DOAS UV/VIS minor trace gases from SCIAMACHY

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ABSTRACT

Analyses presented made in the frame of SCIAMACHY Level 2 product verification activities under leadership of ESA. The initiated verification team consists of members of several european research institutions. The presented work is part of the SUPPRO project funded by ESA (ESAESTEC Contract 13594/99/NL/PR). The goal of the verification team is to analyse Level-2 products with respect to expected precision and accuracy. This is done by comparing Level-2 products with results from independent retrievals applied on calibrated Level-1C spectra, which bases on similar algorithms than the operational processor using similar set-ups. Selected sets of SCIAMACHY data specifically prepared by ESA for this task are used. As a first step it has been analysed if the data considered is consistent and physically meaningful. This paper focusses on BrO and SO2 products, for which data has been made available, but of only very limited extend. Both Level-2 and independently retrieved slant columns obtained are much too large compared to climatology mean values. Large residuals have been observed after the retrieval pointing on severe Level-1B calibration inaccuracies. All SCIAMACHY results presented in this paper are intermediate results from running analyses and are therefore preliminary.

1 OVERVIEW

Two versions of Level-1B spectra and Level-2 trace gas slant columns from SCIAMACHY have been made available by ESA for verification, version V1 and V2, processed using different processor versions and parameter set-ups. Version V1 of verification data consists of 7 selected orbits from the beginning of August, but does not contain any minor trace gas products. Therefore, Level-2 products have been re-calculated from a subset of Orbit 2338 (11th Aug.) using Level-1B spectra generated by the operational prototype processor at DLR-MF. The resulting BrO has been analysed. Version V2 made available on 24th Nov. leaving not much time for analyses. It contains only SO_2 as minor trace gas to be analysed (Orbits 2509 and 2510, 23rd Aug.). For independent retrieval, the DOAS code KVANT (IUP/IFE) was used.

2 BRO FROM ORBIT 2338

For the retrieval of BrO experiences gathered with GOME have been applied [1]. As fitting window the spectral range from 344.7 nm to 359 nm has been used. Highly resolved BrO cross-sections measured using a FTS-spectrometer [2] convolved with the SCIAMACHY slit-function have been used for fitting. For O_3, NO_2, HCHO, and OClO, SCIA-FM spectra have been taken [3]. O_4 absorption-cross-sections [4] have been used, smoothed by FFT transformation to filter artificial step characteristics. The Doppler-shift between radiance and irradiance measurements, taken to be 0.0075 nm has been corrected. A simulated under-sampling spectrum has been fitted. To account for radiance off-sets an inverse solar irradiance spectrum has been fitted simultaneously. The Ring effect has been accounted for by fitting a simulated Ring spectrum [5].

Figures 1 and 2 show maps of BrO slant columns as retrieved by the SCIAMACHY operational processor and by KVANT, respectively. Measurements provided were measured between West-Africa and Antarctica. In the area of the Weddel-Sea increaing BrO values are observed also by other instruments in the same time range. Also the increasing values as a function of latitude are as expected due to enhanced slant pathes with increasing solar zenith angle. However, the magnitude of the observed values is too large from both Level-2 and independent retrievals. The gaps in the data are not foreseen for nominal operations but have been obtained from the data provided.

A 2-D plot of both data sets reveals a mean off-set in slant column of about 1E14 cm^{-2} wrt. KVANT results. The scatter of both data sets is similar, however, results are too large. For the tropical region, a value of the stratospheric BrO-climatology generated at IUP (M. Bruns, private communication) is given for orientation.

Residual spectra averaged over Orbit 2338 and 2509 as obtained after applying KVANT are shown in Figures 4 and 5, respectively. Although the residual structures for Orbit 2509 results are much less intense than for Orbit 2338, values are still too large, as for the absence of systematic spectral errors, averaged residuals are expected to deminish almost completely.

