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First retrieval of global water vapour column amounts from SCIAMACHY measurements

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Abstract. Global water vapour column amounts have been derived for the first time from measurements of the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) on the European environmental satellite ENVISAT. For this purpose, two different existing retrieval algorithms have been adapted, namely the Air Mass Corrected Differential Absorption Spectroscopy (AMC-DOAS) which was originally designed for GOME and the Weighting Function Modified Differential Absorption Spectroscopy (WFM-DOAS) which was mainly designed for the retrieval of CH₄, CO₂ and CO from SCIAMACHY near-infrared spectra. Here, both methods have been applied to SCIAMACHY's nadir measurements in the near-visible spectral region around 700 nm.

Taking into account a systematic offset of 10%, the results of these two methods agree within a scatter of about ± 0.5 g/cm² with corresponding SSM/I and ECMWF water vapour data. This deviation includes contributions from the temporal and spatial variability of water vapour. In fact, the mean deviation between the SCIAMACHY and the correlative data sets is much smaller: the SCIAMACHY total water vapour columns are typically about 0.15 g/cm² lower than the SSM/I values and less than 0.1 g/cm² lower than corresponding ECMWF data. The SCIAMACHY water vapour results agree well with correlative data not only over ocean but also over land, thus showing the capability of SCIAMACHY to derive water vapour concentrations on the global scale.

where it significantly contributes to atmospheric chemistry, weather, and climate. Its large spatial and temporal variability makes water vapour a tracer for tropospheric changes and especially important for global models which aim to predict climate. The high relevance of water vapour has generated the need for global water vapour data. The main sources for these data are currently in-situ radio sonde, ground based or air borne measurements, space borne IR measurements, for example by the TIROS-N Operational Vertical Sounder (TOVS), and microwave soundings, for example by the Special Sensor Microwave Imager (SSM/I), and (recently) also MODIS. Additionally, water vapour total columns have been derived from Global Position System (GPS) observations (see e.g. Dai et al., 2002, and references therein). It has been shown by several studies (e.g. Noël et al., 1999, 2002b; Casadio et al., 2000; Maurellis et al., 2000; Lang et al., 2003; Wagner et al., 2003; Buchwitz et al., 2003) that measurements in the (near-)visible spectral region by the Global Ozone Monitoring Experiment (GOME) (see e.g. Burrows et al., 1999) provide an additional data source for global water vapour concentrations. An extended version of GOME, the SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY), has been successfully launched as part of the atmospheric chemistry payload of ENVISAT in March 2002.

In the current paper first SCIAMACHY water vapour results derived using two different retrieval algorithms are presented. These SCIAMACHY results are then compared with corresponding SSM/I and ECMWF (European Centre for Medium-Range Weather Forecasts) water vapour data.

1 Introduction

Water vapour is one of the most abundant atmospheric constituents and in fact the most important greenhouse gas. More than 99% of water vapour is located in the troposphere

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2 SCIAMACHY measurements

The SCIAMACHY instrument is a national (German/Dutch/Belgian) contribution to ESA's European environmental satellite ENVISAT, which has been launched

successfully in March 2002. SCIAMACHY determines the amount and distributions of a large number of atmospheric constituents by measuring Earthshine radiance and solar irradiance spectra simultaneously from the UV to the NIR (214–2380 nm) in nadir, limb and occultation geometry (see e.g. Bovensmann et al., 1999; Noël et al., 2002a, for details on the SCIAMACHY mission). After extensive tests to assure the correct functioning and performance of the instrument, SCIAMACHY entered nominal measurements mode in August 2002 (Bovensmann et al., 2002, 2003). Since then, mainly alternating nadir and limb measurements have been performed. Both H₂O profiles and vertical column amounts are foreseen as operational SCIAMACHY data products, but due to problems in the operational data processing SCIAMACHY data could not be released to the public until now (September 2003). However, a limited amount of spectral data is already available to selected users. These data typically suffer from a non-optimal radiometric calibration, but as the results of the present paper show, this is not critical for the algorithms used here which rely on differential structures in the spectral region around 700 nm. Nevertheless, it shall be noted that the water vapour results presented here are not based on the official SCIAMACHY Level 2 data products but have been derived from preliminary data.

3 Retrieval methods

3.1 Air mass corrected DOAS

First quantitative amounts of atmospheric water vapour vertical columns have been derived from cloud-free GOME measurements by Noël et al. (1999). The algorithm used is based on the well-known Differential Optical Absorption Spectroscopy (DOAS) approach (Perner and Platt, 1979; Burrows et al., 1999) 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) O₂ absorption features are fitted in combination with H₂O to determine an air mass correction factor which compensates to some degree for insufficient knowledge of the background atmospheric and topographic characteristics, like surface elevation and clouds.

The main equation of this method, which we call Air Mass Corrected (AMC-)DOAS, is given by:

$$\ln\left(\frac{I}{I_0}\right) = P - a \left(\tau_{O_2} + c C_V^b\right) \quad (1)$$

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 O₂ 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 term τ_{O_2} is derived using radiative transfer calculations with and without O₂. 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 scalar parameter a is the above mentioned air mass 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. C_V and a are then derived from a non-linear fit.

The AMC-DOAS method is applied to the spectral region between 682 nm and 700 nm because both O₂ and water vapour absorb in this region. They are the main absorbers in this spectral range, having slant optical depths of similar strength.

The AMC-DOAS method has been further developed to e.g. also allow for a retrieval over cloudy scenes (Noël et al., 2000, 2002b). It could be shown that the introduced cloud correction works well, but that it significantly increases the scatter in the data because the correction requires additional information on atmospheric and cloud properties which is typically not available at sufficiently high quality.

Therefore, it has to be accepted that the ability to derive concentrations of water vapour or other tropospheric gases from measurements in the the UV/Vis/NIR is generally limited by the opaqueness of clouds, although the method of air mass correction provides the possibility to retrieve meaningful H₂O total columns also for partly cloudy scenes.

In fact, the derived air mass correction factor a provides a good quality criterium for the retrieval if no cloud correction is performed. In the ideal case, i.e. if the atmospheric conditions used in the model calculations match the real conditions, the air mass correction factor should be 1. In the presence of clouds, only the atmosphere above the clouds can be probed by the instrument, so the effective amount of both O₂ and H₂O seen by GOME or SCIAMACHY is smaller than the amount used in the model calculations. The air mass factor correction would then try to compensate for this. In this case a would be smaller than 1. A too large deviation of the air mass correction from 1 is thus an indication that the conditions of the reference atmosphere differ too much from reality. In this case the retrieved H₂O columns are considered to be unrealistic. In practice, it could be shown that data retrieved with air mass correction factors larger than 0.8 are reliable, even if the retrieval is only performed using one (tropical) background atmosphere (Noël et al., 2000). The choice of the model surface albedo is – like for most DOAS-type methods – rather uncritical, although some additional errors may arise from this (see the error analysis below).

