Two-parameter model of turbulent transport of admixtures from a line source in the atmospheric surface layer

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Diffusion of passive admixtures from a continuously operating limited-size source, situated on the underlying surface of the neutral atmospheric surface layer, is simulated based on a non-local two-parameter model of turbulence and the equation of transport for the mean concentration. In the proposed diffusion model, the coefficient of turbulent diffusion varies not only with altitude, but also with the distance from the source in the downstream direction according to the data of laboratory measurements [J.E. Fackrell and A.G. Robins, J. Fluid Mech., No. 117, 1–26 (1982); M. Porch and J.E. Cermak, J. Heat Mass Transfer, No. 7, 1083–1095 (1964)]. The results of simulation agree with the measured data on structural peculiarities in transformation of the concentration field.

Introduction

Turbulent diffusion of various impurities plays an important part in atmospheric studies. Since the sources of pollution are often situated near solid boundaries, the study of diffusion in the atmospheric surface layer is of particular interest. This work is aimed at verification of the *K*-theory of turbulent diffusion using the data of the laboratory experiment[1] and new two-parameter Euler model of turbulent diffusion of passive admixtures. In spite of the well-known drawbacks of the *K*-theory (isotropic coefficient of vortex diffusion and local character of the model of "gradient diffusion"), this theory is attractive because of its simplicity (as far as concerned its application to solution of practical problems on dispersion of pollutants in inhomogeneous atmospheric flows near the surface). In this paper, spreading of a pollutant from a line source situated on the surface is numerically simulated for the case of a neutral atmospheric surface layer (the conditions occurring, for example, at high wind). Application of the two-parameter Euler model of diffusion allows us to reproduce the experimentally observed different-power law of decrease of the maximum pollutant concentration with the distance from a source.

1. Euler diffusion model: *K*-theory

Under consideration is the problem on dispersion of passive admixtures from a ground source in the surface sublayer of the atmospheric boundary layer at neutral atmospheric stratification. The equation for the mean concentration of admixtures has the following form:

$$\frac{\partial C}{\partial t} + U_j \frac{\partial C}{\partial x_j} = \frac{\partial}{\partial x_k}\left(D \frac{\partial C}{\partial x_k}\right) - \frac{\partial}{\partial x_j}\langle u_j c\rangle, \qquad (1)$$

where C is the mean concentration of some admixture; D is the molecular diffusion coefficient; $\langle u_j c\rangle$ is the vector of the turbulent flow of the admixture.

As in the laboratory experiment,[2] the problem of admixture dispersion is solved for the case of 2D flow along a smooth solid surface. Equation (1) is written in the form

$$U \frac{\partial C}{\partial x} + V \frac{\partial C}{\partial y} = \frac{\partial}{\partial y}\left[D \frac{\partial C}{\partial y} - \langle vc\rangle\right], \qquad (2)$$

where $\langle vc\rangle$ is the vertical turbulent flow of admixtures; x is the longitudinal coordinate; y is the vertical coordinate; U and V are the mean wind velocity components in the longitudinal and vertical directions, respectively.

Within the framework of the *K*-theory, the turbulent flow of admixtures can be expressed in terms of gradient of the mean concentration

$$-\langle vc\rangle = D_T \frac{\partial C}{\partial y}, \qquad (3)$$

where $D_T = \nu_T / Sm_T$ is the turbulent diffusion coefficient, $Sm_T = 0.72$ is the Schmidt turbulent number, ν_T is the coefficient of vortex (or turbulent) viscosity.

