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METHOD OF DETERMINATION OF THE SOLAR RADIATION EXTINCTION BY THE OXYGEN MOLECULES IN THE ATMOSPHERE

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Abstract: *A method to compute the solar radiation extinction by the molecular oxygen in the atmosphere is developed. Absorption and single scattering towards the observer are included in the extinction model. Plane parallel, 100 km high atmosphere divided into layers with equal thickness is assumed. A computation following the "line-by-line" method is envisaged – the calculations are implemented consecutively for each rotational line from A (0,0) and b (1,0) bands of the oxygen atmospheric system.*

МЕТОД ЗА ОПРЕДЕЛЯНЕ НА ЕКСТИНКЦИЯТА НА СЛЪНЧЕВАТА РАДИАЦИЯ ОТ КИСЛОРОДНИТЕ МОЛЕКУЛИ В АТМОСФЕРАТА

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Резюме: *Развит е метод за пресмятане на екстинкцията на слънчевата радиация от молекулния кислород в атмосферата. В модела на екстинкцията са включени абсорбция и еднократно разсейване в посока към наблюдателя. Разгледана е плоска атмосфера с височина 100 км, разделена на слоеве с еднаква дебелина. Предвижда се пресмятане по метода „линия по линия", при който премятанията се извършват последователно за всяка ротационна линия от ивиците A(0,0) и b(1,0) от атмосферната система на кислорода.*

Introduction

Spectroscopic methods are a powerful tool of atmospheric research. They allow obtaining of information as for the atmospheric species concentration and for the atmospheric processes and parameters, including temperature, as well. For this purpose, in addition to spectroscopic measurements implementation, the processes in the atmosphere are to be modeled.

In this work a method to compute the solar radiation extinction in the atmosphere is developed when the solar radiation is registered at a given angle to the horizon. The term "extinction" means the light loss of a beam passing directly through the atmosphere. Two different mechanisms contribute to the extinction: absorption and scattering. In our model absorption and single scattering by the oxygen molecules towards the observer are included.

The theoretical computation of the shape and intensity of the extinction lines requires the presence of neutral atmosphere and radiation transfer models. Molecular oxygen is one of the main atmospheric constituents and this determines the major presence of its extinction bands in the observed solar spectrum. A number of computations of the oxygen absorption (e.g. in [1, 2, 3, 4]) and studies of the O_2 scattering in the atmosphere [5, 6, 7] have been implemented. The strongest absorption bands in the UV and visible spectral range are the ones of oxygen together with those of ozone and water vapour. The absorption in the visible range is strongest in the atmospheric system of O_2. In this work we examine the A(0,0) and b(1,0) bands of this system.

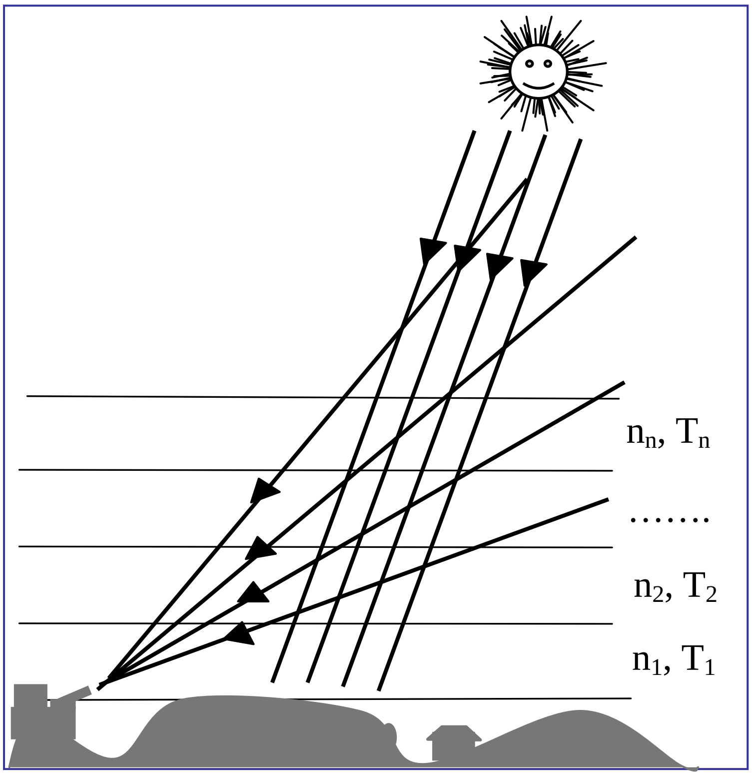

Fig. 1. Sketch of the measurement geometry (single scattering assumed) along different directions below the Sun current position. Thus the scattered light absorption under different angles towards horizon can be registered. The atmosphere is divided into ***n*** layers with equal thickness and given concentration and temperature.

