Correlation function for concentration pulsation of an atmospheric pollutant

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The probability density for gaseous and aerosol atmospheric pollutants' concentration transfer from some initial state to a certain final state is obtained by use of the stationary probability density function which was earlier obtained theoretically and validated experimentally. Using these results, the correlation function for pulsation of pollutant concentration is obtained.

The spread of aerosol and gaseous pollutants in the atmosphere is a random process. When it is simulated by use of semi-empirical equations of turbulent diffusion, one can determine the mathematical expectation of the pollutant concentration $\bar{C}$ and its variance σ^2. However, this information is often insufficient in solving some practical problems. A more complete statistical description of the pollution spread at a given point of the space becomes possible if we know the probability density function for concentration $f_1(C)$, where C is the instantaneous value of concentration. In Ref. 1 this function is obtained under the assumption that variation of pollutant concentration is a Markovian process. In the stationary case, it takes the form

$$f_1(C) = (1-\gamma)\,\delta(C) + \frac{1}{\sqrt{\pi}\beta} \times$$
$$\times \left\{ \exp\left[-\frac{(C-\bar{C})^2}{\beta^2} \right] - \exp\left[-\frac{(C+\bar{C})^2}{\beta^2} \right] \right\}; \quad (1)$$
$$\gamma = \mathrm{erf}(\beta_0); \quad \beta_0 = \bar{C}/\beta,$$

where γ is the concentration intermittence; $\delta(...)$ is the Dirac delta function; β is the second parameter of the probability density function; erf(...) is the error integral. The function is obtained in Ref. 1 under the assumption that the period of concentration averaging T is much longer than the characteristic inner scale of the concentration pulsation τ_e (the Eulerian temporal scale) at a given point of the space. It is in this case that averaging over statistical ensemble can be replaced by "sliding" average over time:

$$\bar{C} = \frac{1}{T} \int\limits_{t}^{t+T} C(t)\,\mathrm{d}t.$$

Then the process $C(t)$ can be treated as approximately Markovian.[2]

The parameter β is related to mathematical expectation of the concentration and its variance σ^2 by the following relation[1]:

$$\frac{\sigma^2}{(\bar{C})^2} = \gamma\left(1 + \frac{1}{2\beta_0^2}\right) - 1 + \frac{1}{\sqrt{\pi}\,\beta_0}\exp(-\beta_0^2).$$

The probability density (1) has been verified in the experiments conducted in a wind tunnel, as well as by data of independent field experiments, and by asymptotics of the theory of turbulent combustion for pollutant concentration at the axis of immersed turbulent jets and at their periphery.[1]

Full statistical description of the Markovian stationary process of the concentration variation at a given point becomes possible if the probability density function for pollutant concentration transfer from one state to another during time t and, as a consequence, the correlation function of the concentration pulsation are known together with the probability density (1). The aim of this paper is to obtain these characteristics.

According to the definition, the correlation function of a stationary random process $C(t)$ is

$$B(\tau) = \iint\limits_{0}^{\infty} C\,C_0\,f_1(C_0)\,f_2(C,C_0,\tau)\,\mathrm{d}C\,\mathrm{d}C_0 -$$
$$-\left[\int\limits_{0}^{\infty} C\,f_1(C)\,\mathrm{d}C\right]^2, \quad (2)$$

where $f_2(C, C_0, \tau)$ is the probability density function of concentration transfer from the state C_0 to the state C during time τ.

Assuming, as before, that variation of concentration is a Markovian process, let us write the Fokker–Planck–Kolmogorov equation for the probability density function[2] of the transfer, f_2,

$$\frac{\partial f_2}{\partial \tau} + \frac{\partial}{\partial C}\,a(C)\,f_2 - \frac{1}{2}\frac{\partial^2}{\partial C^2}\,b(C)\,f_2 = 0. \quad (3)$$

Here we cannot assume that τ_e is much less than T because the transition of concentration from one state to another can occur during time τ, which can be less than τ_e. However, we assume as earlier that the process $C(t)$ is Markovian. The validity of the assumption is

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not evident but some results of studying pollutant diffusion in the near-ground layer of the atmosphere will be given in the end of this paper to confirm this. Nevertheless, we cannot yet start solving equation (2). The matter is that the process $C(t)$ is not continuous due to the effect of concentration intermittence. Actually, at a given point of the space, pollutant concentration can jump from a certain value to zero and to pass, also in a step-wise way, from zero value to a state with non-zero concentration. The equation (3) is inapplicable to description of such continuous-discontinuous processes. At the same time, the inverse Kolmogorov equation[2] related to the initial value of concentration C_0 and initial time moment τ_0 remains correct (the function (1) is also obtained by the use of inverse Kolmogorov equation[1]):

$$\frac{\partial f_2}{\partial \tau_0} + a(C_0)\,\frac{\partial f_2}{\partial C_0} + \frac{1}{2}\,b(C_0)\,\frac{\partial^2 f_2}{\partial C_0^2} = 0. \qquad (4)$$

To determine the coefficients of this equation, let us note that the continuous part of the solution of a similar equation for the probability density function of concentration (1) is formally a difference of two fundamental solutions of the heat transfer equation. This fact demonstrates close connection between the considered problem and the class of normal Markovian diffusion processes.[2] This analogy makes it possible to assume the following form of the coefficients in Eq. (3):

$$a(C) = -\,\frac{C - \bar{C}}{\tau_e}\,; \quad b(C) = \frac{1}{\tau_e}\,\beta^2.$$

The structure of the expression for the probability density function of transfer is evidently similar to the above-mentioned probability density (1). The system of the initial and boundary conditions must be set as follows:

$$f_2(C, \tau_0, C_0, \tau_0) = \delta(C - C_0),$$
$$f_2(0, \tau, C_0, \tau_0) = f_2(\infty, \tau, C_0, \tau_0) = 0. \qquad (5)$$

After solving the problem (4), one should take $\tau_0 = 0$ in Eq.(5).

