Probability of exceeding threshold concentration of an atmospheric admixture

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We propose a statistical approach to achieving the task of calculating the probability of exceeding threshold concentration of an atmospheric admixture. Calculations were made for the case study on the spread of nitrogen dioxide emitted from two power plants in Novosibirsk. The fields of admixture concentration and its variance, as well as the probability of exceeding threshold concentration of an atmospheric admixture at a given point are calculated for different times of a day and wind speeds. In a series of calculations, it was shown that the probability of interest here depends in a complex way on thermal atmospheric stratification and on the concentration field of an atmospheric admixture. In particular, during a summer day the dependence of the probability on threshold concentration looks like a steep "step". Quite the opposite situation is observed at night, when curves of the probability versus admixture concentration are substantially flattened. This is because the probability density function of an atmospheric admixture concentration has a bimodal shape.

Solution of many ecological problems dealing with the atmospheric pollution by industrial gaseous and aerosol admixtures is often reduced to analysis of time-averaged concentrations which, in general, are too unrepresentative characteristics of the random process under study. In particular, actual admixtures may show considerable deviation of the concentration from the measured or calculated mean values in the region under study. Therefore, by making use of information on the probability of exceeding mean or some threshold concentration of an atmospheric admixture value is important in practical applications. In this paper, this problem is studied by simulating the spread of industrial pollutants over an actual industrial center.

The distribution function of an atmospheric admixture concentration $F(C)$ was derived theoretically and tested experimentally in a wind tunnel.[1] It has the form:

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

where C is the instantaneous admixture concentration; $\bar{C}$ is the average concentration; erf(...) is the error function; β is the second parameter of the distribution law related to the variance of concentration σ^2 as

$$\frac{\sigma^2}{\bar{C}^2} = \operatorname{erf}(\beta_0)\left(1 + \frac{1}{2\beta_0^2}\right) - 1 + \frac{1}{\sqrt{\pi}\beta_0}\exp(-\beta_0^2); \quad \beta_0 = \frac{\bar{C}}{\beta}. \quad (2)$$

It is important to note that the distribution law (1) characterizes the intermittency of admixture concentration. Indeed, assuming that $C = 0$ in (1), we obtain the probability of observing zero concentration, $F(0) = 1 - \operatorname{erf}(\beta_0)$. These relations can be used to solve many practical problems (see Refs. 2–6).

Here, analysis will be given for the case of the spread of nitrogen dioxide emitted by closely located power plants TES-2 and TES-3 in Nobosibirsk, each having three 60 to 120-m tall stacks. The effective height of the sources was determined by formulas from Ref. 7. For convenience of presentation and omitting different factors, influencing the calculation and associated with the inhomogeneity of urban underlying surface (such as thermal and orographic inhomogeneity and surface roughness, as well as different types of boundary conditions at the surface), horizontal homogeneity will be assumed throughout the computation.

Under these assumptions, the admixture transport will be entirely determined by wind velocity, thermal stratification of the atmosphere, and intensity of the turbulent exchange. The admixture transport will be assumed a steady-state process. For different times of a day and different wind speeds, we calculated the concentration field, variance of concentration, and probability of exceeding threshold concentration of an atmospheric admixture at a given point. All estimates are made for 2 m height above the ground surface.

The fields of wind velocity and temperature over the computation domain were determined using numerical-analytical method as given in Ref. 8. The admixture concentration was calculated by solving the semiempirical equation of turbulent diffusion and the corresponding equation for the variance of concentration.[9] The obtained fields of the mean and variance values of admixture concentration then were used to calculate the probabilities according to formulas (1) and (2).

