VERIFICATION OF SCIAMACHY NEAR-REAL-TIME AND METEO LEVEL-2 PRODUCTS: O_3 and NO_2 COLUMNS, CLOUDS, AEROSOLS, AND GEOLOCATION

Jan Fokke Meirink(1), **Vincent Soebijanta**(2), **Ankie Piters**(1), **Henk Eskes**(1), **Ronald van der A**(1), **Marc Allaart**(1), **Martin de Graaf**(1), **Jean-Christopher Lambert**(2)

(1) Royal Netherlands Meteorological Institute, P.O.Box 201, 3730 AE De Bilt, The Netherlands. Email: meirink@knmi.nl, piters@knmi.nl, eskes@knmi.nl, avander@knmi.nl, allaart@knmi.nl, graafdem@knmi.nl
(2) Space Aeronomy Institute of Belgium, Avenue Circulaire 3, B-1180 Brussels, Belgium. Email: vincents@oma.be, lambert@oma.be

ABSTRACT

Verification results of some of the SCIAMACHY level-2 near-real-time and METEO products are reported. This paper focuses on geolocation, O_3 and NO_2 columns, clouds, and aerosols. The procedure to extract geolocation information belonging to a certain product from a level-2 PDS file is outlined. Also, a number of bugs in the geolocation product itself are reported. The total ozone column product is generally as expected considering some known implementation bugs. An erroneous dependence of the ozone column on the instrument viewing angle has been detected; the probable cause of this feature is presented. The NO_2 column product shows a reasonable global distribution but has considerable biases compared with GOME. A processor update is needed to improve this situation. The operational cloud products show unphysical patterns but it is demonstrated that the quality of the level-1 data is good enough to allow a reasonable retrieval of the cloud fraction. Finally, the absorbing aerosol index is physically consistent but suffers from errors in the calibrated radiances.

1. INTRODUCTION

The verification results presented here are based on the product files listed in Table 1. Some selected orbits have been disseminated to specific communities (SCCVT and ESABC) specifically for verification purposes, while a larger amount of data has been distributed to wider range of users via CD or FTP. Note that the information for one orbit is often contained in multiple files, and that many of the orbits listed are not complete. It is important to mention the software version when doing verification, since the characteristics of the different products vary between the versions. Therefore, the software version (SV) is also listed in Table 1. The near-real-time (NRT) product contains all tracers considered in the present paper. In contrast, the METEO product contains only ozone vertical column densities retrieved from the UV, together with geolocation.

The outline of this paper is as follows. Aspects of geolocation are discussed in Section 2. The verification of ozone and NO_2 is presented in Sections 3 and 4, respectively. Clouds and aerosols are the subject of Section 5. Finally, the main findings are summarized in Section 6.

2. GEOLOCATION

The geolocation data set of SCIAMACHY NRT files contains the coordinates of the ground pixel along with the viewing geometry (solar zenith, line-of-sight zenith, and relative azimuth angles). In the METEO files only the coordinates of the ground pixel are given. In this section some errors in the pixel coordinates as given in the METEO files are reported (Section 2.2). Bugs in the viewing geometry (viewing angle) were also found; these are outlined in Section 3.2. We start, in Section 2.1, with an explanation of how geolocation information belonging to a certain measurement (for example, an ozone column) should be extracted from a PDS file. The reason for this is that this procedure is not completely trivial and not well documented, and may thus easily be executed erroneously.

2.1 Extracting geolocation information belonging to a measurement

In order to optimize the ground pixel resolution, SCIAMACHY uses integration times (IT) varying with solar elevation

Proc. of Envisat Validation Workshop, Frascati, Italy, 9 – 13 December 2002 (ESA SP-531, August 2003)

Table 1: SCIAMACHY level-2 products distributed until December 2002. The table has been organized according to distribution: SCCVT = to the SCiamachy Calibration and Verification Team, ESABC = to the Envisat Stratospheric Aircraft & Balloon Campaign, CD = distributed to a wider range of users by CD, FTP = idem but by FTP.

	Distribution	Orbits	#	Date	Software Version
NRT	SCCVT	2221, 2222, 2257, 2258, 2302, 2337, 2338	7	3/8, 5/8, 8/8, 11/8	3.52
	SCCVT	2338	1	11/8	3.54
	SCCVT	2509, 2510	2	23/8	4.00
	ESABC	2250, 2355, 2443	3	5/8, 12/8, 18/8	3.53
	CD	1993 – 2098	38	18/7 – 25/7	3.51
	CD	2257 – 2721	116	5/8 – 21/8, 5/9 – 7/9	3.51, 3.52, 3.53
	FTP	3408 – 3861	195	25/10 – 27/11	3.53
METEO	FTP	2445 – 2731	120	18/08 – 07/09	3.52
	FTP	2792 – 3890	568	12/09 – 27/11	3.53

