Effect of atmospheric convection on vertical transport of arid aerosols

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Received November 29, 2000

The processes of transport of arid aerosols under the conditions of developed convection are studied theoretically. The aerosols are wind-driven into the atmosphere due to release of soil particles from bare soil. Further, they ascend due to convection and turbulence. The calculated results are presented for one-dimensional (ignoring convection), two-dimensional, and three-dimensional Large-Eddy-Simulation models (LES) that reproduce convective structures with the scales \geq 100 m.

Introduction

As observations show the arid zones are characterized by an enhanced concentration of arid aerosols. Under conditions of strong wind and high temperature, dust storms often arise. During such storms, the concentration of aerosols is so high that twilight comes in daytime. The mechanism of penetration of fine soil particles into the near-ground air layer is quite thoroughly studied theoretically; it is connected with the processes of saltation and diffusion of aerosol.¹

To describe the processes of aerosol diffusion in the atmospheric boundary layer (ABL), in particular, under convective conditions, numerical models are usually used. Such models include the semiempiric equation of diffusion and some closing hypotheses.^{2,3} In this case, irregular mesoscale processes in the ABL are parameterized as turbulent (subgrid). However, solutions based on this approach do not describe many important peculiarities of the convective ABL structure. This conclusion follows both from the observations^{4,5} and theoretical studies. $^{6-8}$ In eddy-resolving models, the processes of penetrative convection, as well as cloud and precipitation formation are described in the explicit form with the use of the so-called Large Eddy Simulation (LES) models, in which eddies with the scale larger than 100 m are reproduced based on the nonhydrostatic equations of thermohydrodynamics, and smaller eddies are parameterized.

The spread of dust particles under conditions of dry convection in a 2D formulation of the problem (simulated ensemble consisting of thermics) was studied in Ref. 9. The mechanism of aerosol income was not described in detail in Ref. 9 (the turbulent flow of aerosol near the surface was set in an arbitrary way).

In this paper, the sources of atmospheric aerosol are the processes of saltation and deflation (winddriven release of aerosol particles from the surface). Besides, as a basic model, we take the spatial LES model, 10 rather than the 2D model as in Refs. 7 and 9.

Spatial model of a convective ensemble

To describe a convective ensemble, we, as in Ref. 10, use the following set of equations of thermohydrodynamics:

$$\frac{\mathrm{d}u}{\mathrm{d}t} + \omega \frac{\partial U}{\partial z} = -\frac{\partial \pi}{\partial x} + l\upsilon + D_{xy}u + \frac{\partial}{\partial z}K\frac{\partial u}{\partial z} + \frac{\partial}{\partial z}\overline{u}\omega , \quad (1)$$

$$\frac{\mathrm{d}v}{\mathrm{d}t} + w\frac{\partial V}{\partial z} = -\frac{\partial \pi}{\partial y} - lu + D_{xy}v + \frac{\partial}{\partial z}K\frac{\partial v}{\partial z} + \frac{\partial}{\partial z}\overline{vw} , \quad (2)$$

$$\frac{\mathrm{d}\omega}{\mathrm{d}t} = -\frac{\partial\pi}{\partial z} + \lambda\theta + D_{xy}\omega + \frac{\partial}{\partial z}K\frac{\partial\omega}{\partial z},\qquad(3)$$

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} + w \frac{\partial\Theta}{\partial z} = D_{xy}\theta + \frac{\partial}{\partial z}K_{\mathrm{T}}\frac{\partial\theta}{\partial z} + \frac{\partial}{\partial z}\overline{w\theta}, \qquad (4)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 , \qquad (5)$$

$$\frac{\partial U}{\partial t} = l(V - V_{\rm G}) + \frac{\partial}{\partial z} K \frac{\partial U}{\partial z} - \frac{\partial}{\partial z} \overline{uw} , \qquad (6)$$

$$\frac{\partial V}{\partial t} = -l(U - U_{\rm G}) + \frac{\partial}{\partial z} K \frac{\partial V}{\partial z} - \frac{\partial}{\partial z} \overline{vw} , \qquad (7)$$

$$\frac{\partial \Theta}{\partial t} = \frac{\partial}{\partial z} K_{\rm T} \frac{\partial \Theta}{\partial z} - \frac{\partial}{\partial z} \overline{\Theta w} , \qquad (8)$$

where Θ , U, and V are the potential temperature averaged along the horizontal and the components of velocity along the axes x and y; θ , u, v, and w are the convective deviations of temperature and velocity components from their average values; $U_{\rm G}$ and $V_{\rm G}$ are the components of the geostrophic wind; l is the Coriolis parameter; K is the coefficient of vertical turbulent exchange of the subgrid scale; $K_T = K/Pr$, Pr is the turbulent Prandtl number in the ABL;