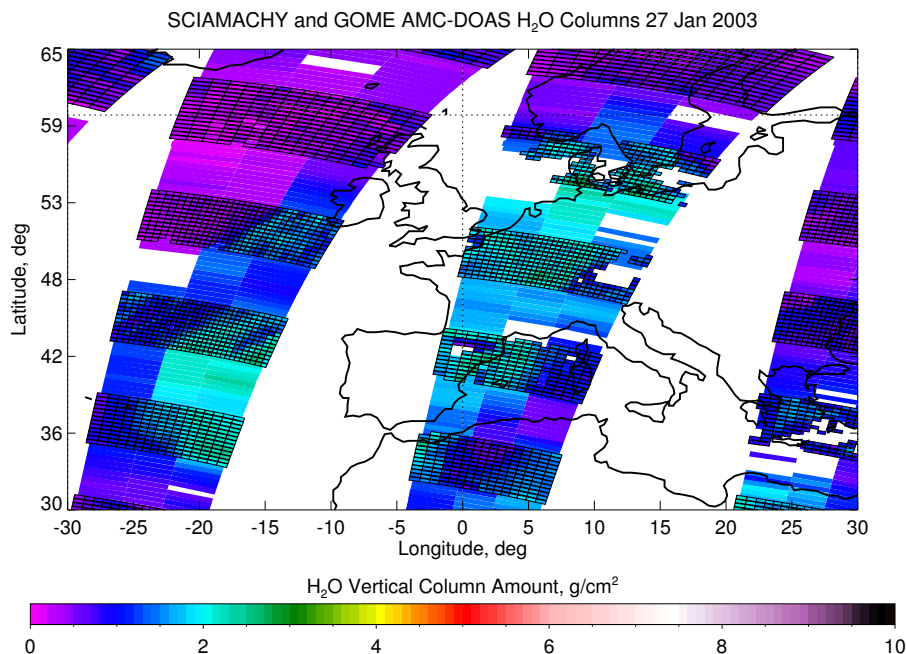


Fig. 1. SCIAMACHY and GOME water vapour total vertical columns for 27 January 2003 over Europe derived with the AMC-DOAS method (data from forward scans only). GOME measurements comprise three ground pixels for one forward scan (across track). The smaller SCIAMACHY ground pixels are marked by boxes.

Therefore, for the present study, all calculations have been performed using a cloud free tropical reference atmosphere assuming an albedo of 5%, and results with an air mass correction factor smaller than 0.8 have been omitted. In addition, measurements performed at high solar zenith angles (larger than 88°) and backscan pixels have been excluded, the latter because of their lower spatial resolution. As GOME, the SCIAMACHY instrument can not see through clouds. However, because the ground pixel size of SCIAMACHY is typically much smaller than for GOME ($30\text{ km} \times 60\text{ km}$ compared to $40\text{ km} \times 320\text{ km}$), the probability for cloud-free scenes is much higher for SCIAMACHY, so less data have to be rejected. The improved spatial resolution of SCIAMACHY can be seen in Fig. 1.

For the present study, the GOME retrieval model has been adapted to handle SCIAMACHY data. The radiative transfer code SCIATRAN (Buchwitz et al., 2000b; Rozanov et al., 2002) has been used instead of its predecessor GOMETRAN (Rozanov et al., 1997), including the latest update of the HITRAN data base (Rothman et al., 2003; Coheur et al., 2003). Recent field tests have shown that especially the 4ν water vapour band around 720 nm used in the present study is well described by HITRAN (Sierk et al., 2003). Furthermore, the grid of solar zenith angles for radiative transfer calculations has been extended to 88° . A Gaussian slit function of full width at half maximum (FWHM) of 0.45 nm has been assumed to fold the highly resolved radiative transfer spectra down to the SCIAMACHY spectral resolution. Be-

cause the SCIAMACHY slit function is close to undersampling at these wavelengths, the chosen value for the FWHM may need revision based on further analysis of in-flight spectra.

3.2 WFM-DOAS

WFM-DOAS (Buchwitz et al., 2000a; Buchwitz and Burrows, 2003) is based on linear least-squares fitting the logarithm of a linearised radiative transfer model plus a low-order polynomial to the logarithm of the ratio of a measured nadir radiance I and solar irradiance spectrum I_0 . The WFM-DOAS equation can be written as follows:

$$\ln\left(\frac{I}{I_0}\right)^{obs} = \ln\left(\frac{I}{I_0}\right)^{mod} + \sum_{j=1}^J \left. \frac{\partial \ln(I/I_0)^{mod}}{\partial V_j} \right|_{\vec{V}_j} \times (\hat{V}_j - \vec{V}_j) + P \quad (2)$$

Here, $\ln(I/I_0)^{obs}$ is the logarithm of the sun-normalised radiance as observed by SCIAMACHY. Terms with superscript *mod* are the WFM-DOAS reference spectra which comprise the computed sun-normalised radiance and its derivatives (also called weighting functions). They correspond to an assumed model atmosphere, surface reflectivity, and viewing geometry, etc. The assumed columns of H_2O and O_2 are denoted \vec{V}_j and the corresponding fit parameters

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.

Background Atmosphere	H ₂ O Reference Column [g/cm ²]	Retrieved H ₂ O 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 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°.

Surface Albedo	H ₂ O Reference Column [g/cm ²]	Retrieved H ₂ O 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

\hat{V}_j . The derivatives refers to the change of the radiance due to changes (scaling) of pre-selected vertical profiles of H₂O and O₂.

In order to avoid time consuming on-line radiative transfer simulations, the reference spectra have been pre-calculated (look-up table approach). A single model atmosphere has been defined (US Standard Atmosphere plus tropospheric maritime and stratospheric background aerosol) and a single surface albedo (0.1). The tabulated reference spectra depend on solar zenith angle (0°–90° in steps of 5°), surface elevation (0, 1, 2, 3 km) and water vapour column (scaling factors: 0.5, 1.0, 1.5, 2.0, 4.0), in total 400 combinations. To account for the temperature dependence of the molecular absorption cross sections, the derivative of the radiance with respect to a temperature profile shift is included in the fit (omitted in Eq. (2) to simplify the notation). WFM-DOAS has been implemented as an iterative scheme, mainly to account for nonlinearities introduced by the high variability of atmospheric water vapour (initial guess: scaling factor 1.0, i.e. unchanged US Standard Atmosphere water vapour profile).

For similar reasons as described in the previous section, O₂ has been included in the fit. The procedure as described above yields retrieved columns $\hat{V}_{\text{H}_2\text{O}}$ and \hat{V}_{O_2} (and their corresponding errors, see Buchwitz and Burrows, 2003). After the fit, the ratio $R_{\text{O}_2} := \bar{V}'_{\text{O}_2} / \hat{V}_{\text{O}_2}$ is computed, where \bar{V}'_{O_2} is the O₂ model column computed in a similar way as \bar{V}_{O_2} but for the actual average surface elevation of the SCIAMACHY ground pixel. To correct for air mass factor differences between the model and the real atmosphere (resulting from, e.g.

partial cloud cover), the retrieved H₂O columns are multiplied by R_{O_2} . This means that each H₂O column is actually divided by the simultaneously retrieved O₂ column (and multiplied by scaling factor \bar{V}'_{O_2} , which only depends on the average surface elevation of the ground pixel). Systematic errors which are common to the retrieved H₂O and O₂ columns will cancel when the ratio is computed (see error analysis given below). As a kind of quality measure and to limit the extent of the air mass factor correction, only retrievals with R_{O_2} larger than 0.7 and less than 1.3 are considered successful and are presented and discussed in this paper.

4 Error Analysis

4.1 AMC-DOAS error analysis

The AMC-DOAS method uses a single set of radiative transfer parameters b , c and τ_{O_2} . These parameters have been computed for different solar zenith angles, but a fixed value of 0.05 for the surface albedo has been taken, and a tropical background atmosphere has been used. In this section, the influence of these two assumptions on the retrieval quality shall be assessed.

For this purpose, various radiance spectra for different atmospheric conditions and surface albedos have been modelled with SCIATRAN. The AMC-DOAS method has then been applied to these spectra, and the difference between the retrieved vertical water vapour column and the vertical water vapour column of the reference atmosphere has been

Table 3. Retrieval errors determined by applying WFM-DOAS to simulated spectra generated using various model atmospheres. For detailed description of the last three columns see Sect. 4.2.1.

