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Description of the AMC-DOAS algorithm

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1 Introduction

This document describes the Air Mass Corrected Differential Optical Absorption Spectroscopy (AMC-DOAS) algorithm used for the retrieval of total water vapour columns from measurements of the Global Ozone Monitoring Experiment (GOME, see e.g. *Burrows et al.* [1999]) and the Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY, see e.g. *Bovensmann et al.* [1999]).

2 Inversion algorithm

The AMC-DOAS algorithm [*Noël et al.*, 1999] is based on the well-known Differential Optical Absorption Spectroscopy (DOAS) approach [*Burrows et al.*, 1999; *Perner and Platt*, 1979] which has been modified to handle effects arising from the strong differential absorption structures of water vapour.

The general features of this modified DOAS method are that

1. saturation effects arising from highly structured differential spectral features which are not resolved by the measuring instrument are accounted for, and
2. O_2 absorption features are fitted in combination with H_2O to determine a so-called air mass factor (AMF) correction which compensates to some degree for insufficient knowledge of the background atmospheric and topographic characteristics, like surface elevation and clouds.

The main equation of the Air Mass Corrected DOAS method is given by:

$$\ln\left(\frac{I}{I_0}\right) = P - a\ \left(\tau_{\mathrm{O}_2} + c\, C_V^b\right) \tag{1}$$

I and I_0 are the measured Earthshine radiance and solar irradiance, respectively. As in standard DOAS, all broadband contributions (resulting e.g. from Rayleigh and Mie scattering or surface albedo) are approximated by a polynomial (P).

The term τ_{O_2} denotes the O_2 optical depth. C_V is the vertical column amount of water vapour, b and c are spectral quantities describing the saturation effect and the absorption. Especially, c contains the effective reference absorption cross section and the air mass factor. The scalar parameter a is the above mentioned AMF correction factor. The quantities τ_{O_2}, b, and c are determined from radiative transfer calculations performed for different atmospheric conditions and solar zenith angles (see section 3). C_V and a

are then derived from a non-linear fit. The error of the vertical column is calculated from the covariance matrix also resulting from the fit. A typical fit result is shown in Fig. 1.

The AMC-DOAS method is applied to the spectral region between 688 nm and 700 nm because both O_2 and water vapour absorb in this region. They are the main absorbers in this spectral range, having slant optical depths of similar strength (see Fig. 2).

The main purpose of the AMF correction factor is to correct the retrieved water vapour column, but beside this the AMF correction factor can be used as an inherent quality check for the retrieved data. The AMC-DOAS retrieval assumes a cloud-free tropical background atmosphere and does not consider different surface elevations. If the derived AMF correction is too large, this is an indication that these assumptions are not valid (most likely because the observed scene is too cloudy or contains a high mountain area). Experience has shown that retrieved water vapour columns for an AMF correction factor of 0.8 or higher are reliable; only these data are distributed.

