Spectroscopic software for an SP-6 sun photometer

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A technique and a computer program have been developed for calculation of atmospheric transmission functions and parameterization of their dependences on the absorbing mass of the atmospheric gases.

Introduction

The Institute of Atmospheric Optics SB RAS is now organizing a regional automated network of SP-6(7) sun photometers for monitoring of the aerosol optical depth of the atmosphere and the total content of some gaseous constituents (H_2O, O_3, and others). The information system is an important component of this network.[1] This paper considers the spectroscopic part of the information system intended for mass calculations of atmospheric transmission functions, their parameterization, and writing this information into a specialized database. The effects of variations in meteorological parameters on the variability of the transmission function are investigated.

Effect of temperature variations on the variability of transmission functions

For solution of the inverse problem of retrieving the total content of a gas and the atmospheric transmittance due to molecular absorption from measurements of the direct solar radiation by the SP-6 radiometer, it is necessary to obtain the functional dependence of the transmittance on the absorbing mass of the gas. In addition, it is desirable that this dependence be represented by a simple parametric equation. It is well-known that the transmittance in absorption bands of atmospheric gases depends not only on the absorbing mass, but also on the vertical profiles of air pressure and temperature.[2] If the atmospheric transmittance depends significantly on these profiles for the used radiometer spectral channel, then it is quite difficult to develop a technique for retrieving the total content of a gas, because the process of measurement of the solar radiation usually is not accompanied by the measurements of temperature profiles.

It should be noted that for wide spectral intervals, which include absorption bands caused by transitions from the ground vibrational state, the atmospheric transmission functions usually have weak temperature dependence, but, nevertheless, it is necessary to carry out such studies for each spectral channel of the SP-6 radiometer. Therefore, for the parameterization of the transmission functions and the study of the effect of variations of meteorological parameters on the accuracy of the approximating equations derived, the transmission functions were calculated for different meteorological situations and solar zenith angles. The following vertical profiles of meteorological parameters were used:

1. Zonal mean AFGL meteorological models[3];
2. Data of aerological sensing of the atmosphere at Novosibirsk weather station, which include the measured pressure, temperature, and specific humidity in winter and summer months for ten years. The total number of observations is 483, in particular, 117 for winter and 366 for summer.
3. Sample of observations at Yuzhnaya weather station (Tomsk) for a year, including the measurement date and time, temperature (°C), and pressure (mm Hg) at the height of 121 m above the sea level.

Figure 1*a* shows temperature variations and Fig. 1*b* depicts variations of the water vapor concentration characteristic of summer in Novosibirsk. Figure 2*a* shows the dependence of the ratio of atmospheric transmittance in two channels of the SP-6 photometer on the absorbing mass of water vapor, calculated by the line-by-line method[4] taking into account all spectral lines in the given region, along with the two-parameter approximating equation. It can be seen from Fig. 2 that for summer and winter in Western Siberia the transmission function in the 0.94 μm spectral range is determined by the dependence on water vapor absorbing mass and almost independent of air pressure and temperature variations, what allows these channels to be used efficiently for determination of the total column water. Analogous results were obtained for SP-6 2 μm channels, which will be used to retrieve the total content of CO_2. It should be noted that the atmospheric transmittance in the 2.06 μm region revealed the dependence on air temperature. Thus, e.g., from Fig. 2*b* we can see that the atmospheric transmittance can vary by 0.01. However, our modeling showed that this error can be decreased, if we take into account the correlation between the transmittance and the surface air temperature. In this case, deviations in the transmittance were as low as 0.006. These results suggest that it is possible to determine the parametric dependence of the transmission

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function on the absorbing mass of atmospheric gases with high accuracy and to neglect variations of atmospheric profiles of meteorological parameters.

