Atmospheric Water Vapor Amounts Retrieved from GOME Satellite Data

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Abstract
A new method for the retrieval of global atmospheric vertical column amounts of water vapor from measurements of the Global Ozone Monitoring Experiment (GOME) is presented. The method is based on a modified Differential Optical Absorption Spectroscopy (DOAS) approach, taking into account the effects arising from strong wavelength dependent absorptions. In this paper the feasibility of this approach is demonstrated and first estimates on the retrieval precision and the accuracy of the H₂O data product are given by comparison with selected Special Sensor Microwave Imager (SSM/I) data.
1. Introduction

The accurate assessment of the impact of present and future anthropogenic pollution and natural phenomena on the atmosphere and the climate-chemistry coupling requires a detailed global knowledge of the temporal and spatial behavior of atmospheric constituents. Water vapor (H\textsubscript{2}O) is one of the most abundant atmospheric gases. More than 90% of water vapor is located in the troposphere where it significantly contributes to atmospheric chemistry and of course to the weather and climate [IPCC, 1996].

Currently, global water vapor concentrations are estimated from satellite-based measurements in the infrared for example with the TIROS-N Operational Vertical Sounder (TOVS) and in the microwave spectral region for example with the Special Sensor Microwave Imager (SSMI) in combination with in situ radio sonde measurements [Chaboureau et al., 1998, and references therein].

In this study it is demonstrated that potentially important additional global information on water vapor can be derived from measurements of the Global Ozone Monitoring Experiment (GOME). The latter has been operating successfully on the ERS-2 satellite since its launch in April 1995. The GOME instrument is a grating spectrometer measuring solar irradiance and earthshine radiances between 240 and 800 nm at a spectral resolution between 0.15 and 0.35 nm. Measurements are performed in nadir viewing geometry with a typical spatial resolution being 320×40 km\textsuperscript{2}. As its name implies, GOME was designed primarily for the determination of global distributions of O\textsubscript{3} and NO\textsubscript{2}, but column amounts of several other atmospheric constituents, for example Br\textsubscript{2}, OC\textsubscript{2}O\textsubscript{5}, SO\textsubscript{2}, HCHO [Burrows et al., 1999, and references therein], have been derived from the data.

In this study an algorithm to retrieve H\textsubscript{2}O vertical column amounts from GOME measurements in the wavelength region around 700 nm is described and a validation for cloud free maritime data is presented.

2. Retrieval Method

2.1. Modified DOAS Approach

The retrieval of vertical H\textsubscript{2}O column amounts is based on the Differential Optical Absorption Spectroscopy (DOAS) approach which was originally developed for ground based long path observations, but has proven to be suitable for ground-based zenith and space-based nadir measurements as well [Burrows et al., 1999, and references therein].

One important and defining assumption of the DOAS technique is that the relative depth of an absorption feature is linearly proportional to the amount of the absorbing species integrated along the light path. This is true for weak absorptions. However, the H\textsubscript{2}O absorption in the spectral region around 700 nm has individual features which are much narrower than the GOME spectral resolution and may be saturated in the Earth’s atmosphere. Thus the measured differential absorption features are nonlinearly dependent on the H\textsubscript{2}O amount and vertical distribution.

To make optimal use of the better signal-to-noise ratio of spectral regions with strong absorption, it is necessary to account for this saturation effect in the retrieval. In this sense an approach for the H\textsubscript{2}O retrieval, similar to the one applied to ground-based occultation measurements by sun photometers operating in the 940 nm band [Halthore et al., 1997], has been selected. The following nonlinear relationship between the slant optical depth \( \tau_{H_2O} \) due to H\textsubscript{2}O absorption and the vertical column amount \( C_V \) is assumed:

\[
\tau_{H_2O}(\lambda) = c(\lambda)C_V^{b(\lambda)}.
\]

(1)

The parameters \( c \) and \( b \) depend on wavelength \( \lambda \), observational geometry (predominantly solar zenith angle), spectral resolution, and atmospheric properties. This approach assumes implicitly that \( c \) and \( b \) do not depend on the total vertical column density. The parameter \( c \) comprises the air mass factor and the differential absorption cross sections for the respective atmospheric temperatures and pressures averaged along the light path, whereas \( b \) is a parameterization of the saturation, where \( b \leq 1 \). The parameters \( b \) and \( c \) are obtained from radiative transfer calculations. The atmospheric conditions during the measurement usually differ from those used for the radiative transfer calculations, for example in pressure, temperature, aerosol loading, cloud coverage, and albedo. This potential error source for the air mass factors can be accounted for by using the atmospheric oxygen (O\textsubscript{2}) absorption, which is measured in the same GOME channel.