and spectral region. Variable integration times result in variable ground pixel sizes, the effective geolocation (pixel corners and center) depending on the molecule and on the solar elevation. The SCIAMACHY level-2 data product contains the geolocations of 'subpixels' corresponding to the shortest IT in the state (= a block of consecutive nadir measurements, usually about 960×400 km). The level-2 product does not contain the effective geolocation for species with larger integration times. By using the appropriate start time of the data set record (DSR time) and the IT provided in the level-2 data, the user is able to compute the effective pixel coordinates of the retrieval by co-adding the component subpixels. Unfortunately, computing is the only manner to get the effective coordinates, viewing geometry and cloud parameters of the retrieved SCIAMACHY product.

As an illustration, Fig. 1a shows what SCIAMACHY ozone forward pixels retrieved in the UV band look like when the extraction of the geolocation information is made without considering the molecule IT. In this particular case, the effective pixel contains two subpixels and only the first of them is plotted. Fig. 1b illustrates the real location of the effective pixels, which are two times larger than when using the erroneous extraction method.

Fig. 1 illustrates the effect of the geolocation misinterpretation. For instance, if we consider a distance of 300 km around a target point (e.g., a satellite, balloon, or ground-based coincident measurement, or a model or assimilation result), different pixels are selected in case the geolocation is extracted correctly or not.

The mistake described above has been made by some validation teams and even by the official product deliverer during the commissioning phase (see the errors in the METEO-BUFR files in the next subsection). EnviView and other conversion tools such as Pds2Ascii and Pds2Hdf, provided by ESA, are presently unable to give the correct geolocation coordinates of the SCIAMACHY retrieved species.

2.2 Problems with geolocation in the METEO files

Fig. 2 illustrates errors in the ground-pixel coordinates reported in the METEO files. In the PDS files (Fig. 2a) four points are given, which should be the four corners. However, the first corner is not present, while the last point is actually the center. This bug has been repaired in SV 4.00. In the BUFR files (Fig. 2b) five points are given, which should represent the four corners and the center. For points 2 to 5 this is correct, but the first point has no relation to the real location of the first corner of the ground pixel.

The BUFR files have additional problems, as can be seen in Fig. 3. Compared to the NRT (see Fig. 4a), large data gaps are present in the BUFR. Also, in the Southern Hemisphere strange ozone variations occur within one nadir state. These are caused by a loss of synchronization between the geolocation and the ozone values, so incorrect matching of geolocation with ozone (see Section 2.1).

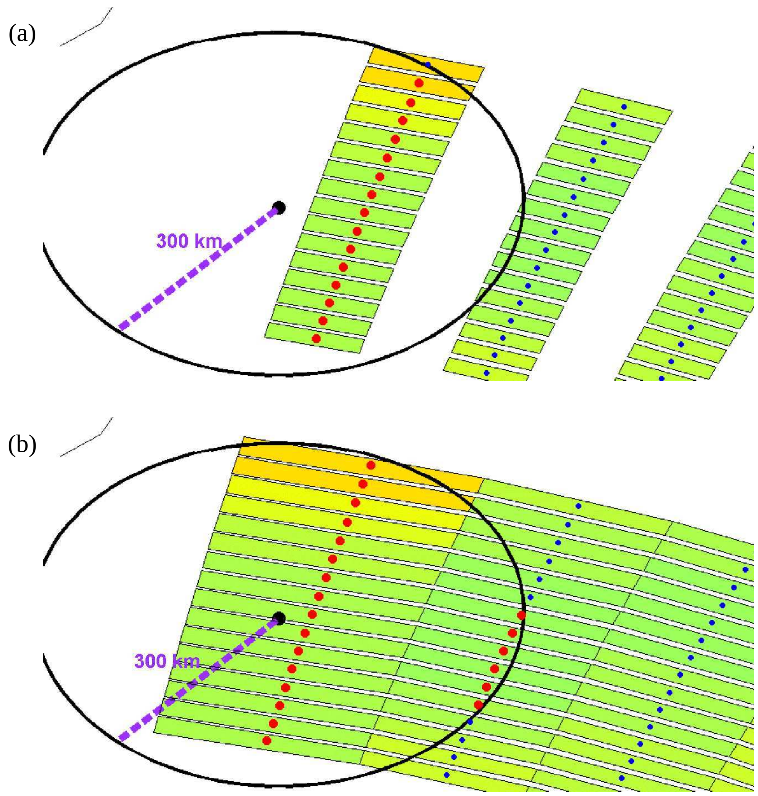

Figure 1: Extraction of the pixel coordinates belonging to a SCIAMACHY measurement (e.g., the total ozone column): (a) erroneous extraction, only the first of a total of two 'subpixels' (rectangles) is selected; (b) correct extraction, both subpixels are selected leading to the effective ozone pixels given by the rectangles. Red dots are pixel centers which are included in a circle of 300 km around an independent correlated data (black dot).

