Determination of the column water vapor from sun photometer measurements

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A method of column water vapor reconstruction from photometric measurements of direct solar radiation is presented. The effect of spectroscopic errors on the accuracy of reconstructing the columnar water vapor amount is estimated. Different methods for processing the data of observations are discussed. The results on the reconstructed column water vapor are compared with the data obtained with a CE-318 photometer that is being operated at the IAO SB RAS as a part of AERONET project.

Introduction

Water vapor is the most important gas component that determines radiative transfer and participates in the formation of the Earth's weather and climate. That is why so much attention is paid to the development of new and improvement of the existing methods of determining the atmospheric moisture content. Optical methods have a lot of advantages over the contact methods of meteorological sounding. Those advantages are the responsiveness, the possibility of measuring integral characteristics, relatively low cost of equipment, etc. Starting from the works by Fowle, Zuev, and Komarov,^{1,2,11} many reserachers use measurement data on the direct solar radiation in the water vapor absorption bands in order to determine the columnar water vapor amount.

As a rule, some models of bands are used to obtain a functional dependence of the atmospheric transmission caused by molecular absorption, on column water vapor. We know several modifications of such approximations. Gates and Harrop³ used one of the Goody's model modifications in the form of transmission function as a square root of column water vapor. To caluclate the transmission function, they used LOWTRAN software package.

Tomasi et al.⁴ divided the changes of the absorbing mass into three intervals: 0.4-1, 1-3, $3-6.1 \text{ g/cm}^2$. In the first interval, the transmission function depends on the absorbing mass to the power of 0.9, in the second one the power is 0.75, and in the last one it is 0.5. Transmission functions were calculated using the LOWTRAN program package.

According to the estimates given by Reagan et al.,⁵ this method can be used in retrieval of column water vapor with the error $\leq 10\%$ as compared to the radiosensing data. The main disadvantage of the model representation of absorption bands is that they give a somewhat idealized description of the absorption spectrum and, as a concenquence, may lead to errors. According to our estimates, with these models daily

behavior of column water vapor can be different. The line-by-line calculations of molecular absorption characteristics provide a higher accuracy. This is proved by the measurements of direct solar radiation performed with a Fourier spectrometer in spectral regions of 0.77 to $1.10 \,\mu\text{m}$ (Ref. 6) and $0.55-0.71 \,\mu\text{m}$ (Ref. 7).

The procedure of photometer calibration is as a rule done by the slow Bouguer method, where it is supposed that the atmosphere keeps stable for the whole measurement period. To find the calibration constant, usually the least-squares method is used,¹² which supposes that only a measurable characteristic has a random normally distributed error, and in factors (arguments of the function to be minimized) there are no errors. Violation of these conditions can yield bias of the estimates of the calibration constant and column water vapor.

Detected signal of sun photometer depends not only on the concentration of the absorbing gases, but also on the distribution of temperature and pressure over the beam propagation path, as well as on the presence of clouds and aerosol, etc. For example, Thome et al.¹² noted that the use of spectral channels centered at 0.87 and 0.94 μ m can bring about noticeable errors in determination of column water vapor. In view of the aforesaid, we need such a calibration procedure, which would allow us to minimize the possible errors including those conditioned by parameterization of the transmission function.

This work aims at improvement of the method of the column water vapor retrieval from the measurement data acquired with sun photometers that are being developed at the Institute of Atmospheric Optics SB RAS. To implement it, we needed to obtain a functional dependence of the atmospheric transmission within the photometer channels on the absorbing water vapor mass, to develop the technique of determining the calibration constant, estimate the column water vapor retrieval errors caused by variations of vertical temperature profiles and surface pressures, by errors in the spectral line parameters, and by errors coming from assignment of the instrumental function, etc.

Description of sun photometer

A detailed description of sun photometers (SP-4m, SP-6) can be found in papers by Kabanov, Sakerin et al.,^{8,9} so we limit our consideration to just their brief overview.

