VERIFICATION OF SCIAMACHY LV1B V6 NADIR DATA

BY RETRIEVALS OF CO, CH4, CO2, O3, NO2, AND BRO

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ABSTRACT

In this paper we report the results of a verification of SCIAMACHY nadir lv1 data version V6.02 undertaken at the University of Bremen. The verification is performed by application of scientific DOAS type retrievals on the data and comparison of the results and residuals with those obtained using data from the previous processor version V5.04. In addition, the effect of using different solar irradiance measurements is investigated and for NO_2 a comparison with operational lv2-data is made.

1. INTRODUCTION

The main products retrieved from measurements of the SCIAMACHY instrument on ENVISAT are columns and vertical profiles of atmospheric species. For most trace gases, retrieval methods based on the Differential Optical Absorption Spectroscopy (DOAS) method are used, usually in combination with other approaches. The only way to validate the results is to compare them quantitatively with independent measurements.

However, the quality of the retrievals depends crucially on the quality of the radiances and irradiances used, and therefore analysis of fitting results can provide indication on how good the lv1 data are. In addition, as the algorithms developed at the University of Bremen are independent of those used in the operational processor, comparison of the lv2 products obtained from the two processors can provide verification for the operational processor.

Here, we present results from application of a number of different algorithms for the retrieval of O_3, NO_2, BrO, CO, CO_2 and CH_4 from SCIAMACHY nadir measurements. For the exercise, subsets of the validation data set provided by ESA have been used and the two lv1 data version V5.04 and V6.02 were compared. In all cases, the program SciaL1C was used to extract calibrated radiances and irradiances (lv1c data). Different settings were used for the calibration as explained in detail in the corresponding sections.

The main question to be answered by this study is whether or not the V6.02 data are an improvement over the current V5.04 data set.

2. RESULTS

2.1. O3

SCIAMACHY Weighting Function DOAS (SCIA WFDOAS) [1] is one of the few DOAS retrievals that is based upon ESM solar diffuser data for sun-normalised radiances. The reason is that radiometrically calibrated radiance data are required for the auxiliary cloud and albedo retrieval. Therefore, full calibration is used in the extraction. The SCIA WFDOAS Version 2 (scaled SCIA FM cross-section by +3.8%, Lamsal O_3 climatology [2]) has been run for one orbit using both L1C versions 5 and 6 (see Figure 1). The results show a 0.5-1% low bias for L1C V6. The spectral fit residuals increased by about 20% as compared to L1C V5.

A possible reason for this change in the residuals may come from the updated keydata that are now interpolated on a finer wavelength grid that may have produced additional differential structures.

In summary, the use of V6.02 data does not improve the retrieval of O_3 but rather increases the RMS. However, the effect on the ozone columns is small.

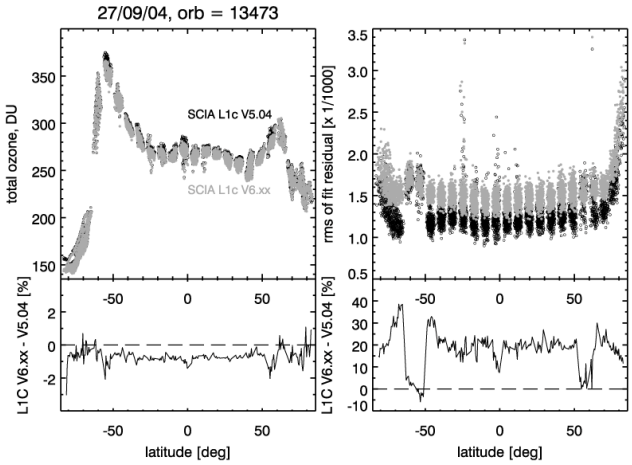

Figure 1 SCIA WFDOAS V2 O_3 retrieval using L1C Versions 5.04 (black) and 6.02 (grey). Left: total column, right: spectral fit residuals.

