On numerical simulation of vertical ozone distribution

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One of the schemes of numerical simulation of the vertical ozone distribution is proposed for the prediction purpose, and sensitivity of the model to variations of the ambient conditions is evaluated. The set of equations most adequately describing the physical processes is derived. Plots illustrating the results of simulation are presented, and the model is shown to be applicable to simulation of a dry stratified atmosphere. The simulation results are assessed.

Regardless of the relatively low ozone content in the atmosphere (if the total ozone is presented in the form of a film around the globe, then the film thickness is only from 1.5 to 6 mm, whereas it is 1560 m for oxygen and 6200 m for nitrogen[1]), it significantly affects the human health and activity.[2] On the one hand, ozone plays the part of a shield against the UV radiation. On the other hand, at a high concentration, ozone is dangerous for human respiratory ducts and can even cause death.[3] Ozone is a very strong oxidant and one of the most dangerous pollutants in the lower atmospheric layer.

In this connection, it is important to study the vertical ozone distribution (VOD) and to try to simulate it. The archives of VOD measurements collected by now are rather extensive.[4]

A sufficient number of VOD models are described in the literature, for example, the Chapman fundamental model of ozone formation,[5] models using the reactions of vibrational and electronic excited states of particles, hydrogen[6] and nitrogen[7] cycles, models using the hypothesis on the vertical advection of ozone,[6] 2D zonally mean photochemical model,[8] etc. At the same time, an ideal model has not been developed yet. In this connection, to study the peculiarities of the vertical ozone distribution, let us consider the model of the stratified dry atmosphere. This is quite reasonable taking into account small values of the horizontal gradients of atmospheric parameters as compared to their vertical gradients. Therefore, neglecting local derivatives with respect to the horizontal coordinates, we can write the main equations of the model in the Cartesian system of coordinates.

1. Equation of motion, which determines the balance of accelerations:

$$\frac{\partial W}{\partial t} + W\frac{\partial W}{\partial z} = -\frac{1}{\rho}\frac{\partial P}{\partial z} - g + \frac{\partial}{\partial z} k_z \frac{\partial W}{\partial z}, \qquad (1)$$

where W is the vertical component of the wind velocity; g is the acceleration of free fall, whose value is altitude-dependent; k_z is the coefficient of turbulent viscosity; t is time; ρ is air density; and P is atmospheric pressure.

2. Equation of continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho W}{\partial z} = 0. \qquad (2)$$

3. Equation of state:

$$P = \rho R T, \qquad (3)$$

where R is the specific gas constant of dry air (R = 287 J/(kg·deg)); T is air temperature in K.

4. Heat transfer equation:

$$\frac{\partial T}{\partial t} + W\frac{\partial T}{\partial z} = \frac{1}{\rho}\frac{\partial}{\partial z} k\left(\frac{\partial T}{\partial z} + \gamma_a\right) - \gamma_a W + \frac{Lm}{c_p}, \qquad (4)$$

where k is the coefficient of turbulent thermal conductivity; γ_a is the dry adiabatic lapse rate; c_p is the specific heat of dry air at the constant pressure (1005 J/(kg·K)); L is the specific evaporation heat for vapor of mass m. Let us assume $m = 0$.

5. Ozone transfer equation:

$$\frac{\partial S}{\partial t} + W\frac{\partial S}{\partial z} = \frac{1}{\rho}\frac{\partial}{\partial z}\rho\, k_z \frac{\partial S}{\partial z} + Q, \qquad (5)$$

where S is the ozone mass fraction in the atmosphere; Q is the ozone inflow.

Thus, the set of equations (1)–(5) consists of five equations for five unknowns: T, W, P, S, and ρ. Because there is no *a priori* information on the sources and sinks of heat, ozone, water vapor, and motion, it is worthwhile checking the predicted profiles for their coordination with each other. For this purpose, we used the equation of conservation of energy, which transforms into the Bernoulli equation

$$(W^2/2) + c_p T + g z = \text{const} \qquad (6)$$

in the adiabatic case.

Since equations (1)–(5) are mutually stipulated, they should be solved by numerical methods. When numerical models are used, certain problems arise as, for example, non-physical oscillations of calculated profiles in the regions of gradient increase, which can lead to negative values of obviously positive parameters. To resolve such problems, one has to use special methods for integration of equations.

