Support to H_2O column retrieval algorithms for GOME-2

O3M-SAF Visiting Scientist Activity

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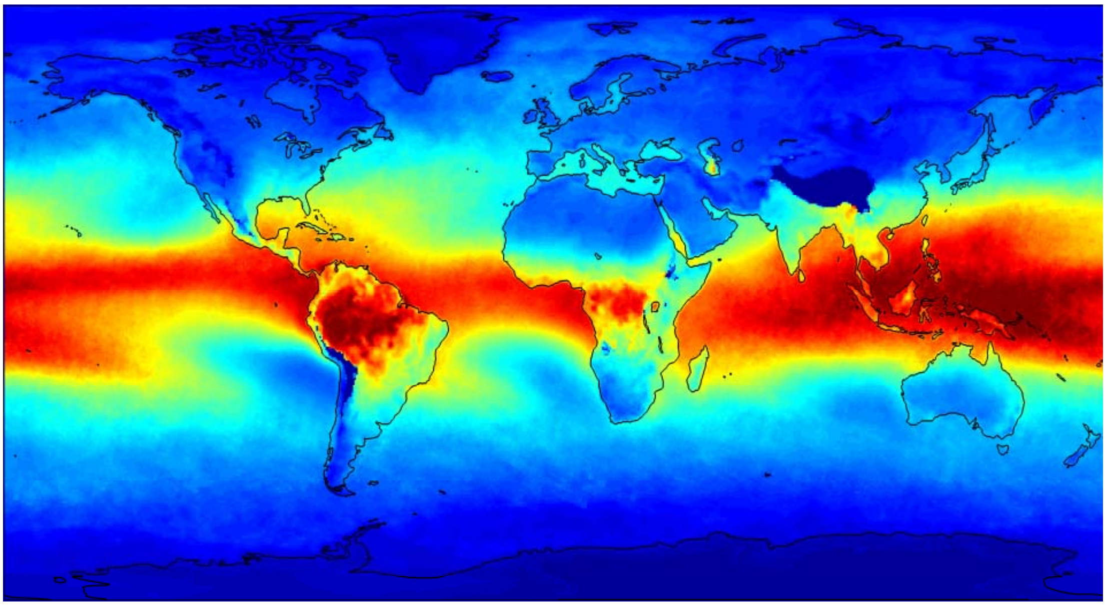

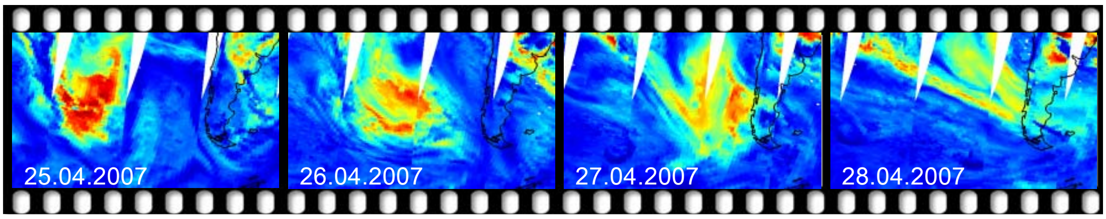

Content

Overview

This report provides an overview on the most important retrieval settings and achievements during the project. More detailed information can be found in the following documents:
a) Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, Minor Trace Gases, and Cloud Properties (ATBD, 2011)
b) GOME-2 H2O total column validation report (Kalakoski et al., 2011)
which can be found at the DLR GOME-2 documentation web site: http://atmos.caf.dlr.de/gome2/documentation.html.

H_2O columns have been retrieved from ERS-2 GOME and ENVISAT SCIAMACHY instruments by various groups using different settings (Noël et al., 1999, 2002, 2004, 2008; Mieruch et al., 2008; Casadio et al., 2000; Maurellis et al., 2000; Lang et al., 2003; 2004; Lang, 2003; Wagner et al., 2003, 2005, 2006).
These algorithms differ not only in the used wavelength ranges, but also in the complexity of the retrievals. Most of the algorithms make use of simultaneously retrieved O_2 or O_4 absorptions to correct for the influence of clouds.
The GOME-2 water vapor retrieval described in this document analyses the H_2O and O_2 absorptions in the red spectral range (614-683nm). This water vapor product was developed with the aim to study time series and temporal trends of the atmospheric water vapor content with high accuracy. Thus no a-priori information or information from external data sets is included in our algorithm.
The fitting parameters used for the processing of GOME-2 spectra are based on those used for the analysis of GOME-1 observations [Wagner et al., 2003; 2005; 2006]. In the chosen spectral range, medium strong absorption lines of H_2O (around 650nm) and O_2 (around 630nm) exist.