Atmosphere	Error of uncorrected H ₂ O column $\hat{V}_{\text{H}_2\text{O}}$ (Retr.-Ref.)/Ref. [%]	Error of O ₂ column \hat{V}_{O_2} (Retr.-Ref.)/Ref. [%]	Error of (O ₂ corrected) H ₂ O column (Retr.-Ref.)/Ref. [%]
Tropical (TRO)	-3.57	-0.07	-3.50
Mid-latitude summer (MLS)	-0.43	-0.26	-0.17
Mid-latitude winter (MLW)	0.33	0.59	-0.26
Sub-arctic summer (SAS)	0.02	-0.34	0.36
Sub-arctic winter (SAW)	-4.17	0.69	-4.83
US-Standard (USS)	0.00	-0.01	0.01

Table 4. Vertical column retrieval errors resulting from aerosol variability and undetected subvisual cirrus clouds at 12 km (OD means scattering optical depth). For detailed description of the last three columns see Sect. 4.2.1.

Aerosol/cloud scenario	Error of uncorrected H ₂ O column $\hat{V}_{\text{H}_2\text{O}}$ (Retr.-Ref.)/Ref. [%]	Error of O ₂ column \hat{V}_{O_2} (Retr.-Ref.)/Ref. [%]	Error of (O ₂ corrected) H ₂ O column (Retr.-Ref.)/Ref. [%]
Aerosol:			
OPAC average continental	-2.07	-1.78	-0.30
Enhanced aerosol in BL	-5.76	0.22	-5.97
No aerosol in atmosphere	-0.90	-1.61	0.72
Clouds:			
Subvisual cirrus (OD 0.01)	-0.54	-0.47	-0.07
Subvisual cirrus (OD 0.02)	-1.11	-0.98	-0.13
Subvisual cirrus (OD 0.03)	-1.71	-1.53	-0.18

computed. All results in this section are valid for a solar zenith angle of 50° and cloud-free conditions.

Table 1 shows the sensitivity of the AMC-DOAS method to different atmospheric conditions including different vertical profile shapes, namely for a tropical (TRO), sub-arctic summer/winter (SAS/SAW), mid-latitude summer/winter (MLS/MLW), and the US standard atmosphere (USS). The surface albedo has always been set 0.05 for these calculations.

For the tropical background atmosphere the exact water vapour column is derived showing the self-consistency of the AMC-DOAS method. Note that even the retrieved AMF correction factor is 1 in this case, as it should be. The maximum relative deviation between the retrieved and the reference water vapour column is about 9%, occurring for the SAW reference atmosphere. This is not surprising as the SAW atmosphere has the lowest H₂O contents and is thus the furthest away from the tropical reference atmosphere assumed by AMC-DOAS. In fact, the absolute deviation is in all cases smaller than 0.1 g/cm², showing that the sensitivity of the AMC-DOAS method to different atmospheric background conditions is considerably low.

The sensitivity to the surface albedo is somewhat higher, as can be seen from Table 2 which lists the results of the AMC-DOAS retrieval for albedos higher than the assumed

0.05 (which is about valid for ocean areas), namely 0.1 (which is the one assumed by the WFM-DOAS method), 0.3 (typical for land surface), and 0.9 (corresponding to ice). Except for the standard 0.05 albedo which shows (as mentioned before) self-consistency, the retrieved column for the other albedos is always too large, and the error increases with the albedo. The maximum relative deviation is about 14%, corresponding to an absolute deviation of about 0.6 g/cm². However, this deviation occurs for a surface albedo of 0.9 which may not be too realistic for a (cloud-free) tropical atmosphere. Nevertheless, the expected deviation over land (albedo 0.3) is only slightly smaller (about 12%, 0.5 g/cm³). It is planned to reduce this albedo dependence in future versions of the AMC-DOAS algorithm by using different parameter sets for different surface conditions.

An additional – maybe even the largest – error source for the retrieval are clouds. In general, the atmosphere below the clouds can not be seen by SCIAMACHY, resulting in a decreased absorption depth for all tropospheric constituents compared to the cloud-free case. The AMC-DOAS method principally accounts for this effect by the derived air mass correction factor, which is usually smaller than 1 for the cloudy case. Clouds may therefore partly compensate the effect of higher albedos, for which the air mass correction factors are usually larger than 1 as can be seen from Table 2. A

Table 5. Vertical column retrieval errors as a function of surface albedo. For an albedo of 0.1 the errors are (nearly) zero because the reference spectra are calculated for albedo 0.1 (note that the small error of -0.01% for oxygen results from wavelength interpolation of the reference spectra). For detailed description of the last three columns see Sect. 4.2.1.

Albedo	Error of uncorrected H ₂ O column $\hat{V}_{\text{H}_2\text{O}}$ (Retr.-Ref.)/Ref. [%]	Error of O ₂ column \hat{V}_{O_2} (Retr.-Ref.)/Ref. [%]	Error of (O ₂ corrected) H ₂ O column (Retr.-Ref.)/Ref. [%]
0.03	-23.40	-18.76	-5.71
0.05	-13.10	-10.57	-2.83
0.10	0.00	-0.01	0.01
0.20	10.45	8.45	1.84
0.30	15.37	12.37	2.67

quantitative estimation of the influence of clouds using simulated data is difficult because of the various types of clouds and the usually inhomogeneous spatial distribution (both horizontally and vertically) within the instrument field of view. At present, a statistical analysis of a comparison with relative measurements (as described in Sect. 5.4) seems to be a more appropriate approach.

4.2 WFM-DOAS error analysis

The fast look-up table approach described in Sect. 3.2 introduces errors. In addition, there are errors resulting from parameters that influence the radiative transfer but are not retrieved by WFM-DOAS, such as aerosols and clouds. In the following, an initial error analysis of the currently implemented version of WFM-DOAS is presented. For this purpose, simulated nadir spectra have been generated with a radiative transfer model for various conditions, such as different model atmospheres and surface albedos. If not stated otherwise, the results shown in this section are valid for a solar zenith angle of 50° and albedo 0.1.

4.2.1 Sensitivity to vertical profiles

The currently implemented look-up table has been generated assuming vertical profiles of pressure, temperature and trace gas and oxygen volume mixing ratios corresponding to the US Standard Atmosphere. In order to estimate the vertical column retrieval error resulting from applying WFM-DOAS to different atmospheres, simulated spectra for several model atmospheres have been generated. The results are shown in Table 3.

The second column of Table 3 shows the relative difference between the uncorrected H₂O column, $\hat{V}_{\text{H}_2\text{O}}$ (see Eq. 2), and the known H₂O column of the model atmosphere. The third column shows the error of \hat{V}_{O_2} . The last column shows the error of the WFM-DOAS retrieved H₂O columns discussed in this paper (i.e., after O₂ correction factor R_{O_2} has been applied to $\hat{V}_{\text{H}_2\text{O}}$, see Sect. 3.2). For a given surface elevation R_{O_2} is a constant divided by the retrieved O₂ column. Therefore this error is identical with the error of the ratio

of the retrieved H₂O and O₂ column, i.e., with the error of $\hat{V}_{\text{H}_2\text{O}}/\hat{V}_{\text{O}_2}$. This error given in the last column has been computed from the errors given in the two previous columns by: $c := ((1+a/100)/(1+b/100)-1) \times 100$, where a denotes the percentage error of $\hat{V}_{\text{H}_2\text{O}}$ and b denotes the percentage error of \hat{V}_{O_2} (note that $c \approx a-b$). For the US-Standard atmosphere the errors are (nearly) zero because this is the WFM-DOAS reference atmosphere (note that the small error of -0.01% for oxygen results from wavelength interpolation of the reference spectra). This demonstrates the self-consistency of the WFM-DOAS method. The retrieval errors mainly reflect the difference in temperature and water vapour profiles of the various atmospheres compared to the US Standard (USS) reference atmosphere (temperatures at sea level in K: USS 288.1, SAW 257.2, TRO 299.7; H₂O columns: see Table 1). To deal with temperature variability the derivative with respect to a temperature profile shift is included in the fit. To deal with water vapour variability the reference spectra have been computed for several water vapour profiles (columns). As can be seen, the error on the retrieved water vapour column is below 5%. For retrievals without allowing for a temperature shift this error could exceed 10%.