In the single-parameter Euler model of diffusion (1)–(3), the turbulent viscosity coefficient ν_T is determined as a function meeting the limiting laws:

(a) in a viscous sublayer, in the immediate vicinity of a wall, the value of $\nu_T^+ = \nu_T/\nu$ increases proportionally to $(y^+)^4$;

(b) further, near the wall, ν_T^+ changes proportionally to the distance from the wall y^+ ($y^+ = (yu_*)/\nu$, where ν is kinematical viscosity, $u_* = (\tau_0/\rho)^{1/2}$ is the friction rate, and τ_0 is the friction stress on the wall);

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(c) in the main part of the flow, except for its outer part, the value keeps almost constant:

$$\nu_T^+ = \kappa \frac{[y^+/y_0^+]^5 \, (1 - \exp(-y^+/\delta_0^+)) \, (\delta_0^+/y_0^+) \, f(x_1)}{1 - (1/y_0^+) \, (y^+/y_0^+)^3}. \quad (4)$$

The parameter y_0^+ characterizes the dimensions of the viscous sublayer, and δ_0^+ characterizes the thickness of the boundary layer:

$$\delta_0^+ = a^{-1} \int_0^\infty (U_0^+ - u^+) \mathrm{d}y_1,$$

where $y_1 = y/L\sqrt{U_\infty L/\nu}$ is the dimensionless coordinate, and L is the characteristic length. The constants y_0^+, κ, and a were chosen from comparison with the experimental data for some simple problems: $y_0^+ = 8$, $\kappa = 0.36$, and $a = 5$. The function $f(x_1) = \exp\{-\gamma[\delta(x)/(x - x_1)]^2\}$ is introduced to describe the transition of the laminar flow to the turbulent flow [x_1 is the coordinate at which the transition begins, $\gamma = 10$ is the numerical coefficient, $\delta(x)$ is the thickness of the boundary layer determined as the coordinate y at which $U/U_0 = 0.99$ (U_0 is the mean speed of the external flow)]. The dynamic problem on determination of the mean wind speed

$$U\frac{\partial U}{\partial x} + V\frac{\partial V}{\partial y} = (\nu + \nu_T)\frac{\partial U}{\partial y},$$

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} = 0 \quad (5)$$

was solved by the implicit three-layer scheme of the second order of accuracy using the sweep method.

Results of numerical simulation of admixture spreading

The profiles of the mean wind obtained by solving the problem (5) are in close agreement with the available measured data and are omitted here. In numerical simulation, the Schmidt molecular number was assumed equal to 0.72 (the Schmidt turbulent number is 0.72). The ammonium gas (NH_3) with the molecular diffusion coefficient $D_{NH_3} \approx 0.236 \cdot Sm = 0.17$ cm^2/s (as in Ref. 2) and the kinematical viscosity coefficient $\nu_{NH_3} = Sm \cdot D_{NH_3} \approx 0.12$ cm^2/s at 25°C was chosen as an admixture emitted into the boundary layer. The position of the admixture source relative to the beginning of the turbulent layer on a plate was chosen the same as in the second series of experiments in Ref. 2, which in numerical calculation corresponded to the Reynolds number $\mathrm{Re}_x = 1.15 \cdot 10^6$.

The results of numerical solution are presented in graphical form. The calculations were performed up to the Reynolds numbers $\mathrm{Re}_x = 4.5 \cdot 10^6$ (by the distance from the beginning of the turbulent boundary layer) and compared with the results of experimental study of NH_3 diffusion from a linear source in the 2D turbulent boundary layer.[2] In the experiment, two zones (intermediate and final) of similarity of the concentration profiles have been detected. The admixture concentration in these zones has, respectively, the developing and completely developed character.

Figure 1 shows the distribution of the admixture concentration referred to the maximum concentration on the plate as a function of the ratio y/λ (where λ is the thickness of the diffusion layer at the place where $c/c_{max} = 0.5$). The dashed lines border the band of experimental points from Ref. 2 for the intermediate zone, and solid lines border the zone of calculated data (cross sections: from $x = 145$ cm, $\mathrm{Re}_x \approx 3.5 \cdot 10^5$ to $x = 1.25 \cdot 10^3$ cm, $\mathrm{Re}_x \approx 3 \cdot 10^6$). Thus, all the similarity zones of the experiment from Ref. 2 are covered. With the distance from the source, the calculated points are grouped near the solid curve corresponding to the final similarity zone ($x \approx 1.25 \cdot 10^3$ cm, closed circles and squares in Fig. 1).