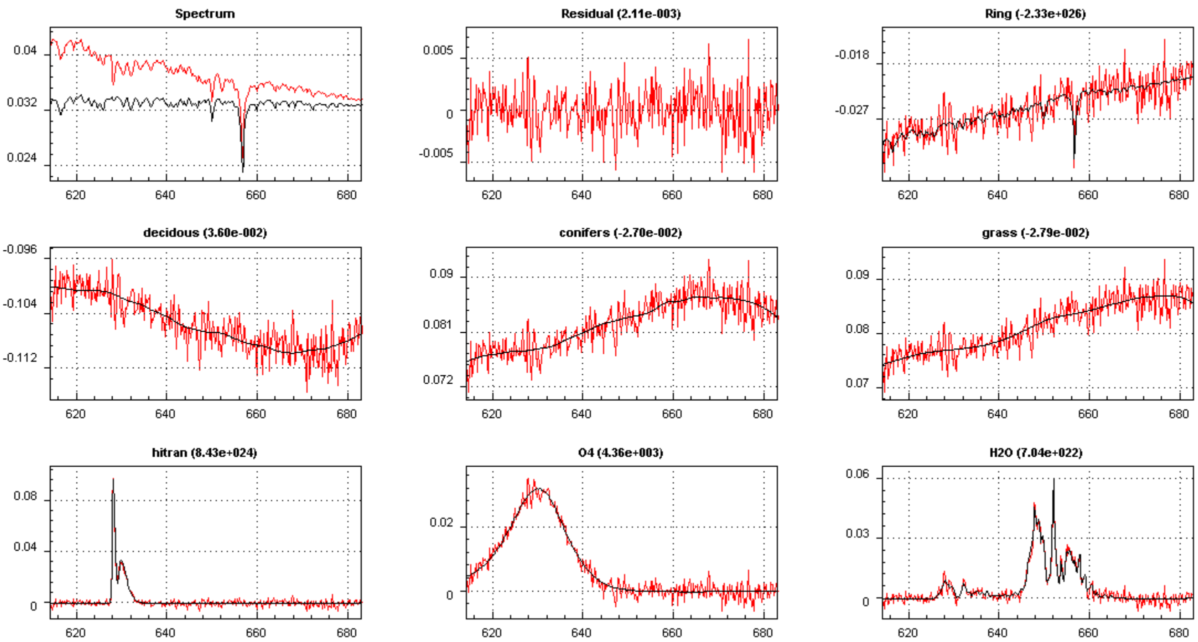

Fig. 1 Example of a spectral DOAS analysis. Displayed are the fitted reference spectra (black lines) scaled to the respective spectral structures in the measured spectrum (red).

Table 1. DOAS settings used for H_2O spectral retrieval

Property	Selected parameter	Remarks
Fitting interval	614-683.2nm nm	
Sun reference	Sun irradiance	
Wavelength calibration	Wavelength calibration of sun reference optimized by NLLS adjustment on convolved Kurucz solar spectrum[1].	
Absorption cross-sections		
H_2O	HITRAN 2006 (Rothmann et al.)	290K, convoluted with wavelength dependent instrument function
O_2	HITRAN 2004 (Rothmann et al.)	290K, convoluted with wavelength dependent instrument function
O_4	Greenblatt et al., 1990	Interpolated
Additional spectra		
Ring spectrum	Synthetic Ring spectrum calculated from sun spectrum using the MFC software (Gomer et al., 1993)	
Conifers	ASTER Spectral Library through the courtesy of the Jet Propulsion Laboratory, California Institute of Technology, http://speclib.jpl.nasa.gov/	Logarithm, interpolated
Grass	ASTER Spectral Library through the courtesy of the Jet Propulsion Laboratory, California Institute of Technology, http://speclib.jpl.nasa.gov/	Logarithm, interpolated
Decidous	ASTER Spectral Library through the courtesy of the Jet Propulsion Laboratory, California Institute of Technology, http://speclib.jpl.nasa.gov/	Logarithm, interpolated
Polynomial	4^{rd} order (5 parameters)	
Intensity offset correction	Inverse solar spectrum[2]	