Note that for this study the errors given in the last column of the tables presented in this section are the most relevant.

4.2.2 Sensitivity to aerosols and subvisual cirrus clouds

Aerosols and clouds mainly scatter but also absorb solar radiation. A large fraction of the water vapour molecules is situated in the lowest kilometres of the atmosphere, i.e., in a region where clouds and aerosols are present in extremely variable type and concentration. The WFM-DOAS reference spectra look-up table used in this study has been generated using a single aerosol scenario only. It is based on the aerosol parameterisation also implemented in the radiative transfer model MODTRAN (Kneizys et al., 1996) and is based on Shettle and Fenn (1979). This (default) scenario can be characterised as follows: Maritime aerosol in the boundary layer (BL), tropospheric visibility and relative humidity 23 km and 80%, respectively, and background stratospheric and normal mesospheric conditions. Aerosol scattering and absorption

vertical optical depth are listed in Table 3 of Buchwitz and Burrows (2003). To a first approximation aerosols increase or decrease the overall (i.e., spectrally broadband) level of solar radiation scattered back to space. This effect is taken into account by the polynomial included in Eq. (2). However, aerosols also determine the relative depth of absorption lines by influencing the (average) photon path.

The retrieval error due to aerosol has been estimated by defining several aerosol scenarios (including two rather extreme ones: (i) extreme aerosol loading of the boundary layer and (ii) no aerosols in atmosphere). The “OPAC average continental” aerosol scenario (Hess et al., 1998) and radiative transfer simulations differ from the default scenario used for the reference spectra in various aspects (Mie phase function instead of Henyey-Greenstein approximation, scattering and extinction profiles). “OPAC average continental” aerosol consists of a mixture of “water soluble aerosol” (small particles mainly originating from gas-to-particle conversion), soot, and “insoluble aerosol” (dust). The “Enhanced aerosol in boundary layer (BL)” scenario contains urban aerosol in the BL with a visibility as low as 2 km and a high relative humidity of 99%. For the “No aerosol in atmosphere” scenario the aerosols have been entirely “switched off” in the radiative transfer simulation. Table 4 shows that the error of the water to oxygen column ratio (last column) is typically below 1%, except for the scenario with extremely enhanced aerosol in the planetary boundary layer where the error can be as large as 6%. The main reason why the systematic errors on the uncorrected water vapour column (second column) and the oxygen column (third column) are not identical (and, therefore, do not perfectly cancel when the error on the column ratio is computed) is that the profile shapes are rather different.

Realistic errors introduced by clouds are difficult to estimate using simulated spectra (because strictly speaking the full three dimensional structure of clouds covering only a part of the ground pixel has to be considered). For this study we have limited ourselves to estimate the vertical column retrieval error resulting from subvisual cirrus clouds. These clouds have been modelled in this study as a scattering layer of 1 km vertical extent centered at 12 km. The assumed scattering vertical optical depths were 0.01, 0.02, and 0.03 (independent of wavelength). Table 4 shows that such a scattering layer near the tropopause is expected to lead to an underestimation of the retrieved uncorrected water vapour columns (shielding of the troposphere lying underneath) by up to nearly 2%. The oxygen column errors are nearly identical with the uncorrected water vapour column errors. Therefore, the error of the column ratio is significantly smaller (below 0.2%) than the error of the uncorrected column.

4.2.3 Sensitivity to surface albedo

The WFM-DOAS look-up table used in this study has been generated assuming a constant (Lambertian) albedo of 0.1.

To a first approximation albedo affects the overall (i.e., spectrally broadband) level of solar radiation scattered back to space. This effect is taken into account by the polynomial included in Eq. (2). However, as aerosols, the albedo also influences the relative depth of absorption lines.

As shown in Table 5 the errors of the O₂ corrected H₂O columns are below 6% for albedos between 0.03 and 0.3.

4.2.4 Other error sources

In this section three additional errors are quantified which are related to the (rather sparse) grid selected for the WFM-DOAS reference spectra look-up table: solar zenith angle interpolation, scan angle correction, and surface elevation (pressure). Note that these errors can be reduced relatively easily, e.g., by extending the look-up table and/or by implementing a better interpolation scheme.

The WFM-DOAS look-up table used in this study has been generated for a range of solar zenith angles from 0 to 90° in steps of 5°. These spectra are (linearly) interpolated to the solar zenith angle of the measurement. The resulting retrieval error is rather small (e.g. less than 0.02% for a solar zenith angle of 52.4°).

The look-up table has been generated for exact nadir observation only, neglecting the ±30° scan around the nadir direction. The columns as determined by the fit are corrected using a simple geometrical approximation Buchwitz et al. (2000a) to account for the enhancement of the depth of absorption lines due to the slant path viewing geometry. The currently implemented correction scheme may result in errors of the water vapour to oxygen column ratio of less than 1%. For the uncorrected water column the error might be as large as 6.5% for the most eastward and westward ground pixels. For oxygen the error is nearly the same and, therefore, the error of the water to oxygen ratio is close to zero.

The look-up table has been generated for a limited number of surface elevations (or surface pressures), covering the range 0–3 km in steps of 1 km. A simple next neighbour approach is currently implemented in order to select the reference spectra for a given ground pixel. This results in retrieval errors of 2–3% for the water vapour to oxygen column ratio.

There are many other potential sources of retrieval errors which are not covered in this study (e.g., calibration errors). A potentially important error source which is difficult to quantify are the spectroscopic data (HITRAN 2000 has been used for this study including all updates available until March 2003 and taking into account the pressure shift of line transitions not considered in earlier versions of the look-up table). Retrieval errors on the order of a few percent can be expected due to, e.g. line intensity uncertainties.

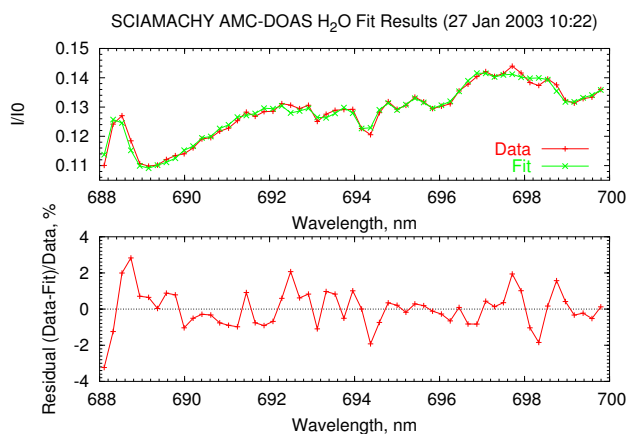


Fig. 2. Example for a fit using the AMC-DOAS method (nadir readout 2568 of orbit 4757 on 27 January 2003 10:22). Top: Sun-normalised SCIAMACHY data and fitted spectrum. Bottom: Corresponding residual.

5 Results

5.1 Fit results

Because of the currently limited amount of available data the present study concentrates on the analysis of SCIAMACHY measurements taken on 27 January 2003 as this is one of the first days for which almost all measured spectra are available in consolidated product files. However, other days have been analysed, too, yielding similar results. Since the solar reference spectra contained in the operational products are currently of limited quality, the analysis uses an elevation diffuser sun reference spectrum measured on 23 January 2003, which has been derived using an improved calibration procedure (J. Frerick, ESA, personal communication).