$$\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + (U+u)\frac{\partial}{\partial x} + (V+v)\frac{\partial}{\partial y} + w\frac{\partial}{\partial z}$$

is the operator of individual derivative;

$$D_{xy} = \frac{\partial}{\partial x} K_x \frac{\partial}{\partial x} + \frac{\partial}{\partial y} K_y \frac{\partial}{\partial y}$$

is the operator of horizontal turbulent exchange; λ is the buoyancy parameter; π is analog of pressure; the averaging operator is defined as

$$\overline{f} = \frac{1}{L_x L_y} \int_0^{L_x} \int_0^{L_y} f \, \mathrm{d}x \, \mathrm{d}y = 0.$$

Here the vector function is $f = (\theta, u, v, w)$; L_x and L_y are the horizontal boundaries of the domain of solution; $0 \le x \le L_x$, $0 \le y \le L_y$. Note that Eqs. (6)–(8) describe the background large-scale flow in the ABL, and Eqs. (1)–(5) model irregular mesoscale convection.

As the boundary conditions along the horizontal, we take the periodicity conditions traditional for the given class of problems. It should be noted that discretization of the ABL area with the dimensions $L_x = L_y = 10$ km on a 128×128 grid allows realization of an ensemble involving up to 100 convective formations of different size and intensity. The periodicity condition has the meaning of statistical homogeneity of the processes along the horizontal. Simultaneously, the problem of boundary conditions along x and y is solved.

We impose the following conditions on the equations of the mean flow in the ABL:

$$U = V = 0, \ \Theta = \Theta_0(z_0, t) \text{ at } z = z_0;$$
$$U = U_G, \quad V = V_G, \quad \frac{\partial \Theta}{\partial z} = \gamma_H \text{ at } z = H, \quad (9)$$

where z_0 is the roughness parameter; H is the upper boundary; $\Theta_0(z_0, t)$ describes the diurnal behavior of temperature near the surface; γ_H is the standard stratification of the free atmosphere. The conditions (9) for Eqs. (6)–(8) were realized with the help of the model of a quasistationary sublayer¹¹ of thickness h. It is assumed that convective pulsations within this layer are small. In this connection, for Eqs. (1)–(5) we take the following conditions:

$$u = v = w = 0; \quad \theta = \theta_0(t, x, y) \text{ at } z = h;$$
$$\frac{\partial f}{\partial t} + C \frac{\partial f}{\partial z} = 0 \text{ at } z = H, \tag{10}$$

where θ_0 are random small-amplitude temperature perturbations. Equations (10) describe radiation conditions at the upper boundary. They approximately set the open boundaries for fast gravitational waves generated in stable layers. The phase velocities *C* are fitted in calculation from analysis of the Brunt–Vaisala frequency.

As the initial conditions, we take

$$U = U_0, V = V_0, \Theta = \Theta_0 \text{ at } t = t_0,$$
 (11)

where U_0 , V_0 , and Θ_0 are the steady-state solutions of Eqs. (6)–(8) in the absence of convection.

According to the theory of 2D turbulence,¹¹ for the coefficients of turbulent diffusion we can write

$$K_x = \alpha_x \Delta x \Delta y \sqrt{D_{\rm T}^2 + D_{\rm S}^2} , \quad K_y = \alpha_y \Delta x \Delta y \sqrt{D_{\rm T}^2 + D_{\rm S}^2} , \quad (12)$$

where $D_{\rm S} = v_x + u_y$ and $D_{\rm T} = u_x - v_y$ are the components of planar deformation; $\Delta x \Delta y$ is the area of an elementary cell; α_x and α_y are dimensionless parameters.

The vertical turbulent exchange is simulated for mean flows based on the equations of semiempiric theory of turbulence.² In the ABL, the equations for the kinetic energy of turbulence b and its dissipation rate has the form

$$\frac{\partial b}{\partial t} = \frac{\partial}{\partial z} K \frac{\partial b}{\partial z} + KJ - \varepsilon , \quad \frac{\partial \varepsilon}{\partial t} = \frac{1}{\sigma} \frac{\partial}{\partial z} K \frac{\partial \varepsilon}{\partial z} - c_1 \frac{\varepsilon}{b} KJ - c_2 \frac{\varepsilon^2}{b} ,$$

$$K = c_k \frac{b^2}{\varepsilon} , \qquad (13)$$

where $J = (U_z^2 + V_z^2) - \frac{\lambda \Theta_z}{\Pr}$ is the source of generation of the turbulent energy; c_k , c_1 , c_2 , and σ are empiric constants.²