Independent retrieval results have been obtained by Andreas Richter (IUP/IFE), using a similar DOAS algorithm but in contrast an earth-shine radiance as the reference, which is assumed not to be influenced by BrO. This method has the advantage to avoid any inconsistencies between radiance and irradiance measurements. Results retrieved as such from

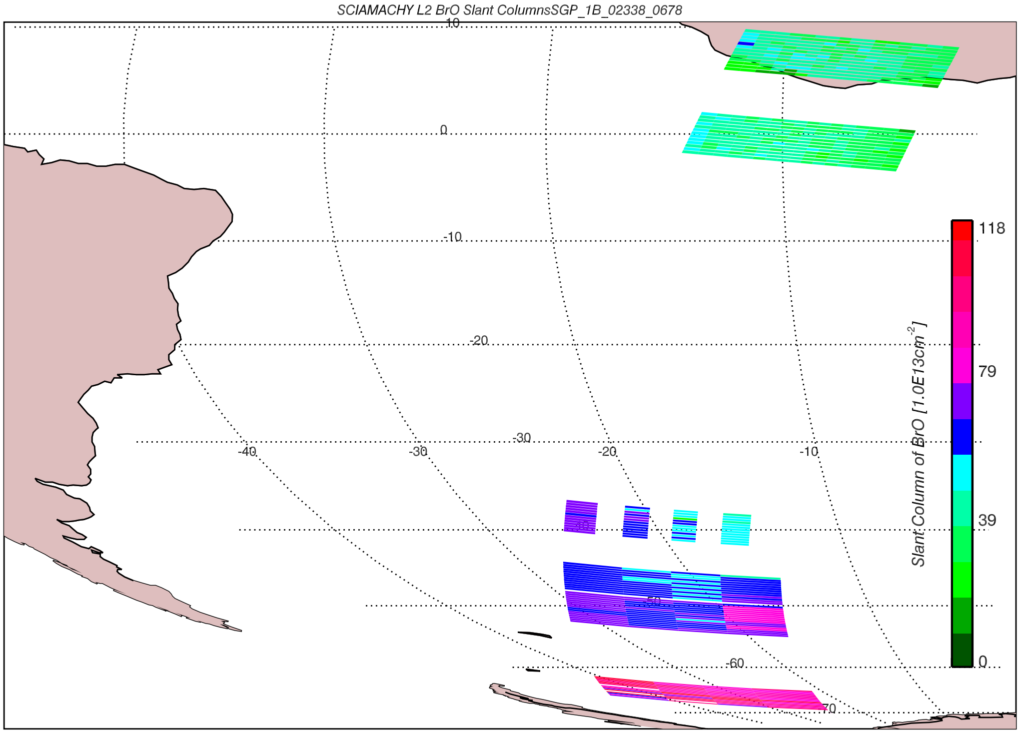

Figure 1: SCIAMACHY Level-2 BrO slant columns from a verification-specifically prepared data set of Orbit 2338 retrievals. Measurements made between West-Africa and the Weddel Sea. Large values compared to climatological background (5E13 cm-2) are obtained. Increasing values to high latitudes are in line with SZA. Gaps originally from L1 product.