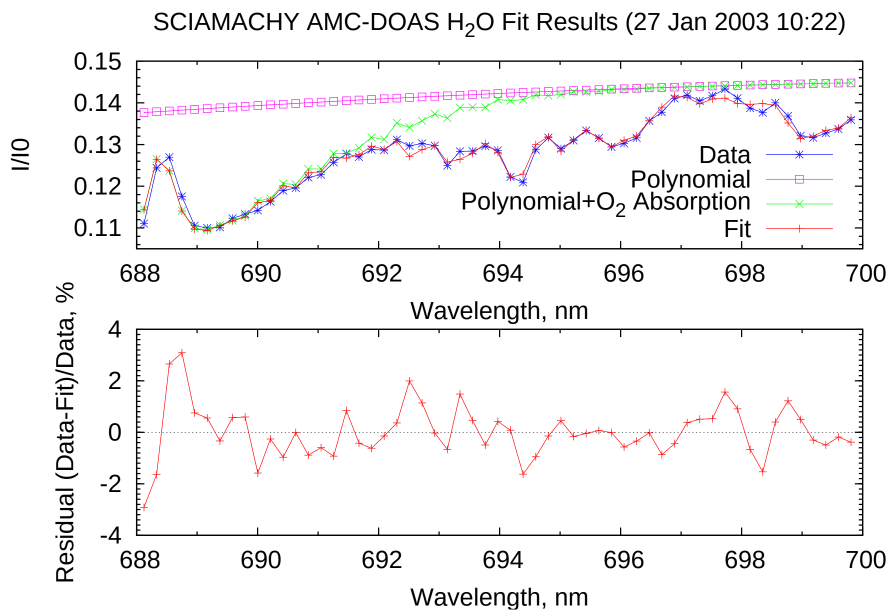

Figure 1: Example for AMC-DOAS fit results. Top: Spectral fit. Bottom: Residual

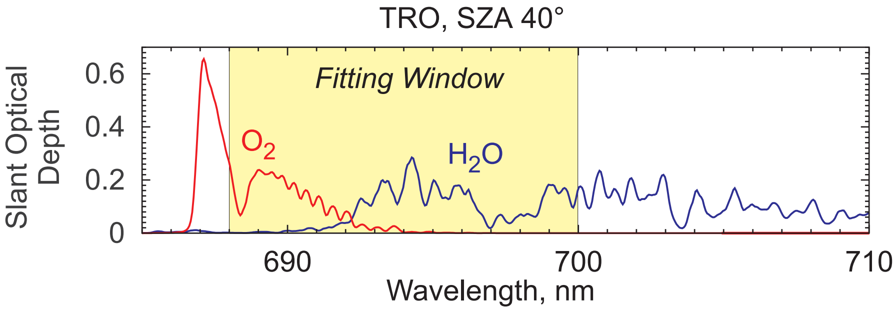

Figure 2: Typical slant optical depths of water vapour and O_2 in the spectral region around the AMC-DOAS fitting window.

3 Forward model and data bases

The parameters τ_{O_2}, b, and c are spectral quantities which are taken from a pre-calculated data base. This data base has been derived using the radiative transfer model (RTM) SCIATRAN [see e.g. *Rozanov et al.*, 2002] as a forward model. The term τ_{O_2} is determined using radiative transfer calculations with and without O_2. The parameters b and c are determined from radiative transfer calculations assuming different water vapour columns C_V [see *Noël et al.*, 1999, for further details].

The spectra for b, c and τ_{O_2} have been calculated for a set of solar zenith angles (SZAs), namely 0°, 20°, 40°, 50°, 60°, 70°, 80°, 85°, and 88°. Based on this data set the b, c and τ_{O_2} spectra are then interpolated during the retrieval for the actual SZA. 88° is therefore the maximum SZA for which the retrieval produces reliable results.

The following assumptions have been made for the radiative transfer calculations:

- tropical background atmosphere (MODTRAN profile)
- no clouds
- surface elevation 0 km

An example for b, c and τ_{O_2} is shown in Fig. 3.

Deviations of the real conditions from these assumptions are handled via the retrieved AMF correction factor a.

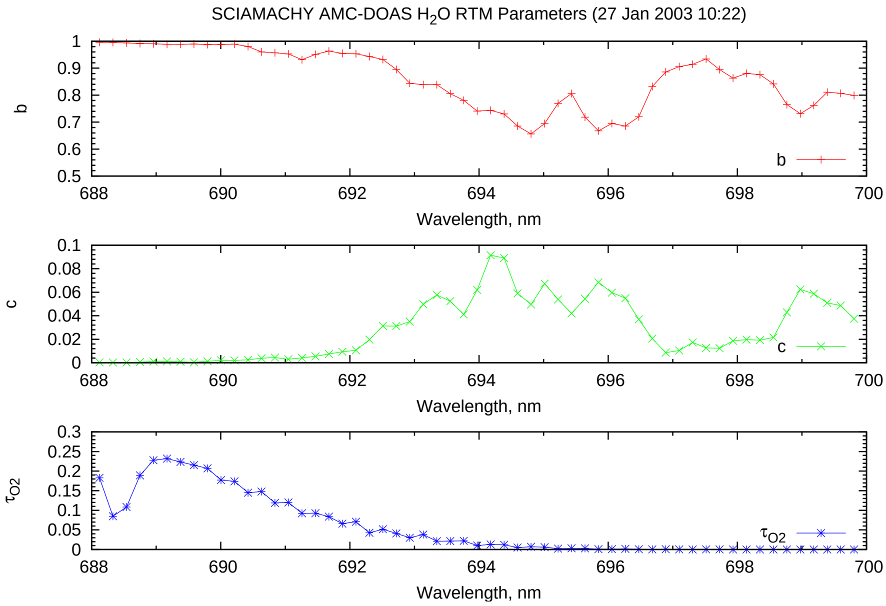

Figure 3: Example for RTM parameters b, c and τ_{O_2}.