[1]Kurucz, R.L., I. Furenlid, J. Brault, and L. Testerman, Solar flux atlas from 296 nm to 1300 nm, *National Solar Observatory Atlas No. 1*, 1984.
[2]from solar spectrum

Besides the trace gas reference spectra, also several other spectra are included in the fitting process. First, a synthetic Ring spectrum to correct for the so called Ring effect caused by inelastic Raman scattering on air molecules. In addition, also three reference spectra for different vegetation types are included: Especially over surfaces with strong vegetation, it turned out that spectral features caused by vegetation show strong interference with the atmospheric absorbers [Wagner et al., 2007]. Also an inverse solar spectrum is included to correct for possible intensity offsets, e.g. caused by instrumental straylight. The parameters for the spectral analysis are summarized in Table 1. An example of the spectral DOAS analysis is shown in Fig. 1. The absorption structures of O_2, H_2O and O_4 are clearly visible. From the spectral retrieval, also the fitting errors are determined.

In the initial phase of the project, the retrieval settings and the prepared reference spectra (see Table 1) were delivered to DLR Oberpfaffenhofen. The implementation in the DLR processor was supported and several details of the procedure (e.g. wavelength calibration) were clarified. Eventually, effectively perfect agreement between the results of our retrieval and the DLR processor was achieved.

Improvement with respect to original algorithm

During the implementation and validation it turned out that several improvements of the original algorithm were necessary. The first improvement was the explicit consideration of the wavelength dependence of the spectral resolution. In channel 4 of the GOME-2 instrument the spectral resolution decreases substantially towards small wavelengths. In particular at the O_2 absorption band (around 630nm) it is 0.54 (FWHM), while at the H_2O absorption band (around 650nm) it is only about 0.51nm. In the updated version of the H_2O retrieval, the spectral resolution is determined as function of wavelength and is used in this way for the convolution of the trace gas reference spectra.
The second improvement was the use of a global albedo map instead of using only one albedo value as in the original retrieval. This turned out to be important because the relative sensitivity of the measured O_2 absorption compared to the H_2O absorption can become quite different for different values of the surface albedo. This leads to a systematic overestimation of the H_2O VCD over regions with high surface albedo (e.g. deserts). In the updated version of the algorithm monthly albedo maps derived from SCIAMACHY and GOME-1 measurements were used (Fig. 2). The respective correction function (Fig. 3) was determined from radiative transfer simulations (Fig. 3).

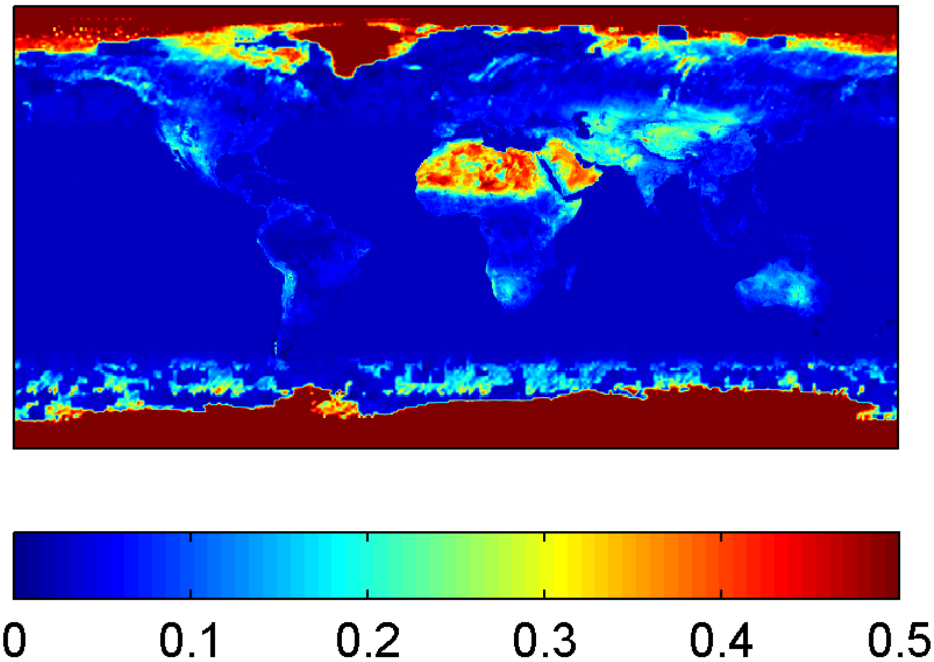

Fig. 2 Surface albedo used for the H_2O retrieval (July). For low and mid latitudes, the surface albedo retrieved from SCIAMACHY PMD measurements were used (Grzegorski, 2009). For high latitudes, the GOME albedo data set from Koelemeijer et al. (2003) was used, because it also takes into account the snow and ice coverage.