2.2. CO, CO2, CH4

The University of Bremen scientific retrieval algorithm Weighting Function Modified DOAS (WFM-DOAS) [3] has been applied to SCIAMACHY operational Level-1 v6.02 and v5.04 near-infrared nadir spectra to retrieve total columns of CO from channel 8, methane from channel 6 and CO_2 from channel 6. The retrieval results obtained with v6.02 have been compared with the results obtained with v5.04 to see if there are any differences, especially if there are any problems with the v6.02 spectra which have not been observed for v5.04.

Initially, at a very early stage, available 6.02 Level 1 orbit files have been investigated which were NOT part of the official verification data set. It has been found that the near-infrared nadir spectra were very "strange", i.e. showed large strange differences compared to v5.04 (not for channel 4 but for channels 6 and 8). A problem report has been sent on 23 June 2006 to eohelp@esa.int. Analysis performed at DLR and SRON have clarified this. It has been found out that the orbits which have been analysed were NOT representative in all aspects for version 6.02. They had been generated with keydata files NOT appropriate for the near-infrared. They had been generated "off line" to investigate the limb pointing problem. In summary: The problems that have been reported in the 23 June 2006 problem report are not representative / not applicable for version 6.02.

After the official version 6.02 verification data set were available the analysis has been repeated, this time with the correct v6.02 orbit files. The results are shown in Figure 2 As can be seen, the columns retrieved using Level 1 v6.02 are basically identical with the columns retrieved using v5.04. This indicates that the near-infrared nadir spectra of version 5.04 and version 6.02 are nearly identical as it should be as only minor changes in v6.02 compared to v5.04 have been implemented for near-infrared/nadir. Some differences have been observed for CO. CO retrieval is however very sensitive to even minor changes of the spectrum. As also shown in Figure 2 the CO is nearly exactly identical for certain ground pixels (here: latitudes less than about 52 deg) but somewhat different for other ground pixels. More studies are needed to find out if CO retrieval using 6.02 is better compared to 5.04. This requires processing and analysis of large amounts of data and is out of scope of the present study but will be investigated in the future. Similar remarks apply to the other gases, e.g. methane, where (small) differences are visible.

In summary: No problems have been identified for version 6.02 near-infrared nadir spectra

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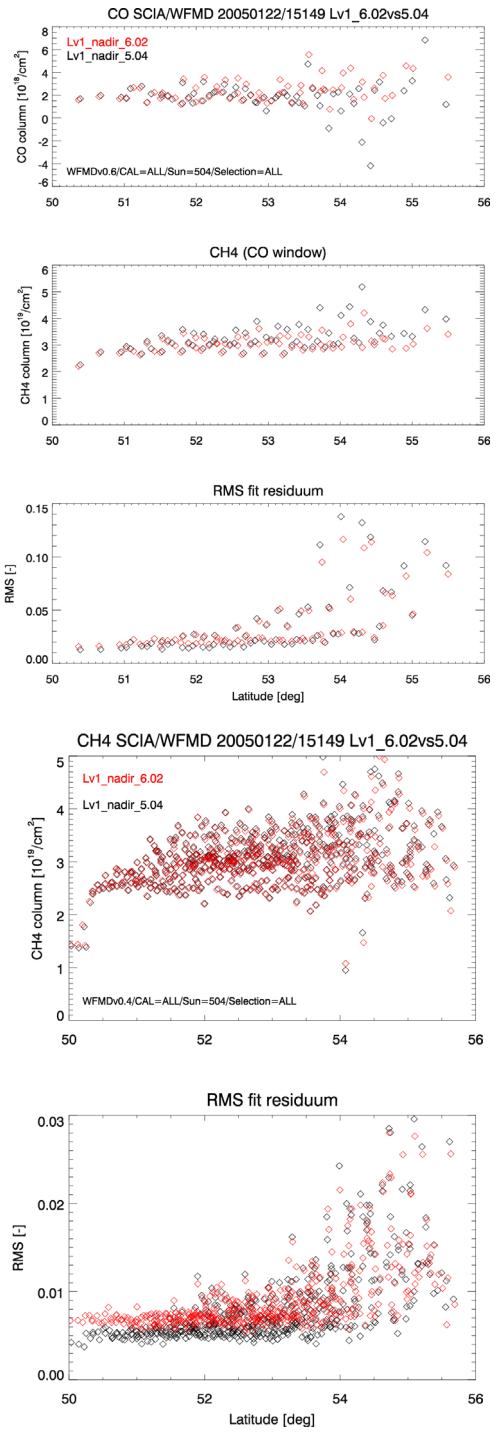

