THREE-DIMENSIONAL MESOSCALE MODEL FOR ANTHROPOGENIC AND CLOUD AEROSOL TRANSFER WITH ACCOUNT OF INTERACTION BETWEEN RADIATIVE AND MICROPHYSICAL PROCESSES AND OROGRAPHY. PART I. PROBLEM FORMULATION

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This paper presents a three-dimensional numerical model for industrial and cloud aerosol transfer in an orographically inhomogeneous atmospheric boundary layer, which makes it possible to study the effect of interacting clouds and aerosols on the radiation regime and the optical char actertistics of the atmosphere, the effect of orography on the microphysical parameters and optical properties of fogs and clouds, and the patterns of anthropogenic aerosol transfer.

INTRODUCTION

Clouds and anthropogenic aerosols have a marked effect on the optical characteristics and radiation regime of the atmosphere[1–4]. These processes have been widely studied in recent years since a physical understanding and description of the interconnection between the cloud-aerosol and optico-radiative parameters of the atmosphere are vital for climatic research, remote sensing of the atmosphere, and various applied problems.

These studies have resulted, in particular, in the development of optico-aerosol[2] and cloud-radiation[1,3,4] model atmospheres. But clouds and aerosols are closely interrelated, as is evident, for instance, from the measurements made by means of airborne photoelectric counters[3,5] and theoretical reseach[6].

The cloud, aerosol, and radiation interaction is particularly intense in zones of anthropogenic aerosol emissions and in the atmospheric boundary layer (ABL). Thus, fog and cloud formation under the impact of radiative and orographic factors entails a localization of inversion layers close to the upper boundary of the fog or cloud, thereby preventing a vertical spread of aerosols that tend to accumulate under the barrier layers and are thus conducive to smogs. As the aerosols interact with the condensate the pollutants undergo diverse transformations, being absorbed by droplets and washed out by precipitations. The aerosol modifies the structure of clouds, with noticeable changes in their optical properties, in the radiation conditions, and the amount of precipitation in the cities.

Numerical simulation is being used with ever greater efficiency to investigate these problems. A one dimensional nonstationary model and a two-dimensional steady-state model were used in Ref. 7 to examine the effect of radiative and river fogs on the spread of pollutants. Three dimensional nonstationary models were used to study the spread of gaseous (weightless) pollutants[8,9] and the transfer of sedimenting aerosols[10–12]; the computations were made for cloudless conditions, without regard to the blocking effect of the radiation inversion that results from the interaction of radiation with clouds and fog.

Three-dimensional models for clouds over land and ocean with an account of the optical parameter evolution in the interaction of microphysical and radiative processes were developed in Refs. 13 and 14, and a three-dimensional model was used in Ref. 15 to study the interaction of clouds with active pollutants (crystals). The models gave no consideration to orography although it often has an appreciable effect on the cloud optical parameters and aerosol transfer[16].

This paper presents a three-dimensional nonstationary mesoscale model for clouds, fogs, and pollution transfer in an orographically inhomogeneous ABL that allows one to study the impact of the interacting clouds and aerosols on the radiation regime of the atmosphere and of the underlying surface, the effect of orography on the microphysical and optical characteristics of clouds, and the patterns of anthropogenic aerosol transfer.

A study of these effects by means of numerical models provides an insight into the cloud-radiation relations and their influence on the optical properties of the atmosphere and on the microclimate in industrial and urban areas. The results of numerical computations can dramatically reduce the time and effort it takes to conduct labor-intensive and costly experiments in the remote sensing of atmospheric optical parameters in the presence of clouds, fogs, and anthropogenic aerosol pollution.

MODEL FORMULATION

A system of equations for the model includes dynamic equations for a thermally and orographically inhomogeneous ABL, equations of cloud thermohydrodynamics and microphysics, transfer equations for long-wave radiation (LWR) and soil heat transport, and equations describing aerosol transfer and sedimentation in a turbulized flow.

The model equations are solved in a curvilinear coordinate system associated with the local topography whose function has the form $z_{10} = \delta(x, y)$. The orthogonal coordinate system $x_1y_1z_1$ is replaced by the curvilinear coordinates xyz: $x = x_1$; $y = y_1$; $z = z_1 - \delta(x, y)$. In the new coordinate system xyz, the motion and continuity equations are reduced to a form different from that used in Refs. 8 and 9. Note that the equations are solved not for meteorological element perturbations but for total values; the geostrophic wind at the ABL top is given as the background value. Hence

$$\frac{\partial u}{\partial t} + \mathrm{di}V_a Uu + (w-u\delta_x-v\delta_y)\frac{\partial u}{\partial z} = -\frac{\partial \pi'}{\partial x} + \frac{\partial \pi'}{\partial z}\delta_x + \hat{\Delta}u + f_c(v-V_b) + \frac{DU_b}{Dt} \quad (1)$$

