SCIAMACHY H₂O column validation by the Atmospheric Chemistry Validation Team

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ABSTRACT
Comparisons have been performed for two non-operational SCIAMACHY H₂O products with sonde measurements performed at different stations, ECMWF Reanalysis data (ERA) and ATOVS satellite measurements. Both retrieval methods show water vapour columns that are systematically lower than correlative measurements. The main reasons for this offset are thought not to be algorithm related.

1. INTRODUCTION
Due to the built up of ice in channels 7 and 8, the operational SCIAMACHY water vapour product is not mature enough for validation.

However, several institutes have been working on scientific (non-operational) algorithms to retrieve water vapour columns from the SCIAMACHY measurements in the visible channels. Currently two of these retrievals deliver scientific products available for validation: The AMC-DOAS (Air Mass Corrected Differential Optical Absorption Spectroscopy) retrieval by IFE-Bremen and the SSP (Spectral Sampling Parameterization) retrieval by MPI-Mainz.

In this paper both scientific products will be compared to integrated radiosonde measurements and water vapour columns from ECMWF or the ATOVS satellite instrument.

The SCIAMACHY data used in the validation exercises are for the SCIAMACHY validation reference dataset containing about 1900 states from July to December 2002.

2. SCIENTIFIC PRODUCTS

2.1 AMC-DOAS
The so-called Air Mass Corrected Differential Optical Absorption Spectroscopy (AMC-DOAS) approach has been originally developed for the analysis of GOME data. Recently, it has also been successfully applied to SCIAMACHY's nadir measurements in the near-visible spectral region around 700 nm. For details see [1].

Similar as the standard DOAS approach, AMC-DOAS determines the amount of an absorber from the differential structures in the measured spectrum, but the method additionally includes:

1) A parametrisation of the saturation effect: The strongly wavelength dependent absorption of water vapour is not resolved by the measuring instrument (SCIAMACHY), which results in a non-linear relation between the differential absorption and the absorber amount.

2) An Air Mass Factor (AMF) correction derived from O₂ absorption in the same spectral region where H₂O absorbs. This is why the AMC-DOAS fitting window has been chosen to be 688 - 700 nm where spectral structures of both O₂ (B band) and water vapour with similar strength are present.

For the AMC-DOAS water vapour retrieval a cloud-free tropical atmosphere is assumed. Using the AMF correction it is possible to derive water vapour total columns also for partly cloudy scenes and other regions than the tropics.

However, especially over clouds the quality of the retrieved water vapour columns is naturally limited by the amount of information reaching the instrument; because SCIAMACHY cannot see through clouds missing information from below the clouds will be estimated from climatological information used in the radiative transfer calculations. In this context, the AMF correction is used as a quality criterium:

A large deviation of the AMF correction factor from 1 is an indication for a large deviation between the real conditions and the model atmosphere used in calculating the AMF.

Experience has shown that retrievals resulting in an AMF correction factor larger than 0.8 are reliable for solar zenith angles up to 88°.

All SCIAMACHY validation data have been processed using the (uncalibrated) ASM diffuser solar spectrum.
as reference (marked by "D9" in the validation master set data). To be compliant with the ASM diffuser spectrum, except for a wavelength calibration the SCIAMACHY spectra have only been corrected for dark current. All measurements of the validation data set have been processed, but the distributed AMC-DOAS data set contains only result results, which passed the AMC-DOAS inherent quality check, i.e. data with an air mass correction factor larger than 0.8 and solar zenith angle up to 88°.

First comparisons with SSM/I and ECMWF data indicate that the SCIAMACHY AMC-DOAS water vapour columns are systematically about 10% lower than these correlative data. This systematic offset is currently under investigation and has not been corrected for the validation data set.