Photometers consist of two separate cableconnected parts. An optical-electronic unit on the X-Y (azimuth/zenith) positioner is set outside. A power supply, a remote control unit, and a computer are indoor. The optoelectronics unit of SP-4m device includes two measurement channels: a short-wave and a long-wave channel. The SP-6 photometer has also a UV channel (0.306–0.37 μ m). Measuring complexes also involve a light sensor (a usual photodiode with a scattering attachment) used for automatic activation of the photometer Sun-tracking system when the Sun is not covered by clouds.

The main technical characteristics of SP-4m, whose measurement data were used for calculating the results we present here, are summarized in the Table.

Technique of calculation and parameterization of the atmospheric transmission functions for an SP-4m sun photometer

To solve the inverse problem on the columnar gas content retrieval using data acquired with an SP-4m photometer of direct solar radiation, we need to know the functional dependence of transmission on the absorbing gas mass. Thus, we performed calculations of the transmission functions by a direct method for different solar zenith angles and different meteorological situations that take place in Western Siberia. In simulations, we have found out that the transmission function in the spectral region around 0.94 and 0.87 µm depends on the absorbing mass of water vapor and is almost independent of the variations of temperature and air pressure.¹⁴ Our estimates show that the error of the optical thickness is caused by fluctuations of meteorological parameters $\Delta \tau / \tau \sim 1\%$ (where $\tau = -\ln(T_{0.94}/T_{0.87})$, $T_{0.94}$ and $T_{0.87}$ stand for the atmospheric transmission in spectral channels of 0.94 and $0.87 \mu m$, respectively). This fact has enabled us to develop an effective method of calculating transmission functions.¹⁴ It is based on the archive of the narrow-band functions of atmospheric transmission with spectral resolution of 5 cm^{-1} , calculated by the direct method with the use of 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 zenith angles and four seasons (polar winter, mid-latitude winter and summer, tropics) of the AFGL model. In calculating transmission function the initial altitude was set at 120 m, which corresponds to the elevation of Tomsk above sea level. We set spectral resolution 5 cm^{-1} to make it much smaller than the spectral width of the instrumental function. The transmission function for the specified spectral channel (within the region of $\lambda_1 - \lambda_2$) of the sun photometer was calculated as follows:

$$T(\theta, \{W_i\}_{i=1}^0) =$$

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

where $T_0(\lambda, \theta, W_i)$ is the value of the narrow-band transmission function, which was taken from the archive for the wavelength λ , solar zenith angle θ , and the absorbing *i*th gas mass W_i (with the total of six gases considered); $F(\lambda)$ is the instrumental function of the considered spectral channel of the sun photometer; $I_0(\lambda)$ is the solar constant. In Eq. (1),

Characteristic	Short-wave channel	Long-wave channel
Central observation angle, degrees	1.38	1.48
Number of wavelengths	10	4
Light filter transmission band maxima, µm	0.371; 0.408;	1.246; 1.557;
	0.438; 0.475;	2.20; 3.97
	0.500; 0.547;	
	0.675; 0.871;	
	0.938; 1.052	
Bandpass transmission filter half-width, nm	5-12	15 - 40
Type of photodetector	FD-24k	MG-32
Photometry error, %	0.3	0.7
Sun tracking error, degrees	0.2	
Spectrum measurement duration (1 drum rev.), s	5	
Range of pointing angles (zenith \times azimuth), degrees	90×300	
Thermostat temperature, °C	32 ± 0.3	
Range of ambient temperatures, °C	from -50 to 35	
Total photometer weight (estimated), kg	30	
Considered characteristics (range/error):		
aerosol optical thickness;	0-1/0.01	
atmospheric water vapor content, g/cm^2 ;	0-6/0.07	
direct, total, scattered radiation, W/m^2	0-1500/6%	

Characteristics of the SP-4m sun photometer (Ref. 8)

for the calculation of transmission functions we used the approximation of the transmission function product, which at a mean spectral resolution gives good results. Moreover, at averaging over the spectrum, which is done in Eq. (1), the error of this approximation decreases further and becomes lower than 1% because these errors are oscillating.