Figure 2 Comparison of retrieved gas columns using version 6.02 spectra (red) and version 5.04 spectra (black) for orbit 15149 from 22-Jan-2005. From the top: CO from channel 8, CH_4 from ch.8, RMS. Methane from channel 6 and RMS Nominal calibration has been used (-cal 0,1,2,3,4,5,6,7) and the same solar reference spectrum (nominal ESM v5.04 SMR). Retrieval results for all pixels are shown without any filtering for clouds etc.

2.3. NO2

For NO_2 which is retrieved in channel 3, the following verification activities have been performed:

1. Comparison of slant columns and residuals of NO_2 DOAS fits using Level-1 v6.02 and v5.04 data covering the full validation data set
2. Study of the impact of using different solar spectra in the retrieval (2003 data only)

In all cases the extraction of the master set data was performed using scial1c_rev1.23. The DOAS settings for the NO_2 fit are those used in the NRT scientific DOAS product produced at the IUP Bremen [4] (wavelength window 425 – 450 nm, including O_3, NO_2, O_4, H_2O, Ring, Undersampling, constant offset, and a polynomial with 3 coefficients). All tests were performed with calibration settings 0 1 2 5.

Although a large number of data points are included in these tests (about 900 000), it should be noted that as result of their non-random distribution over the globe, the results are probably not representative for the global dataset provided by SCIAMACHY. The test will therefore have to be repeated with a more representative data set as it becomes available.

Comparison of fits using V6.02 and V5.04 lv1 data

n the first exercise, data retrieved from the two Lv1 versions are compared. For this comparison, the fixed ASM solar spectrum A1 was used. The results are summarized in Figure 3
The main results are that

- Chi-square improves significantly with V6.02 for many situations.
- Largest improvements at small chi-square => memory effect or stray light correction?
- NO_2 columns vary mostly less than 5% but at small columns, differences are larger

It is interesting to investigate the geographical distribution of the fits which have improved in the new data version. In Figure 4, the difference in Chi-Square is shown for all verification data from December 2003. Clearly, only the results in some special states have improved and in addition some localised pixels. Some of the improvements can be linked to bright clouds, and all the others occur over ice and snow. However, not all data over bright surfaces are affected, and it is not at all clear from these results what the reason for these sporadic but significant improvements is.

Overall, from these results we conclude that the V6.02 Lv1 data are clearly an improvement over V5.04.

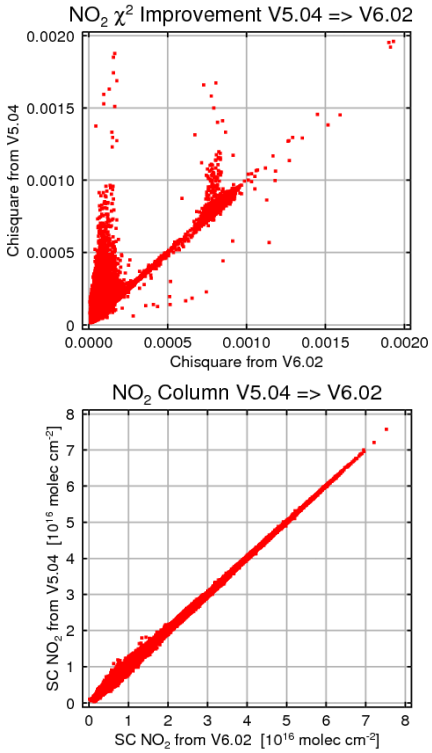

Figure 3 Change in chi-square (top) and NO_2 column (bottom) when moving from V5.04 to V6.02 Lv1 data