$$\frac{\partial v}{\partial t} + \mathrm{di}V_a Uv + (w-u\delta_x-v\delta_y)\frac{\partial v}{\partial z} = -\frac{\partial \pi'}{\partial y} + \frac{\partial \pi'}{\partial z}\delta_y + \hat{\Delta}v - f_c(u-U_b) + \frac{DV_b}{Dt} \quad (2)$$

$$\frac{\partial w}{\partial t} + \mathrm{di}V_a Uw + (w-u\delta_x-v\delta_y)\frac{\partial w}{\partial z} = -\frac{\partial \pi'}{\partial z} + \hat{\Delta}w \quad (3)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \quad (4)$$

To complete the ABL equation system, we used Kolmogorov's approximate similarity hypothesis, solved the balance equation for the turbulent kinetic energy b, and expressed the vertical turbulent exchange coefficient k_z and the rate of the turbulent energy dissipation into heat ε_T in terms of b and the turbulence scale 1:

$$\frac{\partial b}{\partial t} + \mathrm{di}V_a Ub + (w-u\delta_x-v\delta_y)\frac{\partial b}{\partial z} = \hat{\Delta}_a b + \frac{\partial}{\partial z}k_b\frac{\partial b}{\partial z} + k_b\left[\left(\frac{\partial u}{\partial z}\right)^2 + \left(\frac{\partial v}{\partial z}\right)^2 - \beta\frac{\partial \theta}{\partial z} - \beta\frac{\partial q}{\partial z}\right] - \varepsilon_T \quad (5)$$

$$k_z = lb^{1/2};\quad \varepsilon_T = cb^2/k_z;\quad l = -\kappa\, c^{1/4}\, b\left[k_z\frac{\partial}{\partial z}(b/k_z)\right]^{-1};$$
$$k_b = 0.73k_z \quad (6)$$

In equations (1)–(6), U is the three-dimensional wind velocity vector, $\pi' = \pi - c_b$, where π is an analog of pressure $\left(\pi = \dfrac{C_p\theta_0 T}{A\theta}\right)$, A is the thermal equivalent of work, θ is the mean potential temperature, π' is the departure from the background pressure (Π_b), C_p is the specific heat at constant pressure, U_b and V_b are the horizontal components of the background wind, $\mathrm{di}V_a$ is the horizontal advection operator, δ_x and δ_y are the surface slopes along the x and y axes;

$$\hat{\Delta}_a = \frac{\partial}{\partial x}k_x\frac{\partial}{\partial x} + \frac{\partial}{\partial y}k_y\frac{\partial}{\partial y};$$

$$\hat{\Delta} = \hat{\Delta}_a + \frac{\partial}{\partial z}k_z\frac{\partial}{\partial y};$$

k_x and k_y are the horizontal turbulent diffusion coefficients, and f_c is the Coriolis parameter.

The heat and moisture transfer equations read:

$$\frac{\partial w}{\partial t} + \mathrm{di}V_a UT + (w-u\delta_x-v\delta_y)\left(\frac{\partial T}{\partial t} + \gamma_a\right) = \frac{1}{C_p}\varepsilon_c + \hat{\Delta}T - u\gamma_a\delta_x - v\gamma_a\delta_y + R_L + \frac{DT_b}{Dt} \quad (7)$$

$$\frac{\partial q}{\partial t} + \mathrm{di}V_a Uq + (w-u\delta_x-v\delta_y)\frac{\partial q}{\partial z} = -\varepsilon_c + \hat{\Delta}q \quad (8)$$

where ε_c is the specific condensation rate, R_L is the radiative heat influx, and γ_a is the dry adiabatic temperature lapse rate. The thermohydrodynamic equations are supplemented with transfer equations for droplet concentration N_L, water content q_L, and mean droplet radius r_L (on the assumption that the droplet spectra are approximated by the gamma size distribution), and the distribution function $f(r_L)$ becomes

$$f(r_L) = \frac{N_L\beta_L^{P_L}}{\Gamma(P_L)}\, r_L^{P_L-1}\exp(\beta_L r_L)$$

where

$$\beta_L = P_L/r_L$$

$$\frac{\partial N_L}{\partial t} + \mathrm{di}V_a UN_L + (w-u\delta_x-v\delta_y-w_{N_L})\times\frac{\partial N_L}{\partial z} = I_{N_L} + \hat{\Delta}N_L \quad (9)$$

$$\frac{\partial q_L}{\partial t} + \mathrm{di}V_a Uq_L + (w-u\delta_x-v\delta_y-w_{q_L})\frac{\partial q_L}{\partial z} = I_{q_L} + \hat{\Delta}q_L \quad (10)$$