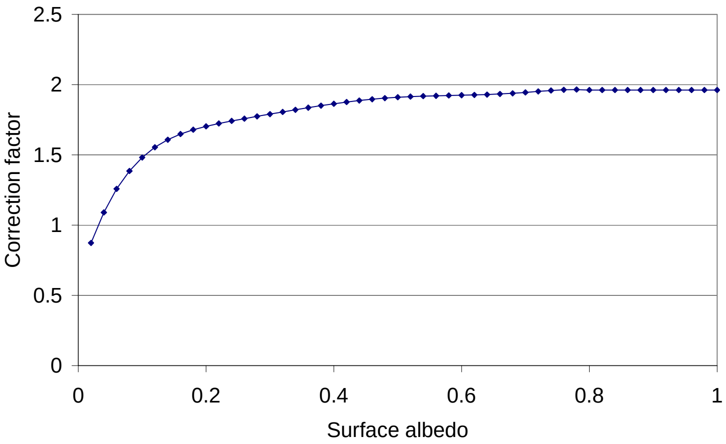

Fig. 3 Correction function taking into account the influence of the surface albedo. The H_2O VCDs of the original algorithm are divided by this function.

Another (and connected) improvement was the implementation of a line of sight dependent correction. The GOME-2 instrument has a much wider swath compared to GOME-1 and SCIAMACHY. Thus the dependence of the albedo correction had explicitly to be considered for the GOME-2 H_2O retrieval. The respective correction factors (Fig. 4) were determined by radiative transfer simulations. The correction factors and the correction procedure were sent to DLR and were successfully implemented in their system.

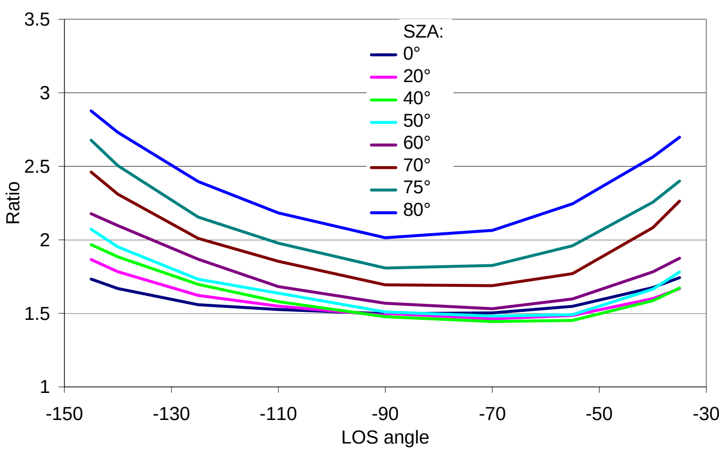

Fig. 4 Dependence of the correction factor on the line of sight (LOS) angle of the satellite instrument for different solar zenith angles. Here only values for a relative azimuth angle of zero are shown for simplicity. In the retrieval, however, the actual relative azimuth angle of individual measurements is taken into account. Note that for SCIAMACHY (and GOME-1), only LOS between about –120 and –60° occur. Larger deviations of the LOS angles from -90° occur for GOME-2.

Finally, a detailed error estimate was developed and implemented. Since our H_2O data product is not based on explicit radiative transfer calculations for individual measurements, a straightforward estimation of the product uncertainty is not possible. Instead, the influence of the main error sources is estimated. The uncertainty of the final product depends mainly on the following parameters:

• the fit error of H_2O
• the fit error of O_2
• general uncertainties of the spectral retrieval, e.g. related to uncertainties of the spectroscopic data.
• uncertainties related to radiative transfer effects, especially due to clouds.

