DEVELOPMENT OF SCIAMACHY OPERATIONAL ESA LEVEL 2 PRODUCTS TOWARDS VERSION 5 AND BEYOND

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ABSTRACT

Since the foundation of the SCIAMACHY Quality Working Group (SQWG) in a joint ESA-DLR-NIVR inter-agency effort in late 2006, the ESA operational Level 2 processor was significantly improved w.r.t. data quality and product range. During the last two years the product list was substantially enhanced by new (total columns of SO_2, BrO, OClO, H_2O, CO, Limb BrO profiles, Limb cloud flags) and improved products (total columns of O_3, NO_2, Absorbing Aerosol Index, Limb O_3 profiles, Limb NO_2 profiles).

For example, important improvements were achieved in the O_3 and NO_2 profile calculation by implementing an upgraded retrieval scheme and using now Level 1b version 7.0 data with an improved pointing correction. Nadir products of total column O_3 and Absorbing Aerosol Index were improved by applying a radiometric degradation correction (m-factors) in the Level 1 to 2 processing step.

1. INTRODUCTION

This paper will shortly summarise on the new Level 2 offline processor SGP (SCIAMACHY ground processor) version 5 ESA products to be released in autumn 2009 and the expected data quality. The new SGP combines several types of retrieval algorithms which are actively developed by the members of the SQWG. The algorithms were implemented by DLR-IMF or were - in the case of AMC DOAS and SACURA – delivered by IUP and integrated into the SGP.

The new Level 2 version 5 contains the following retrieval schemes (in brackets the names of the developing institutions):

- Nadir O_3, NO_2, BrO: SDOAS (BIRA)
- Nadir SO_2, OClO: SDOAS (BIRA, IUP-UB retrieval settings)
- Nadir H_2O: AMC DOAS (IUP-UB)
- Nadir CO: BIRRA (DLR-IMF)
- Cloud top height & optical depth: SACURA (IUP-UB)
- Cloud fraction: OCRA (DLR-IMF)
- AAI: SC-AAI (SRON/KNMI)
- Limb O_3, NO_2, BrO: DRACULA (DLR-IMF, retrieval settings IUP-UB)
- Limb Cloud Flags: SCODA (IUP-UB)

The SGP v5 will also be used for the future fast delivery service by ESA that aims to deliver Level 2 products within 24 h after sensing, using unconsolidated Level 1 near real time data.

2. IMPROVEMENTS OF THE OPERATIONAL LEVEL 1 PROCESSOR VERSION 7

- The new operational Level 2 processor version 5 will run on Level 1 data version 7. The operational Level 1 product version 7 will have the following features in comparison to earlier version:

- Off-line m-factor data base 2002 - 2008
- Improved dynamic dead bad pixel mask (SciCal)
- Uniform stray light correction in channel 2 replaced with matrix approach to better reflect changes of the stray light with wavelength
- Implementation of correction for an onboard software/electronics error that lead to intermittently wrong geolocations on rare occasions
- Handling of Mesosphere states (OCR37)

ESA plans to switch to the operational L1 processor version 7 in autumn 2009.

3. IMPROVED AND NEW PRODUCTS OF THE SGP v5 FOR NADIR VIEWING GEOMETRY

3.1. Absorbing aerosol index

An improved product was implemented, based on the SC-AAI, the scientific absorbing aerosol index algorithm developed at SRON/KNMI [1]. The algorithm uses the absolute reflectance at 340 and 380 nm as input. Improvements w.r.t. the previous version are (1) the use of look-up tables of reference reflectances which were calculated without neglect of polarisation, (2) an improved theoretical algorithm background leading to higher accuracy and increased performance, (3) improved surface height calculation, and finally, (4) usage of m-factors to correct for instrument degradation. Full agreement with the SC-AAI based reference algorithm was achieved.