$$\bar{r}_L = \left[\frac{3\,q_L P_L^2}{N_L 4\pi\rho_L(P_L+1)(P_L+2)}\right]^{1/3} \quad (11)$$

where w_{N_L} and w_{q_L} are the sedimentation rates for droplet concentration and mass, I_{N_L} and I_{q_L} are their sources, and P_L is the gamma-distribution factor. Condensation and evaporation processes for a collection of droplets are calculated by the MacDonald method (see Ref. 1). At the instant when saturation is reached over water, I_{N_L} droplets are activated at a given point, and the mass of condensed water is calculated subject to the heat and moisture balance condition at condensation.

Long-wave radiation (LWR) transfer processes are calculated in a two-flow approximation as in Refs. 1, 13–15. The water vapor absorption spectrum was schematized[18] by division into two areas: 1) an atmospheric transparency window at 8–-13 μm with water vapor and droplet absorption coefficients α_v = 0.1 cm^2/g and α_L = 450–650 cm^2/g, respectively, and 2) an area outside the window, where LWR spectral flows approach black-body radiation fluxed.

The transfer equations for integrated flows in the window $F_w^{\uparrow,\downarrow}$ total flows $F_1^{\uparrow,\downarrow}$, and influx R_L can be given as

$$\frac{dF_w^{\uparrow}}{dz} = \beta_1 \rho_a (\alpha_v q + \alpha_L q_L + \alpha_{pi} m_{pi})(F_w^{\uparrow} + P_w B) \tag{12}$$

$$\frac{dF_w^{\downarrow}}{dz} = \beta_1 \rho_a (\alpha_v q + \alpha_L q_L + \alpha_{pi} m_{pi})(F_w^{\downarrow} - P_w B) \tag{13}$$

$$F_1^{\uparrow\downarrow} = F_w^{\uparrow\downarrow} + (1 - P_w)B \ ;$$

$$C_p \rho_a R_L = (F_1^{\uparrow} + F_1^{\downarrow} - 2B) \ ; \tag{14}$$

$$\alpha_L = \alpha_0 \left[1 - \frac{P_L + 4}{P_L + 1} r c + \frac{(P_L + 4)(P_L + 5)}{(P_L + 1)^2} r_L^2 c_L \right] \tag{15}$$

where $\alpha_L$and α_{pi} are the mass absorption coefficients for droplets and aerosol particles, m_{pi} is the aerosol mass, $B(T)$ is the black-body radiation flow, $P_w = 0.27$ is its fraction in the transmission window 8–13 μm, β_L is the diffusion coefficient, and α_0 = 550 cm^2/g.

To take into account the diurnal temperature variations, the soil heat conductivity equation is solved:

$$\frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x_{sj}} k_{sj} \frac{\partial T_s}{\partial x_{sj}} \tag{16}$$

where x_{sj} is the vertical coordinate in the soil depth, and k_{sj} is the thermal diffusivity of different soil layers. To relate the atmospheric thermohydrodynamic equations with the soil heat transfer equation, we use the heat balance equation for the underlying surface:

$$c_p \rho_a k_z \left[\frac{\partial T}{\partial z} + \gamma_a \right] - L \rho_a k_z \frac{\partial q}{\partial z} -$$

$$- c_s \rho_s R_s \frac{\partial T_s}{\partial x_{sj}} + R_0 = 0 \tag{17}$$

where ρ_a and ρ_s are the air and soil densities, L is the latent vaporization heat, and R_0 is the underlying surface radiation balance.

The neutral sedimenting aerosol tranfer is described by the semiempirical turbulent diffusion equation[7,8,11]:

$$\frac{\partial S}{\partial t} + \mathrm{div}\, V_a US + (w - u\delta_x - v\delta_y - w_s(R_e))\frac{\partial S}{\partial z} =$$

$$= \hat{\Delta} S - \alpha_s S + I_s \tag{18}$$

where $w_s(R_e)$ is the aerosol sedimentation rate for a particle with a mean effective radius R_e, I_s on the right side of Eq. (18) describes the aerosol sources and sinks, and $\alpha_s S$ specifies the aerosol sink due to absorption by droplets. According to Ref. 7,

$$\alpha_s S = \int_0^{\infty} P(r_L)\, f(r_L)\, dr_L \tag{19}$$

where $P(z_L)$ is the number of aerosol particles absorbed by the r_L I-radius droplets per unit time, and $f(z_L)$ is the droplet size distribution function.