The first two terms are simply determined from the spectral retrieval. For the third term, an overall value of 10% is used, which mainly represents the uncertainties of the spectral data for H_2O and O_2. For the fourth term, an empirical formula taking into account the measured O_2 SCD is used:

$$err_{RTM} = (SCD_{O2,meas} - SCD_{O2,max}(SZA)*1.16)/2 \cdot 10^{25} molec/cm^2$$

This error increases with decreasing O_2 SCD (indicating strong cloud shielding). From sensitivity studies (e.g. Wagner et al., 2005, 2006) it was shown that for measurements with low O_2 SCDs the retrieved H_2O VCDs systematically underestimate the true H_2O VCD.
The total (relative) error is derived from the individual error terms by the following formula:

$$err_{rel,total} = \sqrt{fit_{H2O}^{\ 2} + fit_{O2}^{\ 2} + 0.1^2 + err_{RTM}^{\ 2}}$$

Validation

We compared the GOME-2 water vapor columns to three different data sets: Radio sondes, SCIAMACHY observations and SSM/I observations. Each of these data sets has its own advantages and disadvantages. From the different comparisons, different properties of the GOME-2 data set can be studied: The comparison of GOME-2 water vapor VCDs versus radio sonde data yields mainly information over land, but also some data over ocean are available. The comparison of the GOME-2 water vapor VCDs versus SCIAMACHY observations is possible over land and ocean with similar coverage. The comparison of the GOME-2 water vapor columns versus SSM/I observation is restricted to measurements over the ocean.
In the following, the main findings from the different comparison studies are summarised. More details can be found in validation document (Kalakoski et al., 2011).
From the comparison with radio sondes, a mean positive bias of 1.1 kg/m2 (6.1% of mean sonde data) is found, with a standard deviation of ~6 kg/m2. The correlation coefficient between both data sets is 0.92. The bias of the GOME-2 water vapor columns depends on surface albedo: Positive biases are found for low surface albedo and negative biases are found for high surface albedo. In general, the bias increases strongly for SZA > 80±. Also a seasonal dependence of the bias was found with the highest values in the winter hemispheres. The seasonal dependence is probably related to changes in the SZA, surface albedo and cloud cover.
From the comparison with SCIAMACHY data, overall a good consistency is found (also with GOME-1). One important (and expected) result of this comparison is that sampling effects have a great influence on the comparison results: if only collocated measurements are compared, the standard deviation decreases from 4.37 to 2.27 kg/m2, and the mean difference decreases from -1.11 to -0.01 kg/m2. It was also found that the bias between GOME-2 data and SCIAMACHY depends on latitude, with higher biases in the southern hemisphere. The effects of the differences in spatial and spectral resolution are small.
From the comparison with SSM/I data it was found that GOME-2 H_2O columns are in general larger than the SSM/I data: from correlation analyses, slopes between 1.05 and 1.10 kg/m2 and biases between 1.7 and 2.0 kg/m2 were found, with a standard deviation of ~5 kg/m2, for

global averages. These findings are in good agreement with the validation results based on radio sondes. The comparison between GOME-2 and SSM/I data also revealed systematic spatial patterns of the differences with negative biases over regions with low clouds. For one month in northern summer (July 2007), particular high biases at high latitudes were found. The reasons for these high biases are not yet clear.
Based on the validation with ground-based measurements, we conclude that the current GOME-2 OTO/H2O product fulfils the user requirements in terms of accuracy for most conditions (especially for climatologically relevant averaged data), as stated in the Product Requirements Document (target accuracy: 25%; threshold accuracy: 10%).

Documentation

The algorithm and its implementation is described in the Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, Minor Trace Gases, and Cloud Properties (ATBD, 2011).
The Validation is described in detail in the GOME-2 H2O total column validation report (Kalakoski et al., 2011).
Both documents are available from the official O3M SAF site
http://o3msaf.fmi.fi/products/ouv.html and the DLR GOME-2 documentation web site:
http://atmos.caf.dlr.de/gome2/documentation.html.

Future improvements.

The GOME-2 OTO/H2O product was developed to fulfil the needs of the climate community; the rather simple and robust retrieval does not rely on explicit a-priori assumptions and additional information. These restrictions may cause relatively high uncertainties for individual observations and for specific measurement conditions. While this product is well suited for trend analyses (and other ‘relative’ comparison studies like e.g. the effect of ENSO), the rather high uncertainties of individual measurements might limit its use for other applications. It is thus recommended to develop a second H_2O product from UV/vis sensors, which explicitly takes into account a-priori information, e.g. a latitudinal and seasonal (or even daily) varying H_2O profile. Also cloud information (at least cloud fraction and cloud top height) for individual observations should be considered.

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