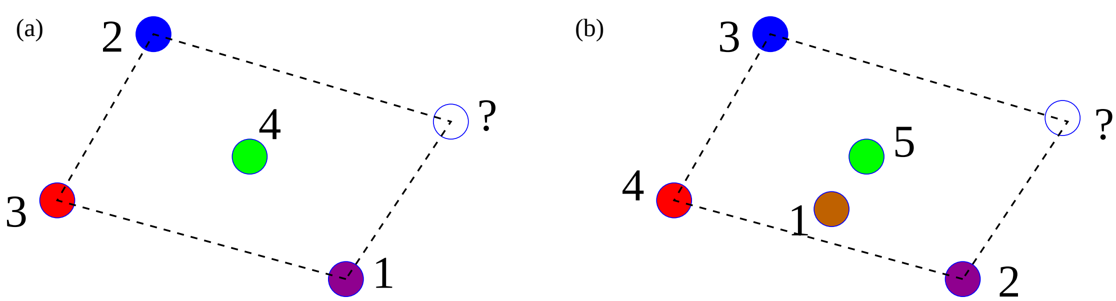

Figure 2: Coordinates of the ground pixels in a forward scan as reported in the METEO files: (a) PDS, (b) BUFR.

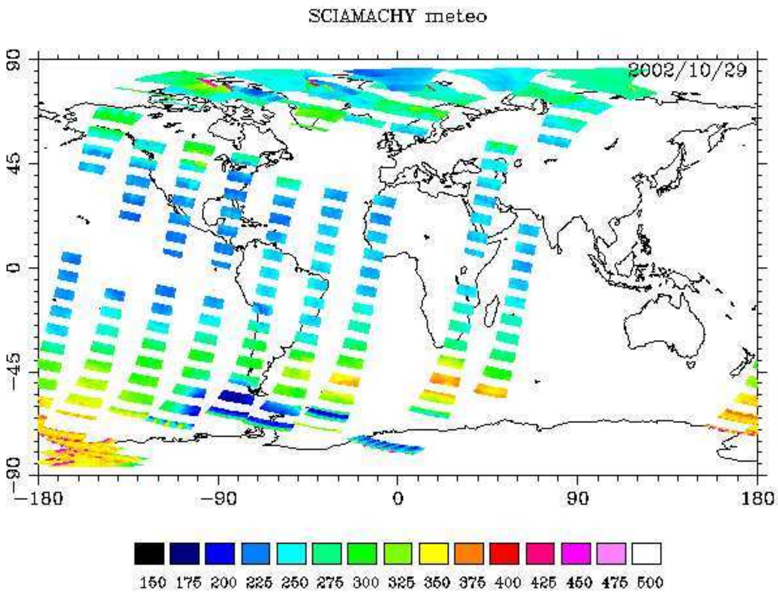

Figure 3: Ozone data from the METEO-BUFR files on 29 October 2002.

3. OZONE

A general verification of the ozone column product is given in Section 3.1. Specific problems related to the viewing angle are reported in Section 3.2.

3.1 General verification

The total ozone column density has been retrieved from the SCIAMACHY measurements in two different wavelength regions: in the UV (325-335 nm, channel 2, DOAS fitting window 0) and in the VIS (425-450 nm, channel 3, DOAS fitting window 1, as a by-product of the NO_2 retrieval). Here, the data retrieved from the UV is analysed. The ozone columns retrieved from the VIS are far too high, and will not be further discussed.

Qualitatively the ozone column from the operational product appears to be quite good. Fig. 4 compares SCIAMACHY ozone columns with an assimilated ozone field from GOME. The main features seen by GOME (e.g., the ozone hole and the ozone maximum West of the hole) are well reproduced by SCIAMACHY. A general undesirable feature is that at solar zenith angles larger than around 90 degrees the air mass factor (AMF), and thus the vertical column, is zero (the black pixels in Fig. 4a are actually all zeroes). For solar zenith angles around 90 degrees, the column is often unrealistically large or negative.

More quantitative comparisons, e.g., with GOME observations [1, and others] or with ground-based observations [2], have shown that SCIAMACHY underestimates the ozone column compared to GOME by 20-25 DU (6-9%) over most of the globe. This low bias was expected, based on the fact that up to SV 3.53 GOME-FM cross sections were used in the retrieval [3]. From SV 3.54 the SCIA-FM cross sections are used. The impact of this change is shown in Fig.5. Although up to now only a small number of pixels are available with this new software version, the figure suggests a systematic increase of the ozone column density by more than 20 DU due to the updated cross sections. Hence, it is expected that most of SCIAMACHY's negative bias will disappear.