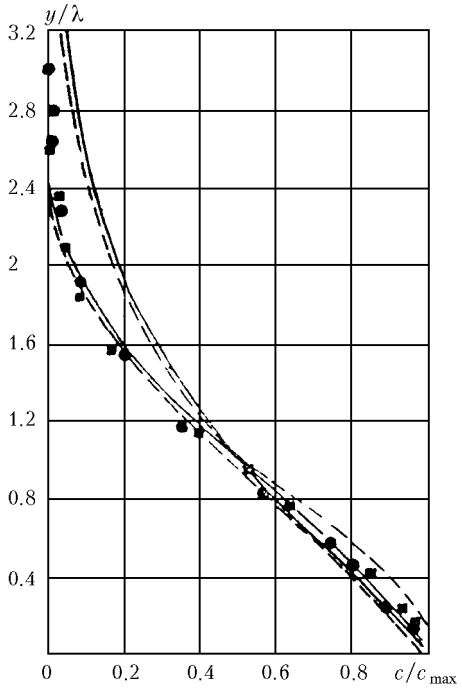

Fig. 1. Profiles of admixture concentration c/c_{max} as functions of the vertical coordinate y/λ (c_{max} is the maximum concentration on the surface; λ is conditional width of diffusion plume). Points are the calculated values of concentration in the final similarity zone.

Figure 2 shows the distribution of c/c_{max} as a function of y/δ, where δ is the thickness of the boundary layer at the place where $u/U_\infty = 0.99$. The dashed lines border the band of experimental points from Ref. 2 in the final zone. The calculated points at different distance from the source are shown as well.

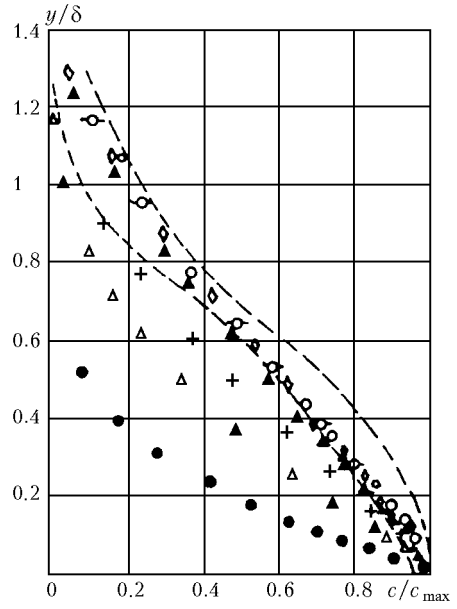

Fig. 2. Profiles of admixture concentration c/c_{max} as functions of the vertical coordinate y/δ (δ is the thickness of the boundary layer). Points show the calculated concentration profiles at different distance from the source: x = 145 (●) and $1.25 \cdot 10^3$ cm (○), intermediate cross sections (Δ, , +, and ◊).

Figure 3 shows how the admixture concentration decreases along the wall downstream from the source. Curves *1* and *2* correspond to the intermediate and final similarity zones from Ref. 2 (result of joining Figs. 6 and 9 from Ref. 2). The decrease of concentration on the wall in the intermediate zone (curve *1*) is described by the power law: $c_{max} \sim x^{-0.9}$, and that in the final zone (curve *2*) is $c_{max} \sim [U_\infty \cdot \delta]^{-1}$, where U_∞ is the speed in the oncoming flow. Crosses label the calculated dependence. It is seen from Fig. 3 that the experimental dependence from Ref. 2 cannot be described only by the power law.