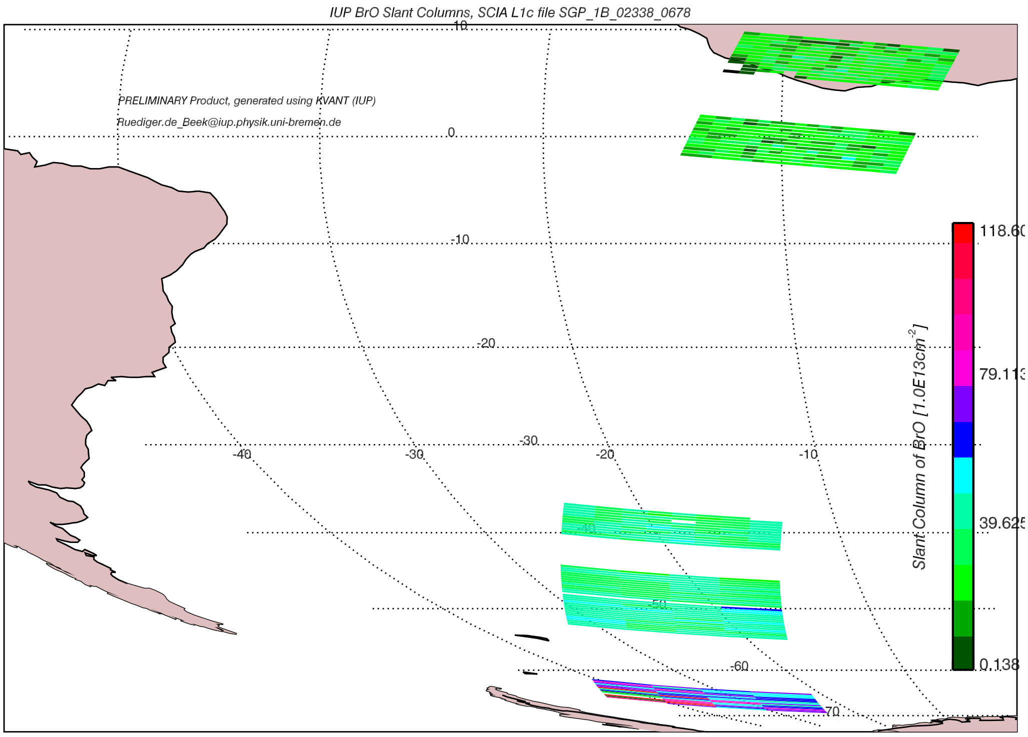

Figure 2: IUP retrievals of BrO slant columns (SCIAMACHY Orbit 2338). Slightly smaller values than Level-2 (Fig. 1), but also much too large compared to climatology.

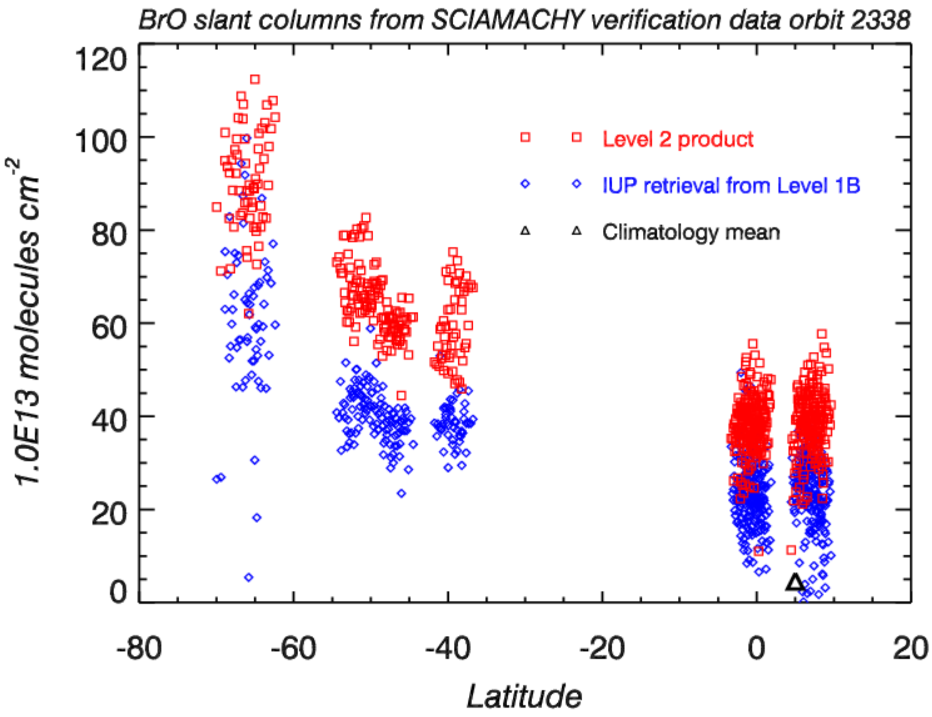

Figure 3: SCIAMACHY Level-2 and IUP BrO (Orbit 2338). Similar scatter for both data sets and a mean off-set of about 1E14 cm-2 are observed. Too large values compared to climatological mean (triangle)!