Because there is now a new version of HITRAN-2004 database,¹⁶ we have performed test calculations for these two spectral channels, which have demonstrated that the transmissions calculated using the new database version and those calculated using the version of the year 2000 are actually identical. So, we did not do any recalculations of the narrow-band functions. However, to estimate the calculation error for transmission functions, we used HITRAN-2004, where the spectral line error data are more adequate. To obtain such estimates, we calculated the transmission functions with those values of line halfwidths and intensities, which are given in the database. Then, for every spectral line, we increased its intensity by the error value and calculated again. For halfwidths, we performed the same calculations. Finally, we obtained the range of the spectroscopic error $\Delta \tau / \tau \sim 2 - 3\%$. Note that this value is overstated. This is because all the line intensities were simultaneously increased, i.e., this error is a systematic one. Another limiting case is when all the errors are random. Firsov et al.¹⁵ showed that in this situation, for the transmission function with resolution lower than 5 cm^{-1} the errors are negligibly small.

In calculations of transmission function, we needed to take into account spectral dependence of the instrumental function, which was a convolution of spectral dependences of the interference filter transmittance, receiver sensitivity, and transmittance of the sun photometer window. These spectral dependences of the window and the optical filter were experimentally recorded with an SF-46 spectrometer, whose error in determining the wavelength is ≤ 0.5 nm, and the measurement error in transmission does not exceed 1%.

Thus, the calculation errors of transmission function for the photometer channels used in sensing of the column water vapor are due to:

1) spectroscopic error $\Delta \tau / \tau \sim 2-3\%$,

2) the error that comes from fluctuations of meteorological parameters $\Delta \tau / \tau \sim 1\%$,

3) the error of spectral transmittance of optical filter $\Delta T \sim 1\%$.

If we assume that these errors are non-correlated, then the total error in τ will not exceed 3–4%. To solve an inverse problem of the column water vapor retrieval and photometer calibration, we needed to obtain a parametric dependence of the transmission function on the absorbing mass. One of the most common ways was to use band models, when transmission ratio in photometer channels is approximated as follows:

$$T_{0.94} / T_{0.87} = e^{-(\alpha + \beta (mW_0)^n)},$$
 (2)

where W_0 is the absorbing mass of the vertical atmospheric column (cm ppw); *m* is the optical mass, which for small zenith angles θ is expressed by the formula $m = 1/\cos\theta$; *n*, α , and β are the model parameters found via adjustment to the calculated transmission function. The equations like Eq. (2) are convenient, because they allow us to apply linear regression in calibration. For the case of n = 0.5, we used linear regression to determine the model parameters $\alpha = 0.01634 \pm 0.00606$, $\beta = 0.47626 \pm 0.00241$.

Figure 1 shows the results of line-by-line calculation and calculation by Eq. (2), wherefrom it follows that the approximation error at large and medium absorbing masses reaches 5%, and at low masses it can be as large as 10%. Since the optical thickness and the absorbing mass are related by a square root relation, then the error in the column water vapor retrieval will, respectively, reach 10 and 20% just because of parameterization.

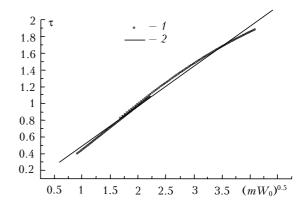
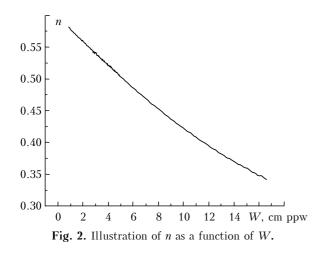


Fig. 1. Optical thickness as a function of the columnar water vapor amount in the Earth's atmosphere: transmission functions are calculated using the fast method for the midlatitude summer and winter (the AFGL meteorological model, ¹⁰ $W_0 = 0.82$ cm ppw for winter and $W_0 = 2.81$ cm ppw for summer, while *m* varied from 1 to 5.85) (*1*); approximation of τ by Eq. (2) (2).