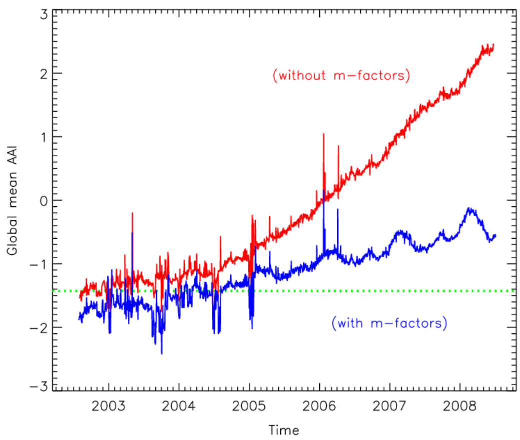

Figure 1. Global mean AAI as a function of time, for the case without m-factors (in red), and for the case where m-factors are applied (in blue). The increase is caused by instrument degradation. The m-factors correct most of the effects of instrument degradation.

Shown in Fig. 1 is the global mean AAI as a function of time, for the case without m-factors (given in red), and the case with m-factors applied (given in blue). The global mean AAI is defined the mean of all AAI measurements between 60°N and 60°S, and is regarded as almost constant, showing only a very mild seasonal variation (+/-0.2 index points at most). The dotted green line shows the level of the global mean AAI at the start of the mission. The global mean AAI for the case without m-factors has increased by more than 4 index points over the last years. For the case with m-factors applied, the increase is much lower, showing that the m-factors are able to effectively correct for most of the instrument degradation in the UV.

3.2. Cloud fractions

The cloud fraction calculation using OCRA by DLR IMF [2] was improved. The reflectance database that is used to determine the colour of the ground pixel was updated to the latest available data measured by SCIAMACHY.

3.3. O_3 total columns

The ozone total column product is based on the retrieval algorithm SDOAS developed at BIRA-IASB. Fig. 2 shows mean relative differences between the columns provided by SGP v3.01 and total O_3 measurements from OMI (OMI_TOMS), GOME (GDP 4.1) and ground-based instruments. These comparisons indicate a decreasing trend in the SCIAMACHY columns of about 0.5%/year.

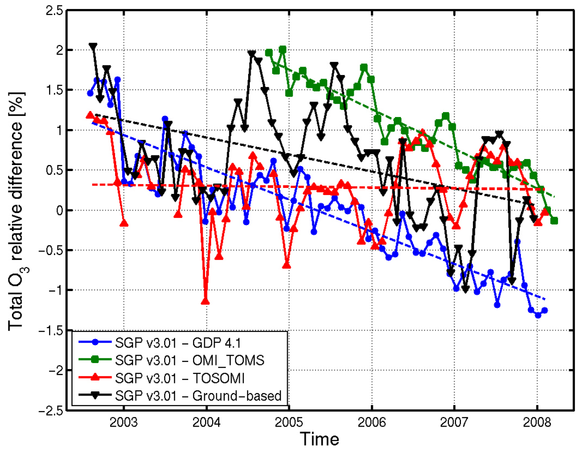

Figure 2. Comparisons of the SGP v3.01 total O_3 product with independent measurements from OMI, GOME and ground-based instruments.

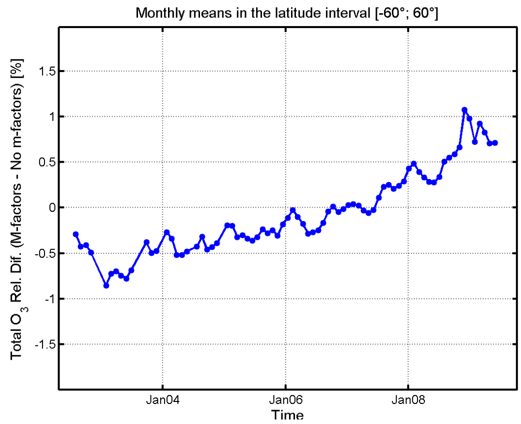

Figure 3. Meridian mean of the relative differences between the total O_3 columns retrieved with application or not of the m-factors.

Fig. 2 also compares the SGP columns to the SCIAMACHY product from KNMI (TOSOMI) based on the same level-1 version. This product is also characterized by a similar trend which indicates that it originates from radiometric calibration inaccuracies in the level-1. More details about these comparisons can be found in [3].

Fig. 3 shows the mean relative differences between the total O_3 columns retrieved with and without application of the m-factors. A slight positive trend is clearly visible in the differences. So, applying the m-factors during the calibration helps to greatly improve the temporal stability of the SCIAMACHY total ozone product. These degradation correction factors will be implemented in the SGP v5, so that one can expect a better total O_3 product.