SCIAMACHY Orbit 2509 measurements have been compared to those from coincident GOME measurements using the average of results according to the related GOME pixels. Similar settings were used for the fitfings for both instruments. Results are given in Fig. 6. An off-set of 2E14cm-2 has been added to the results obtained from SCIAMACHY. Apart from this correction, good agreement is obtained at low latitudes. Discrepancies observed for high latitudes can be related to differences in SZA and geo-location for both instruments. Similar results were obtained for orbit 2510.

3 SO_2 from Orbit 2509

Although the recommended fitting window for SO_2 is 314–327 nm, the fitting window used in the operational processing was between 321 nm and 327 nm. The reason was an unexpected software complication when trying to use a fitting window which extends over the SCIAMACHY spectral cluster boundary at about 321 nm. For the fitting, SO_2 and O_3 absorption cross-sections from SCIA-FM [3] have been taken as is foreseen for the operational processing. Although mandatory, no undersampling correction has been applied for this analysis, as by now this has been omitted in the operational processing of the verification products, but nevertheless has to be done for future processing. As for BrO, the Ring spectrum applied has been simulated by the radiative transfer model SCIATRAN.

Figures 7 and 8 give a picture of the SO_2 slant columns taken from SCIAMACHY Level-2 and KVANT results, respectively. Values are too large as for BrO. Negative values were obtained and filtered out, especially from KVANT, leading to gaps in the data set.

The 2-D plot of the unfiltered data sets (Fig. 9) reveals many negative results and larger values at the northern high latitudes for KVANT compared to Level-2.

For the IUP retrievals again fit residuals are available. Fig. 10 shows all residuals obtained averaged over Orbit 2509 and plotted versus a SO_2 differential optical depth spectrum for a typical situation. The fitting window chosen independently from recommendations after optimisation studies appears to avoid most of the spectral information contained mainly in the left half of the spectrum (see blue line). The mean residual shown in Fig. 11 has been obtained in the same way but by including the mean spectral residual from Fig. 10 in the fitting. First, the strongly reduced residual shows the systematic character of the spectral error. Secondly, the fit results are positively affected as the fitting is numerically stabilized. Results of KVANT are then more similar to Level-2 slant columns, which is shown in Fig. 12. However, errors

