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SCIAMACHY delta-Validation Report for the ESA operational Level 1b Version 7 and Level 2 Version 5 Products

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1 INTRODUCTION

In the beginning of 2010, a new SCIAMACHY processing baseline was delivered and implemented in the ESA ground segment. Both for Level 1b and Level 2 important changes were included in the upgrade

1.1 Level 1b Upgrade Version 6 to Version 7

The changes in the Level 1b data include:

- Improved spectral straylight correction for channel 2
- Mesospheric Limb Measurements MDS

No format change has been introduced in the new Level 1b product.

The degradation correction using m-factors is available from the new Level 1b Version 7 processor. M-factors are not part of the Level 1b product and are not used in the Level 0-1b processing itself. The m-factor correction will be applied in the Level 2 data processing.

1.2 Level 2b Upgrade Version 3 to Version 5

The Level 2 processor Version 5 is a major upgrade from previous versions. It includes a number of new datasets, both for the limb and the nadir viewing geometry.
In order to accommodate the new products, the format has been changed and documented in the SCIAMACHY Product Specification Version 3L, available on the ESA web site.

1.2.1 Nadir Product Improvements

The following trace gases have been included in the new baseline:

- SO_2 nadir total columns for normal conditions (anthropogenic sources) and "volcanic" conditions (two MDS, one new)
- BrO nadir total columns
- OClO nadir slant columns (new MDS)
- H_2O nadir total columns
- CO nadir total columns

In addition important improvements on the existing products have been implemented:

- M-factor correction, impacting nadir ozone retrievals and AAI retrievals
- Change of NO_2 retrievals now using not radiometrically calibrated data
- New AAI algorithm
- Cloud fraction improvements
- New forward model in limb retrievals using Picard iteration

1.2.2 Limb Product Improvements

For the limb viewing geometry BrO profiles and Limb cloud flags for PSC, tropospheric clouds (new MDS) are now available in the new processor version.

In addition the following improvements have been included:

- Optimised settings for limb profile retrieval of NO_2 and O_3
- Usage of in the Limb Cloud Flag in Ozone profile retrieval
- Update of the usage of aerosols in Ozone profile retrieval

2 VALIDATION RESULTS

In order to allow the SCIAMCHY Quality Working group and the validation teams organised in SCIAVALIG a first investigation on the products quality, as Level 2 validation dataset was processed and provided. This includes approximately 1900 orbits processed with the Version 5.01 of the ESA operational Level 2 processor. In addition as dedicated validation dataset for SO_2 containing 513 orbits was provided. These datasets were defined in close cooperation with the validation scientists.
Beginning of September 2010, the SCIAMACHY validation team, SCIAVALIG, met to discuss the validation results based on the Level 1b reprocessed and the Level 2 validation dataset. In some cases a validation was not possible and a verification with reference datasets was provided. Input was provided by the following institutions:

Level 1b: SRON/KNMI, IUP
Ozone: IUP, IASB-BIRA, RIVM
NO_2: IUP, IASB-BIRA
BrO: IASB-BIRA, IUP
SO_2: IUP
Clouds: KNMI, IUP
CTH: IUP
H_2O: IUP, MPI Mainz, DLR-IMF
OClO: IUP
CO: DLR-IMF, IASB,-BIRA, IUP, University of Liege, MPI Mainz, SRON

2.1 NADIR PRODUCTS

2.1.1 Cloud Top Height

The SCIAMACHY Level 2 v5.01 cloud product is in good shape and many features have been documented in the ATBD, and the product quality disclaimer. SCIAMACHY Level 2 v5.01 cloud height is higher than FRESCO+, which is well-known and explained by the difference in definition of cloud top. SACURA cloud heights are retrieved only for cloud fractions greater than 0.05 and estimates geometric cloud top while FRESCO delivers an

effective cloud height representative of light path. The quality of CTH over snow/ice surfaces (for example Greenland) needs to be carefully assessed.

2.1.2 Cloud Fraction

The operational cloud fraction was changed and improved compared to V3.01, in particular at small cloud fractions. There is broad agreement with MICROS (cloud fraction derived from MERIS data at SCIA pixel size, Schlundt et al. 2010) but shows a low bias and large scatter. The V5.01 data shows more compact correlation with MICROS but has lower values. There are some yet unexplained effects at very high MICROS cloud fractions where all kind of cloud fractions can be found in the operational data. Good agreement for low cloud fractions should be beneficial for the retrieval of tropospheric trace gas abundances.

2.1.3 Total Column O_3

Both SCIAMACHY Ground Processor (SGP)[1] 3.01 and SGP 5.01 generate O_3 column data consistent with GAW ground-based data records. There are slight differences between the two SGP versions, usually in the form of a bias < 0.6%. Drifts noticed with SGP 3.01 at numerous but not all stations persist with SGP 5.01. Uncertainties increase at large SZA and at low Total Column O_3. The introduction of the degradation correction improves on the drift in the tropics, but not on mid to high latitudes and is it questioned whether such a zonally structured is preferred over a zonally more homogeneous trend. More quantitative validation awaits full SCIAMACHY data record.