3.4. NO_2 total columns

The already good quality of this product has been maintained during the SQWG project. In addition, the retrieval settings have been slightly changed (e.g. solar reference spectrum) so as they are more consistent with the settings used for other trace gases. These changes have even improved the quality of the DOAS fits.

3.5. BrO total columns

The BrO total column is a new product implemented in the SGP v5, which is based on the retrieval settings recommended by BIRA-IASB. The stratospheric air mass factor calculations are based on a-priori stratospheric BrO profiles provided by a climatology also developed at BIRA-IASB [4]. Using the improved retrieval settings and the new climatology, a good consistency was found between the SCIAMACHY BrO columns and the measurements from other satellite instruments (see Fig. 4).

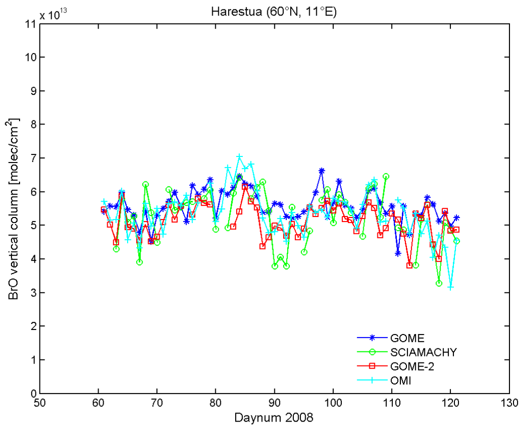

Figure 4. Comparisons of BrO vertical measurements retrieved from different satellite instruments.

3.6. SO_2 total columns

The SO_2 retrieval is based on an IUP-UB algorithm. A world map showing some hot spots of SO_2 total columns is shown in Fig. 5.

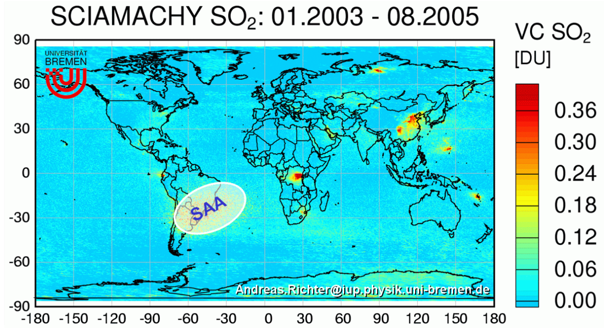

Figure 5. World map with SO_2 events between 2003 and 2005.

In the SGP v5 the SCD is at first corrected for offsets by subtraction of the SCD retrieved at the same latitude over a clean Pacific reference sector. After that, it is converted to a VCD using two types of airmass factors, simulating “anthropogenic pollution” and “volcanic eruption” scenarios. Both SO_2 data sets are placed in the operational Level 2 Product and users will have to select the more appropriate for their application. More details on the SO_2 retrieval from the SCIAMACHY data can be found in [5]. Fitting residuals agree quite well, when compared to the IUP-UB algorithm.

3.7. OClO slant columns

The OClO slant column concentration is a new product implemented in the SGP v5 and based on an IUP-UB algorithm developed for GOME data [6] and later adapted for SCIAMACHY. Since OClO is a photochemical unstable species which can only be observed at low sun, only slant columns are computed and a higher SZA cut-off (95°) was introduced for this product. Fig. 6 shows OClO slant columns for the northern winter hemisphere.

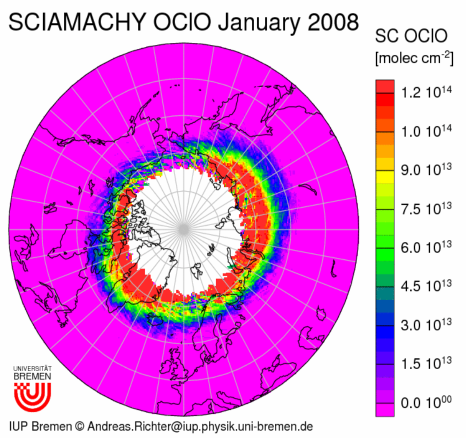

Figure 6. OClO slant columns for the northern hemisphere for January 2008 showing enhanced OClO at the polar vortex edge.