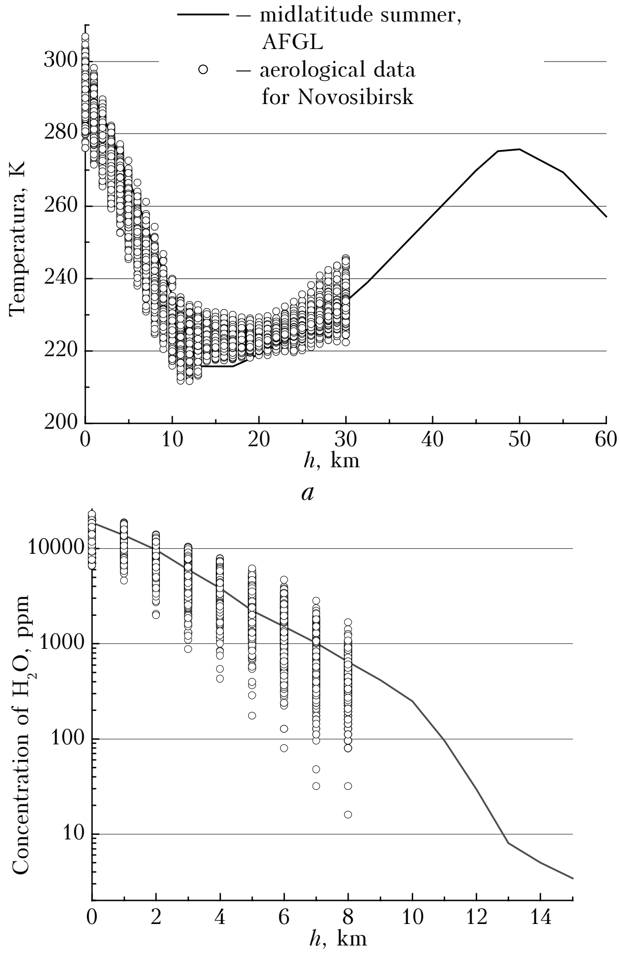

Fig. 1. Vertical profiles for summer: atmospheric temperature (*a*) and water vapor concentration (*b*).

Parameterization of the transmission function of atmospheric gases

For parameterization of the atmospheric transmission function, it is needed to pre-calculate the set of transmittance values for different solar angles and absorbing masses, which are observed in the experiments. In addition, this data set should have a representative sample for the regression method to be used for determination of the parameters. The most consistent way of obtaining such a sample is the calculation of transmission functions by the line-by-line method based on the aerological sounding data described in the previous section. However, such calculations are time-expensive even on modern computers, despite the computer program we used is one of the fastest. This circumstance is not a restriction, when scientific research is carried out, but for the sun photometer network, which is now organized in Western Siberia,[1] such calculations are to be conducted periodically for every radiometer, because interference filters can age and change their spectral characteristics with time. If we take into account that the SP-6 sun photometer has 16 spectral channels, then the time needed for calculation of the transmission functions becomes unacceptable for practice.

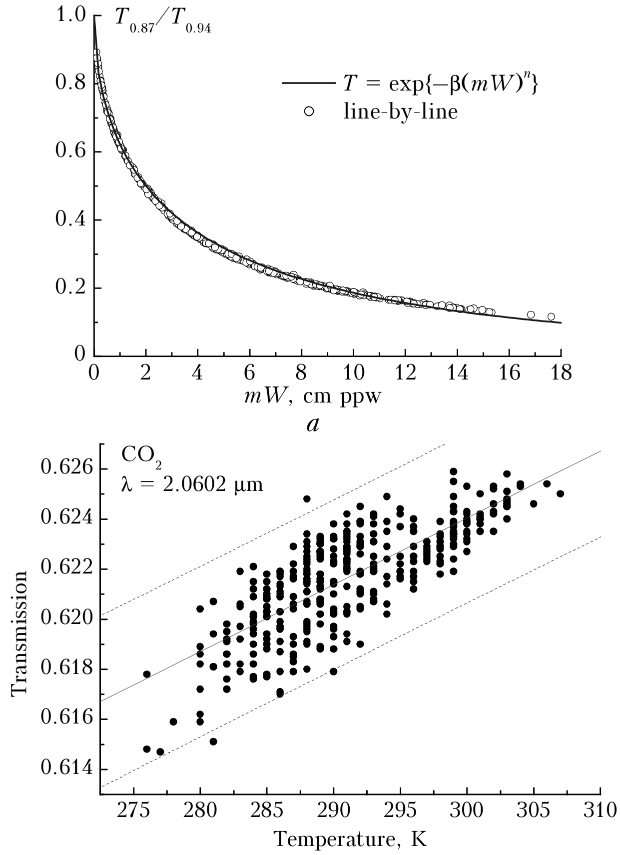

Fig. 2. Ratio of atmospheric transmittance in two SP-6 channels as a function of water vapor absorbing mass, calculated by the line-by-line method and by the approximating equation (*a*); transmittance as a function of air temperature (*b*). Temperature varies according to Fig. 1*a*; linear regression is shown by the solid line.