Following the recommendations given in Ref. 9, we introduced an artificial viscosity to the numerical scheme. Taking this into account, we integrated the set of equations (1)–(5) using the method of time steps (15 min) in the altitude range from 0 to 60 km. The solution was sought with the use of Matsuno conforming semi-implicit two-step two-level scheme (Euler scheme with recalculation) of the first order of accuracy in time (Δt) and the second order in space (Δr), that is, $O[\Delta t, (\Delta r)^2]$:

$$f_q^{s+1,(*)} = f_q^s + F_q^s \Delta t ,$$
$$f_q^{s+1} = f_q^s + F_q^{s+1,(*)} \Delta t , \qquad (7)$$

where f_q is the sought function; F are the terms containing no time derivatives; s is the number of a time layer; q is the number of a point at a space mold.

As is seen, the scheme (7) consists of two parts: a predictor scheme (first equation) and a corrector scheme (second equation). Tentative values are calculated with the use of the predictor scheme, and then they are refined using the corrector scheme. The main criterion in selecting the finite-difference scheme was the condition of stability assuming the fulfillment of the Courant–Friedrichs–Levi (CFL) criterion. In this case, the scheme suppresses the relative amplitude of high-frequency oscillations and is unconditionally stable and dissipative.

To increase the computational viscosity and to suppress the computational modes, the numerical scheme was supplemented with frequency filters and iterations, which allowed restriction of possible amplitudes of predicted values of the simulated profiles. The computational error was monitored at every time step by comparing the current and previous profiles of the simulated function. When constructing the filters, we took, as a basis, the time filter proposed by Rober and Asselin[9]:

$$\bar{f}_{ij}^{\,s} = f_{ij}^{s} + 0.025\,(f_{ij}^{s-1} - 2\, f_{ij} + f_{ij}^{s})^{s+1}, \qquad (8)$$

where $s = t/\Delta t$.

To solve the equation of motion (1), we had to break the time steps in order to obtain actual values of the vertical speed. To enhance the stability of solution, we used the assumption that the equation is quasistationary in time at every step with the allowance made for variations of the parameters included in Eq. (1).

The algorithm of the model uses the method of successive approximations. At the first stage, the variables, arrays, and constants used in the model were set. Then the initial profiles of temperature, air density, acceleration of free fall, vertical mixing coefficient, and partial pressure of the atmospheric ozone at the preset levels were entered. The initial profile W was set based on the assumption that $W = 0$ over the entire integration domain. Then the values of W, ρ, T, and S were calculated by the predictor scheme, first for the inner area and then for limiting points. Calculations were made by the method of successive approximations with the discrepancy set to be $\varepsilon = 0.001$. Once each parameter is calculated, short-wave noise was filtered out. After calculation of T and ρ, they were put in consistency with the use of Eq. (6). Then similar calculations were made by use of the corrector scheme. Finally, the newly obtained profiles were assigned to the parameters, and calculation passed to the next time step.

The results of observation and climatic information for Tateno, Japan (36.0°N, 140.1°E) were used as the initial data. These data included the air density and temperature, acceleration of free fall in the standard atmosphere,[10] air temperature and density in the reference atmosphere,[2] the vertical mixing coefficient in accordance with Ref. 11, and the ozone partial pressure.[2]

As an example, several VOD profiles obtained in Tateno in January 1981 (Ref. 4) were used. Figure 1 shows the actual VOD profiles recalculated to the 2-km altitude step with the use of linear interpolation and extrapolation, as well as long-term “climatic” VOD profile for this latitudinal zone.[2]

The time step of integration was chosen taking into account the conditions of stability and convergence, as well as the altitude step equal to 2 km. Thus, the time step was taken to be 15 min. The profiles of vertical mixing coefficients were set according to Ref. 12.