4 Auxilliary data

Except for the RTM data base described in section 3, the AMC-DOAS method does not rely on any other external data, e.g. calibration factors derived from comparisons with ground based radio sonde measurements as it is the case for e.g. Special Sensor Microwave Imager (SSM/I) data. The retrieved water vapour columns therefore provide a completely independent data set.

5 Sensitivity, error analysis and validation

GOME and SCIAMACHY water vapour data retrieved using the AMC-DOAS method have been compared with SSM/I measurements and model data from the European Centre for Medium-Range Weather Forecasts (ECMWF) [see *Noël et al.*, 2005, and references therein]. In addition, *Timmermans et al.* [2004] performed comparisons between SCIAMACHY AMC-DOAS water vapour columns and ATOVS satellite results and radiosonde data.

Whereas the GOME water vapour product validation has been performed on an orbital basis, SCIAMACHY validation has been done globally, based on all (at that time) available data for the year 2003.

All inter-comparisons with correlative data sets show an overall good agreement, although a large scatter of about 0.5 g/cm^2 is usually observed. This scatter is mainly caused by atmospheric variability which in general makes a validation of water vapour columns very difficult.

The global mean SCIAMACHY AMC-DOAS water vapour columns for the year 2003 tend to be slightly lower than SSM/I and ECMWF data (see Figs. 4 and 5). The agreement of SCIAMACHY results with ECMWF data is somewhat better than with SSM/I data.

Comparisons of SCIAMACHY monthly mean water vapour columns with corresponding ECMWF monthly means showed in general a good agreement, although there are some discrepancies especially over ocean and desert areas which are possibly related to albedo effects and require further investigation (see Fig. 6, also taken from *Noël et al.* [2005]).

Sensitivity studies (see Tables 1 and 2, taken from *Noël et al.* [2004]) revealed that the AMC-DOAS algorithm is quite insensitive to different atmospheric conditions, which are generally handled quite well via the AMF correction factor. However, there is some sensitivity to the surface albedo which may cause deviations of up to about 15%, or 0.6 g/cm^2, which is in the order of magnitude of the typically observed scatter between AMC-DOAS results and correlative data.

Note that the validation results and sensitivity studies mentioned above are based on AMC-DOAS products V0.9.1. Recently, a new AMC-DOAS product version (V1.0) has been produced which uses an updated HITRAN spectroscopic data base and is derived from (partly reprocessed) SCIAMACHY V5 and V6 data products. The resulting AMC-DOAS V1.0 water vapour columns are typically lower than previous versions but in fact compare quite well with more recent SSM/I data (see *Noël et al.* [2007]).

Background Atmosphere	H_2O Reference Column (g/cm^2)	Retrieved H_2O Column (g/cm^2)	Retrieved AMF Correction Factor	Relative Deviation (Retr.-Ref.)/Ref. (%)	Abs. Deviation (Retr.-Ref.) (g/cm^2)
Tropical (TRO)	4.18	4.18	1.00	0.0	0.00
Mid-latitude summer (MLS)	2.96	3.05	1.01	3.0	0.09
Mid-latitude winter (MLW)	0.89	0.85	1.06	-4.7	-0.04
Sub-arctic summer (SAS)	2.11	2.17	1.03	3.1	0.06
Sub-arctic winter (SAW)	0.42	0.38	1.08	-8.6	-0.04
US-Standard (USS)	1.43	1.47	1.04	3.0	0.04

Table 1: Deviation of water vapour columns retrieved by the AMC-DOAS algorithm from atmospheric spectra computed with SCIATRAN for different background atmospheres. The solar zenith angle is 50°, the surface albedo 0.05 in all cases.