Equations (13) must meet the following boundary conditions:

$$\frac{\partial b}{\partial z} = 0, \quad \varepsilon = c_k \frac{b^2}{K_h} \text{ at } z = h,$$
$$\frac{\partial b}{\partial z} = 0, \quad \frac{\partial \varepsilon}{\partial z} = 0 \quad \text{at } z = H.$$
(14)

Model of the aerosol spread

$$\frac{\partial S}{\partial t} - w_0 \frac{\partial S}{\partial z} = D_{xy}S + \frac{\partial}{\partial z}K_S \frac{\partial S}{\partial z}, \qquad (15)$$

where *S* is the aerosol concentration; $w_0(d)$ is the acceleration due to gravity of a spherical particle having the diameter *d*; $K_S = K/Sm$, where Sm is the Schmidt number.

The surface concentration S is determined from the equation¹¹:

$$K_{S} \frac{\partial S}{\partial z} + w_{0}S = \beta S - \Gamma \text{ at } z = z_{0},$$
 (16)

where Γ is the mass of dancing particles torn away from the surface due to saltation; β is the rate of their entrainment into turbulent diffusion. The source intensity was calculated according to the technique proposed in Ref. 1, which studied processes of saltation and diffusion in the surface winddriven sand flow. The process of sequential lifts and falls of particles in a turbulent flow (saltation) is described in Ref. 1 based on equations of discontinuity and conservation of momentum in a two-component medium. The dynamic characteristics of the surface layer were calculated based on the assumption that after being lifted the particle is subject to the forces of gravity and resistance, and the latter is assumed proportional to the squared absolute value of the relative velocity. A parameter distinguishing small obstacles from sand particles is the ratio of their size to the Kolmogorov microscale of turbulence.

The critical velocity of the initial release is a function of the particle size and the friction velocity of the flow. In the process of transport, large particles fall onto the surface, whereas small ones become suspended and migrate due to turbulent pulsations. The criterion of distinguishing between saltation and diffusion is formulated in the terms of the Froude number $Fr = \rho u_*^2 / \rho_d g d$ for aerosol particles, where ρ_d is the density of particles; u_* is the friction velocity. Based on the equation of conservation of energy, the equation was obtained¹ for the mass Γ of particles torn from the unit area in the unit time interval as a function of the wind velocity at the level $z_2 = 2$ m and the particle size spectrum.

Figure 1 demonstrates the values of Γ obtained in Ref. 1 for sand-dust particles with the size of 10–50 µm versus wind speed. We can see that the critical speed of sand release depends on the size of sand particles and ranges from 3 to 5 m/s; at a lower wind speed, $\Gamma = 0$ and release does not occur. The rate of gravitational sedimentation calculated by the Stokes equation increases as the particle size increases, varying from 0.03 to 0.3 m/s for the considered values of *d*.



Fig. 1. Mass of particles involved in diffusion as a function of the wind speed at the level of 2 m for the fractions with $d = 10, 20, 30, 40, \text{ and } 50 \ \mu\text{m}$ (curves 1, 2, 3, 4, and 5).

The condition (16) is written at the level of roughness; to use it in the ABL model, we should reformulate it to the first computational level, which coincides with the upper boundary of the layer of constant flows (LCF) z = h. Toward this end, let us write the equations of transport while applying usual simplifications of the LCF theory in the form

$$-w_0 \frac{\partial S}{\partial z} = \frac{\partial}{\partial z} K_S \frac{\partial S}{\partial z}.$$
 (17)

Integrating Eq. (17) from z_0 to z and using Eq. (16), we obtain

$$K_{\rm S} \frac{\partial S}{\partial z} = -w_0 S + \Pi_0 , \qquad (18)$$

where $\Pi_0 = \beta S_0 - \Gamma$, S_0 is the concentration at $z = z_0$. The sought analytical equation for S(z) can be obtained from Eq. (18) on the assumption that $K_{\rm S} = \alpha_{\rm S} K$ $(\alpha_{\rm S} = 1/{\rm Sm})$ in terms of the variable ς defined by the equality $dz = K_{\rm S} d\varsigma$. Finally, the exact analog of Eq. (16) takes the form

$$K_{\rm S} \frac{\partial S}{\partial z} = w_0 \frac{(\beta - w_0)S - \Gamma}{\beta - (\beta - w_0)\exp(-w_0\varsigma_h)} \exp(-w_0\varsigma_h)$$

at $z = h$, (19)

where ς_h corresponds to the level z = h, and the dependence $\varsigma(z)$ is determined through the LCF parameters based on the accepted system of universal functions.

