NUMERICAL-ANALYTICAL MODEL OF THE AEROSOL TRANSPORT IN A THERMALLY STRATIFIED BOUNDARY LAYER OF THE ATMOSPHERE

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This paper deals with a model of admixture dispersal in the atmospheric boundary layer. The model developed is to be used in IBM-compatible computers. The wind field is determined by analytically solving three-dimensional non-stationary linear system of the atmospheric boundary layer equations that allow for orographic and dynamic inhomogeneity of the underlying surface and for the quasi-stationary sublayer. Admixture concentration is found by numerically solving semiempirical turbulent diffusion equation. To set the diffusion coefficients they are assumed to be proportional to the corresponding components of the Reynolds stress tensor. The results obtained using this model have been compared with the observational data and with those obtained using other models.

Reduction, into practice, of modern methods of simulating the dispersal of gas and aerosol admixtures in the boundary atmospheric layer needs for the development of corresponding software in order to use PCs. However, this inevitably imposes certain restrictions on the software. On the one hand, it must be “fastB, convenient, and sufficiently simple for users. On the other hand, the mathematical models used should rely on real physical processes. The model proposed in the present paper satisfies this contradictory requirements to a certain extent.

1. MODEL OF THE BOUNDARY LAYER DYNAMICS

The model has a two-layer structure consisting of the near-surface layer $z_0 \le z \le h$ and the rest part of the boundary layer $h < z \le H$, where z_0 is the roughness parameter, h is the height of the near-surface layer, H is the height of the boundary layer.

The system of equations[1] taking the following form after linearization will be considered as the initial one:

$$\frac{\partial U}{\partial t} = lV + \alpha\lambda\theta + \nu_h \frac{\partial^2 U}{\partial z^2}\ ;\quad \frac{\partial V}{\partial t} = -\,lU + \beta\lambda\theta + \nu_h \frac{\partial^2 V}{\partial z^2}\ ;$$

$$\frac{\partial \theta}{\partial t} = -\,S(\alpha U + \beta V) + \nu_h \frac{\partial^2 \theta}{\partial z^2}\ ; \qquad (1)$$

$$\frac{\partial q}{\partial t} = -\,S_q(\alpha U + \beta V) + \nu_h \frac{\partial^2 q}{\partial z^2}\ ;\quad \frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} = 0\ .$$

The initial conditions for $t = t_0$ and the boundary conditions for $z = h$ and H are as follows (below we suppose that $H \to \infty$):

$$t = t_0:\quad U = U_0\ ,\quad V = V_0\ ,\quad \theta = \theta_0\ ,\quad q = q_0\ ; \qquad (2)$$

$$z = h:\quad -\,\nu_h \frac{\partial U}{\partial z} = \tau_U\ ;\quad -\,\nu_h \frac{\partial V}{\partial z} = \tau_V\ ;$$

$$-\,\nu_h \frac{\partial \theta}{\partial z} = \tau_\theta\ ;\quad -\,\nu_h \frac{\partial q}{\partial z} = \tau_q\ ;$$

$$z = H:\quad -\,\nu_h \frac{\partial U}{\partial z} = -\,\nu_h \frac{\partial V}{\partial z} = 0\ ;\quad -\,\nu_h \frac{\partial \theta}{\partial z} = 0\ ;$$

$$-\,\nu_h \frac{\partial q}{\partial z} = 0\ ;\quad W = 0.$$

Theoretically, all the unknowns entering into the system of equations (1) and (2) are the averages over certain statistical ensembles.[2] However, in practice the averaging over an ensemble is changed by averaging over a temporal interval approximately 20 minutes long.

The equations (1) are written in a generalized orthogonal coordinate system. The axes x and y are curvilinear in the terrain surface and oriented to the east and to the north, respectively, the axis z is directed vertically upwards. The terrain whose inclination angles α and β are supposed to be small is described by the function $\delta(x,y)$, $\alpha = \frac{\partial \delta}{\partial x} \ll 1$, $\beta = \frac{\partial \delta}{\partial y} \ll 1$. Other designations are as follows: U and V are deviations of the horizontal wind velocity components from their background values U_b and V_b, respectively; θ and q are deviations of the potential temperature and specific humidity from their background values θ_b and q_b, respectively; S is the stability parameter; S_q is the gradient of the background specific humidity; ν_h is the coefficient of vertical turbulent exchange at $z = h$; λ is the convection parameter, and l is the Coriolis

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parameter. According to Ref. 1, we suppose that the background values are known, the velocity components U_b and V_b coincide with the geostrophic wind are constant, the background temperature and humidity correspond to the standard atmosphere.

The system of equations (1) describes nonstationary thermohydrodynamic processes in the boundary atmospheric layer over a thermally and orographically inhomogeneous underlying surface. Horizontal inhomogeneities are assumed to be small. In this case the nonlinear advective summands of the initial system of equations (1) are not the decisive ones as compared with the Coriolis force, buoyancy force, and the vertical turbulent exchange entering into the right-hand part of the first two equations in the system (1). So the nonlinear terms can be neglected. For this same reason, we also neglect a part of the horizontal pressure gradient; from which, because of the curvilinear coordinate system, used are only the summands with the Archimedes force whose components act along the slant terrain surface.