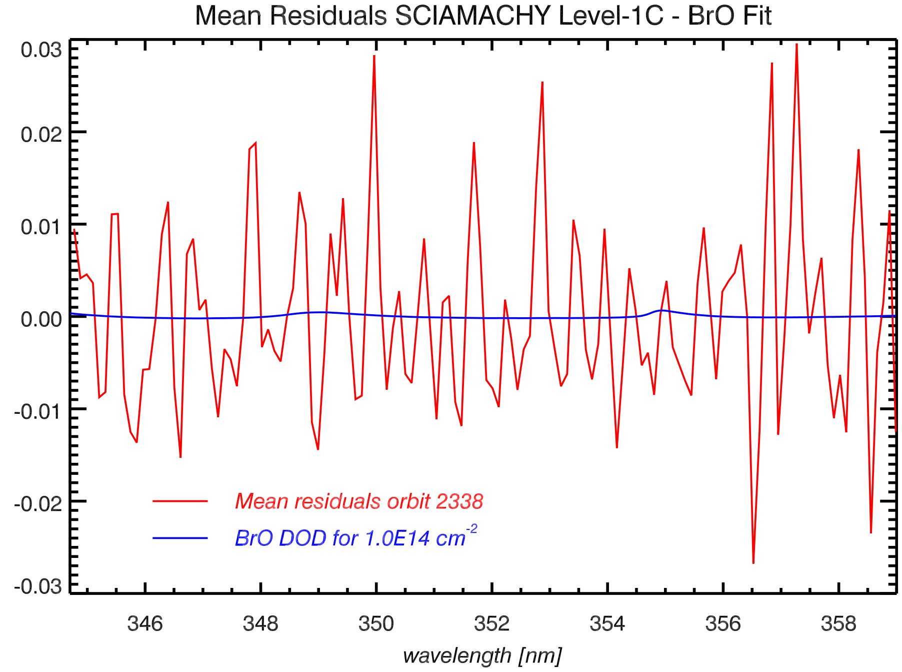

Figure 4: Residuals after IUP fit averaged over orbit 2338 (red) compared to expected differential optiical depth (blue). Residuals are expected to deminish when averaged as such. In contrast, the obtained residual is far too large.

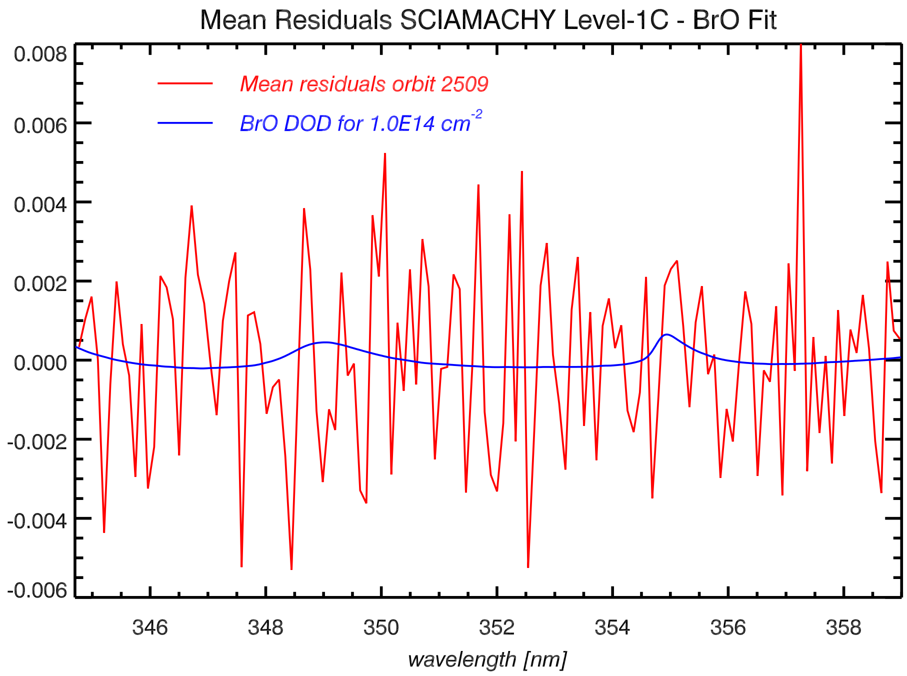

Figure 5: Smaller residuals for Orbit 2509 than for Orbit 2338 (Fig. 4). Very similar residuals for Orbit 2510 are obtained (not shown; data from V2 retrievals, no Level-2 product available).