3.2 Viewing angle dependence

The ozone columns in the SCIAMACHY level-2 NRT files have a significant dependence on the line-of-sight zenith angle

(a)

(b)

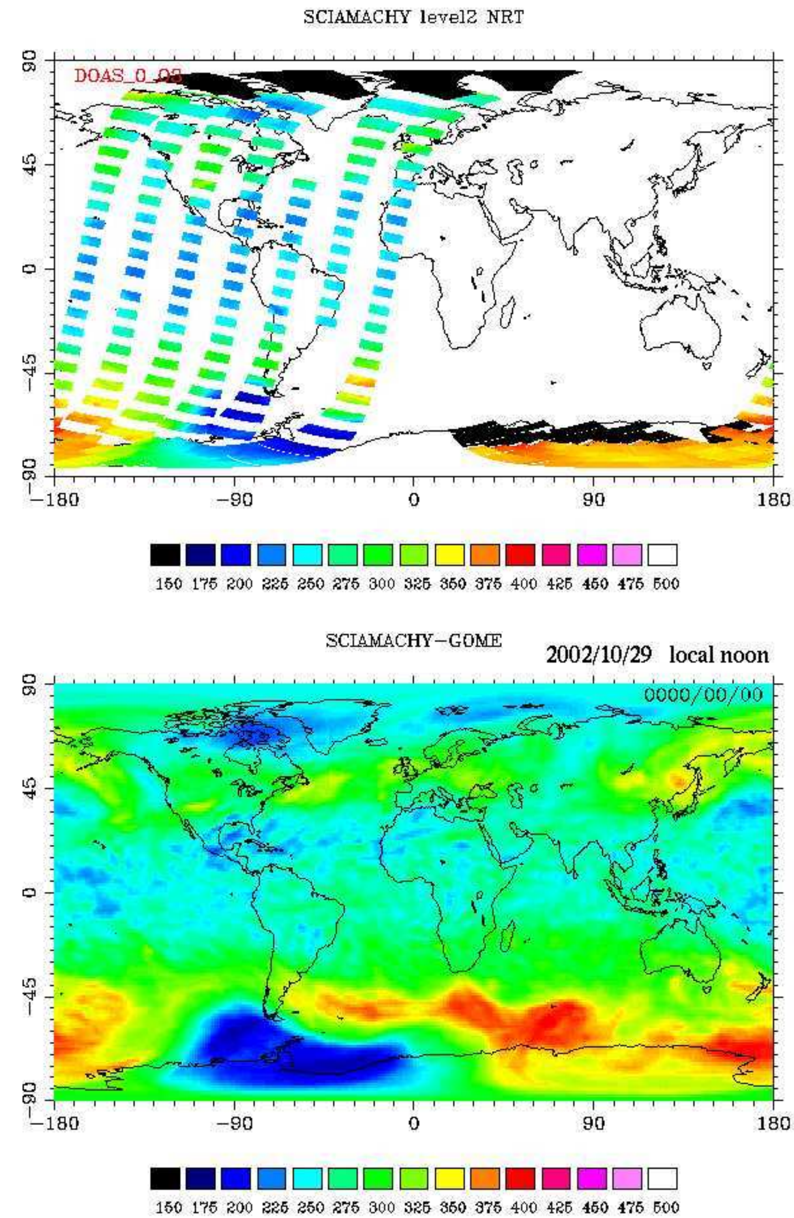

Figure 4: Comparison of (a) SCIAMACHY ozone column density (29 October 2002, SV 3.53) with (b) assimilated GOME ozone field (same day, local noon), both in Dobson Units (DU). For more information on the assimilation system, see [1].

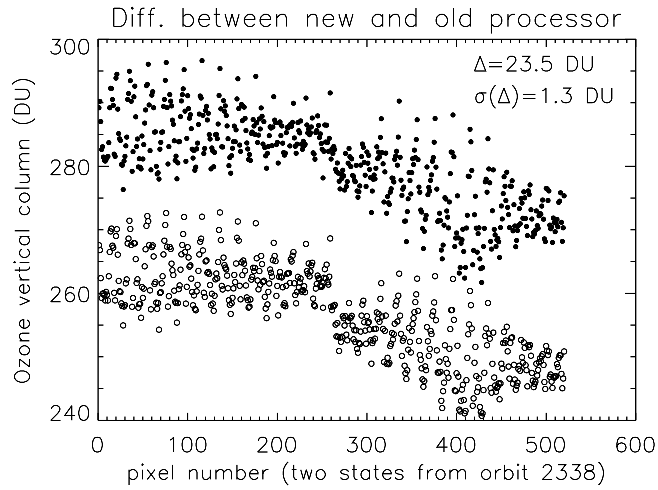

Figure 5: Comparison of vertical ozone column density for SV 3.52 (open dots) and SV 3.54 (filled dots): the plot shows all pixels from two states around the equator in orbit 2338 on 11 August.