Note that it was not necessary to include a “shift and squeeze” correction for the spectral calibration in the fitting process, as it could be verified that such a correction has no significant influence on the retrieval results. Therefore, it has been omitted for processing speed reasons.

First retrieval results using the AMC-DOAS algorithm with SCIAMACHY data revealed systematically about 10% lower water vapour columns derived from SCIAMACHY data in comparison with corresponding SSM/I data over ocean. This is consistent with the results of the WFM-DOAS method. To compensate for this systematic effect, all AMC-DOAS and WFM-DOAS water vapour columns presented in this paper have been multiplied by 1.1. The reason for this systematic under-estimation by SCIAMACHY is currently unclear. Since different algorithms (both AMC-DOAS and WFM-DOAS) derive approximately the same offset, errors in the algorithms or their implementation seem to be unlikely. The following possible systematic error sources are currently under discussion:

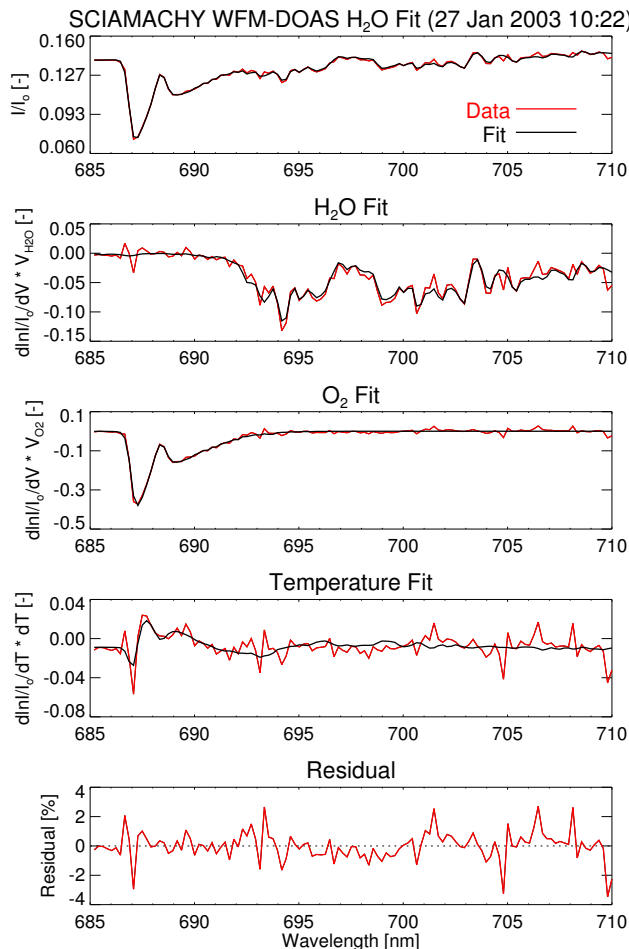


Fig. 3. Typical example of a WFM-DOAS fit. Top panel: Sun-normalised radiance as measured by SCIAMACHY (red) and WFM-DOAS model after the fit (black). Following three panels: (i) H₂O fit: fitted (i.e. scaled) H₂O weighting function (black) and H₂O fit residuum (red). The H₂O fit residuum is defined as the sum of the scaled H₂O weighting function plus the fit residuum (i.e. the difference between measurement and model, see bottom panel). Retrieved column: $1.54 \pm 0.07 \text{ g/cm}^2$. (ii) O₂ fit: $5.00 \times 10^{24} \text{ molecules/cm}^2 \pm 1.8\%$. (iii) Temperature fit: retrieved temperature profile shift: $24 \pm 4 \text{ K}$. Bottom panel: relative difference measurement-model (RMS: 0.96%).

1. Systematic errors arising from the currently insufficient radiometric calibration of SCIAMACHY. This can be assessed as soon as re-processed data are available (probably mid of 2004).
2. An error due to insufficient knowledge of the instrument slit function. This needs further investigation using in-flight monitoring measurements.
3. Potential errors in the spectral data base (absolute cross sections). This error is considered to be small, because the water vapour band used seems to be well described

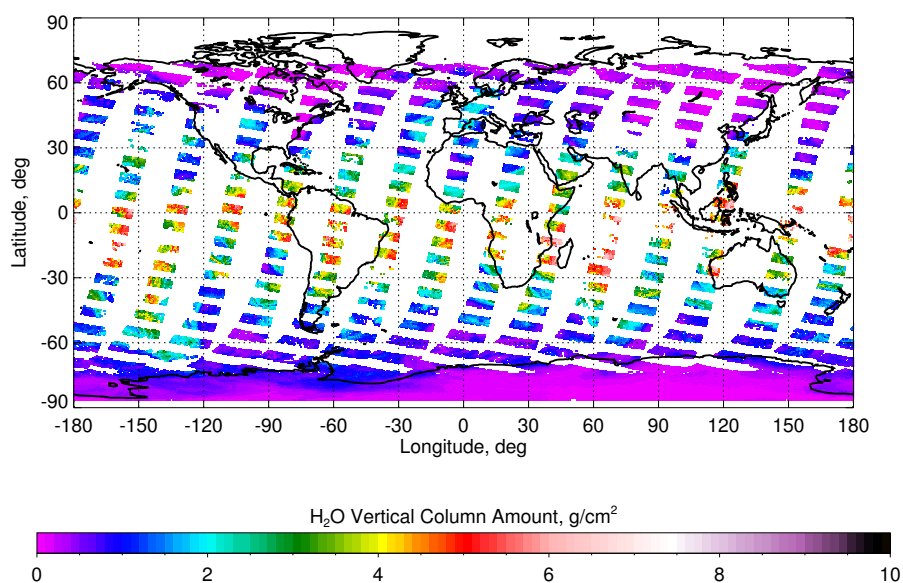


Fig. 4. Gridded SCIAMACHY water vapour total vertical columns for 27 January 2003 derived with the AMC-DOAS method.

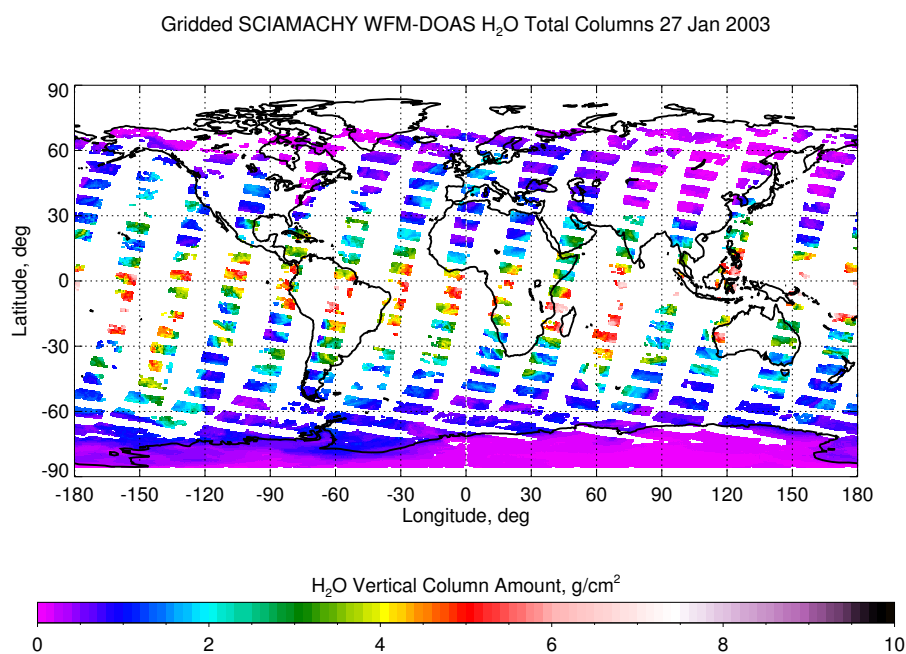


Fig. 5. Gridded SCIAMACHY water vapour total vertical columns for 27 January 2003 derived with the WFM-DOAS method.

by HITRAN. Nevertheless, transferring the algorithm to other spectral regions where water vapour absorbs (further in the infrared) may give more information on this contribution.