It is clear that this approximation is not effective. But other approximation techniques, when the parameter α is set zero and *n* and β are varied, do not give good results either.

Our simulation showed that approximation (2) is correct, if *n* is made dependent on the absorbing mass *W*, i.e., if the optical thickness is approximated by the expression $\tau = \beta W^n$, where *n* is variable. The value of *n* is easy to find using the formula $n = d(\ln \tau)/(dW)$. Figure 2 illustrates the dependence of *n* on *W*. Here we see that *n* varies from 0.35 to 0.6 for the summer and winter conditions of the AFGL model. If we calculate it for the polar and tropical latitudes, the range will be wider. From the aforesaid, it becomes clear why approximation (2) is so ineffective.



That is why we decided to use an implicit dependence of τ on $W = mW_0$, though it complicates the calibration procedure, because linear regression is no more applicable.

Calibration of the SP-4m photometer and retrieval of the atmospheric water vapor content

To determine the calibration constant, we minimized the following functional:

$$\sum_{i} \left(m_{i} W_{0} - \tau^{-1} (\ln(S_{0.94} / S_{0.87})_{i} - \ln C) \right)^{2} w_{i} \to \min, \quad (3)$$

where *i* is the experiment number; w_i is the weighting function.

This functional was obtained with the following transformations. The ratio of the signals $S_{0.94}/S_{0.87}$, if we neglect molecular and aerosol scattering in two photometer channels at the wavelengths of 0.94 and 0.87 µm, is determined by the equation

$$S_{0.94} / S_{0.87} = C \exp[-\tau(mW_0)].$$
 (4)

Then

$$mW_0 = \tau^{-1} (\ln(S_{0.94} / S_{0.87}) - \ln C).$$
 (5)

Where τ^{-1} is the function inverse to τ .

For the weighting function we used $w = 1/\tau^2$.

This form of the functional allowed us to avoid many problems that are typically connected with the use of linear regression:

1) the use of an implicit function $\tau(W)$ excluded the errors connected with parameterization of transmission function;

2) the errors in coefficients are minimized, for the error in the signals is small;

3) introduction of the weighting function allowed us to reduce the weight of those errors which arise at large zenith angles.

Now, there remains only one problem: W_0 is a non-stationary quantity and it can vary considerably

within a day. We know¹³ that in summer distribution of the atmospheric humidity is close to lognormal. Besides, we can observe a daily behavior of W_0 . So, to estimate the influence of these factors on the calibration constant C, we performed numerical simulation, for which we set a linear trend $W_0 = W_{00} + k(m - m_0)$, while W_{00} was varied as a lognormal quantity using the random number generator. Using AERONET data in analysis of the column water vapor we used in simulation the following values of the parameters: $W_{00} = 1.8$, the variation coefficient of W_{00} was 0; 3; 5%, $m_0 = 1.2$, i.e. m varied within 1.2–5.7, which corresponded to photometer measurement range, and k assumed the values of ± 0.02 ; ± 0.03 ; ± 0.04 .

In the simulation, we found that with the trend growth (the coefficient k was positive) there was a growth in the calibration constant (up to 5–6%), while with reduction of the trend, the constant decreased approximately by the same value. Introduction of a random component lognormally distributed with the variation coefficient 5% did not result in any considerable changes in the calibration constant, and the error did not exceed 1%.

For photometer calibration, we used the results of measurements on July 4, 2003, from 6:00 to 16:00 and August 28, 2004, from 6:00 to 13:00. From Eq. (3) we obtained the calibration constant C = 1.37. The column water vapor was retrieved by the direct method with and without regard to molecular scattering using the equation

$$W = \frac{1}{m} \left[\frac{\ln \left(C \frac{S_{0.94}}{S_{0.87}} \right) + m\Delta \tau}{\beta} \right]^{\frac{1}{n}},$$

where $\Delta \tau$ determines the contribution of molecular and aerosol scattering. Transmission ratio at the two wavelengths gives a non-compensated value for molecular scattering: $\tau_{0.94} - \tau_{0.87} = -0.005m$ (at $\Delta \tau = 0$ molecular scattering was neglected).

