1.72
1.00	1.00 ± 0.20	1.03 ± 0.33	1.15 ± 0.69	1.76 ± 1.93
10.00	10.00 ± 1.48	10.00 ± 1.72	10.01 ± 2.33	10.05 ± 4.11
100.00	100.00 ± 10.0	100.01 ± 13.1	100.04 ± 15.2	100.10 ± 19.4

FIG. 1.   *Distribution function of the time interval in which the integral concentration reaches a preset threshold value at* $a_1 = 1$, $a_2 = 0.125$, 0.25, 0.5 1, 2, *and* 4 *(curves 1, 2, ... , 6, respectively)*

One can see that mathematical expectation of time is always greater or equal to a_1. The maximum deviations occur at minimum values of a_1 and I_c. The deviation of mathematical expectation of time from its estimate increases with increasing I_c. However the opposite behavior is characteristic of the case with increasing a_1. Standard deviation of time grows with the increases in a_1 and I_c. Significant, more than 10%, standard deviations are observed for $a_1 < 10$ and $I_c > 0.25$.

Thus, statistical nature of the integral concentration has a significant effect on time in which the concentration reaches a preset threshold value. This is of basic importance, for instance, in estimation of maximum permissible, for people, time of staying in a contaminated zone. Although the trivial estimate of the mathematical expectation, a_1, is approximately equal to time in which the integral concentration reaches a preset threshold value, we have a strong spread in the instantaneous values of time in which the integral concentration reaches a preset threshold value when the intensity of concentration pulsation becomes higher. This demonstrates the necessity to revise modern guides that regulate the time admissible for people to stay in zones dangerous for health. Corresponding theoretical grounds have been described in this paper. According to the above consideration, in the general case, one ought to consider the probability of time interval in which the integral concentration reaches a preset threshold value instead of the trivial estimate of the time a_1.

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