4. Systematic effects of surface albedo and clouds (see also error analysis in Sect. 4). Especially this point requires further studies.

Figure 2 shows a typical fit result of the AMC-DOAS method for one individual nadir measurement. The solar zenith angle for this measurement is about 43° , the retrieved column $1.85 \pm 0.25 \text{ g/cm}^2$. The measured data are reproduced quite well, with an average residual of about 2%. The WFM-DOAS method essentially yields the same results for the residual (see Fig. 3), although the retrieved column is actually lower ($1.54 \pm 0.07 \text{ g/cm}^2$).

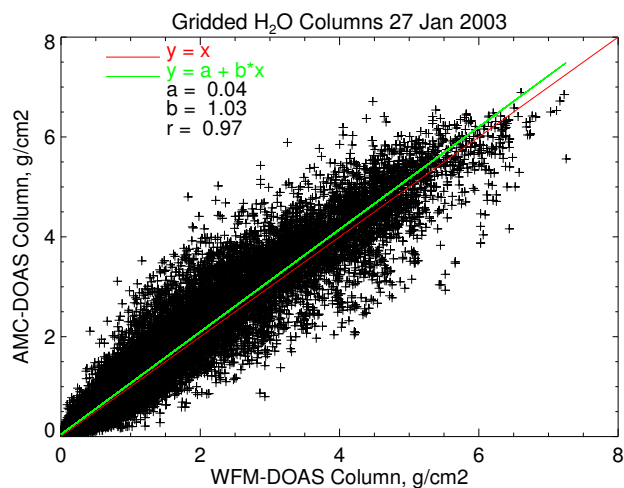


Fig. 6. Correlation between gridded SCIAMACHY/AMC-DOAS and SCIAMACHY/WFM-DOAS water vapour total vertical columns for 27 January 2003. Red line: 1:1 correlation. Green line: Linear fit. The resulting linear Pearson's correlation coefficient r is also specified.

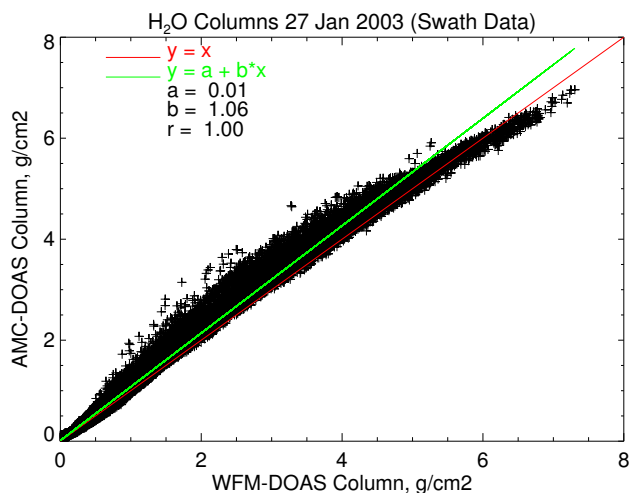


Fig. 7. Correlation between SCIAMACHY/AMC-DOAS and SCIAMACHY/WFM-DOAS water vapour total vertical columns for 27 January 2003 (swath data). Red line: 1:1 correlation. Green line: Linear fit. The resulting linear Pearson's correlation coefficient r is also specified.

The complete data sets derived for 27 January 2003 by the AMC-DOAS and WFM-DOAS methods are displayed in Figs. 4 and 5. The data have been gridded to $0.5^\circ \times 0.5^\circ$ to facilitate a comparison with SSM/I and ECMWF data (see below). Note that the regular gaps between blocks of nadir measurements along the orbits are caused by SCIAMACHY's standard measurement mode involving alternating limb and nadir measurements. Taking this into account, it can be seen that not many data are rejected by the inher-

ent quality check of both retrieval algorithms. In fact, both algorithms reject data in the same areas, mainly within the tropical regions where usually extended cloud coverage is expected. In addition, the AMC-DOAS quality check rejects data over high surface altitude regions, like the Himalaya, because in this case air mass correction can not compensate for the largely different atmospheric conditions. The WFM-DOAS method considers different surface elevations (using an appropriate data base) and thus has less problems here.

The direct correlation between the two methods (see Fig. 6) shows an almost perfect agreement (linear Pearson's correlation coefficient $r=0.97$), although the scatter of the data is high. As can be seen from the comparison of ungridded swath data in Fig. 7 most of this scatter is caused by gridding. For the ungridded data the correlation is perfect (1.0), although there seem to be systematic deviations depending on the water vapour column. Most likely, these deviations are caused by the different retrieval methods: The AMC-DOAS method only uses a tropical reference atmosphere, whereas the WFM-DOAS method relies on a large input data base for surface elevation, etc., and retrieves not only the water vapour column in an iterative way, but other atmospheric parameters as well (O_2 column, temperature profile shift). Therefore, the observed differences are not surprising.

5.2 Comparison with SSM/I data

In contrast to SCIAMACHY, the SSM/I instrument is capable to measure under all illumination conditions, but only over water surface. For the comparison with SCIAMACHY data measurements of the SSM/I instrument on-board DMSP-14 during the descending part of the orbit have been selected, because in this case the difference in local time between SCIAMACHY and SSM/I are smallest (ENVISAT has an equatorial crossing time of 10:00 LT whereas DMSP-14 crosses the equator at about 08:00 LT).

Figure 8 shows the gridded total precipitable water columns derived from SSM/I measurements on 27 January 2003. Clearly, the same water vapour structures as in the SCIAMACHY data can be seen. The correlation between SSM/I and SCIAMACHY water vapour is for both methods (AMC-DOAS, see Fig. 9, and WFM-DOAS, see Fig. 10) quite good. At the lower edge of the plots, SSM/I data show some extraordinarily high columns which are probably due to water regions in the northern area covered with ice which have not been masked out.

5.3 Comparison with ECMWF data

SSM/I data are only available over open water. To assess the quality of the derived SCIAMACHY water vapour columns also over land a comparison with assimilated global water vapour data provided by the European Centre for Medium-Range Weather Forecasts (ECMWF) has been performed.

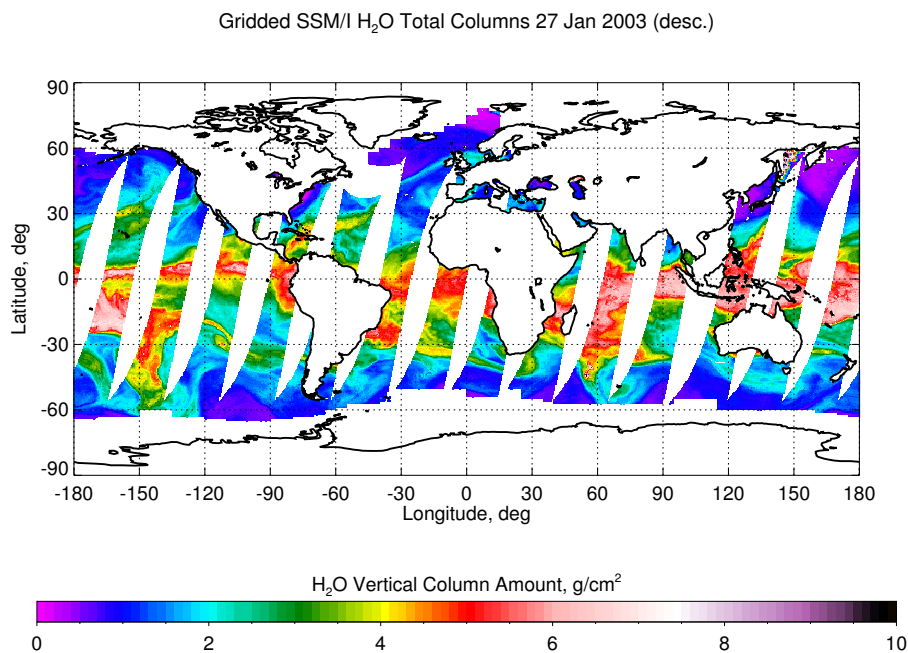


Fig. 8. DMSF-F14 SSM/I water vapour total vertical columns for 27 January 2003 (descending orbit part only).