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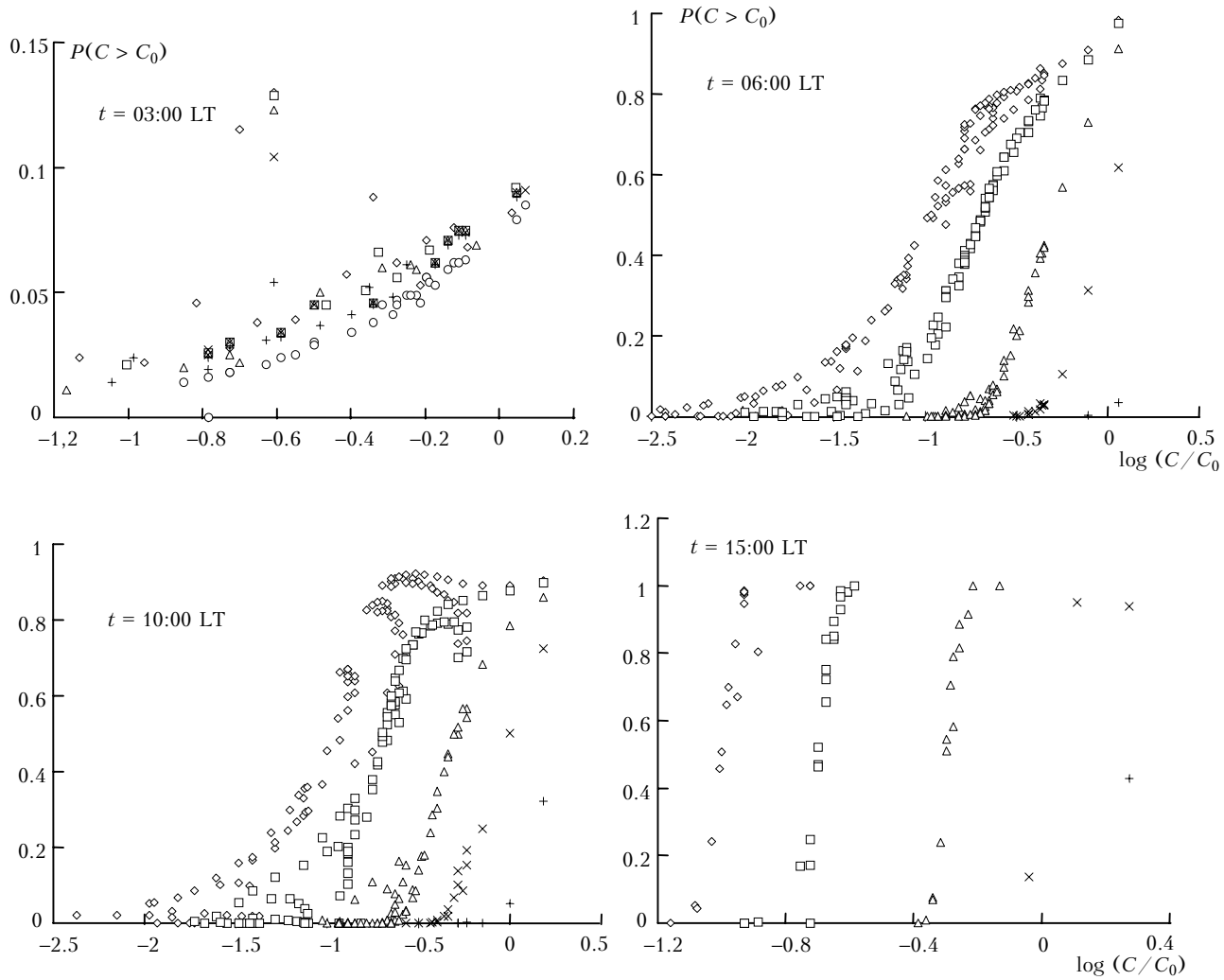

Fig. 1. Probability of exceeding the nitrogen dioxide concentration threshold C_0 at 03:00, 06:00, 10:00, and 15:00 LT; computations are made for C_0 = 0.1 (◊); 0.2 (□); 0.5 (Δ); 1 (×); 2 (+); 5 (○).

Figure 1 presents the probabilities of exceeding threshold concentration of nitrogen dioxide C_0 calculated for 03:00, 06:00, 10:00, and 15:00 Local Time (LT) and wind speed 2 m/s at a height 2 m above the ground surface. All quantities in units of concentration are normalized to the maximum permissible concentration of nitrogen dioxide that was assumed to be $C_0 = 0.85 \cdot 10^{-4}$ g/m^3 in this paper. The vertical turbulent exchange is absent during night; for this reason, the calculated concentrations at height 2 m are typically several orders of magnitude lower at night than during daytime. For the ease of comparison of calculated nighttime concentrations at 2 m height with their daytime counterparts, the level of nighttime aerosol emission was taken three orders of magnitude higher than usual, which, due to the linear dependence of admixture concentration and its variance on source strength, has little influence on the resulting β_0 value.

During daytime, (15:00 LT), the curve of the probability versus concentration is very steep. When $C = C_0 = \bar{C}$, the concentration may exceed C with the probability of 0.5. At this locality, an increase of concentration by only 10% causes more than 30% growth in the probability. This finding is very important for practical applications. For instance, when at a given location the mean concentration is calculated/measured to be equal to or lower than the maximum permissible concentration, this does not mean that the situation is so much fine. In fact, with the probability of 0.5 the concentration may exceed considerably the maximum permissible level. Moreover, considering that the relative measurement error often exceeds 10%, in practice the pollution level at a given location may considerably exceed the maximum permissible one with the probability in excess of 80%.

For 06:00 and 10:00 LT, the excess probability vs. concentration dependence has a less steep slope, probably because of a weaker turbulent exchange and, hence, smaller variance and, consequently, smaller parameter β_0 at this time. It is remarkable that the

scatter in the probability vs. concentration dependence, is most pronounced at 10:00 LT. Probably, this is because that at this location the variance of concentration depends on the spatial gradients of concentration, and not only on the mean concentration. As a consequence, regions with the identical mean values while different variances of the concentration may have different excess probabilities. Moreover, with the increase of the threshold concentration, the excess probability may even decrease. This is evident from the data presented here for 10:00 LT.