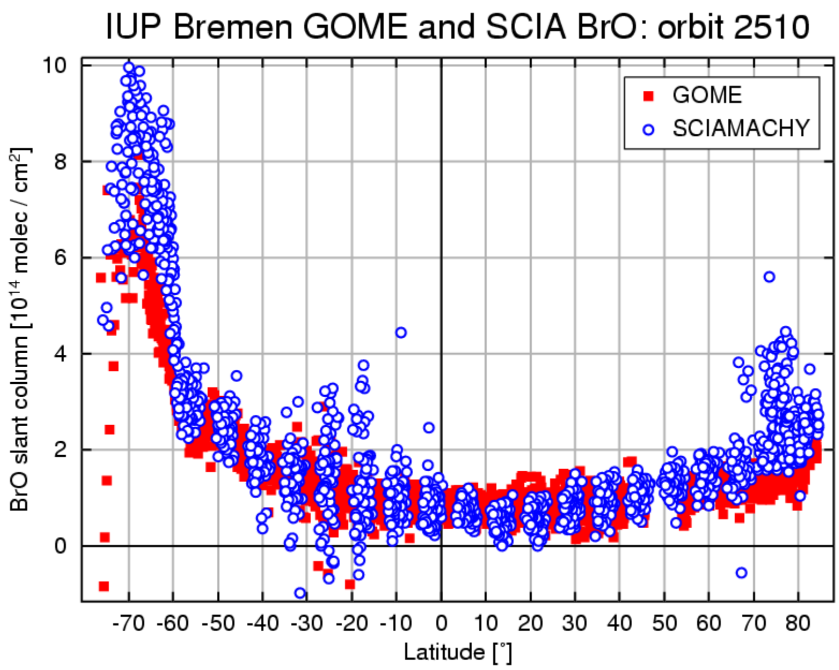

Figure 6: Results of Andreas Richter (IUP/IFE), using earth-shine radiance as the reference. An off-set of 2E14cm-2 has been added to the results obtained from SCIAMACHY. The average of results according to the related GOME pixels were used for comparison. Similar settings for fit for both instruments. Good agreement at low latitudes. Discrepancies at high latitudes related to differences in SZA and geo-location. Similar results were obtained for orbit 2510.

are only partly reduced, as the residual structure is by definition orthogonal to any other spectral structure fitted and is therefore only an indication for inconsistencies. The source of the discrepancies has to be revealed to avoid errors due to correlations with absorption cross-sections.

One source clearly is not to include a simulated spectral interpolation (under-sampling) error pattern in the fitting [6]. The magnitude of the residuals suggest that there is an additional problem, which could be e.g. related to the spectral calibration and diffuser indused spectral characteristics as seen already for GOME [7]. This has to be further investigated.

Finally, an impressive result obtained by Andreas Richter (IUP) using SCIAMACHY Level-0 data obtained near Sicily two days after the 2002 Ätna erruption is shown in Fig. 13 to demonstrate the potentials of trace gas retrievals using SCIAMACHY measurements, pointing to the high accuracy and spatial resolution. The plotted values speak for themself!