– or viewing angle (VA) – as is shown in Fig. 6a. The dependence is approximately parabolic with the highest values appearing at the largest VA. An additional feature is that the backscan pixels are above the forward scans on the West side, while they are below the forward scans on the East side. Finally, there is a strange kink in the curve at the most westerly forward pixel. We have investigated these features in some detail, and conlude that they are due to errors in the VA used for calculating the AMF, which then leads to wrong ozone column densities.

The first error is that the VA at the satellite (SAT) is used for the calculation of the AMF, whereas the VA should be evaluated at the top of the atmosphere (TOA). This can be easily corrected for with the following relation:

$$\frac{\sin\alpha_{\mathrm{TOA}}}{\sin\alpha_{\mathrm{SAT}}} = \frac{R+H_{\mathrm{SAT}}}{R+H_{\mathrm{TOA}}}, \tag{1}$$

where α is the VA, R the radius of the Earth and H the height above the Earth's surface. Based on the corrected VA we calculate the ratio of old and new geometrical AMF's, and multiply the ozone vertical column densities with this ratio. The result is shown in Fig. 6b: the parabolic dependence has disappeared but the forward and backward scans are still different.

A second error appears to be that the VA used for the calculation of the AMF is not the VA at the centre of the pixel. Instead, the value at a PMD slightly before the centre seems to have been taken. In the corrections we have made, we have assumed that the forward-scan VA's are shifted by 0.5 degrees, while the back-scan VA's are shifted by 2 degrees (in opposite direction). Note that the Scia retrieval algorithm calculates three AMF's at three different VA's and then takes a weighted average of these. We cannot reproduce this more complex derivation but seem to be able to characterize the error quite satisfactorily. Correcting again the vertical columns leads to Fig. 6c: forward and backward scans are now consistent.

However, there is still an increase in the column going frow East to West. This can be partly due to natural variations of ozone with latitude, since on the NH (SH) the West pixels within a scan have a consistently higher (lower) latitude than the East pixels. By comparing the ozone columns with independent measurements, such dependences can be ruled out. In Fig. 6d assimilated GOME ozone columns have been subtracted from the SCIAMACHY columns (for details see [1]). Indeed, the resulting variation with viewing angle is smaller than in Fig. 6c. A significant feature remaining unexplained is the 'kink' at the most westerly forward pixel. We note that this pixel causes problems in many retrievals [4].