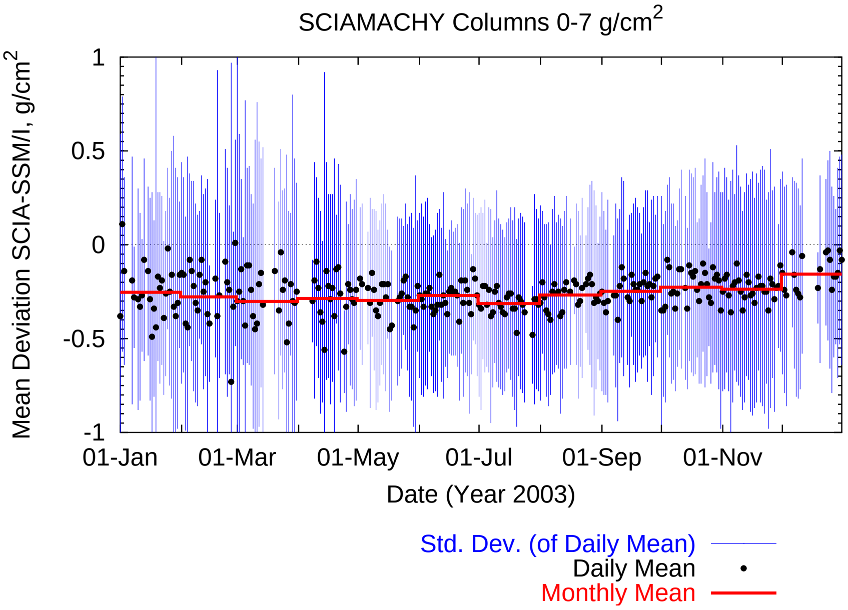

Figure 4: Global mean and standard deviation of the difference between collocated SCIAMACHY and SSM/I water vapour columns for the year 2003.

6 Recommendations for product validation

The large spatial and temporal variability of water vapour makes a validation of the derived water vapour columns in general very difficult. Depending on the correlative measurements, a typical scatter in the order of 0.5 g/cm^2 can be expected from differences in spatial and temporal resolution and sampling.

Therefore, large data sets are required to derive statistically relevant information. Experience has shown that global satellite water vapour data (as those derived via the AMC-DOAS method from GOME and SCIAMACHY measurements) are validated best by comparisons with other global satellite data sets.

Because the AMC-DOAS method uses data from the visible spectral region, comparisons should reveal the best results during cloud-free conditions, although too cloudy data are masked out by the inherent AMC-DOAS quality check via the AMF correction factor.

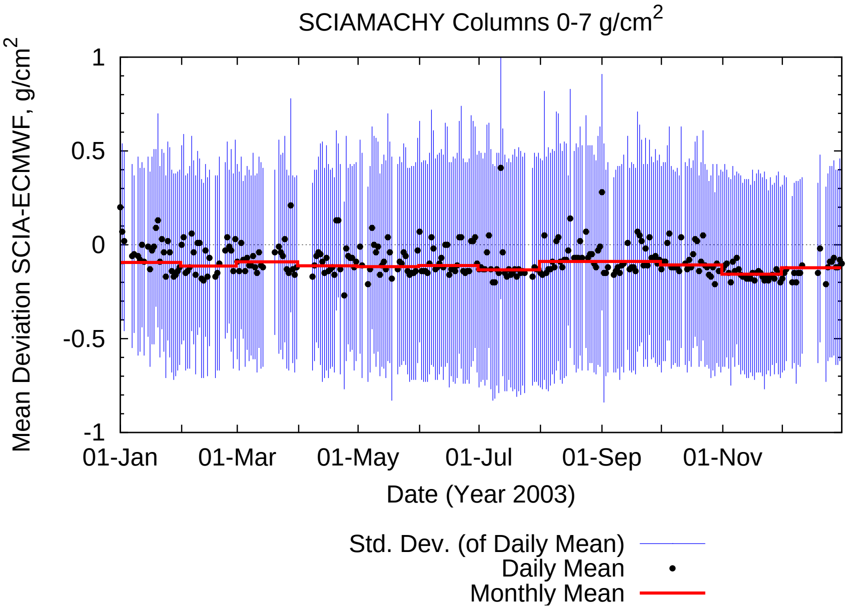

Figure 5: Global mean and standard deviation of the difference between collocated SCIAMACHY and ECMWF water vapour columns for the year 2003.