Atmospheric model and geometry of the indirect measurements

In fig.1 the geometry of the measurements for which the method was developed, is shown. A plane parallel atmosphere was assumed. As upper limit the height of 100 km was taken, and above it the absorption was neglected. The atmosphere was divided into 50 parallel levels. Every level was considered as homogenous and was characterized by a single value of the parameters ***n***, ***T*** and ***p*** in the middle of the level. The concentration ***n***, the temperature ***T*** and the pressure ***p*** were determined from the used atmospheric model.

Sunlight was considered as a parallel beam. During observations under different directions below the Sun current position (different angles towards horizon) and assuming single scattering in every observation direction rays scattered at different altitudes in the atmosphere are registered.

Theory

The attenuation of the solar light in the atmosphere is due mainly to absorption and scattering. In the common case after the Bouguer law:

(1) $$I(\lambda) = I_0(\lambda)\exp(-\tau(\lambda)/\cos\theta)$$

where $I_0(\lambda)$ is the flux with wavelength λ at the upper edge of the atmosphere, $I(\lambda)$ is the flux reached the Earth (or any other considered height) , θ is the zenith angle of the Sun, and $\tau(\lambda)$ is the optical depth. It is important that $\tau(\lambda)$ can be constituted of several components and generally it is given by the expression:

(2) $$\tau(\lambda) = \tau_R(\lambda) + \tau_a(\lambda) + \tau_g(\lambda)$$

where $\tau_R(\lambda)$ is the Rayleigh optical depth, $\tau_a(\lambda)$ is the aerosol optical depth, and $\tau_g(\lambda)$ is the optical depth due to the gases absorption. Absorption optical depth at a height z is given by:

(3) $$\tau(\lambda, z) = \frac{1}{\mu}\int_z^\infty n(z')\sum_J S_J\left[T(z')\right] f\left[n(z'), T(z'), \ldots\right] dz'$$

It depends on the vertical profiles of the concentration $n(z')$ and the temperature $T(z')$, on the air mass factor μ, and on the individual rotational lines intensities $S_J(T)$ and profiles f.

The molecular Rayleigh scattering at wavelength λ is:

(4) $$I = I_0 \frac{8\pi^4\alpha^2}{\lambda^4 R^2}(1 + \cos^2\vartheta)$$

where α is the polarizability of the molecule, R is the distance to it, and ϑ is the scattering angle.

In a lot of investigations a precise estimate of the Rayleigh scattering in the Earth atmosphere is needed. For that reason the parameters, characterizing this type of scattering were well studied and defined [5]. A number of theoretical calculations [6, 7, 8] and experimental measurements [9, 10, 11, 12, 13] were published.

The Rayleigh scattering by a molecule can be defined as well by the total cross section *σ(λ)[cm2)*:

(5) $$\sigma(\lambda) = \frac{24\pi^3}{\lambda^4 N^2} \frac{(n_{(\lambda)}^2 - 1)^2}{(n_{(\lambda)}^2 + 2)^2} F_{k(\lambda)}$$

where *λ[cm]* is the wavelength, *N[cm3]* is the molecular density, $n_{(\lambda)}$ is the refractive index, and $F_{k(\lambda)}$ is the King correction factor. The factor $(n_{(\lambda)}^2 - 1)^2 \big/ (n_{(\lambda)}^2 + 2)^2$ is an effect of the local electrostatic field, known as Clausius-Mossotti or Lorentz-Lorenz factor, and it is proportional to *N*. The King correction factor is defined by:

(6) $$F_{k(\lambda)} = \frac{6 + 3\rho_n}{6 - 7\rho_n}$$

where ρ_n is the depolarization factor of the natural or non-polarized light taking into account the anisotropy of the non-spherical molecules.