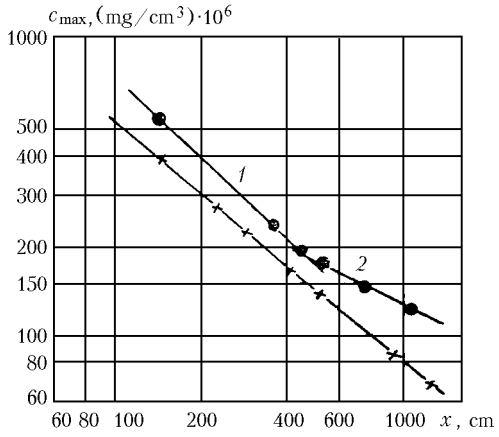

Fig. 3. Distribution of admixture concentration on the surface as a function of the distance from the source; curve marked by crosses corresponds to experimental results.

Conclusions from the results of verification of single-parameter Euler diffusion model

Thus, Fig. 3 presents the results of numerical simulation of diffusion of an aerosol (polluting admixture) from a ground-based source in the atmospheric surface layer. It is seen that, although the model of the vortex diffusion coefficient (1) (K-theory) closely reconstructs the concentration distribution along the vertical (see Figs. 1 and 2), nevertheless it proves to be insufficient for careful pre-calculation of the behavior of the maximum surface concentration (see Fig. 3) with the distance from the source. This drawback of the model (1) can be eliminated by using more accurate two-parameter model of turbulent diffusion, in which the coefficient of vortex diffusion is determined by two parameters: kinetic energy of turbulence (KET) and its spectral flux (KET dissipation). As follows from the experimental results of Ref. 2, in this case the vortex diffusion coefficient is not only a function the vertical coordinate, but, as in Eq. (1), a function of coordinate in the mean wind direction.

2. Two-parameter Euler diffusion model

To describe the evolution of the concentration field of a plume from a ground-based source, the E–ε-model (Ref. 3) is used for calculation of the mean wind velocity distribution in the atmospheric surface layer. This model adequately reproduces all structural peculiarities of a turbulent flow near the surface under the conditions of neutral stratification (conditions in the surface layer at high wind). This is due to the fact that the turbulent viscosity coefficient, based on the two parameters E and ε, is a function varying not only with height, but also with the mean wind direction. The kinetic energy of turbulence E and the rate of its dissipation ε are calculated from the differential equations of transfer. This, in fact, allows us to take into account the non-local character of evolution of these parameters. Actually, in an inhomogeneous turbulent flow, liquid particles from different regions of flow pass through a given point, and the parameters E and ε averaged over the expanding region of space backward along the mean trajectories of particles depend on the flow prehistory.

The Euler two-parameter diffusion model includes the equations of transfer for the kinetic energy of turbulence $E = 1/2 \langle u_i u_i \rangle$ and its spectral flux ε, as well as the equations of transfer for the mean concentration of an admixture (1).

The explicit algebraic anisotropic model for the vector of turbulent flow of the concentration $\langle u_j c \rangle$ in Eq. (1) can be obtained from the differential equation of transfer:

$$\frac{D \langle u_i c \rangle}{Dt} = - \langle u_i u_j \rangle \frac{\partial C}{\partial x_j} - \langle u_j c \rangle \frac{\partial U_i}{\partial x_j} - $$

$$- D_{ic} - 1/\rho \langle c \frac{\partial P}{\partial x_i} \rangle, \qquad (6)$$

where ρ is the mass density, and the model for correlation "pressure fluctuations – gradient of concentration fluctuations" is taken in the form[4]

$$\frac{1}{\rho}\left\langle c\,\frac{\partial P}{\partial x_i}\right\rangle = -\frac{c_{1c}}{\tau}\langle u_i\, c\rangle + \frac{c_{2c}}{\tau}\langle u_k\, c\rangle\frac{\partial U_i}{\partial x_k}, \qquad (7)$$

where $\tau = E/\varepsilon$ is the time scale of turbulence; c_{1c} and c_{2c} are constants determined from experimental data; $D_{ic} \equiv (\partial/\partial x_j)\langle u_i\, u_j\, c\rangle$ is a term of turbulent transfer.