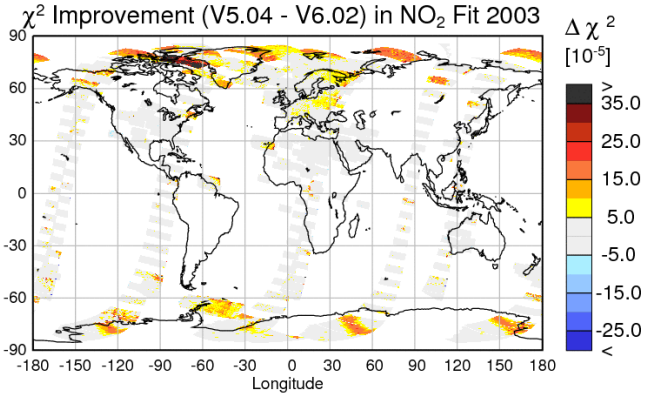

Figure 4 Difference in chi-square between the NO_2 fits on the two lv1 data versions. Reddish colors indicate an improvement in V6.02 as compared to V5.04.

Impact of different solar irradiance files

The second exercise analysed the impact of the different solar spectra available in the product. The following options were tried:

1. A1 fixed ASM solar spectrum
2. A0 daily uncalibrated ASM solar spectrum
3. daily uncalibated ASM solar spectrum from IUP Bremen lv0 extractor
4. E0 and E1 uncalibrated solar spectra
5. calibrated ASM and ESM spectra on fully calibrated (0 – 7) data

Although the SCIAMACHY instrument is very stable, small changes in performance over time still accumulate, and therefore it is foreseen to use the daily solar measurements as background in the DOAS analysis. This should provide the best fit and the smallest dependence on instrumental drifts. However, in previous lv1 data versions, the respective solar measurements were not included and therefore a fixed solar measurement (A1) had to be used.

The tests gave an unexpected result: The best fits could be produced using the fixed ASM spectrum A1, and not the daily ASM or ESM spectra. The differences are quite large as is sown in Figure 5, where the relative change in chi-square between using the A1 and A0 spectra is shown and compared to the same change but with the daily solar spectra from the IUP Bremen lv0 extractor.

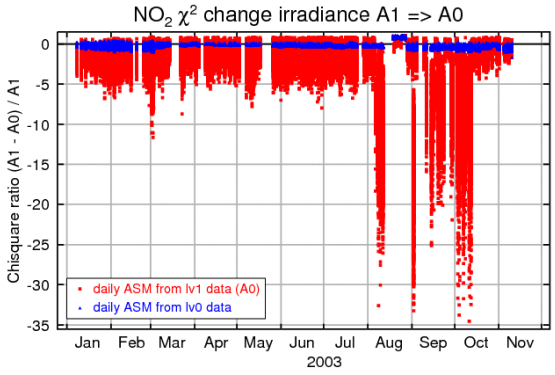

Figure 5 Relative change in chi-square of the NO_2 fit when replacing the A1 solar spectrum by the A0 daily ASM (red points) or the daily ASM spectra from the IUP Bremen lv0 extractor (blue points). Negative values correspond to worse results.

In Figure 6, the change in chi-square is shown for different solar spectra, highlighting the degree of scatter between different (groups of) data and the overall better performance of the A1 spectrum.

As was the case for the improvements between the two versions of the lv1 data, the differences are clearly not distributed randomly but rather in groups, indicating systematic differences for some parts of the verification data set. This is an unexpected and unexplained result and should be followed up.

In summary, the fixed A1 solar ASM spectrum results in the best fits for unknown reasons. The daily ASM solar spectra (A0) produce much worse fits, in contrast to the same spectra extracted from raw data at the IUP Bremen. Therefore we conclude that something is wrong with these files. The better performance of ASM compared to ESM has already been shown in previous studies.