The intensity I_0 of aerosol sedimentation on the underlying surface and the total sediment F_s are determined from the formulas

$$I_0 = 4/3\ \pi\ \rho_s\ R_e^3\ S_0 ;$$

$$F_s = \int_0^t I(t')\, dt' \tag{20}$$

where S_0 is the aerosol concentration on the underlying surface and ρ_s is the aerosol density.

SOLUTION APPROACH

Equations (1)–(3), (5), (7)–(10) and (18) are solved by the variable component separation technique for spatial coordinates and physical processes. The equations of motion are solved by a combination of the matrix and scalar pass techniques, as in Ref. 11 and through matching the wind velocity fields with pressure gradients by the over relaxation method. To ensure the monotonicity and conservative character of the finite-difference scheme in solving Eq. (18), use is made of hybrid self-regulating algorithms with an improved order of accuracy[17].

The number of grid nodes is 21×21×31; ABL dynamics is calculated by means of a variable height fine-structure meshwidth many vertical discrete points (151 level). Mesometeorological-scale processes with a horizontal extent of 15–400 km (the horizontal step varies from $\Delta x = \Delta y$ = 0.75 km to 20 km) were simulated. The x-axis is oriented towards the east and the y-axis – towards the north. The background (geostrophic) wind velocity along the x-axis (V_F = 0) was assumed to be $U_F = G$ = 5 m/s. In studying the ABL evolution over an orographically inhomogeneous underlying surface the local topography profile was taken to be

$$\delta(x,y) = h \sin\left[\pi \frac{x'}{D_x}\right] \sin\left[\pi \frac{y'}{D_y}\right] \tag{21}$$

where $x' = (0, \bar{D}_x)$; $y' = (0, \bar{D}_y)$; $D_x = 8\Delta x$; $D_y = 8\Delta y$, i.e., we examined the flow around a domelike, round-based hill centered in the middle of the estimated area with a height h and a base diameter $D_x = D_y$; H_p is the ABL height.

The boundary conditions for the equations of motion are the reattachment conditions for the underlying surface wind velocity while those for the horizontal substance transfer are the free-flow conditions on the boundaries of the estimated area. The boundary conditions for the turbulent energy balance equation are: $\partial b/\partial z = 0$ $(z = 0)$, $b = 0$ $(z = H_p)$. The boundary condition for q on the underlying surface with due account of variable soil humidity is derived by joining the molecular and turbulent moisture flows near the surface[1].

$$k_z \rho_a \frac{\partial q}{\partial z} = \alpha_{ef} \rho_a \frac{v_v}{4} (q_s - q_0) \tag{22}$$

where α_{ef} is the effective condensation (evaporation) factor, v_v is the velocity of water vapor molecules, and q_s is the saturation value of the specific humidity.

The boundary conditions for the long-wave radiation transfer equation are of the form: $F^{\uparrow}_{\omega,0} = P_{\omega} B(T_0)$; $F^{\downarrow}_{\omega,Hp} = F^{\downarrow}_{\omega}(H_p)$. The value of $F^{\downarrow}_{\omega}(H_p)$ is obtained by formula through integration from the tropopause, where $F^{\downarrow}_{\omega}(H_{tr}) = 0$, to the ABL top $z = H_p$.

In solving Eq. (18) it is important to estimate the amount of aerosol particles reaching the underlying surface. Therefore, the relevant boundary condition is an equation for the particle balance at the height of the underlying surface:

$$k_{sz} \frac{\partial S}{\partial z} + (w_s - u_s \delta_x - v_s \delta_y - w_s(R_э))\, S = \beta_s S - I'_s \tag{23}$$

where u_s, v_s, w_s and k_{zs} are the wind velocity components and the turbulence coefficient at the height of the source z_s; β_s is the absorptance of aerosol particles by the underlying surface, and I'_s describes the pollution sources at the roughness level.

A point source with coordinates (x_s, y_s, z_s) is described by the δ-function:

$$I_s = M\, \delta(x-x_s)\, \delta(y-y_s)\, \delta(z-z_s) \tag{24}$$

where M is the source power.

To describe a vertically extended aerosol emission source with lower and upper level heights z_{s1} and z_{s2}, we introduce the θ function and reduce the right side of Eq. (18) to obtain:

$$I_s = M\, \delta(x-x_s)\, \delta(y-y_s)\, \delta(z-z_s) \times (\theta(z-z_{s1}) - \theta(z-z_{s2})) \tag{25}$$

CONCLUSION

The proposed model describes cloud-aerosol relations on a mesometeorological scale with account of the interaction between radiation and condensate and changes in the optical characteristics of an aerosol atmosphere in an orographically inhomogeneous atmospheric boundary layer. Its usage allows the anthropogenic environmental pollution effects to be evaluated and recommendations for optical remote sensing to be worked out. The results obtained with this model are presented in Part 11 of this paper.

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