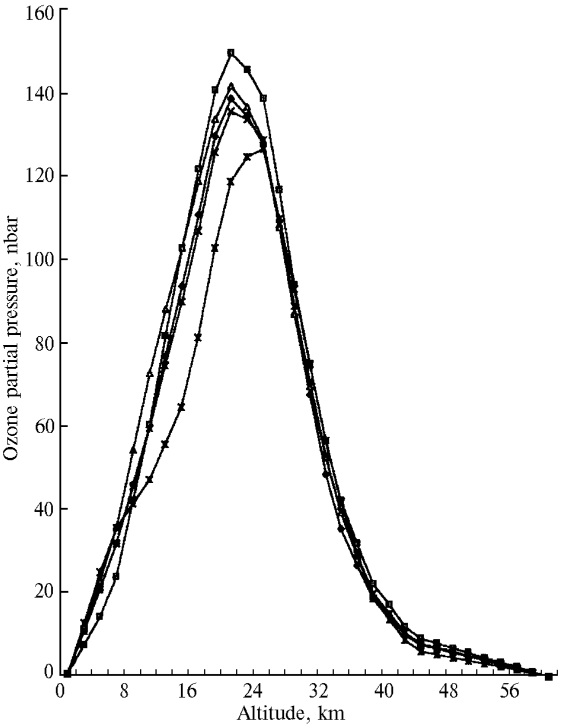

Fig. 1. Actual VOD profiles for Tateno extrapolated to a 2-km grid based on the data of ozone sounding: January 15, 1981 (–◆–), January 16 (– –), January 17 (–▲–), and January 18 (–×–); mean climatic profile (–∗–).

In the numerical experiment, we studied the changes in the profile three days after the model was started at different combinations of the initial conditions, as well as at heating in the ground layer and in the layer of 30–40 km, at the change in the speed of the vertical air motion.

Figure 2 shows the VOD profile simulated with the use of the climatic ozone profile and under conditions of standard and a reference atmosphere. The profile was calculated for the forecast range of three days. The analysis shows that on the whole both of the models adequately describe the ozone profile. At the same time, the tendency to the anomalous ozone distribution in the 6–10-km layer should be noted, as well as rather large deviations at the level of 2 km and above 30 km. The maximum deviations reach 40% of the ozone partial pressure in nanobars. In the 9–23-km layer both of the models somewhat underestimate the result and overestimate it in the layer above 23 km. At the same time, in the 24-km level, where the ozone partial pressure was maximum, the deviation of the model values from the climatic mean ones was about 3%.

The VOD profiles calculated with the use of the initial data for the reference and standard atmosphere differ insignificantly, except for the layers of 0–12 and 50–56 km, where the maximum deviation reaches 19% in the lower layer and 10% in the upper one. In different levels both models alternatively turn out to be closer to the mean climatic profile. The data of the reference atmosphere[2] turned out to be preferable for use in calculations, since with them the optimal result was achieved in 67% of levels.

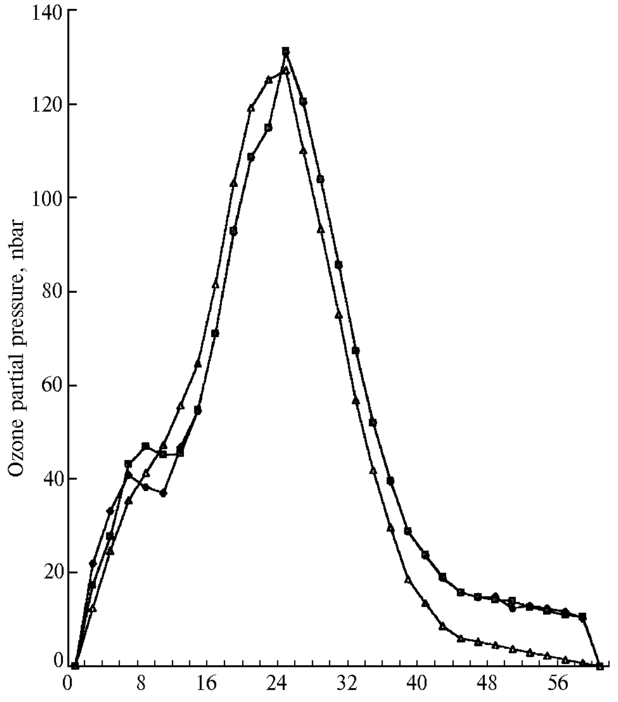

Fig. 2. Simulated VOD after three days from the data of the reference atmosphere (—◆—) and standard atmosphere (— —) and mean climatic profile (–△–).

The comparison of the actual VOD profile on January 18, 1981 (recalculated to a 2-km grid) with the profile calculated by the model with the use of data on actual VOD on January 15, 1981, showed their very close agreement (up to the altitude of 30 km the deviation did not exceed 4%). As in the initial profile, the level of maximum ozone content remained at 20 km, what is 4 km below the mean climatic level.

To study the model sensitivity, the numerical experiments were conducted on introducing perturbations in thermal conditions and increasing the vertical air speed.