The situation is quite different at 03:00 LT. The dependences of the probability of exceeding the concentration threshold are flat. As seen, within the entire concentration range under study, of exceeding the concentration threshold C_0 has the magnitude less than during daytime hours. Even in the cases with the mean concentration many times larger than C_0, at this location, the probability of concentration in excess of C_0 is small and weakly depends on the admixture concentration. Although surprising at the first sight, this is a consequence of the bimodal probability density function of concentration, i.e., the intermittency of the concentration values occurrence. When the parameter β_0 is small, most of the constituents of the ensemble of instantaneous concentrations are close to zero value. For this reason, at low β_0 values, the distribution function of concentration rapidly reaches its maximum at the unity value and then remains almost unchanged; i.e., the corresponding probability that $C > 0$, expressed as $P(C > 0) = \mathrm{erf}(\beta_0)$, is near unity and weakly depends on the concentration $C > 0$.

Table 1 presents typical (for this case) values of the studied characteristics at the same finite-difference grid points. As the wind speed increases from 2 to 7 m/s, for the six stacks considered here the height of the initial plume ascend decreases on the average by approximately 8 times, while the rate of the vertical turbulent exchange increases by a factor of 50 at night and 1.2 during daytime. As a result, the nighttime concentrations at the height of 2 m become very close to daytime values at the wind speed of 2 m/s, while the dependence of the excess probability vs. concentration for nighttime conditions become more and more like those for the daytime hours at the identical source strengths. Under daytime conditions, the increase in the wind speed from 2 to 7 m/s leads to no significant changes in the concentration field at the 2-m height. The probability vs. concentration dependences become steeper. Values of the studied characteristics, typical for the cases considered here, are summarized in Table 1.

It could be expected that, for the cases with a significantly inhomogeneous underlying surface, the field of the probability of concentration in excess of some preset threshold will be very patchy, and that its prediction will be almost impossible without the knowledge of the variance of concentration and probability density function.

Table. Nitrogen dioxide concentration, parameter β_0, and the probability of exceeding the maximum permissible concentration (C_0) at two times of a day and two wind speeds

$\bar{C}$, g/m^3	β_0	$P(C>C_0)$	$\bar{C}$, g/m^3	β_0	$P(C>C_0)$
03:00 LT			15:00 LT		
Wind speed is 2 m/s					
$0.138\cdot10^{-5}$	0.01	0.01	$0.541\cdot10^{-6}$	1.56	0.00
$0.221\cdot10^{-4}$	0.03	0.03	$0.840\cdot10^{-5}$	6.24	0.46
$0.880\cdot10^{-5}$	0.03	0.03	$0.105\cdot10^{-4}$	3.16	0.81
$0.173\cdot10^{-4}$	0.10	0.11	$0.446\cdot10^{-4}$	3.08	0.99
Wind speed is 7 m/s					
$0.842\cdot10^{-6}$	3.27	0.00	$0.110\cdot10^{-5}$	2.71	0.00
$0.626\cdot10^{-5}$	7.35	0.00	$0.793\cdot10^{-5}$	10.14	0.12
$0.692\cdot10^{-5}$	4.19	0.09	$0.134\cdot10^{-4}$	3.82	0.96
$0.19\cdot10^{-4}$	5.64	1.00	$0.415\cdot10^{-4}$	4.04	1.00

To solve many problems dealing with the assessment of the effect of pollution on the public health, persistence, and not only the magnitude of concentration in excess of some threshold may be required. This characteristic can be estimated using the intermittency concept, interpreted as the probability of finding nonzero concentrations, i.e., the probability of exceeding the zero threshold of the admixture concentration. If the intermittency concept is generalized formally, and a concentration $C_* \neq 0$ is used as a basis, the reference value with respect to which the concentration is measured, then the probability of exceeding this threshold of concentration will be[1]

$$P(C > C_*) = \frac{1}{2}\left[\mathrm{erf}\left(\frac{C + C_*}{\beta}\right) + \mathrm{erf}\left(\frac{C - C_*}{\beta}\right)\right]. \quad (3)$$

On the other hand, under ergodicity conditions of the admixture spread this generalization of the intermittency concept can be interpreted as the ratio of the time during which nonzero concentrations are measured to the total measurement time. The ergodicity condition will be exactly satisfied only for a steady state processes. In reality, for this condition to be approximately satisfied, it is necessary and sufficient that the concentrations be averaged over period much longer than the characteristic timescale of concentration variations, and much less than the characteristic time of variations of the ensemble mean values. These conditions are quite realizable in observations of concentration variations in the atmosphere.[1] Therefore, formula (3) for the probability of exceeding some concentration threshold can also be used to estimate the relative time during which this excess concentration is being observed.

Thus, under real conditions of an admixture spread the probability of concentration of atmospheric admixture in the excess of some threshold can strongly vary not only in time but in space also. For instance, any two regions may have equal mean concentrations but drastically different probabilities of exceeding the threshold concentration. In some cases insignificant

alterations of the threshold concentration may cause abrupt drops/jumps of the excess probability. The results of this study suggest that, for reliably solving many applied problems, the statistical nature of the process of atmospheric admixture dispersal must be correctly taken into account.

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