2.2 SSP

For the purpose of water vapour retrieval from GOME and SCIAMACHY the Spectral Sampling Parameterization (SSP) [2,3] retrieval technique has been developed. The algorithm aims at performing the spectral sampling of the usually highly non-linear water vapour absorption response in an accurate and computationally efficient way. The technique is therefore useful for instruments that measure in the visible and IR spectral regions at relatively high resolution. SSP spectrally samples the exponent of the optical thickness in a way that provides straightforward implementation in solutions of the equation of radiative transfer by preserving the vertical impact of pressure and temperature on the spectroscopy. The only a priori information used for SSP retrievals in the visible bands of SCIAMACHY and GOME are pressure and temperature profiles which are currently taken from a climatology but will be taken directly from ECMWF starting with an new, improved version of the retrieval code, which is currently implemented and tested. Water vapour subcolumn-profiles (WVSCP) are retrieved simultaneously with the surface or cloud/aerosol albedo. From the WVSCP either a total water vapour column (TWVC) can be calculated or a regularized profile using a Phillips-Tikhonov-Twomey regularization (SSP-TIKH) [3]. For the purpose of this paper only TWVC retrievals from SSP in the visible bands of SCIAMACHY and GOME are pressure and temperature profiles which are currently taken from a climatology but will be taken directly from ECMWF starting with an new, improved version of the retrieval code, which is currently implemented and tested. Water vapour subcolumn-profiles (WVSCP) are retrieved simultaneously with the surface or cloud/aerosol albedo. From the WVSCP either a total water vapour column (TWVC) can be calculated or a regularized profile using a Phillips-Tikhonov-Twomey regularization (SSP-TIKH) [3]. For the purpose of this paper only TWVC retrievals from SSP in the visible bands of SCIAMACHY and GOME are considered (hereafter referred to as SSP-TIKH). SSP-TIKH is also used to deliver realistic retrieval-error estimates from contributions of shot-noise and systematic model biases. Mean pixel cloud-top pressure is simultaneously retrieved from the strong (O$_2$)$_2$ absorption signals around 580 or 620 nm depending on which water vapour absorption band is employed for the retrieval. So far, only global clear-sky retrievals (cloud-cover fraction less than 10%) have been considered. No attempts have been made for the current versions of SSP to account for higher cloud-coverage. For SSP, the retrieval accuracy is better than 0.5 cm for all cloud-free (or above cloud) and all surface cases including the "worst-case" impact of aerosols (around 0.3 cm for moderate aerosol-impact scenarios) based on more than 300 representative GOME retrievals from the weak 590 nm WV-absorption band.

Comparisons with SSM/I data reveal differences in total WVC below 30% [3]. First inter-comparisons of the total water vapour column retrieved from GOME with data from the DMSP SSM/I microwave sounder series, ECMWF and radiosondes have already been performed with correlation coefficients as high as 0.79 for pixels with low cloud-cover. Comparisons of global monthly mean GOME retrievals with NVAP (NASA water vapour project) show the capability of water vapour retrievals from the visible region of the spectra to deliver good results over all surface types.

3. RESULTS

3.1 AMC-DOAS

For the comparisons of AMC-DOAS with radiosondes measurements, colocated measurements are used on the same day and within 1000 km of the center of the SCIAMACHY pixel. Data from 17 stations (l’Aquila, Belgrano, De Bilt, Hohenpeissenberg, Jokioinen, Lauder, Legionowo, Marambio, Ny Alesund, Orland, Paramaribo, Payerne, Scoresbysund, Sodankyla, Thule, Uccle and Yakutsk) has been retrieved from the NILU calval database.

Fig. 1 shows a comparison between the AMC-DOAS SCIAMACHY measurements and integrated radiosonde measurements from the station Legionowo in Poland (52.2°N, 20.6°E). The SCIAMACHY measurements are in the same order of magnitude as the sonde measurements and follow the large-scale fluctuation in time. The mean difference between the SCIAMACHY and sonde measurements is -15% (SCIAMACHY being lower than the integrated sonde measurements) with a standard deviation of 38%.

In Fig. 3 we have plotted the relative difference as function of distance between the center of the SCIAMACHY pixel and the launch site of the sonde. No clear relationship can be seen from this figure.
Fig. 1. AMC DOAS SCIAMACHY water vapour columns [cm] (magenta squares) and integrated sonde water vapour measurements [cm] (blue diamonds) for Legionowo station as function of the date in 2002.

Fig. 2. Relative difference between the water vapour columns from SCIAMACHY (AMC-DOAS) and sondes for Legionowo as function of the date.
Fig. 3. Relative difference between the water vapour columns from SCIAMACHY (AMC-DOAS) and sondes as function of the distance between the center of the SCIAMACHY pixel and the sonde measurement.

Fig. 4 and 5 show the sonde measurements at Jokioinen station in Finland (60.8°N; 23.5°E), colocated SCIAMACHY measurements and the relative difference between them.

The mean difference between the SCIAMACHY and sonde measurements for this station is 0.2% with a standard deviation of 35%. Next to these 2 stations, we had data from 5 other stations (de Bilt, Hohenpeissenberg, Sodankyla, Uccle, and Payerne) with more than 20 colocations. All these 7 stations are located within 46°N and 68°N. The mean difference between the SCIAMACHY and sonde measurements for these 7 stations is –10.8% with a standard deviation of 34.6%. For all 17 stations used in this study, the mean difference is –6.6%.

For the comparisons with ATOVS measurements, colocated measurements are used on the same day within 200 km, and only the closest colocation for each SCIAMACHY pixel has been used.

Fig. 6 shows the relative difference between the AMC-DOAS SCIAMACHY measurements and colocated ATOVS water vapour columns as function of the solar zenith angle.

Table 1 gives the mean differences and standard deviation for different solar zenith angles.
Fig. 4. AMC DOAS SCIAMACHY water vapour columns [cm] (magenta squares) and integrated sonde water vapour measurements [cm] (blue diamonds) for Jokioinen station as function of the date in 2002.