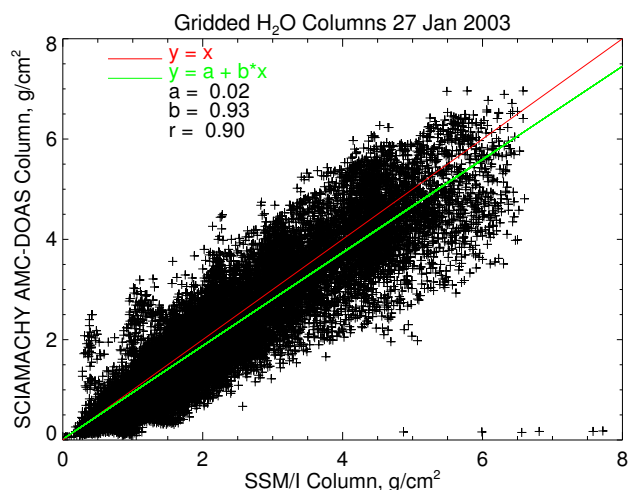


Fig. 9. Correlation between SSM/I and SCIAMACHY/AMC-DOAS water vapour total vertical columns for 27 January 2003. Only the descending part of the SSM/I data has been used. Red line: 1:1 correlation. Green line: Linear fit. The resulting linear Pearson's correlation coefficient r is also specified.

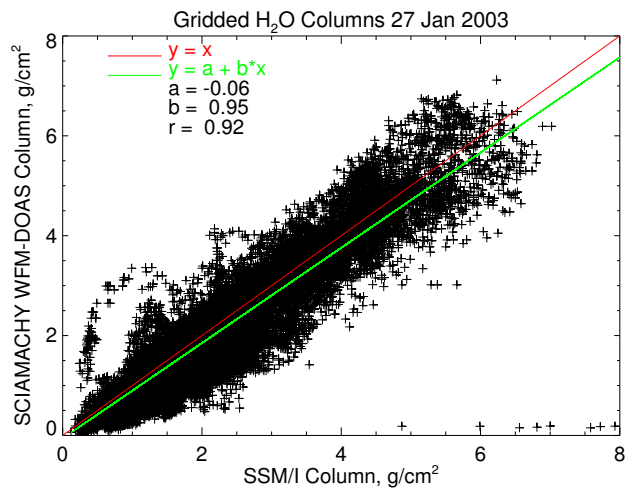


Fig. 10. Correlation between SSM/I and SCIAMACHY/WFM-DOAS water vapour total vertical columns for 27 January 2003. Only the descending part of the SSM/I data has been used. Red line: 1:1 correlation. Green line: Linear fit. The resulting linear Pearson's correlation coefficient r is also specified.

Note that the ECMWF data at least partly rely on SSM/I data, such that no large differences are expected over ocean areas.

The data set of analysed meteorological fields provided by ECMWF that has been used for this study comprises geopotential height, temperature, pressure, and specific humidity on a $1.5^\circ \times 1.5^\circ$ latitude/longitude grid on 60 model altitude levels. From these data the water vapour column in g/cm²

has been computed for each grid point by numerical integration. For each day a daily average column field has been calculated from the original six-hourly fields (0:00, 6:00, 12:00, 18:00, and 24:00 UTC). These data have then been remapped on a $0.5^\circ \times 0.5^\circ$ latitude/longitude grid by assigning to each grid point the corresponding value of its lower resolution grid box, thereby avoiding any interpolation.

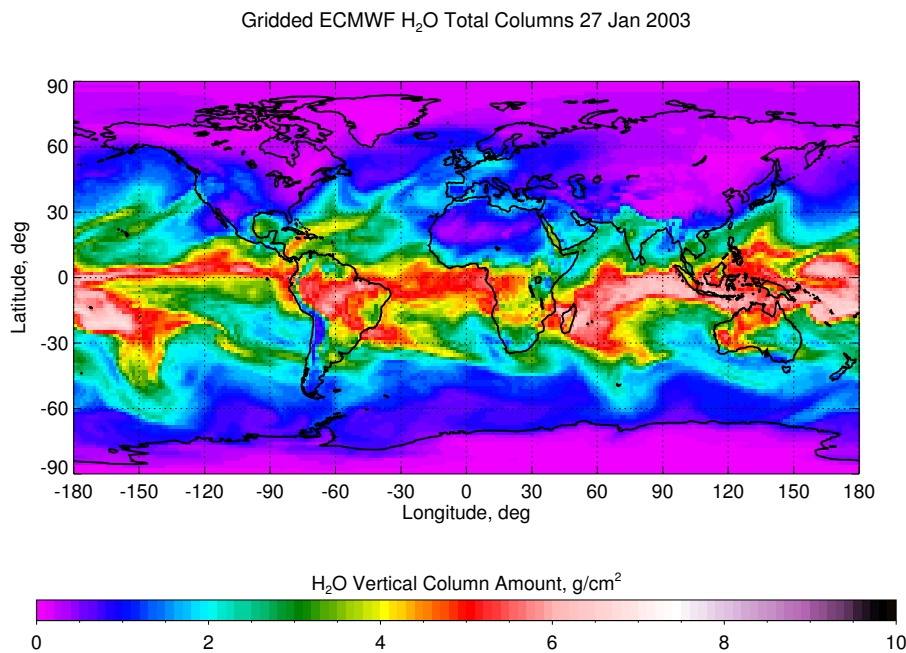


Fig. 11. ECMWF water vapour total vertical columns for 27 January 2003.

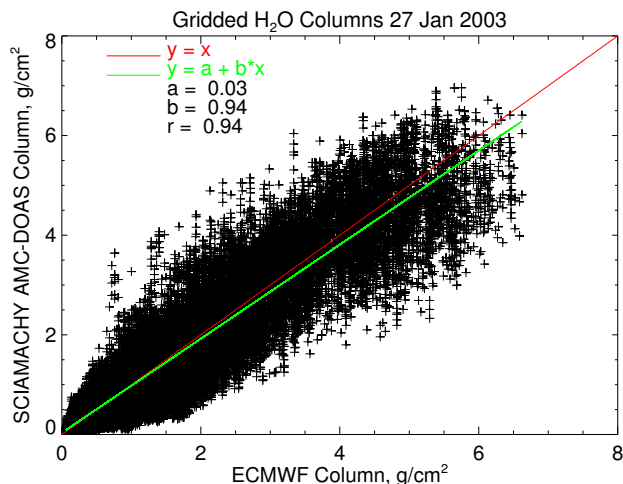


Fig. 12. Correlation between ECMWF and SCIAMACHY/AMC-DOAS water vapour total vertical columns for 27 January 2003. Red line: 1:1 correlation. Green line: Linear fit. The resulting linear Pearson's correlation coefficient r is also specified.