Extending the DOAS technique to take into account the above results in the following equation:

\[
\ln \left( \frac{I(\lambda)}{I_0(\lambda)} \right) = P(\lambda) - A \left( \tau_{O_2}(\lambda) + c(\lambda)C_V^{b(\lambda)} \right)
\]

(2)

\( I \) and \( I_0 \) are the earthshine radiance and the solar irradiance, respectively, both measured by GOME. \( P \) is a polynomial taking into account all broadband spectral features. \( \tau_{O_2} \) is the O\textsubscript{2} slant optical depth. \( A \)
is a wavelength-independent correction factor, which compensates for incorrect air mass factors. As a first order approximation, it is assumed that the air mass correction factor for both O$_2$ and H$_2$O is identical in spectral regions, where these absorbers have similar absorption strength and the wavelength distance between their absorption features is small. As can be seen from the slant optical depth shown in Figure 1, this is fulfilled for the spectral window between 685 and 710 nm, which has been selected in this study for this reason.

For a given set of parameters $b$, $c$, and $\tau_{O_2}$, the H$_2$O vertical column is retrieved from (2) by a non-linear fitting procedure. The fit parameters are the polynomial coefficients, $A$, and $C_V$. To correct for small differences in the wavelength scale of reference spectra and measurements, two additional parameters describing the relative spectral shift and squeeze are taken into account.

### 2.2. Determination of Parameters $b$, $c$, and $\tau_{O_2}$

The first step in the determination of $b$ and $c$ is the derivation of the slant optical depth $\tau_{H_2O}$. For a given scenario, two radiative transfer calculations are performed: one for an atmosphere which contains H$_2$O and one without H$_2$O. Then $\tau_{H_2O}$ is given by:

$$\tau_{H_2O}(\lambda) = \ln \left( \frac{I_{\text{without}}(\lambda)}{I_{\text{with}}(\lambda)} \right)$$  \hspace{1cm} (3)

By taking the logarithm of (1) a linear relation between the logarithms of the vertical column density and the slant optical depth is obtained:

$$\ln \tau_{H_2O}(\lambda) = \ln c(\lambda) + b(\lambda) \ln C_V$$  \hspace{1cm} (4)

Varying the vertical column density and computing the corresponding slant optical depths yields a set of $C_V$ and $\tau_{H_2O}$ values from which $b$ and $c$ are determined for each wavelength by using a linear regression. To retrieve parameters, which are specific for a given model atmosphere, the shape of the water vapor profile is kept constant in this process. This is achieved by scaling the assumed H$_2$O profile of the model atmosphere by factors from 0.2 to 1 without changing the other atmospheric parameters.

The parameter $\tau_{O_2}$ is computed from

$$\tau_{O_2} := -\ln \left( \frac{I_{\text{without}}(\lambda)}{I_0(\lambda)} \right)$$  \hspace{1cm} (5)

using $I_{\text{without}}$ for the appropriate scenario. Note that this quantity differs from the O$_2$ slant optical depth by a broadband contribution which is taken into account by the polynomial $P$ in (2).

In this study, all radiative transfer calculations are performed with GOMETRAN [Rozanov et al., 1997; Buchwitz et al., 1998] in the wavelength range between 685 and 710 nm. The simulated spectra are computed at a spectral resolution of 0.05 nm and then convolved to the GOME spectral resolution (about 0.35 nm in this spectral range). Parameter sets of $\tau_{O_2}$, $b$ and $c$ are computed for solar zenith angles between 0° and 80° and the six LOWTRAN [Anderson et al., 1995] reference atmospheres (tropical, mid-latitude summer/winter, sub-arctic summer/winter, and 1976 US standard atmosphere). GOMETRAN calculations are performed in multiple scattering mode, assuming no clouds/precipitation and no aerosols. The surface albedo is set to 0.05, which is representative of ocean scenes.

### 3. Results

#### 3.1. Algorithm Verification

The water vapor retrieval algorithm has been successfully verified by the use of synthetic radiance data. In all cases, the input vertical water vapor columns could be reproduced within 0.6% provided the appropriate reference atmosphere was selected. This supports the parameterization (1). However, choosing a wrong reference atmosphere may produce significant deviations between the retrieved and the reference H$_2$O vertical column. The largest discrepancies occur when a parameter set based on a reference atmosphere with a small H$_2$O column is applied to a spectrum which corresponds to a large H$_2$O amount. In this case an underestimation of the column density of up to 50% may occur. This is most likely due to the fact that an extrapolation of H$_2$O amounts may produce unphysical results such as relative humidities larger than 100%. Using a parameter set for a high reference H$_2$O column is less critical; in this case deviations are typically <10%.

For the use of the retrieval algorithm with real measurements, the selection of an appropriate model atmosphere is thus of crucial importance. The following procedure is used. For each of the six reference atmospheres, a retrieval is performed. The result which has the smallest residual, that is, the one which reproduces the measurements best, and for which the retrieved column does not exceed the column of the
reference atmosphere is selected. Performing the retrieval for each reference atmosphere is not the most efficient method from a computation time point of view, but it is adequate for the present study, as it succeeds in selecting the proper reference atmosphere for each of the simulated spectra. Other, more sophisticated algorithms will be subject to future investigations.