Scattered light per unit volume is characterized by the coefficient of total volume Rayleigh scattering *β[cm-1].* At height *z´* it is given by the formula:

(7) $$\beta(\lambda, z') = N(z')\sigma(\lambda)$$

Then the Rayleigh optical depth at height z is defined by the integral:

(8) $$\tau(\lambda, z) = \int_z^\infty \beta(\lambda, z')dz'$$

The angular distribution of scattered light is described by the Rayleigh phase function:

(9) $$P_{ray}(\vartheta) = \frac{3}{4(1+2\gamma)}\left[(1+3\gamma) + (1-\gamma)\cos^2\vartheta\right]$$

γ is defined by

(10) $$\gamma = \frac{\rho_n}{2 - \rho_n}$$

where ρ_n is the depolarization factor.

Then the angular coefficient of volume Rayleigh scattering is:

(11) $$\beta(\vartheta, \lambda, z) = \frac{\beta(\lambda, z)}{4\pi} P_{ray}$$

Methods of computation

The principal scheme to implement the computations for the assumed atmosphere model is shown in fig.2. The observation is carried out from point *A* under angle *α* towards horizon, in direction l_1. The line of observation intersects the upper limit of the atmosphere in point L_1. The zenith angle of the Sun is *θ*, the direction to the Sun from the point of observation *A* (*l*) crosses the upper limit of the atmosphere in point *L*. All columns with section unity from point *L* to point L_1 are included in the calculations, with step *c* in horizontal direction. Their number depends on the angle of observation *α* and the step chosen for the calculations.

Let's consider such a column starting from point *B* at the upper limit of the atmosphere (fig.2). The computations can be divided into 3 principal parts: 1) calculation of the O_2 absorption from the