The simulation showed that the retrieved value of column water vapor slightly varies if we take into account molecular scattering (Figs. 3 and 4). Dependence of the aerosol extinction on the wavelength can be approximated by the Angström formula $\tau \sim \lambda^{-\delta}$, where δ is the Angström parameter, whose typical values lie within the interval from 0.5 to 1.5. When this parameter has its maximum value, we observe the largest error $\tau_{0.94} - \tau_{0.87} = -0.11 \tau_{0.87} m$. By setting a typical value of 0.03 of the aerosol optical thickness at a 0.87 μ m wavelength⁵ it is easy to obtain the estimate $\tau_{0.94} - \tau_{0.87} = -0.003m$. This value is 1.5 times smaller than the contribution of molecular scattering. That is why at this stage, we neglected aerosol scattering. However, in the future we are going to consider it via measurements in the spectral channels in the regions of 0.53 and 1.06 μ m.

 $W_{\rm H_2O}$, cm ppw 1.2 08.28.04 AERONET Without the account of scattering With the account of 1 molecular scattering 0.8 14 16 6 8 10 12 Time, h

Fig. 3. Retrieval of the water vapor amount in a vertical atmospheric column using the sun photometer SP-4m and the photometer CE-318 of AERONET (2004).

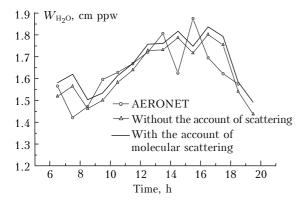


Fig. 4. Comparison of the absorbing mass of water vapor averaged over August 2004 and retrieved by direct method with the AERONET data.

The results of retrieving the columnar water vapor amount are presented in Fig. 3. Figure 4 shows comparison of the absorbing water vapor mass averaged over the values of August 2004 with the AERONET data (http://www.aeronet.gsfc.nasa.gov).

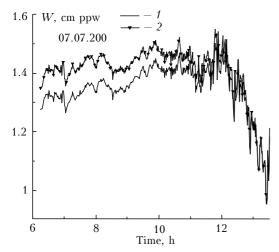


Fig. 5. Comparison of the column water vapor retrieved from the SP-4m data using different techniques of inverse problem solution: implicit dependence of transmission on the absorption mass (1); a common parameterization method of transmission function of the type $T = \exp(-(\alpha + \beta W^{0.5}))$ (2).

As is seen from Fig. 3, at small zenith angles, the value of $W_{\rm H_{2O}}$ is in a good agreement with the AERONET data. But at large zenith angles we observe a divergence, which grows with the growth of the zenith angle.

In conclusion, to demonstrate the boundedness of the band models, we compared the column water vapor retrieved with the use of the technique described in this paper with that obtained using the approximation of transmission function (2). From the results shown in Fig. 5, with the growth of the solar zenith angle, Eq. (2) overstates the columnar water vapor amount.

Conclusions

1. The analysis we have performed shows that HITRAN database allows a high-precision calculation of the functional dependence of transmission on the absorbing mass. The estimates show that a typical model error does not exceed ~ 2-3% of the optical thickness which leads to the error in the columnar water vapor amount of no more than 5%.

2. It has been demonstrated that fluctuations of meteoparameters (temperature and pressure) for summer and winter conditions do not result in significant changes of the atmospheric transmission functions.

3. The use of an implicit dependence of the transmission function on the column water vapor allows us to simplify the calibration procedure and avoid the errors connected with parameterization of transmission function.

4. Comparison of the retrieved value of water vapor shows a good agreement with the AERONET data.

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