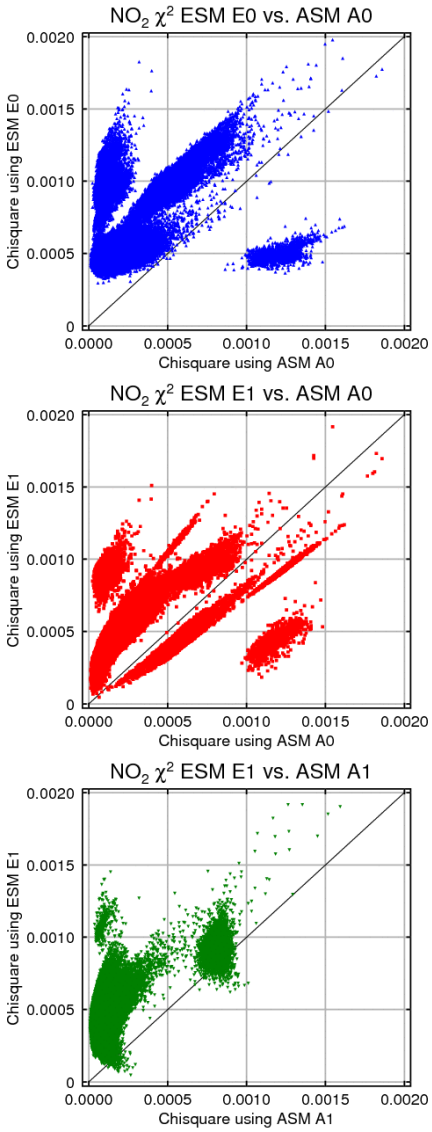

Figure 6 Comparison of chi-square obtained in NO_2 fits with different solar spectra. Comparison of AO to E0 (top, blue), of A0 and E1 (middle, red) and A1 and E1 (bottom, green). While E1 is performing better than E0, A1 is significantly better than E1 for nearly all fits.

Comparison of UBremen and operational lv2 data

As a verification of the operational NO_2 slant and vertical columns, they were compared to the columns from the scientific NO_2 product produced at the University of Bremen. As the settings used are very similar, the results should also agree well. However, as both are based on the same measurements, this can not be taken as data validation.

The results are shown in Figure 7 for both slant and vertical columns. As can be seen from the graph, there is an offset of about 1 10^{15} molec cm^{-2} by which the operational slant columns are larger. In addition, there is a scatter of about the same size within measurements from one day. According to the Product Quality Disclaimer, an offset of 1 10^{15} molec cm^{-2} is added to the operational slant columns to correct for "known calibration problems". From this comparison it appears that this offset is not necessary.

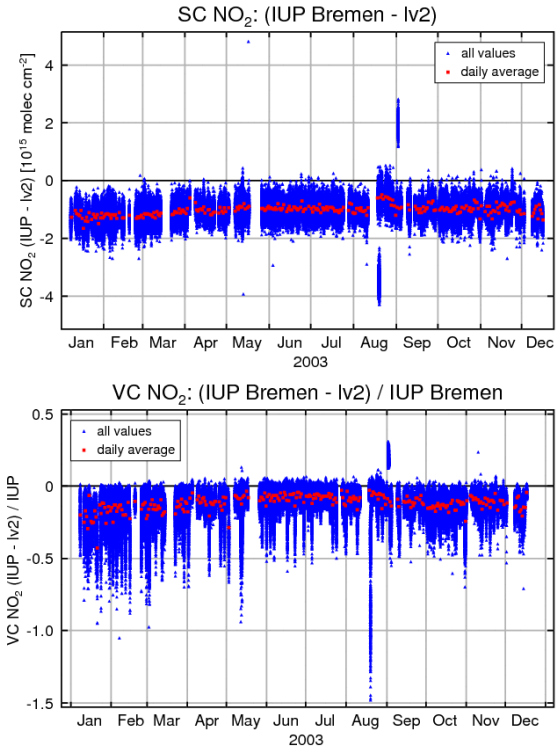

Figure 7 Comparison of NO_2 slant columns (difference, left) and vertical columns (relative difference, right) between the operational OLv3.0 product and the scientific product from the University of Bremen. Blue points are all values, red points are daily averages.

The differences for the vertical NO_2 columns are also moderate (of the order of 10 – 20% for daily averages but much larger for individual points) and are dominated by the differences in the slant columns which depending on airmass factor have different effects on the vertical columns.

In contrast to previous verification results, the airmass factor in the current version OLv3.0 are very well with those used in the scientific product (see Figure 8) which is based on a simple US standard profile without tropospheric contribution. No unexpected cloud effects have been found, and the remaining differences can be linked to the use of a more elaborate NO_2 profile climatology in the operational data product.