3.8. H_2O total columns

This is a new product implemented in the SGP v5 and is based on the AMC-DOAS algorithm from IUP-UB [7]. Fig. 7 shows as an example the annual mean total water vapour column derived with the scientific algorithm for the year 2008. Comparisons of the water vapour column between the operational and the scientific algorithm show good agreement.

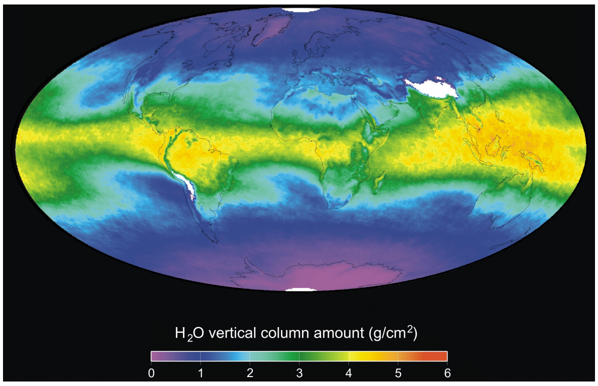

Figure 7. Annual mean water vapour total columns for 2008 derived from SCIAMACHY nadir measurements with the AMC-DOAS algorithm.

3.9. CO total columns

The operational SCIAMACHY carbon monoxide vertical columns (see Fig. 8) uses the direct fitting "Beer InfraRed Retrieval Algorithm" (BIRRA) developed by DLR-IMF [8]. Retrieval settings (nb. fitting window channel 8) are similar to those used by the scientific processors and were refined using Bremen's and SRON's recommendations for, e.g., additional masked water lines in the DBPM and wavelength shift.

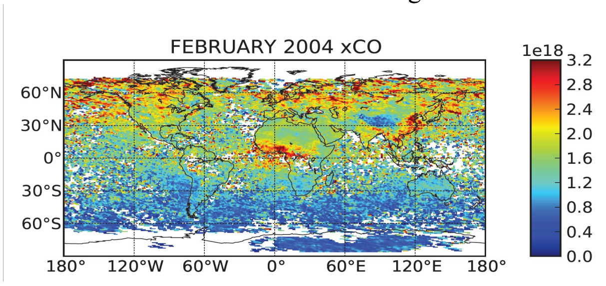

Figure 8. Averaged CO value for February 2004.

As the CO retrieval suffers from so-called "bad" detector pixels, the masking of those pixels is crucial for the quality of the retrieval. Studies by IUP-UB showed that additionally to these bad pixels, some strong water lines in the retrieval window should be masked. Following this recommendation, these lines will also be masked in operational retrieval.

The scientific WFMDv0.6 data product has been compared with MOPITT [9] and ground-based Fourier Transform Spectroscopy (FTS) measurements [10].

The comparison with the FTS data has shown that the scatter of the WFMDv0.6 CO product relative to the FTS retrievals is typically 20% for daily averages around the FTS sites. The bias (accuracy) is typically about 10%. The operational product has been compared with the results of the scientific SCIAMACHY CO column data product as generated with the WFM-DOAS version 0.6 (WFMDv0.6) retrieval algorithm [8]. Further intercomparisons with SRON's carbon monoxide product (IMLM algorithm) as well as validation using spaceborne thermal infrared sounding data (e.g., AIRS, MOPITT) and ground based FTIR data is ongoing. Recently SCIAMACHY CO has been assimilated into a global model [11] and it has been found that assimilation of the SCIAMACHY CO significantly improves the agreement of the model with the highly accurate aircraft observations given additional confidence in the good quality of the SCIAMACHY WFMDv0.6 CO column data product.

4. IMPROVED AND NEW PRODUCTS OF THE SGP v5 FOR LIMB VIEWING GEOMETRY

4.1. O_3 profiles

The Limb retrieval of trace gas profiles is based on the DRACULA algorithm by DLR-IMF [12] and uses retrieval settings from IUP-UB. The ozone profile retrieval was optimised in SGP v5. Aerosols and clouds were also taken into account to improve the accuracy towards the troposphere to about 10% in the whole stratosphere (see Fig. 9).