At the height of the near-surface layer $z = h$, the turbulent flux of the momentum τ_U, τ_V, heat τ_θ, and moisture τ_q are supposed to be known and obtained by solving the equations for the constant flux layer.[3] Turbulent processes weaken towards the upper boundary of the boundary layer, and the vertical turbulent transfer of the momentum, heat, and moisture equals zero at $z = H$.

Following Ref. 3, we use the similarity theory,[4] empirical functions,[5] and the balance equation for the energy flows on the underlying surface[3] in order to describe the structure of the near-surface layer.

The system (1) under the initial and boundary conditions (2) admits an analytical solution. After the introduction of new functions and integro-differential transforms described in Ref. 6, we obtain the following expressions for the wind velocity, temperature, and humidity in the upper part of the boundary layer ($z \geq h$):

$$U = -\left\langle \frac{A\cos[\gamma(t_j-\eta)]}{\gamma^2} + \frac{B\sin[\gamma(t_j-\eta)]}{\gamma} - \frac{D\beta}{\gamma^2} \right\rangle ;$$

$$V = -\left\langle \frac{M\cos[\gamma(t_j-\eta)]}{2} + \frac{N\sin[\gamma(t_j-\eta)]}{\gamma} + \frac{D\alpha}{2} \right\rangle ; \quad (3)$$

$$\theta = -\left\langle S \left\{ \frac{F\cos[\gamma(t_j-\eta)]}{\gamma^2} + \frac{Q_1\sin[\gamma(t_j-\eta)]}{\gamma} \right\} + \frac{E}{\gamma^2} \right\rangle ;$$

$$q = -\left\langle S_q \left\{ \frac{F\cos[\gamma(t_j-\eta)]}{\gamma^2} + \frac{Q_1\sin[\gamma(t_j-\eta)]}{\gamma} \right\} + \frac{S_q E}{S\gamma^2} + E_1 \right\rangle ,$$

where

$$\langle \{\ldots\} \rangle = \sum_{j=1}^{n} \frac{1}{(\pi \nu_h^j)^{1/2}} \int_{t_{j-1}}^{t_j} \frac{\{\ldots\}}{(t_j-\eta)^{1/2}} \times \exp\left[\frac{-z^2}{4\nu_h^j (t_j-\eta)}\right] d\eta ;$$

$$\gamma^2 = l^2 + \lambda S (\alpha^2 + \beta^2) ;$$

$$F = l(\alpha\tau_V - \beta\tau_U) + (\alpha^2 + \beta^2)\lambda\tau_\theta ;$$

$$Q_1 = -\alpha\tau_V - \beta\tau_U; \quad E = -l[S(\alpha\tau_V - \beta\tau_U) - l\tau_\theta] ;$$

$$E_1 = \tau_q - \frac{S_q}{S}\tau_\theta ;$$

$$A = -l^2\tau_U + \lambda S(\alpha^2\tau_U + \alpha\beta\tau_V) - \beta l\lambda\tau_\theta ;$$

$$B = l\tau_V + \alpha\lambda\tau_\theta ; \quad D = \lambda S(\alpha\tau_V - \beta\tau_U) - \lambda l\tau_\theta ;$$

$$M = l^2\tau_V + \lambda S(\alpha\beta\tau_U + \beta^2\tau_V) + \alpha l\lambda\tau_\theta ;$$

$$N = -l\tau_U + \beta\lambda\tau_\theta .$$

Thus the formulas (3) allow one to obtain the values of meteoelements at the height of the near-surface layer and in the boundary layer.

It should be noted that, in order to determine the wind velocity at $h \leq z \leq H$ by formulas (3), it is, necessary to know their background values U_b and V_b which are supposed to be given in the problems dealing with the boundary layer. Experimental determination of U_b and V_b at the height $z = H$ is connected with certain technical difficulties. Therefore, in this model, they are obtained from measurements of the wind velocity in the near-surface layer with the use of Newton iteration method.

2. THE ADMIXTURE TRANSPORT MODEL

To calculate the concentration of an admixture the semi-empirical equation of turbulent diffusion[2]