Surface Albedo	H_2O Reference Column (g/cm^2)	Retrieved H_2O Column (g/cm^2)	Retrieved AMF Correction Factor	Relative Deviation (Retr.-Ref.)/Ref. (%)	Abs. Deviation (Retr.-Ref.) (g/cm^2)
0.05	4.18	4.18	1.00	0.0	0.00
0.10	4.18	4.45	1.07	6.5	0.27
0.30	4.18	4.67	1.13	11.7	0.49
0.90	4.18	4.77	1.16	14.2	0.59

Table 2: Deviation of water vapour columns retrieved by the AMC-DOAS algorithm from atmospheric spectra computed with SCIATRAN for different surface albedos and a tropical background atmosphere. The solar zenith angle is 50°.

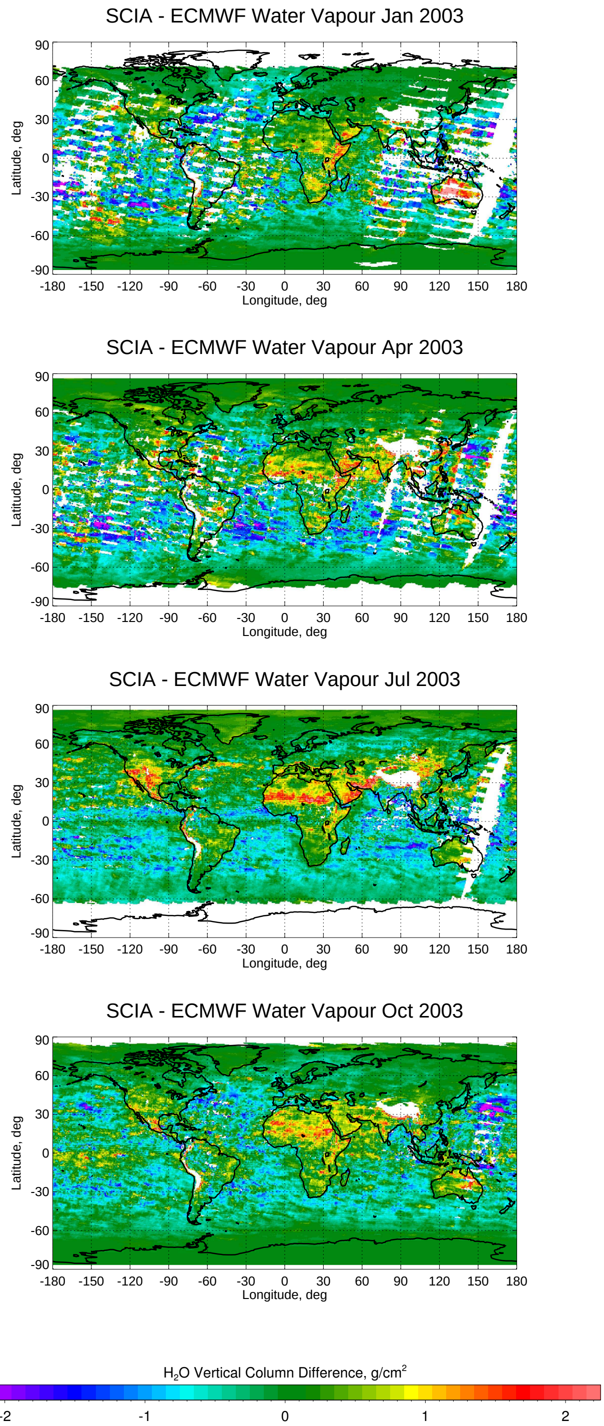

Figure 6: Difference between SCIAMACHY and ECMWF monthly means of total water vapour columns for the year 2003.

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