According to the results presented in the previous section, variations of temperature and pressure profiles have almost no effect on the variability of the transmission functions. This circumstance allowed us to develop the fast technique for calculation of the transmission functions for the sun photometers, which is based on the archive of narrow-band atmospheric transmission functions with the spectral resolution of 5 cm^{-1}, calculated by the line-by-line method with the use of the HITRAN-2000 database of spectral line parameters (http://www.hitran.com) and modern models of continuum absorption (http://rtweb.aer.com/continuum_code.html) for different solar zenith angles and four seasons (polar winter, mid-latitude winter and summer, and tropics) of the AFGL meteorological model. The initial altitude for calculation of the transmission function was set equal to 120 m – it is the height of Tomsk above the sea level. The calculations were carried out for gaseous H_2O, CO_2, O_3, CH_4, N_2O, and other absorbing gases, which were taken into account in sum. For every gas, the archive includes the value of the absorbing mass of the vertical atmospheric column. The spectral resolution of 5 cm^{-1} was selected so that it is much smaller than the spectral width of the instrumental function. The transmission function for the given spectral channel of the sun photometer was calculated as follows:

$$T(\theta,\{W_i\}_{i=1}^{6}) = \int_{\lambda_1}^{\lambda_2} F(\lambda)I_0(\lambda)\prod_{i=1}^{6} T_0(\lambda,\theta,W_i)\,d\lambda \Big/ \int_{\lambda_1}^{\lambda_2} F(\lambda)I_0(\lambda)\,d\lambda, \quad (1)$$

where T_0 is the narrowband transmission function taken from the archive at the wavelength λ with the solar zenith angle θ and the absorbing mass of the ith gas W_i; $F(\lambda)$ is the instrumental function of the considered spectral channel of the sun photometer; $I_0(\lambda)$ is the solar constant. In calculating the transmission function by Eq. (1) the approximation of the product of transmission functions, which gives good results at a moderate spectral resolution, was used. In the case of spectral averaging, which is performed by Eq. (1), the error of this approximation becomes even smaller, less than 1%, because these errors have the oscillating behavior.

To calculate the atmospheric transmission functions for the SP-6 photometers and their parameterization, a dialog computer program has been developed. This program allows an operator to perform multiversion calculations and to browse the results in the graphic mode. In processing the SP-6 measurements, it is necessary to have several types of the functional relation between the transmittance and the absorbing mass, which are given in the Table.

Approximation	Purpose
$\ln T_w = f(mW)$	Photometer calibration
$mW = f(\ln T_w)$	Calculation of water content for measurements in main radiometer channels, in which H_2O absorbs
$T_\lambda = f(\ln T_w)$	Allowance for H_2O in all other channels
$T_\lambda = f(mX)$	Allowance for O_3 and other gases

Note. $T_w = T_1/T_2$ is the ratio of transmission functions in two radiometer channels; T_λ is the transmission function in one radiometer channel; mW is the water vapor absorbing mass; mX is the absorbing mass of O_3 and other gases.

To retrieve the total content of water vapor and other greenhouse gases, the transmission function should be parameterized so that the absorbing mass is one of the explicit parameters and the number of parameters is minimum with the acceptable accuracy of the approximation. For approximating the tabulated dependences, an operator has an optimal set of equations, which are presented below.

1. Dependence of the transmission function on the absorbing mass of one gas for a particular filter is described in three ways:

$$\text{a) } y_i = a_0 + a_1\exp(a_2x_i) + a_3\exp(a_4x_i); \quad (2)$$

$$\text{b) } y_i = a_0 + a_1\exp(a_2x_i); \quad (3)$$

$$\text{c) } y_i = \exp(a_0x^{a_1}), \quad (4)$$

where y_i are the transmittance values at the given values of the absorbing mass x_i ($x_i = m_iW$), $m_i = 1/\cos\theta_i$ is the optical mass for the zenith angle θ_i. The absorbing mass is measured in cm ppw (precipitable water) for water vapor and in atm·cm for other gases.