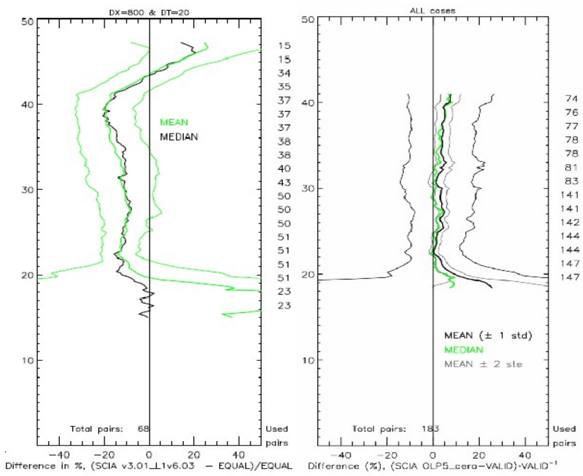

Figure 9. Comparison of SGP v3.01 and v5 ozone profiles with independent data from LIDAR and sondes. Left: Mean of differences of SGP v3.01 and EQUAL data. Right: The same for SGP v5 and VALID data (Comparisons done by A. v. Gijsel).

4.2. NO_2 profiles

The NO_2 profile retrieval model [12] was optimised in SGP v4 and verified with independent satellite data, e.g. from HALOE. The accuracy is expected to be 10% in the stratosphere (see Fig. 10). The version 4 algorithm will be used unchanged in the SGP v5.

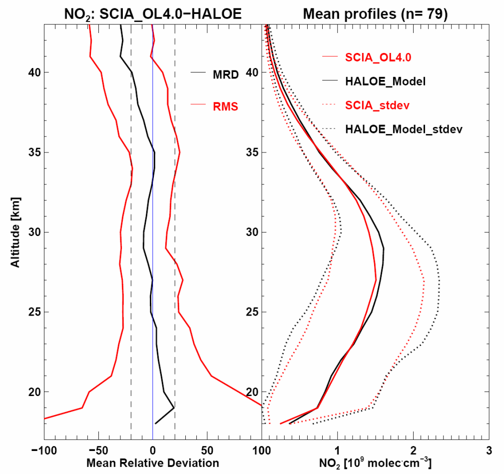

Figure 10. Validation of SGP Limb NO_2 profiles with HALOE measurements. The agreement especially below 25 km is within 7% for up to 37 km. Note that the retrieval method is only well constrained below 40 km. Together with the low densities of NO_2 this leads to higher relative deviation above that height.

4.3. BrO profiles

The BrO profile algorithm is a new product [12] implemented in SGP v5. It has been evaluated in a comparison with the BrO algorithm V3.2 from IUP-UB. An accuracy of 30% is expected (see example Fig. 11).

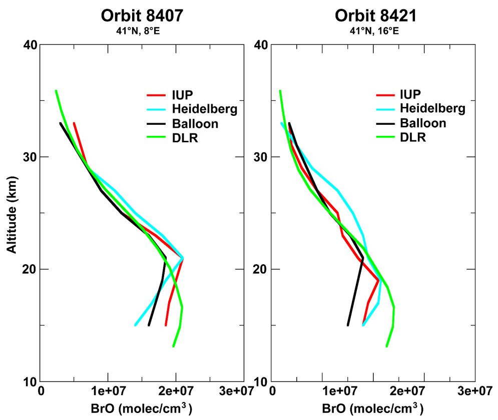

Figure 11. Comparison of different retrievals using SCIAMACHY data and airborne DOAS (black). The retrievals are from DLR (green), IUP/IFE (red; see e.g. [13]) and the University of Heidelberg (cyan [14]).

4.4. Cloud flag and top heights

The new product giving cloud flags and top heights for tropospheric clouds, ice clouds and PSCs is based on the SCODA algorithm [15] developed at the IUP-UB and has been implemented in the SGP v5. These parameters are needed to further refine the accuracy of the limb products towards the troposphere. Fig. 12 gives an example of the cloud top heights along an orbit.