In the approximation of weakly equilibrium turbulence, it is assumed that

(a) there is a similarity between the transfer of $\langle u_i\, c\rangle$ determined according to Eq. (6) as $\frac{D\langle u_i\, c\rangle}{\partial t} - D_{ic}$ and the transfer of E and its analog for the scalar field – the dispersion of concentration $\langle c^2\rangle$:

$$\frac{D\langle u_i\, c\rangle}{D\tau} - D_{ic} = \frac{\langle u_i\, c\rangle}{E}(P-\varepsilon) + \frac{\langle u_i\, c\rangle}{\langle c^2\rangle}(2P_c - \varepsilon_c), \quad (8)$$

where D is the KET generation; $P_c = -\langle u_i\, c\rangle\frac{\partial C}{\partial x_i}$ is the generation of $\langle c^2\rangle$; $\varepsilon_c = \left\langle \frac{\partial c}{\partial x_k}\frac{\partial c}{\partial x_k}\right\rangle$ is the destruction of turbulent fluctuations of concentration;

(b) the transfer of $\langle u_i\, c\rangle$ determined by the left-hand side of Eq. (8) is negligibly small in this approximation. Then it follows from Eq. (8) that

$$-\langle u_i\, c\rangle = \frac{1}{c_{1c}}\sqrt{\frac{E}{\varepsilon}\frac{\langle c^2\rangle}{\varepsilon_c}}\times$$

$$\times\left(\langle u_i\, u_k\rangle\frac{\partial C}{\partial x_k} + (1-c_{2c})\langle u_k\, c\rangle\frac{\partial U_i}{\partial x_k}\right). \qquad (9)$$

To obtain the completely explicit model for the vector of the turbulent flow of concentration, the models

$$-\langle u_i\, u_k\rangle = \nu_T(U_{i,k} + U_{k,i}) - \frac{2}{3}\delta_{ij}E,$$

$$-\langle u_i c\rangle = D_T\,\partial C/\partial x_i,$$

are used, which then are substituted into the right-hand side of Eq. (9). Besides, it is assumed that the ratio of the time scales of the dynamic and scalar fields $R = \tau/\tau_c$ (where $\tau_c = \langle c^2/\varepsilon_c\rangle$) is a constant as confirmed by measurements for translation turbulent flows.

In the final form, the explicit algebraic model for the turbulent flow of concentration is written as

$$-\langle u_i c\rangle = D_T\frac{\partial C}{\partial x_i} - \frac{1}{c_{1c}}\frac{E^2}{\varepsilon}\{[2\nu_T + (1-c_{2c})D_T]S_{ik} +$$

$$+ (1-c_{2c})D_T\,\Omega_{ik}\}\frac{\partial C}{\partial x}, \qquad (10)$$

where

$$S_{ik} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_k} + \frac{\partial U_k}{\partial x_i}\right);\quad \Omega_{ik} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_k} - \frac{\partial U_k}{\partial x_i}\right);$$

$$\nu_T = C_\mu f_\mu\frac{E^2}{\varepsilon};\quad D_T = \frac{\nu_T}{Sm_T},$$

$f_\mu = (1 + 3.45/\sqrt{\mathrm{Re}_t})\,[1 - \exp(-y^+/70)]$ is a damping function introduced for integration of the model equations down to the surface in order to meet the asymptotically correct behavior of turbulent parameters near the surface. The values of constants in the model are the following: $Sm_T = 0.9$, $c_{1c} = 3$, $c_{2c} = 0.4$. The model (10) for the vector of turbulent flow of concentration takes into account not only anisotropy of the turbulent transfer (the longitudinal flow $\langle uc\rangle \neq 0$ even if $\frac{\partial C}{\partial x}$ is zero; x is the longitudinal coordinate coinciding with the mean wind direction), but also the dependence of the coefficient of turbulent diffusion of a substance $D_T = \nu_T/Sm_T$ on the distance from the source.

Such more realistic model of turbulent transfer of a scalar property can reproduce the different-power law of decrease of the maximum surface concentration (see Fig. 3) in contrast to the model (3), which uses the coefficient of vortex diffusion only along the vertical.

Acknowledgments

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