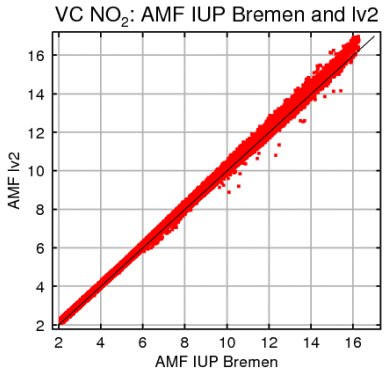

Figure 8 Comparison of NO_2 airmass factors from the operational OLv3.0 product and the scientific product from the University of Bremen. Operational airmass factors were computed by taking the ration of VC and SC from the files and therefore include the effects of clouds.

In summary, the operational lv2 slant and vertical NO_2 columns are much improved over previous versions and are reasonable agreement with the scientific product from the University of Bremen. A remaining offset of 10^{15} molec cm^{-2} in the slant columns introduced artificially in the operational processing still needs some investigation.

2.4. BrO

As result of lack of time, only a limited verification could be performed by comparison of slant columns and residuals of BrO DOAS fits using Level-1 v6.02 and v5.04 data covering the full validation data set

In all cases the extraction of the master set data was performed using scial1c_rev1.23. The DOAS settings for the BrO fit are those used in the NRT scientific DOAS product produced at the IUP Bremen [5,6] (wavelength window 336 - 347 nm, including O_3 (2 temperatures), NO_2, BrO, Ring, Undersampling, constant and linear offset, and a polynomial with 4 coefficients). All tests were performed with calibration settings 0 1 2 5.

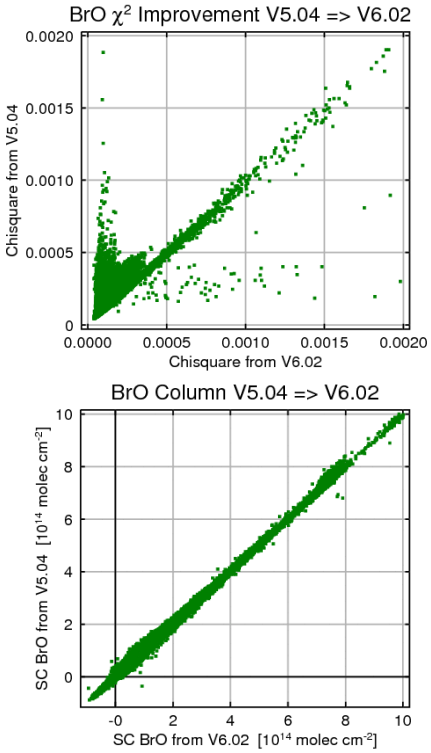

Figure 9 Change in chi-square (top) and BrO column (bottom) when moving from V5.04 to V6.02 Lv1 data.

The main results are shown in Figure 9 and can be summarized as

- Chi-square improves significantly with V6.02 for many situations.
- Largest improvements at small chi-square => memory effect or stray light correction?
- BrO columns vary mostly less than 10% but at small columns, differences are larger

The results are very similar as those found for NO_2 and it is to be expected, that the same changes to the lv1 data are responsible for the observed improvements. Again, it is not clear why only a subset of data is affected.

As in the case of NO_2, the conclusion from these results is that the V6.02 Lv1 data are clearly an improvement over V5.04.

3. Summary

The verification data set of SCIAMACHY lv1 radiances from two data versions (V5.04 and V6.02) were used to derive nadir columns of O_3, NO_2, BrO, CO, CO_2, and CH_4. The results were compared to investigate the difference in lv1 data quality between the two versions. The main results are that no significant differences exist for the IR species, slightly larger residuals but small changes in the column for O_3 and significant improvements for a subset of data for NO_2 and BrO.
A study of the effect of different solar irradiance data on the NO_2 retrieval showed that the daily ASM spectra (A0) saved in the file behave unexpectedly and result in poorer fits than when using the fixed A0 irradiance or the daily ASM spectra extracted with the IUP Bremen software. This indicates a remaining problem in the V6.02 data product.
Comparison of the IUP Bremen and the operational OLv3.0 NO_2 columns shows very good overall agreement with the exception of an offset which is explicitly introduced in the operational data and a surprisingly large scatter of the values.

4. References

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