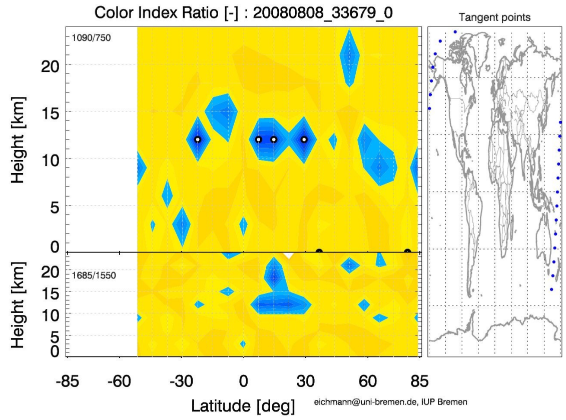

Figure 12. The color index ratio is plotted along an orbit of SCIAMACHY limb measurements during the outbreak of the Kasatochi volcano. Blue colors remark the cloud top heights for water clouds (upper panel) and ice clouds (lower panel). The right panel shows the tangent points of the measurements.

5. SUMMARY AND OUTLOOK

A summary of all improvements from Level 2 version 3.01 to version 5 and a roadmap of potential improvements and new products for future versions are shown in the tables 1-4.

Table 1. Improvements of the Nadir processor

Product Improvements Level 2	**V 3.01 2007**	**V4.0 2008**	**V5.0 2009**
Nadir Products		***not activated***	
Absorbing Aerosol Index	quality not sufficient	improved algorithm and usage of degradation corrections	no changes
Ozone total column evolution	slight trend over time (< 0.5% per year), GDP 4	degradation correction taken into account	smaller trend
NO_2	offset removed	reference spectra	no changes
BrO		SCD	VCD
SO_2		SCD, reference sector	VCD, volcanic and pollution
OClO			SCD
H2O			VCD
CO / xCO			VCD xCO quality tbc
Cloud parameter evolution	OCRA/SACURA	improvements due to degradation correction	new minimum reflectance data base improved OCRA CF

Table 2. Roadmap for the Nadir processor

Product Improvements Level 2	***V6.0 2010***	*V7.0 2011*	*V8.0 2012*
Nadir Products			
Absorbing Aerosol Index	Maintenance	*Maintenance/ Scan Angle dependent degradation*	*Maintenance*
Ozone total column evolution	Maintenance	*Maintenance / GDP 5*	*Maintenance*
trop. O3			*new product*
NO_2	Maintenance	*Maintenance*	*Maintenance*
trop. NO2		*new product*	*Maintenance*
BrO	AMF Improvements	*Maintenance*	*Maintenance*
SO_2	VCD, AMF improvements	*Maintenance*	*Maintenance*
OClO	Maintenance	*Maintenance*	*Maintenance*
HCHO		*new product*	*Maintenance*
CHOCHO		*new product*	*Maintenance*
H2O	Maintenance	*Maintenance*	*Maintenance*
CO / xCO	xCO improvements	*Maintenance*	*Maintenance*
xCH4	new product	*Maintenance*	*Maintenance*
xCO2			*new product*
Cloud parameter evolution	**ice/snow/ clouds**	*Maintenance*	*Maintenance*

Table 3. Improvements of the Limb processor

Product Improvements Level 2	**V 3.01 2007**	**V4.0 2008**	**V5.0 2009**
Limb Products		***not activated***	
Ozone profile evolution	TH offset removed, maximum of 4 limb O3 profiles per tangent height	improved forward model, optimised retrieval settings, => substantially smaller low bias	clouds and aerosol improvements lower stratosphere
NO_2 profile evolution	TH offset removed	improved forward model, optimised retrieval settings => improved lower strat.	clouds taken into account
BrO profile implementation			product newly implemented
Limb cloud flagging (NLC, PSC, etc.)			product implemented, verfied and used in O3, NO2 and BrO retrieval

Table 4. Roadmap for the Limb processor

Product Improvements Level 2	***V6.0 2010***	*V7.0 2011*	*V8.0 2012*
Limb Products			
Ozone profile evolution	extension to **upper stratospher and lower mesosphere**	*Maintenance*	*Maintenance*
NO_2 profile evolution	aerosol	*Maintenance*	*Maintenance*
BrO profile implementation	lower stratosphere improvements	*Maintenance*	*Maintenance*
Limb clouds	**cloud identification**	*Maintenance*	*Maintenance*
H2O profile			*New Product*

6. References

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