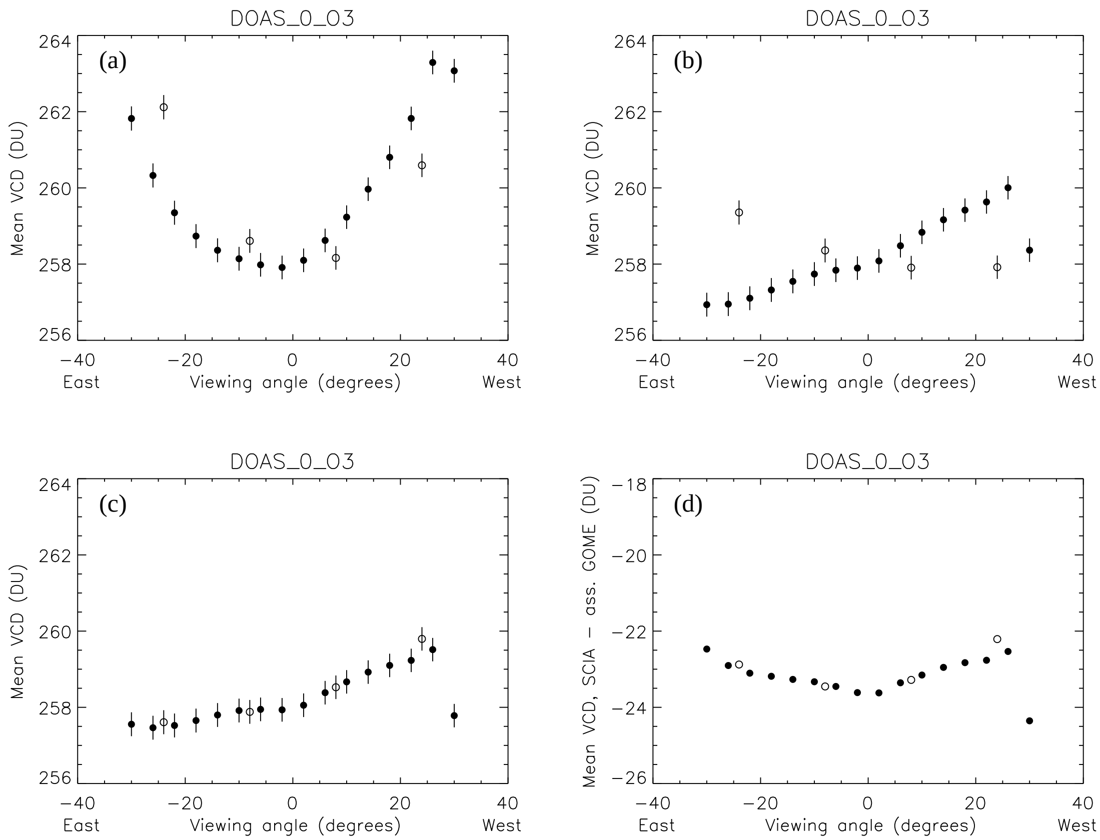

Figure 6: Mean ozone vertical column density as a function of viewing angle for all pixels with 1/4 second integration time from 25 October until 6 November (SV 3.53): (a) from level-2 product, (b) with viewing angle corrected for top-of-atmosphere, (c) with correction for viewing angle shift, (d) with assimilated GOME column subtracted. Filled dots are forward-scan pixels; open dots are backscans. The error bars reflect $\pm\sigma/n^{1/2}$, where n is the number of pixels on which the mean vertical column is based and σ the standard deviation.

4. NO_2

The total column of nitrogen dioxide (NO_2) is retrieved from SCIAMACHY measurements in the wavelength range 425-450 nm (channel 3, DOAS fitting window 1). Fig. 7 shows SCIAMACHY measurements at the end of October. In comparison with GOME (not shown here) the general global distribution appears to be captured reasonably well. However, comparisons with ground-based observations [2] have shown that considerable latitude-dependent biases are present. In particular, NO_2 is overestimated by SCIAMACHY in the Northern Hemispheric midlatitudes. By contrast, SCIAMACHY's NO_2 seems to be too low in the Tropics and most of the Southern Hemisphere. Around the Equator negative values are present (dark blue in Fig. 7a). These features are at least partly explained by the fact that the processor used for the retrieval is similar to GDP version 2.4. Known artefacts of this processor are negative NO_2 columns in the Tropics and too large tropospheric signals.

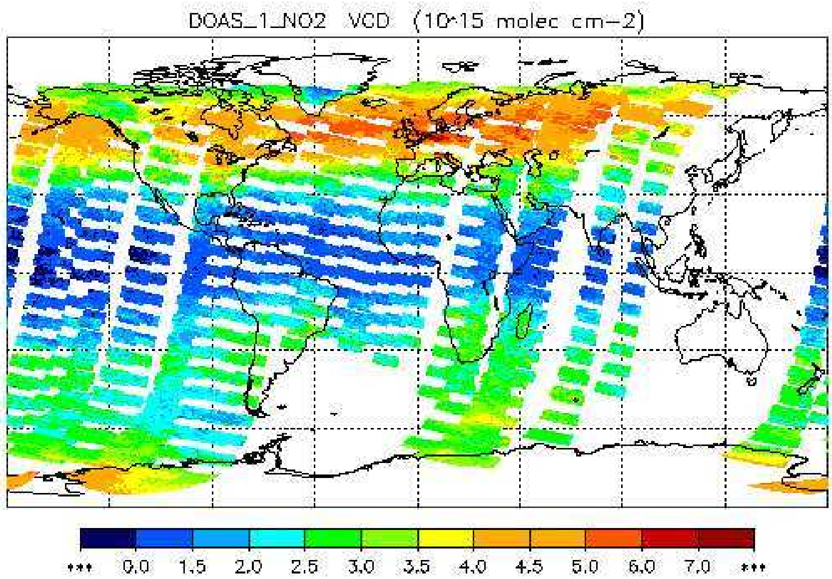

Figure 7: SCIAMACHY measurements of NO_2 column density from 25 to 31 October 2002 (SV 3.53).

As was the case for ozone, the NO_2 column becomes negative, unrealistically large or zero for solar zenith angles larger than around 90 degrees (these measurements have been omitted in Fig. 7a).

Up to SV 3.53 GOME-FM cross sections were used in the retrieval. From SV 3.54 the SCIA-FM cross sections are used. The impact of this change is shown in Fig.8. The figure suggests an average decrease of the NO_2 column density by around 4×10^{14} molecules cm^{-2} (25 %) due to the updated cross sections. Although this will improve the situation in the NH midlatitudes, the underestimation will become even larger on the SH. Clearly, an update of the processor to at least GDP version 2.7 is needed.