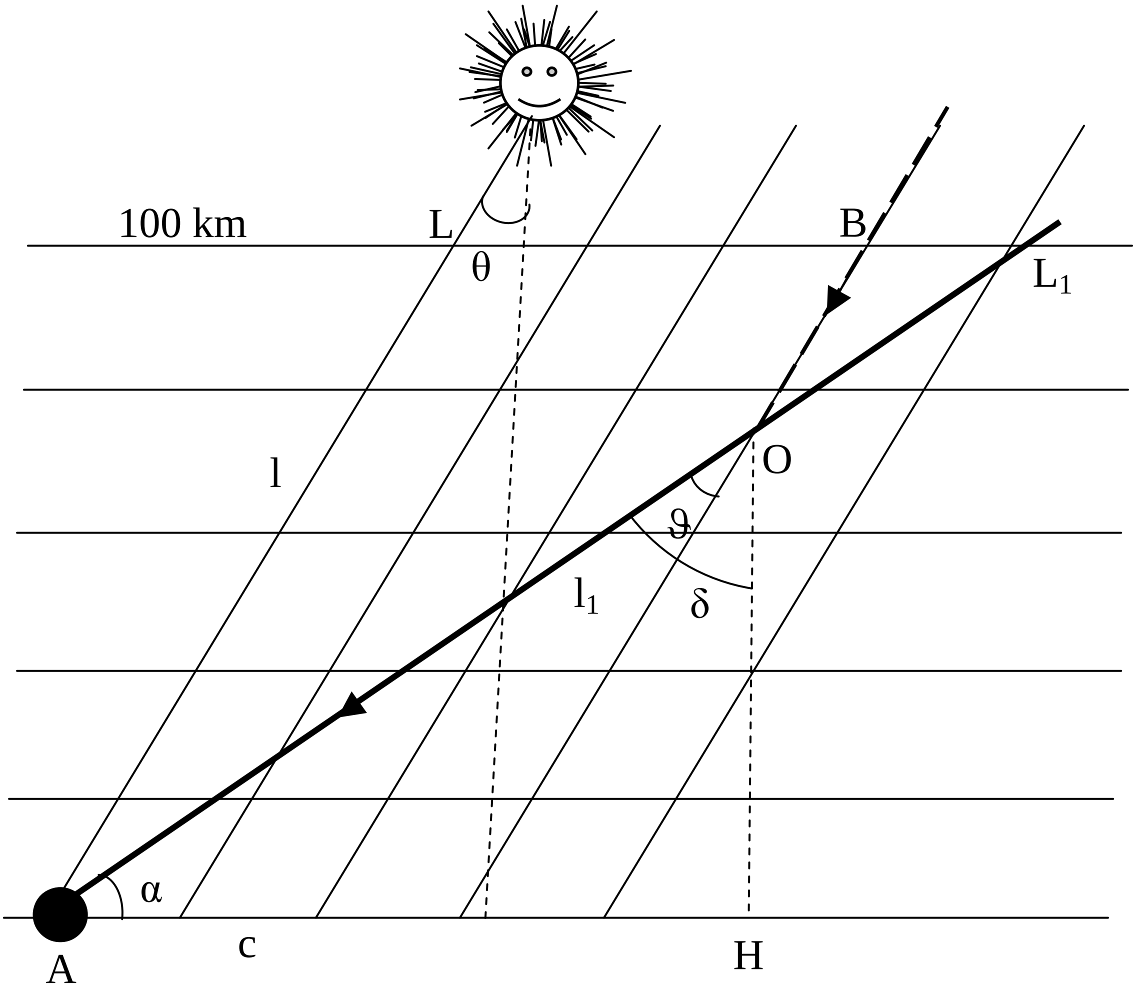

Fig. 2. Principal scheme of the O_2 extinction computations assuming observation under angle *α* towards horizon. The calculations for every considered ray are divided into 3 parts: calculation of the absorption from the upper edge of the atmosphere to the crossing point *O* of the ray with the direction of observation, single scattering in the direction of observation l_1 and absorption of the obtained radiation from that point to the Earth in the direction of observation.

upper limit of the atmosphere to point *O*, where the solar rays reach the direction of observation; 2) calculation of the single scattering of the transmitted radiation in the direction of observation; 3) calculation of the absorption of the received up to here radiation from point *O* to the observer.

Computing the O_2 absorption from the upper limit of the atmosphere to the direction of observation

The computation of the absorption from the upper limit of the atmosphere to the line of observation is carried out as for direct observation of the Sun. Detailed calculations of the A(0,0) and b(1,0) bands absorption bands from O_2 atmospheric system and plane parallel atmosphere are described in [3,14]. The absorption spectra are computed by the so-called line-by line calculations method [1]. The intensity and profile of every rotational line are determined for every specified atmospheric layer. The needed parameters for every rotational transition at standard conditions are taken from HITRAN 96 data base [15]. Temperature and concentration profiles from U.S. Standard Atmosphere 1976 are used. The computations are implemented with a step of 0.01 cm^{-1} for the intervals 12880 ÷ 13190 cm^{-1} (7580÷ 7760 Å) and 14280 ÷ 14590 cm^{-1} (6850 ÷ 7000 Å) which cover completely the spectral ranges of the bands A(0,0) and b(1,0). The water vapour absorption in the (1,0) band range can be included as well, because the O_2 and H_2O spectra are superimposed for high values of the rotational quantum number *J* [16].

Computing the single scattering of the transmitted radiation in the direction of observation

The scattering cross section computed for certain wavelengths, from 200 nm to 4000 nm was presented in tables by Bucholtz [7]. For the scattering cross section for λ>500 nm, where the examined O_2 bands lie, the following dependence on λ was obtained by the least squares method:

$$\sigma(\lambda) = A\lambda^{-(B+C\lambda+D/\lambda)} \quad (12)$$

where A=4.01061x10^{-28}, B=3.99668, C=1.10298x10^{-3}, D=2.71393x10^{-2}. Thus the scattering cross section can be obtained with an accuracy of 0.1%. The total volume Rayleigh scattering β at height $z'=OH$ is obtained by formula (7). The density at that height is defined by the used atmospheric model U.S. Standard Atmosphere 1976. The scattering in the direction of the line of observation is under angle $\vartheta = 90^\circ - \alpha - \theta$ and the angle coefficient of volume scattering is calculated by (11). The phase function is computed by (9). For γ a value obtained by linear approximation of the presented in tables in [7] values is used. For single scattering, $\tau(\vartheta,\lambda,z')=\beta(\vartheta,\lambda,z')$ is applied.

Computing the absorption after the scattering, in the direction of observation

These calculations are carried out for the layers from point *O* to point *A* as the ones in the first part. In this case the angle $\delta=\beta+\theta$ is assumed as light source zenith angle, β being the angle of scattering in the direction of observation and θ – the zenith angle of the Sun.

Conclusions

A method to compute the extinction of the solar radiation from the molecular oxygen in the Earth atmosphere is presented. The (0,0) and (1,0) bands of the atmospheric system of O_2 are envisaged. Absorption and single scattering are included in the computations and described in detail. The indispensable parameters are specified.

In a future work the program realization of the method will be completed and the results will be analyzed.

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