The largest H₂O column of the six reference atmospheres used is 4.1 g/cm² (in the tropical case). This currently limits the applicability of the algorithm to the retrieval of columns, which are smaller than this value. An extension of the atmospheric data base is required to cover regions having higher H₂O column amounts, but this is not a general constrain of this method.

3.2. Comparison with SSM/I Results

As a result of the limited availability of appropriate in situ measurements, a comparison with other satellite remote sensing data is most appropriate to assess the quality of the GOME water vapor retrieval algorithm. The spatial and temporal coverage of such data is generally more optimal for comparison than sonde measurements. Therefore GOME total water vapor columns are compared with daily gridded Integrated Water Vapor (IWV) data produced by the Global Hydrology Resource Center (GHRC), which have a spatial resolution of 0.5° × 0.5°. These IWV data are based on measurements of the Special Sensor Microwave Imager (SSM/I) from the Defense Meteorological Satellite Program (DMSP) F-14 satellite. Data are available on a global scale but as a result of limitations of this retrieval method only above the ocean. For further information the reader is referred to the GHRC web site (http://ghrc.msfc.nasa.gov).

For the comparison a SSM/I water vapor data set obtained during the descending orbits on 14 June 1998 was arbitrarily selected. For each GOME ground pixel the average of all SSM/I data covering the same area was computed. The data set was further reduced by only considering GOME pixels with a cloud fraction less than 0.1. Furthermore, no data with a H₂O column amount larger than 4.1 g/cm² were used. This leaves approximately 800 GOME measurements for which the total water vapor column has been retrieved and compared with the corresponding SSM/I data.

In Figure 2 a typical result of the water vapor retrieval algorithm is given. The top part of the figure shows the logarithm of the ratio of the GOME measured earthshine radiance and extraterrestrial irradiance and the corresponding result of the fit. The retrieved H₂O vertical column of 3.75 g/cm² is only slightly smaller than the corresponding SSM/I result of 3.79 g/cm². The residual, i.e. the difference between the two curves of the upper plot, is shown in the bottom part of the figure. This residual can be interpreted as a slant optical depth and is in the order of 0.02. This is at least one magnitude larger than the expected instrumental noise level. Comparing results of several retrievals reveals systematic structures in the residuals. This indicates that the fit may possibly be improved by introducing improved line parameters and additional model atmospheres.

The results for the complete data set are compared in Figure 3. Good agreement between GOME and SSM/I total water vapor columns is obtained. Fitting a straight line to the data reveals a negligible bias and a small underestimation of the SSM/I columns <3%. The scatter of the data is about 18%. This is larger than the statistical error of approximately 4% arising from averaging several SSM/I measurements over one GOME ground pixel. However, taking into account that SSM/I measurements show a scatter of up to 20% when compared with radio sonde data (Chaboureau et al., 1998), the SSM/I and GOME results agree within the accuracy of SSM/I. Therefore most of the scatter is attributed to atmospheric variations over the GOME ground pixel.

4. Summary and Conclusions

For the first time vertical H₂O column amounts have been determined from GOME measurements. These columns are in good agreement with SSM/I results. Thus a new global water vapor data set can be generated from GOME measurements, which is expected to have a high precision, because it is derived directly from atmospheric absorption measurements. This is of great importance not only for users of other GOME data products but also for numerical weather prediction and global atmospheric models, which aim to predict the future climate.

Several improvements of the retrieval algorithm are being developed. These include the optimization of the fitting window and the extension of the atmospheric data base to large H₂O column amounts. The applicability and accuracy of the retrieval algorithm for measurements over land and for partially cloudy scenes will be investigated in a subsequent study. In addition, the sensitivity of the retrieval to different
H₂O profile shapes has to be investigated further. This may be used to derive information about the vertical distribution of water vapor.

Acknowledgments. GOME data are provided by ESA. SSM/I data have been obtained from the Global Hydrology Resource Center (GHRC). Part of this work was funded by the BMBF under grant 07 UF 12/8 and the University of Bremen.

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Received February 12, 1999; revised April 23, 1999; accepted April 28, 1999.

This preprint was prepared with AGU's LATEX macros v4.
Figure 1. Slant optical depths at GOME spectral resolution of H\textsubscript{2}O (solid line) and O\textsubscript{2} (dashed line) for a tropical atmosphere and a solar zenith angle of 40°.

Figure 2. Example of water vapor retrieval for a GOME measurement located at (8°S, 80°E) in the tropics for a solar zenith angle of 38.9°. Top: The logarithm of the ratio of the earthshine radiance and extraterrestrial irradiance, measured by GOME, and the fit result. Bottom: Resulting residual (GOME measurements – Fit).

Figure 3. Correlation of GOME and SSM/I total water vapor columns. The dotted curve shows the result of fitting a straight line to the data.