For the equations like Eq. (4), of the parabolic type with a negative diffusion coefficient, the solution of Cauchy problem exists not for arbitrary initial conditions. In the cases when the solution's existence is established, the Cauchy problem is ill-posed in the Hadamard sense. This manifests itself in the fact that a decrease of the perturbations' wavelength in the initial conditions leads to an increase in the acceleration of their amplitude. As a result, the solution is quickly distorted. However, the theorem about uniqueness of the solution to Cauchy problem is valid for such equations if it exists.[3] Thus, if an exact solution is obtained, one can be sure that it is unique.

The exact analytical solution of the problem at $\tau_0 = 0$ has the form

$$f_2(C, C_0, \tau) = (1 - \gamma_2)\delta(C) + \frac{1}{\sqrt{\pi g(\tau)}} \times$$
$$\times \left\{ \exp\left[-\,\frac{(C - \bar{C} - (C_0 - \bar{C})\exp(-\tau/\tau_e))^2}{g(\tau)} \right] - \right.$$
$$\left. - \exp\left[-\,\frac{(C + \bar{C} + (C_0 - \bar{C})\exp(-\tau/\tau_e))^2}{g(\tau)} \right] \right\};$$
$$g(\tau) = \beta^2\,[(1 - \exp(-2\tau/\tau_e)];$$
$$\gamma_2 = \mathrm{erf}\left[-\,\frac{\bar{C} + (C_0 - \bar{C})\exp(-\tau/\tau_e)}{\sqrt{g(\tau)}} \right]. \qquad (6)$$

This can be shown directly by substituting Eq. (6) into Eq. (4). In order to return to f_2 as a function of τ_0, one should change τ by $\tau - \tau_0$. If τ tends to infinity, we obtain the stationary probability density function (1). At the same time we see that the conditions (5) are satisfied.

Now, according to Eq. (2), we obtain the correlation function of concentration pulsation

$$B(\tau) = \sigma^2 \exp(-|\tau|/\tau_e). \qquad (7)$$

Owing to this formula, the density of spectral power of concentration pulsation $S(f)$ has the form[2]

$$S(f) = 2\int_0^\infty B(\tau)\cos(f\tau)\,d\tau = \frac{2\sigma^2\,\tau_e}{1 + (f\tau_e)^2}\,, \qquad (8)$$

where f is the frequency of concentration pulsation.

The validity of the above-stated assumption that the process $C(t)$ is approximately Markovian can be demonstrated using data from Ref. 4. As was shown in that paper, one can observe two fluctuation regimes of pollutant concentration in the near-ground layer of the atmosphere: "transition" and "equilibrium." The transition regime is characterized by the fact that, together with the part of spectral power of concentration pulsation which corresponds to the equilibrium law $f \sim -5/3$, one can observe the pulsation obeying the law $f \sim -2/3$. The latter works at the values of the dimensionless frequency $-\ \tau_e f$ of the order of two, and the law of "five thirds" at the dimensionless frequency greater than seven. The Figure 1 presents the dimensionless density of spectral power (8) as a function of dimensionless frequency. The straight lines corresponding to the laws of "five thirds" and "two thirds," which were discussed above, are also presented in the Figure. We see that the density of spectral power which was obtained theoretically under the assumption that the process $C(t)$ is Markovian satisfactorily corresponds to $S(f)$ observed as a function of frequency in the experiments conducted in the near-ground layer of the atmosphere.

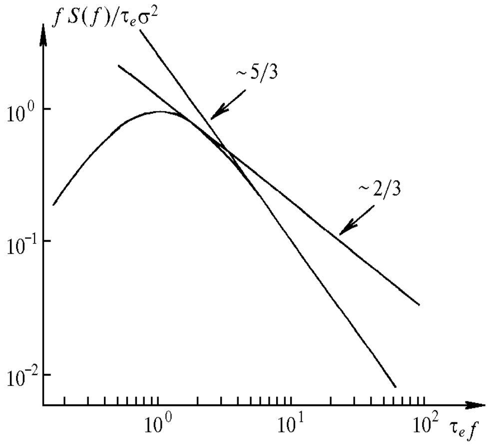

Fig. 1. The density of spectral power $f\,S(f)/(\tau_e\,\sigma^2)$ as a function of $\tau_e f$.

Thus, we have obtained a complete statistical description for the Markovian stationary process of atmospheric pollutant concentration variation at a given point. To make use of the obtained results, one has to know all three statistical characteristics of the process: the mathematical expectation of concentration, its variance, and Eulerian temporal scale of the concentration pulsation.

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