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + (W + V_S)\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}K_x\frac{\partial C}{\partial x} + \frac{\partial}{\partial y}K_y\frac{\partial C}{\partial y} + \frac{\partial}{\partial z}K_z\frac{\partial C}{\partial z} - \alpha C + R \quad (4)$$

with the initial and boundary conditions

$$C\big|_{t=0} = 0, \quad C\big|_{\substack{x=0,X \\ y=0,Y}} = 0, \quad C\big|_{z=H} = 0,$$

$$\left(K_z\frac{\partial C}{\partial z} + V_S C\right)\bigg|_{z=0} = \beta\, C\big|_{z=0} .$$

is used. Here C is the average value of the admixture concentration over the interval of twenty minutes; t is time; x, y, z are the spatial coordinates; U, V, and W are the components of the wind velocity field; V_S is Stokes sedimentation rate of aerosol particles; K_x, K_y, and K_z are coefficients of horizontal and vertical turbulent diffusion; X, Y, H are horizontal dimensions and the height of the calculational domain; α is the logarithmic coefficient of the admixture decay; R is the function simulating the work of the source; β is the coefficient of admixture interaction with the underlying surface. The process of an admixture dispersal in the atmospheric boundary layer is supposed to be local. So the admixture concentration equals zero at a sufficiently large distance from the source at the horizontal boundaries of the domain and at the upper boundary, as well. The turbulent and gravitational flows of the admixture are proportional to its concentration at the lower boundary. The coefficient β is the empirical value depending on the size of aerosol particles, their state (liquid or dry), the type of the underlying surface, and other characteristics.

The equation (4) can be reduced to a system of one-dimensional equations by its splitting into physical processes and directions.[7] These equations can be solved by the finite difference method with the use of Krank–Nikolson[8] and Fromm–Van-Leer[9,10] schemes.

The hypothesis that the coefficients K_{ij} are proportional to the corresponding components of the Reynolds stress tensor[11] was used in order to set the coefficients of turbulent diffusion. To apply this hypothesis, it is also necessary to set the ratio of the kinetic energy of turbulence, b^2, to its dissipation rate, ε. These parameters were calculated in correspondence with a simple algebraic model[11,12] from the known fields of the mean wind velocity and temperature. The hypothesis was verified in the experiments performed under the conditions of turbulence in the near-surface layer,[13] and the possibility of its successful application to the calculation of the admixture dispersal was demonstrated. The method for measuring coefficients K_{ij} was based on the "recursiveB approach proposed by Galkin.[14]

The parameters b^2 and ε obtained in the above-described way were used in order to approximate the term describing the dissipation in the equation for the concentration dispersal.[11] The empirical constants for the algebraic model were taken from literature data.

3. COMPARISON OF THE RESULTS OBTAINED WITH THE DATA FROM OBSERVATIONS AND FROM OTHER MODELS

To compare the calculational results obtained by the given model with the experimental data, the data of observations[15] during the period from 15 h August, 24, 1953 to 13 h August 25, 1953, (near the city of O'Neil, State of Nebraska, USA) were used.

The values of the input parameters were set in accordance with Refs. 16, 17, and the components of the mean value of wind velocity were taken from the data[15] of observations for the height of 16 m. Figure presents the isolines of the wind velocity module which were constructed using calculational results (dashed lines) and experimental data (solid lines) for the period from 15 h August 24 to 13 h August 25 up to the height of 300 m. One can see that the maximum discrepancy is observed at the transition period nearly 21 h August 24. The analysis of the data from Ref. 15 made in Ref. 16 demonstrates that the presence of the cool advection along the x axis and heat advection along the y axis in the background flow nearly 21 h ignored in the model seems to be the cause of such a discrepancy. Additional analysis of relative errors (calculation–experiment) shows that they are close to measurement errors of wind velocity.

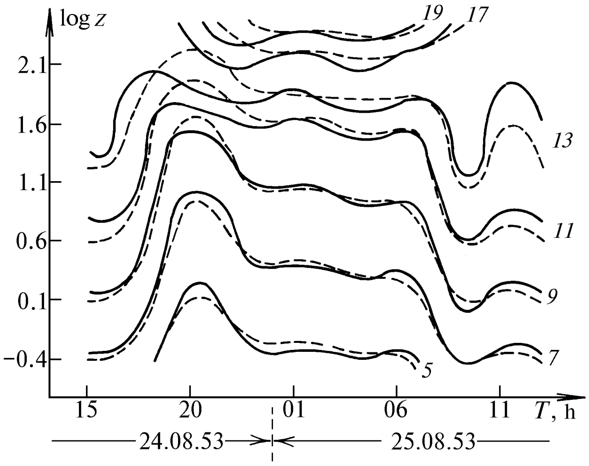

FIG. 1. Isolines of the absolute value of wind velocity: solid lines are for the observational data, dashed lines are for the results of calculations; numbers at the isolines indicate the wind velocity, m/sec.

Let us compare the results of calculations by the above model with the calculations by similar models (see, for instance, Ref. 18) where, based on the data of observations, the author compares fourteen different models of turbulent exchange from the simplest one with a constant coefficient of vertical turbulent exchange to the model using the balance equation of turbulent energy. The values of rms deviations of the calculated values and experimental data for wind velocity obtained by all fourteen models and averaged over the whole observation period[18] for different heights fall within the range from 1.67 to 5.28 m/sec. Similar value averaged over the whole observation period for the 300 m layer and obtained by our model equals 1.43 m/sec. It is obvious that better coincidence is achieved by using the measurement data of wind velocity near the underlying surface in contrast to the data of Refs. 16, 17, and 18 requiring information about U_b and V_b at the height H.

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