Fig. 5. Relative difference between the water vapour columns from SCIAMACHY (AMC-DOAS) and sondes for Jokioinen as function of the date.
Table 1. Mean relative difference and standard deviation between water vapour columns from AMC-DOAS SCIAMACHY and integrated sonde water vapour measurements.

<table>
<thead>
<tr>
<th>Solar zenith angle (sza)</th>
<th>Mean difference</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>All sza</td>
<td>-15.8%</td>
<td>41.5%</td>
</tr>
<tr>
<td>&lt; 30º</td>
<td>-5.3%</td>
<td>23.4%</td>
</tr>
<tr>
<td>30º-60º</td>
<td>-15.2%</td>
<td>31.9%</td>
</tr>
<tr>
<td>&gt;60º</td>
<td>-16.9%</td>
<td>48.2%</td>
</tr>
</tbody>
</table>

These results are in agreement with previous validation of the AMC-DOAS H₂O product (not based on the SCIAMACHY validation reference set) with SSM/I and ECMWF data, where a systematic offset of 10% was found, SCIAMACHY being lower. The same results were found using a different retrieval method, the WFM-DOAS method, indicating that this is a systematic effect and probably not related to the algorithm. Possible reasons given for the offset are:
- Calibration errors.
- Insufficient knowledge of slit function.
- Potential errors in spectral data base (cross sections).
- Systematic effects of clouds and/or surface albedo.

3.2 SSP

Fig. 7 shows the two-monthly averaged SCIAMACHY water vapour columns from the SSP-TIKH algorithm and those from the ECWMF Reanalysis dataset for July and August 2002. The cloud mask derived from SSP has also been applied to the ERA dataset. The employed SCIAMACHY validation dataset is focussing on the northern hemisphere and regions with high density in high quality sonde measurements. Therefore, and due to cloud masking, there are significant gaps in this dataset concerning the tropics, Asia and the southern hemisphere.

SSP-TIKH resembles the variational pattern of the ERA data quite well, however, with a significant negative bias with respect to the ERA total column values.

Figs. 8 and 9 show the correlation between the monthly averaged SCIAMACHY water vapour columns from the SSP algorithm and ECMWF and radiosonde measurements, respectively. Here again, only the cloud-free or low-cloud fraction SCIAMACHY measurements have been considered.

The SCIAMACHY measurements show systematically lower values by 20-25% for both comparisons. These results are in agreement with previous validation of the SSP H₂O product (not based on the SCIAMACHY validation reference set) with SSM/I, radiosonde and ECMWF data [3]. For comparison Fig. 10 shows correlations between SSP-TIKH retrievals from the GOME instrument and radiosonde data from the operational ECMWF radiosonde network. The comparisons show correlations up to 0.7 with standard deviations of 0.4 cm - which can predominantly be explained by spatial variational differences - and very small offsets below 2% (Fig. 10). In contrast, the standard deviations for both comparisons in Fig. 8 and 9 are between 0.5 and 0.7 cm with a negative offset of 20 to 25%, both significantly above values that can be achieved by GOME SSP-TIKH retrievals. For the presented comparisons using SCIAMACHY retrievals one has also to keep in mind that both TWVC, as well as cloud-top pressure retrievals, are usually affected simultaneously by problems with calibrated level 1 data. Comparisons with other datasets relying on “cloud-free” pixel are therefore also influenced by problems with the retrieval of an appropriate cloud-mask.

We conclude that for the observed offsets for SCIAMACHY/SSP-TIKH TWVC retrievals compared to independent measurements similar reasons can be given as for the SCIAMACHY/AMC-DOAS algorithm. Due to the success of the high quality GOME TWVC retrievals using SSP-TIKH, it is expected that the results can be improved after forthcoming significant improvements of the quality of the level 1 calibrated SCIAMACHY dataset.

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References

Fig. 7. Two-monthly averaged SCIAMACHY water vapour columns from the SSP-TIKH algorithm and ECWMF (ERA) for July and August 2002.
Fig. 8. Correlation between SCIAMACHY water vapour columns from the SSP-TIKH algorithm and ECWMF for July and August 2002.

Fig. 9. Correlation between SCIAMACHY water vapour columns from the SSP-TIKH algorithm and ECMWF operational radiosonde network for July and August 2002. Only sondes lying within the area covered by a SCIAMACHY ground pixel and correlated in time within 3 hours are considered. Stars surrounded by a purple circle are results from Asian sondes, whereas those marked by a green circle are from Europe. Other results are from unclassified regions.
Fig. 10. Same as Fig. 9 but for correlation between GOME water vapour columns from the SSP-TIKH algorithm and ECMWF operational radiosonde network for Augst 1995 to 2000. Stars surrounded by a yellow circle are results from North-American sondes.