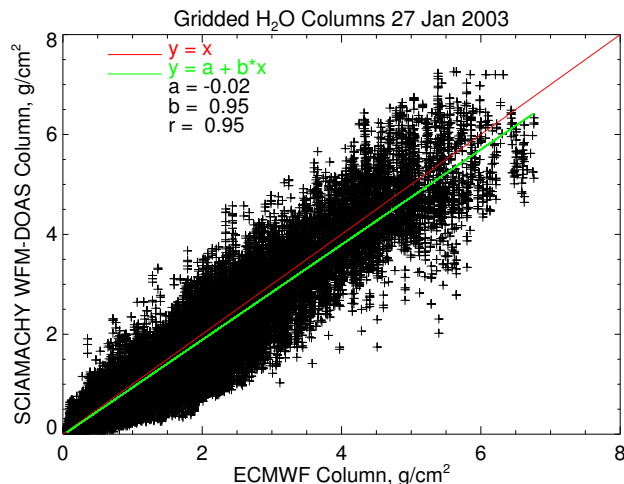


Fig. 13. Correlation between ECMWF and SCIAMACHY/WFM-DOAS water vapour total vertical columns for 27 January 2003. Red line: 1:1 correlation. Green line: Linear fit. The resulting linear Pearson's correlation coefficient r is also specified.

Figure 11 shows a global map of the ECMWF water vapour data, which in fact agrees well with both SSM/I and SCIAMACHY results. As mentioned before, the resolution of the ECMWF data used is $1.5^\circ \times 1.5^\circ$ which is slightly coarser than for SSM/I and SCIAMACHY. However, for the statistical analysis described here it is sufficient to match each ECMWF grid point to (up to) nine SSM/I or SCIAMACHY data points.

The correlation between the ECMWF data and the SCIAMACHY total water vapour column amounts are shown in Fig. 12 for AMC-DOAS data and Fig. 13 for WFM-DOAS data. The agreement in both cases is very good. The Pearson's r correlation is better than 0.94; there is almost no bias, and the slope of the fitted linear curve is 0.94 for AMC-DOAS and 0.95 for WFM-DOAS. The scatter of the data is high but not much higher than for ocean scenes. Most of

Table 6. Deviation of retrieved water vapour columns from reference data for different column intervals. The last line gives the average deviations for the complete columnar range from 0 to 7 g/cm².

Column Range (g/cm ²)	AMC-DOAS – SSM/I		AMC-DOAS – ECMWF		WFM-DOAS – SSM/I		WFM-DOAS – ECMWF	
	Mean Dev. (g/cm ²)	Std. Dev. (g/cm ²)	Mean Dev. (g/cm ²)	Std. Dev. (g/cm ²)	Mean Dev. (g/cm ²)	Std. Dev. (g/cm ²)	Mean Dev. (g/cm ²)	Std. Dev. (g/cm ²)
0.00–1.00	−0.35	0.51	−0.07	0.26	−0.30	0.58	−0.08	0.24
1.00–2.00	−0.17	0.44	−0.09	0.47	−0.21	0.43	−0.18	0.46
2.00–3.00	−0.06	0.70	0.08	0.67	−0.07	0.54	−0.04	0.56
3.00–4.00	−0.08	0.75	0.12	0.88	−0.03	0.54	0.07	0.64
4.00–5.00	−0.00	0.74	0.12	0.83	−0.03	0.55	0.02	0.66
5.00–6.00	0.53	0.61	0.59	0.68	0.30	0.63	0.40	0.67
6.00–7.00	0.63	0.40	0.90	0.47	0.73	0.47	0.91	0.57
0.00–7.00	−0.14	0.62	−0.03	0.45	−0.16	0.54	−0.08	0.39

the scatter can be attributed to the large temporal and spatial variability of water vapour.

5.4 Statistical analysis

For each of the comparisons described above a statistical analysis has been performed. For this purpose, all SCIAMACHY data shown in Figs. 9 to 13 have been binned into water vapour vertical column intervals from 0–1 g/cm² up to 6–7 g/cm². For each of these intervals and for each comparison the following quantities have been determined:

1. The mean deviation between the SCIAMACHY column and the reference column (either from SSM/I or ECMWF); this is a measure for systematic offsets between the data sets.
2. The standard deviation of the difference between the SCIAMACHY column and the reference column; this is a measure for the deviation between correlative data points. The results of this analysis are shown in Table 6.

The results for AMC-DOAS and WFM-DOAS are quite similar, although WFM-DOAS seems to perform slightly better especially for smaller columns, probably because the real atmospheric conditions are better adapted by the iterative approach. AMC-DOAS only uses one (tropical) reference atmosphere for the whole Earth, nevertheless the columns retrieved by this method agree remarkably good with both SSM/I and ECMWF data.

Smaller columns are typically underestimated, larger columns overestimated by SCIAMACHY. The agreement between the SCIAMACHY results and both SSM/I and ECMWF data is best in the columnar range from 2 to 5 g/cm² where the mean deviations vary between −0.08 and 0.12 g/cm². The maximum average deviation is 0.91 g/cm² at very high columns. Largest relative discrepancies occur for very small columns, especially when compared to SSM/I. The latter is partly caused by those extraordinarily

high SSM/I values probably obtained over ice which have been mentioned before.

The standard deviation of the data sets is typically about 0.5 g/cm² and varies between about 0.4 and 0.8 g/cm². The scatter is quite independent from the water vapour column amount, although of course it becomes smaller for very small columns. This is in line with the assumption that most of the scatter is produced by the spatial and temporal variability of water vapour.

Both the AMC-DOAS and the WFM-DOAS results agree on average better with ECMWF data than with SSM/I data. This indicates that both methods are not only applicable over ocean scenes but also over land, and that they benefit from the enhanced signal over land caused by the higher albedo.

6 Conclusions

For the first time, global total water vapour column amounts have been retrieved from SCIAMACHY data in the spectral region around 700 nm using two different methods, AMC-DOAS and WFM-DOAS. These methods have been successfully applied on GOME data in previous studies and have been adapted for the analysis of SCIAMACHY data. Both algorithms include inherent methods to assess the quality of the retrieved columns. Comparisons of the derived SCIAMACHY water vapour columns with corresponding SSM/I and ECMWF data have shown an excellent correlation for both methods. This is the case not only for ocean scenes but also over land, which is an advantage with respect to SSM/I. However, both methods compensate for a currently unexplained systematic deviation of 10% which needs further investigation. Looking at the slope of a fitted straight line, the average agreement between the different data sources is better than 5%, irregardless of ground scene, although there is a significant scatter (in the order of 0.5 g/cm²) in the data which can be mainly attributed to the high spatial and temporal variability of water vapour. The water vapour

columns derived from SCIAMACHY measurements are typically slightly smaller than those of the correlative data sets; the mean deviation between SCIAMACHY and SSM/I data is about 0.15 g/cm^2 ; the mean deviation from ECMWF data is less than 0.1 g/cm^2 .

Due to the currently reduced availability of consolidated SCIAMACHY data, the algorithms have up to now only been applied to a small amount of data. In this sense the promising results presented here are only valid for a rather limited time interval. However, first investigations using SCIAMACHY data for other days show similar results, and it is planned to extend the analysis range in further studies.

Therefore it can be concluded that both the AMC-DOAS and the WFM-DOAS method are able to retrieve reasonable total water vapour columns from SCIAMACHY data not only over ocean but also over land. The algorithms are reliable and in principle fast enough to allow for an operational processing and are thus good candidates for a future “visible water vapour” data product of SCIAMACHY which is currently under discussion.

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