Figure 2 shows the horizontal distribution of the concentration of the fine aerosol with $d = 20 \,\mu\text{m}$ at the level of 300 m above the quasistationary sublayer. The fields of the rates and coefficients of turbulent exchange were obtained from numerical simulation of Eqs. (1)–(8), in which it is taken that $U_{\rm G} = 10 \,\text{m/s}$. The physical time corresponds to 2 h after the beginning of deflation.



Fig. 2. Isolines of the field *S* in the horizontal cross section at z = 300 m.

It is seen from Fig. 2 that the specific concentration is characterized by significant spatial inhomogeneity and varies from 0.09 to 0.27 g/m³, i.e.,

by three times (the value \overline{S} averaged over x and y at this level is 0.14 g/m³). With height, the contrast of the spatial distribution of aerosol becomes more pronounced, and the increased values of the concentration correspond to upwelling flows of warm air.

The "spotty" structure of the concentration shown in Fig. 2 is caused by the irregularity of the spatial distribution of convective cells, as well as by the peculiarities of vertical transport due to powerful upwelling motions in thermics, whose speed in this calculation reaches 3.5 m/s (negative extreme of w is roughly twice as small). Since $w_0 \approx 0.07 \text{ m/s}$ is much less than positive w, aerosol particles involved in convective flows are lifted up almost to the upper boundary of the mixing layer, thus forming pronounced zones of increased convection. Downwelling flows along with the sedimentation processes favor the local decrease of the aerosol content and partial removal of aerosol from the atmosphere. The presence of the mean wind leads to formation of the extended structure of pulsations of the concentration field. The structure extended along the x axis can be seen in Fig. 2. These factors cause complex spatiotemporal dynamics of aerosol parameters in the convective ABL.



Fig. 3. Vertical profiles of the mean concentration in 1D (curve t), plane zx (curves 2 and 2'), and spatial (curve 3) problems.

The concentration profile averaged over the horizontal is shown in Fig. 3, curve 3. This figure also shows the distribution S obtained within the framework of the one-dimensional model, i.e., model ignoring convection (curve 1). Comparing curves 1 and 3, we can see that in the lower layers the difference in the

concentrations is small, while at z = 300 m the convective transport leads to the more than twofold increase of \overline{S} , and at the level z = 600 m – to the tenfold increase. The diffusion processes, described based on 1D *K*-model, are practically confined within this layer, whereas the effect of convective factors manifests itself at the heights up to 800-1000 m. The total mass of particles involved in air flows due to the purely diffusion mechanism was 42 g/m^2 by the given time, whereas that with allowance made for convective exchange was 94 g/m^2 , i.e., 2.2 times as large.

Analyzing the profile 3 in Fig. 3, note the tendency to formation of a layer with the values of Svarying slightly along the vertical at 300 < z < 700 m. This peculiarity of the convective ABL is confirmed by the observations,⁴ according to which the turbidity of the lower 1-km atmospheric layer increases in clear summer days. The mixing layer is more pronounced in curve 2' (Fig. 3), which was obtained within the plane model with the longitudinal flow about convective waves. The qualitatively similar results were obtained in Refs. 6 and 9 when solving similar problem in a 2D formulation and simplified description of aerosol interaction with the surface. In a 2D problem with the cross orientation of waves relative to the wind, the mixing layer, on the contrary, is smeared and the profile of S is close to linear (see Fig. 3, curve 2). Comparison of curves 2 and 2' suggests that to reproduce correctly the ABL structure based on a 2D LES-model, it is necessary to set correctly the direction, along which the processes are assumed uniform.

Summarizing the above-said, let us note that the convection in the ABL play a significant part in the upward transport of sand-soil aerosol to the upper layers.

The calculations by use of a 3D nonstationary eddy-resolving model showed good qualitative agreement with the earlier theoretical results, as well as with the known meteorological phenomena: turbidity of the mixing layer in summer days and penetration of heavy particles up to the altitudes of 1 km.

It is important to note that in the short-term field observations a significant inhomogeneity may arise in the spatial distribution of the fields of atmospheric aerosol, especially, if these observations fall on different phases of the eddy convective formations. The zones of convergence and divergence cause the appearance of the areas with an enhanced aerosol concentration. In this case, the distribution of a passive admixture above the surface layer is inadequately reproduced if using an ordinary diffusion model.

Thus, the maximum in the concentration of an admixture involved in a circulation cell can several times exceed its mean value. This circumstance should be taken into account when interpreting observations and setting the intervals of time averaging of the data. V.A. Shlychkov et al.

Acknowledgments

The work was partially supported by the Russian Foundation for Basic Research, Grants No. 99–05–64678 and No. 99–05–64735.

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