5. CLOUDS AND AEROSOLS

5.1 Cloud fraction

Up to SV 3.53 all cloud fractions reported in the operational product were equal to 1. From SV 3.54 this is no longer the case. However, Fig. 9a shows that unphysical regular patterns are present. Fig. 9b gives an indication of what the cloud fraction should be based on the FRESCO retrieval algorithm [5] applied to GOME radiances. Application of this algorithm to SCIAMACHY level-1 data results in Fig. 9c. Panels (b) and (c) compare reasonably, which shows that it is indeed possible to derive the cloud fraction from the SCIAMACHY measurements. Note that the wrong cloud fraction in

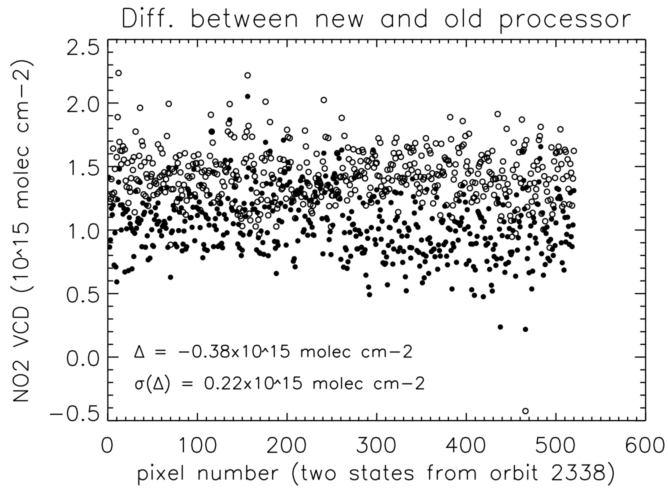

Figure 8: As Fig. 5 but for NO_2.

the operational product gives rise to errors of a few percent in the total columns of ozone and NO_2.

5.2 Cloud-top height

The cloud-top height should be a climatology but shows unrealistic regular patterns with zeroes at some locations.

5.3 Absorbing aerosol index

The AAI is discussed in detail in [6]. The AAI in the operational product (SV 4.00) is consistent with the location of clouds as seen from PMD measurements but the range over which the AAI varies is far too wide. This is probably caused by errors in the calibration of the radiances.

6. SUMMARY

The main findings presented in this paper are:

- Geolocation
  - The extraction of geolocation information belonging to a measurement from a PDS file is not completely trivial. A short explanation on this topic is included in this paper.
  - In the METEO files (PDS and BUFR format) the coordinates of the ground pixel are incorrectly specified. Additionally, in the BUFR files an erroneous matching of ozone with geolocation has been performed.
- Ozone total column
  - Based on SV 3.53, the ozone vertical column density, retrieved from the UV, was found to have a negative bias of 20 to 25 DU (6 to 9%) with respect to GOME over most of the globe, while towards the poles the bias becomes smaller (see, for example, [1,2]).
  - This underestimation was to be expected given that GOME-FM cross sections were used in SV 3.53. In SV 3.54 the SCIA-FM cross sections have been introduced: preliminary data available from this version indicate an increase by approximately 8%, which will remove most of the bias mentioned above.
  - A significant viewing angle dependence is present in the ozone vertical columns. This can be explained by the use of erroneous viewing angles for the calculation of the air mass factors. If these errors are corrected, it is expected that the viewing angle dependence will largely disappear. An anomalous value remains in the most westerly forward pixel. The reason for this still has to be identified.