Figure 3 shows the VOD profile, for calculation of which the ground temperature in the initial data was increased by 5°, the temperature at the level of 2 km was increased by 0.5°, and that at the level of 4 km was increased by 0.1°. The mean climatic profile and the profile constructed for the standard atmosphere and the mean climatic ozone profile are also shown for a comparison. After three days significant differences in the simulated profiles manifested themselves in the 2–10-km layer and resulted in an up to 20% decrease in the ozone partial pressure at all these levels.

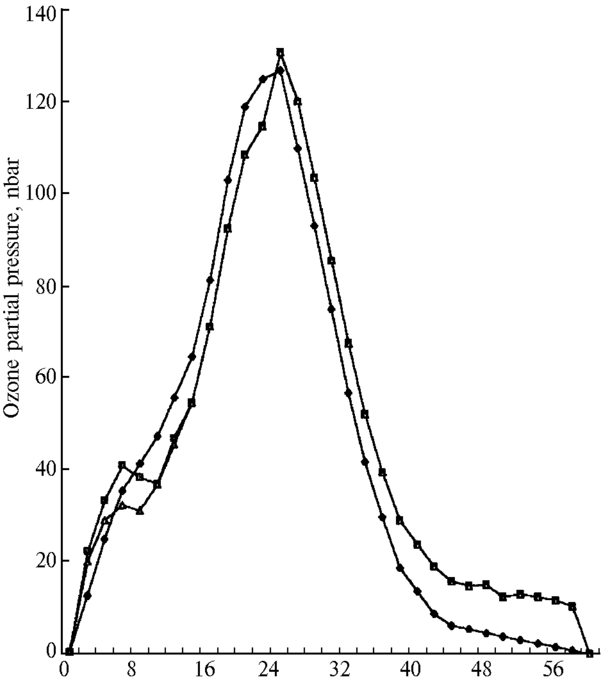

Fig. 3. Simulated VOD after three days from the data of the reference atmosphere (— —), profile calculated with the allowance for additional heating (–△–), and mean climatic profile (—◆—).

Figure 4 shows the mean climatic profile, the profile constructed with the use of the reference atmosphere[2] and the mean climatic ozone profile, and the VOD profile, in calculating of which the speed of vertical air motion was increased by 0.1 m/s during 10 h. In this case, a significant decrease in the ozone partial pressure (by up to 62%) was revealed in the 2–9-km layer.

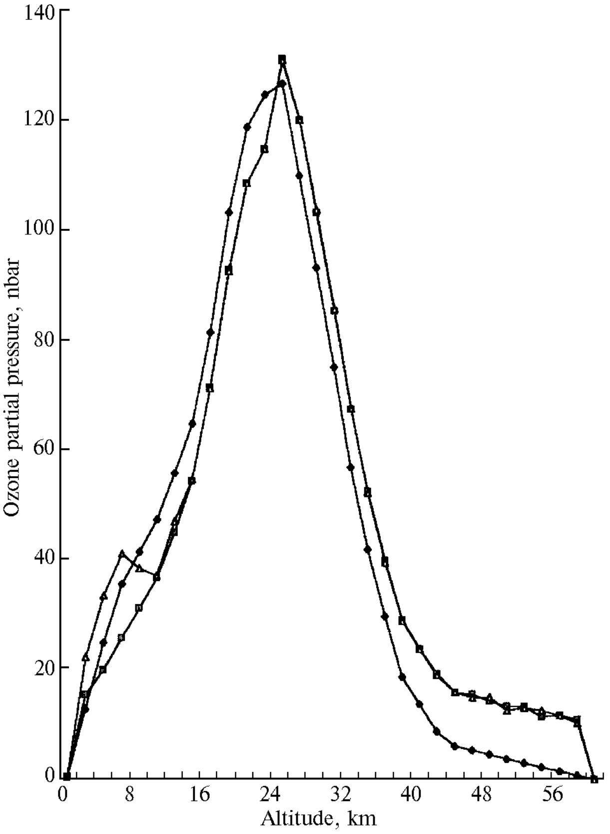

Fig. 4. Simulated VOD after three days from the data of the reference atmosphere (–∆–), profile calculated with the allowance for changes in the speed of vertical motion (— —), and mean climatic profile (–♦–).

Thus, it should be noted that the applied model adequately represents the physics of the processes. Analysis of the results obtained is indicative of a insignificant influence of the change in the speed of vertical motion and temperature in the lower and middle troposphere on the concentration and partial pressure of ozone. It demonstrated the priority of the actual VOD profile in simulation. For the further study of the problem on VOD prediction assuming different forecast range, a statistically significant number of the VOD profiles should be collected.

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