2. The dependence of water vapor absorbing mass mW on the ratio of atmospheric transmission functions (T_1/T_2) for two channels of the photometer is described by the equations:

a) direct dependence for calculation of the atmospheric water content

$$mW = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4,$$

where

$$x = \ln(T_1/T_2); \quad (5)$$

b) inverse dependence for calibration of the photometer–hygrometer

$$y = a_0 + a_1x^{a_2},$$

where

$$y = \ln(T_1/T_2),\ x = mW. \quad (6)$$

3. Dependence of the water vapor transmission function T_3 on the ratio of the transmission functions T_1/T_2, where T_1, T_2, and T_3 are calculated taking into account three different spectral filters of the sun photometer:

$$y = y_0 + a_1\exp(-(x - x_0)/t_1) + a_2\exp(-(x - x_0)/t_2), \quad (7)$$

where $y = T_3$; $x = T_1/T_2$; y_0, x_0, a_1, a_2, t_1, t_2 are the parameters of fitting.

The operator can select the needed approximation, then the calculation is performed and the parameters of the transmission function are displayed along with the mean sum of squared deviations, the maximum absolute error, and the maximum relative error, based on which the operator can judge on the quality of the parameters obtained.

For illustration, we present below the results of simulation for the 0.87, 0.94, and 1.047 μm spectral channels of the SP-6 sun photometer. Figure 3 depicts the dependence of the transmission function at $\lambda = 0.94$ μm on the water vapor absorbing mass with the use of different approximating equations.

The best result was achieved when using Eq. (2): the mean sum of the squared deviations $S/n = 6.93 \cdot 10^{-7}$ (where n is the number of transmission functions in the calculated sample, $n = 200$), the maximum absolute error of $1.45 \cdot 10^{-3}$, and the maximum relative error of 0.28%. Hereinafter the parameters of the functional dependence of transmittance on the absorbing mass were determined with the aid of the Marquardt least-squares method.[5]

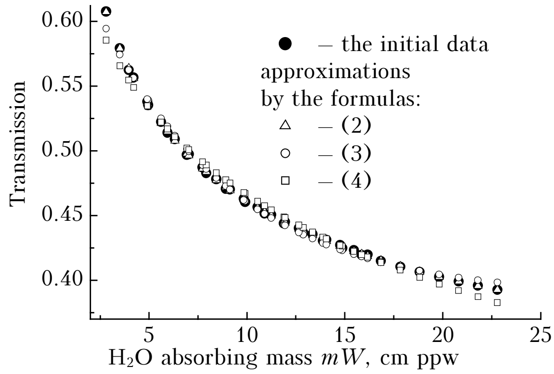

Fig. 3. Atmospheric transmission function vs. the absorbing mass mW at the wavelength of 0.94 μm; meteorological conditions: mid-latitudinal summer and tropics.

The simulation was carried out for two spectral channels of the SP-6 photometer: at 0.87 and 0.94 μm wavelengths. The considered range of variations of the water vapor absorbing mass is characteristic of meteorological models of mid-latitudinal summer and tropics. In approximating by Eq. (5), the mean sum of squared deviations was $S/n = 1.14 \cdot 10^{-2}$, the maximum absolute error was 0.22, and the maximum relative error was 2.4%. In approximating by Eq. (6), the mean sum of squared deviations was $S/n = 2.65 \cdot 10^{-5}$, the maximum absolute error was 0.014, and the maximum relative error was 3%. The error of approximation can be decreased considerably, if we take a narrower range of mW variations, for example, calculate the transmission functions only for the mid-latitudinal summer. In this case, the maximum relative error of approximation by Eq. (5) was as low as 0.9%, and that in the case of approximation by Eq. (6) was 1.5%.

The dependence of the transmission function T_3 for the wavelength of 1.047 μm on the transmittance ratio T_1/T_2 (for the wavelengths of 0.94 and 0.87 μm) is well described by Eq. (7). For this case, the maximum absolute error was 0.0004, and the maximum relative error was 0.014%.

Conclusions

The parameterization of the dependence of the transmission function on the absorbing masses of atmospheric gases has been carried out for the spectral channels of the SP-6 photometers. It has been shown that the parameters of the transmission function weakly depend on temperature variations in the entire atmospheric column and on variations of the surface air pressure. The technique and the computer program have been developed for calculation and parameterization of the bandpass transmission functions caused by the absorption by atmospheric gases in the spectral range of 0.4–5 μm. This program allows fast calculations of broadband transmission functions to be made with the allowance for the spectrophotometer instrumental function and different meteorological conditions and solar zenith angles.

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