2.1.4 Total Column NO2

Both SGP 3.01 and SGP 5.01 generate NO2 column data consistent with NDACC and GOME GDP 4.1 data records. Slight differences between the two SGP versions, usually in the form of a low bias a few 10^{-13} to 10^{-14} molec.cm^{-2} (close to detection limit of NDACC UV-VIS spectrometers). Global maps show areas with challenges such as the bright and elevated surface of Greenland.
SCIAMACHY SGP 5.01 remains low biased with respect to NDACC and GOME GDP 4.1 in Southern Hemisphere, by about $5x10^{-14}$ molec.cm^{-2}. This negative bias exhibits a seasonal cycle. Validation was performed only against sites at pristine locations hence the results are representative of the stratospheric column or total column under clean conditions.

2.1.5 Total Column BrO

The data shows reasonably good agreement between SCIAMACHY nadir and ground-based BrO observations for the years 2003 to 2006 (relative difference: -17.1+/- 20.4%). For 2002 the BrO columns are substantially too low with a lot of negative values. It is recommended not to use the BrO data in 2002 in its current quality.

[1] The SCIAMACHY Ground Processor, SGP, is equivalent to the operation ESA Level 2 processor.

2.1.6 Total Column SO_2

The operational SO_2 product picks-up all relevant volcanic signals. There is a problem in the fit leading to a low bias in the slant columns over continents. There are also very high values encountered in some areas of the Northern Hemisphere in spring. At high latitudes, strongly negative values are found, presumably as result of problems with the reference sector subtraction method. Sometimes there are individual days having poor results. Due to these uncertainties in the data it is recommended not to use the current version of the Slant Column and anthropogenic Total Column for quantitative studies. Usage of the volcanic Total Column as indicator of large volcanic eruptions seems to be feasible.

2.1.7 Total Column H_2O

The data shows an average standard deviation of around 0.4-0.5 g/cm^2 compared to ECMWF and SSMI, the latter only available over oceans. A low bias exists (-0.4/-0.2 g/cm^2) compared to both, SSMI and ECMWF. The bias to ECMWF is smaller, presumably because of offsetting effect of a small high bias over land. There are indications for seasonal modulations in the bias. A detailed validation needs to be performed.

2.1.8 Slant Column OClO

The operational OClO slant column product provides a good indicator for chlorine activation. There is indication for a globally uniform low bias of about $3x10^{-13}$ molec cm^{-2} in the data which also leads to negative values over the majority of the globe.

2.1.9 Total Column CO

Due to erroneous retrieval settings in the operational software, the CO product from Level 2 v5.01 is recommended not to be used.

2.2 LIMB PRODUCTS

2.2.1 O_3 Profiles

The ozone profile product of Level 2 v5.01 is a clear improvement over Level 2 v3.01. SGP 5.01 ozone profiles have a correct vertical shape, and capture well the seasonal cycle and meridional structure. Differences reveal no significant drift, except at a few stations, but this should be confirmed over entire SCIAMACHY lifetime. When compared to GB network data, O_3 profiles retrieved with SGP 5.01 are of equivalent or better quality than those retrieved with SGP 3.01. The low bias in v3.01 is significantly reduced. In the tropics a positive bias in SCIAMACHY v5.01 (5 to 23%) is observed, which has a pronounced maximum around 18 km, which needs further investigation. In the mid-latitudes SCIAMACHY v5.01 matches validation instruments within 5% up to 38 km altitude. In polar regions a variable bias exists ranging from -10% to +7% in the altitude range 15 to 35 km, increasing rapidly above (magnitude depending on validation instrument) is observed for the validation data set. Due to the pronounced deviation in the tropics around 18 km, it is currently recommended to use data only above 20 km in the tropics.

2.2.2 NO_2 Profiles

No initial validation was performed for limb NO_2.

The comparison of the NO_2 scientific with operational retrieval show good agreement with Level 2 v5.01 with a mean difference of better than 10% between 20 and 37 km. Higher differences exist for large SZAs in the NH. The higher scatter is driven by the polar Northern Hemisphere.

2.2.3 BrO Profiles

Comparisons to data from ground based MAX-DOAS measurements at Harestua (60°N, 11°E) indicate that for the 15-27 km partial columns there is an overestimation of 32 ± 31 % on average by Level 2 v 5.01. Also vertical BrO profiles of SCIAMACHY seem to be larger than profiles derived from ground-based in the 15-21 km altitude range (up to 50%) at Harestua (60°N, 11°E).

The comparison of the BrO scientific retrieval with the operational retrieval shows good agreement with L2 v5.01 with a mean difference of 20-30% for altitudes between 20 and 30 km in the NH. There are indications that the mean difference shows some seasonal effect. Larger differences and much higher scatter are observed in the Southern Hemisphere.

2.2.4 Limb Cloud Flag

Independent comparisons of SCODA and a MIPAS limb cloud retrieval (data from Harjinder Sembhi, University of Leicester) show good agreement with respect to cloud top height assignment (mean difference -1.2 km, standard deviation 3-5 km).

3 CONCLUSION

In particular the deficiencies in CO and SO2 do require a modification of the processor and processing baseline. The investigations for the SO2 slant and anthropogenic column will require an in-depth analysis. It is foreseen that the products will be considerably improved in the next processor version.
For CO it is considered that a minor upgrade on the processing baseline will significantly improve the product. As a consequence, it was decided to interrupt the ongoing reprocessing of the SCIAMACHY Level 2 dataset until the corresponding patch for CO is provided.