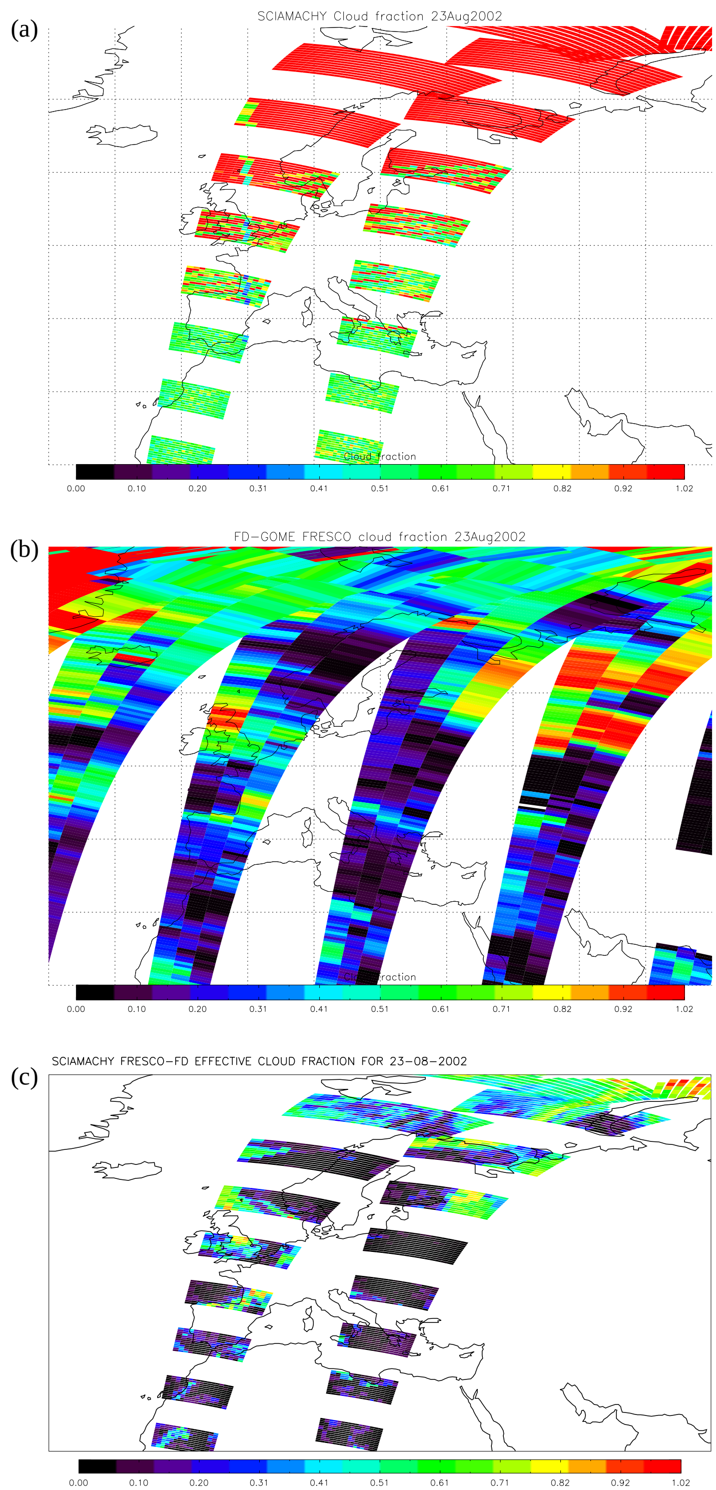

Figure 9: Cloud fraction on 23 August 2002: (a) SCIAMACHY level-2 product (orbits 2509 and 2510, SV 4.00), (b) retrieved by the FRESCO algorithm from GOME data, (c) retrieved by FRESCO from SCIAMACHY level-1 data.

- After correction, no systematic difference is found between forward and backward scans.
- Ozone columns for solar zenith angles larger than ≈ 90 degrees are either equal to 0, negative or far too high.
- Ozone retrieved from the VIS is far too high.

- NO_2 total column
  - The global distribution of NO_2 is reasonable, but considerable biases are present (see [2]).
  - The use of SCIA-FM cross sections (SV 3.54 and SV 4.00) gives lower values.
  - The processor is similar to GDP version 2.4. Known artefacts of this processor are negative NO_2 columns in the Tropics and too large tropospheric signals.
  - NO_2 columns for solar zenith angles larger than ≈ 90 degrees are either equal to 0, negative or far too high.

- Clouds and aerosols
  - For SV 3.53 and lower all cloud fractions were equal to 1. From SV 3.54 cloud fractions below 1 are present but these exhibit unphysical regular patterns. Wrong cloud fractions lead to errors of a few percent in the ozone and NO_2 columns.
  - At KNMI the cloud fraction has been retrieved using the FRESCO algorithm applied to SCIAMACHY level-1 data. The results compare reasonably with GOME.
  - The cloud-top height should be a climatology; however, at some locations this field shows unrealistic regular patterns with zeroes.
  - The spatial distribution of the absorbing aerosol index is consistent with the location of clouds as seen from PMD measurements but the range of values is too large. For a proper retrieval the level-1 data will have to be improved.

ACKNOWLEDGEMENTS

Part of this work is funded by the NIVR and OSTC. Gijsbert Tilstra is thanked for giving suggestions on the bugs related to the viewing angle. Robert Koelemeijer is acknowledged for providing the FRESCO code. José Granville is thanked for discussions about geolocation-related problems.

7. REFERENCES

1. Eskes H., et al., these proceedings.

2. Lambert J.-C., et al., these proceedings.

3. Von Bargen A., General status of level 2 product - Part 1, Envisat Calibration Review, ESTEC, Noordwijk, The Netherlands, 9 – 13 September 2002.

4. Richter A., personal communication.

5. Koelemeijer R. B. A., Stammes P., Hovenier J. W., and De Haan J. F., A fast method for retrieval of cloud parameters using oxygen A-band measurements from GOME, *J. Geophys. Res.*, Vol. 106, 3475 – 3490, 2001.

6. De Graaf M., et al., these proceedings.