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Modeling 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 was developed. Absorption and single scattering towards the observer were included in the extinction model. Plane parallel, 100 km high atmosphere divided into layers with equal thickness was assumed. A computation following the "line-by-line" method was applied – the calculations were implemented consecutively for each rotational line from A (0,0) and b (1,0) bands of the oxygen atmospheric system. The radiation extinction at different angles of observation was computed and the obtained spectra were analysed.

Atmospheric model and quantities, assumed for the calculations:

- Plane-parallel atmosphere;
- Upper limit at 100 km;
- 50 parallel homogeneous layers with 2 km thickness;
- Indirect measurements;
- Line-by-line calculations;
- U.S.Standard atmosphere 1976;
- HITRAN 96 data base.

Geometry of the indirect observations



Measurementgeometry(singlescatteringassumed)alongdifferentdirectionsbelowtheSuncurrentposition.Thusthescatteredlightabsorptionunderdifferentanglestowardshorizonbe registered.

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

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

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

 $\tau_R(\lambda)$ 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:

$$\tau(\lambda, z) = \frac{1}{\mu} \int_{z} n(z') \sum_{J} S_{J}[T(z')] f[n(z'), T(z'), ...] dz'$$

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:

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

where α is the polarizability of the molecule, R is the distance to it, and ϑ is the scattering angle. The Rayleigh scattering by a molecule can be defined as well by the total cross section $\sigma(\lambda)[cm^2)$:

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

where $\lambda[cm]$ is the wavelength, $N[cm^3]$ is the molecular density, $n_{(\lambda)}$ is the refractive index, and $F_{k(\lambda)}$ is the King correction factor. The factor $(n_{(\lambda)}^2 - 1)^2 / (n_{(\lambda)}^2 + 2)^2$ 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:

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

where ρ_n is the depolarization factor of the natural or non-polarized light taking into account the anisotropy of the non-spherical molecules. The scattering cross section for λ >500 nm, where the examined O₂ bands lie, can be determined by

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

where A=4.01061x10⁻²⁸, B=3.99668, C=1.10298x10⁻³, D=2.71393x10⁻². Scattered light per unit volume is characterized by the coefficient of total volume Rayleigh scattering $\beta[cm^{-1}]$. At height z' it is given by the formula: $\beta(\lambda, z') = N(z')\sigma(\lambda)$

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

$$\tau(\lambda, z) = \int \beta(\lambda, z') dz'$$

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

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

 γ is defined by $\gamma = \frac{P_n}{2-\rho}$

where ρ_n is the depolarization factor.

 $\beta(\vartheta,\lambda,z) = \frac{\beta(\lambda,z)}{\lambda-z}$



The angular coefficient of volume Rayleigh scattering is:

Methods of computation



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 layer where the ray crosses the direction of observation l_1 (point O), absorption and single scattering in the direction of observation l_1 in

this layer and absorption of the obtained radiation from this layer to the Earth in the direction of observation under angle $\vartheta = 90^{\circ} - \alpha - \theta$.

Computation results for O₂ (0,0) band

Absorption, $\theta = 30^{\circ}$

Absorption&scattering, θ =30°, α =20°



Computation results for O₂ (0,0) band



Conclusions

- A method to compute the extinction of the solar radiation from the (0,0) and (1,0) bands of the atmospheric system of the molecular oxygen in the Earth atmosphere was developed;
- Absorption and single scattering are included in the computations and described in detail. The indispensable parameters are specified;
- The radiation extinction at different angles of observation was computed and the obtained spectra were analysed.
- The computations coincide well with the measured spectra at similar conditions;
- In the future we envisage to explore the possibility to evaluate the temperature profile based on such observations and computations.