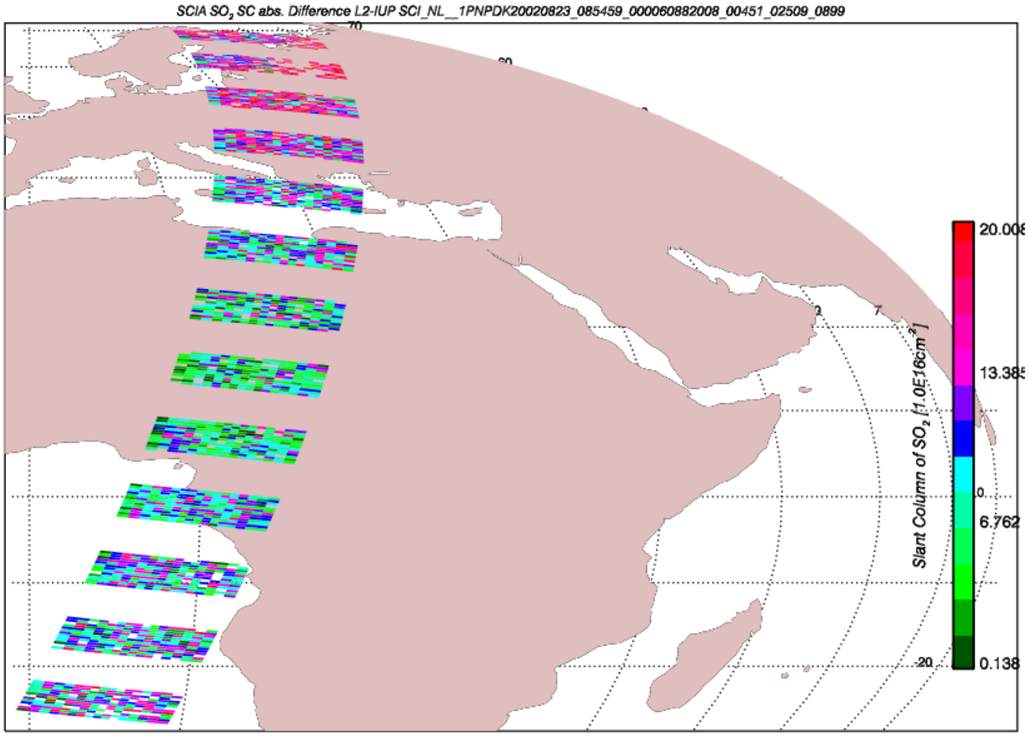

Figure 7: SCIAMACHY Level-2 SO_2 from verification Orbit 2509. Large values compared to climatological background (5E15 cm-2). Increasing values to high Latitudes in line with SZA.

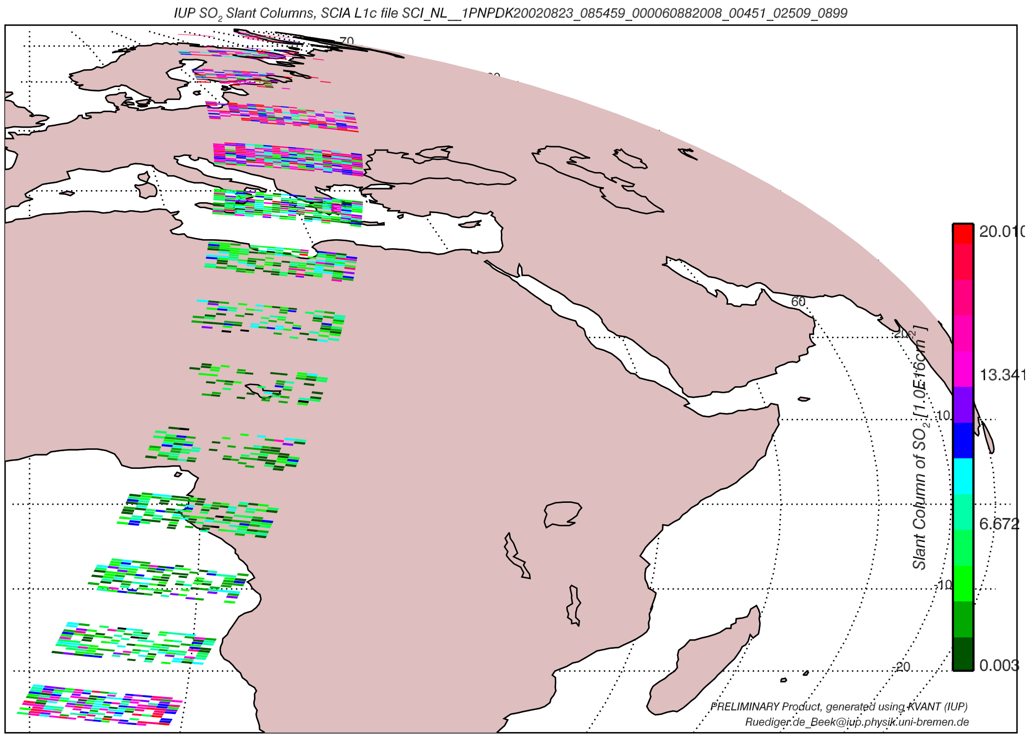

Figure 8: IUP SO_2 slant columns for Orbit 2509. Similar to SCIAMACHY Level-2 (Fig. 7), but many gaps due to negative values.

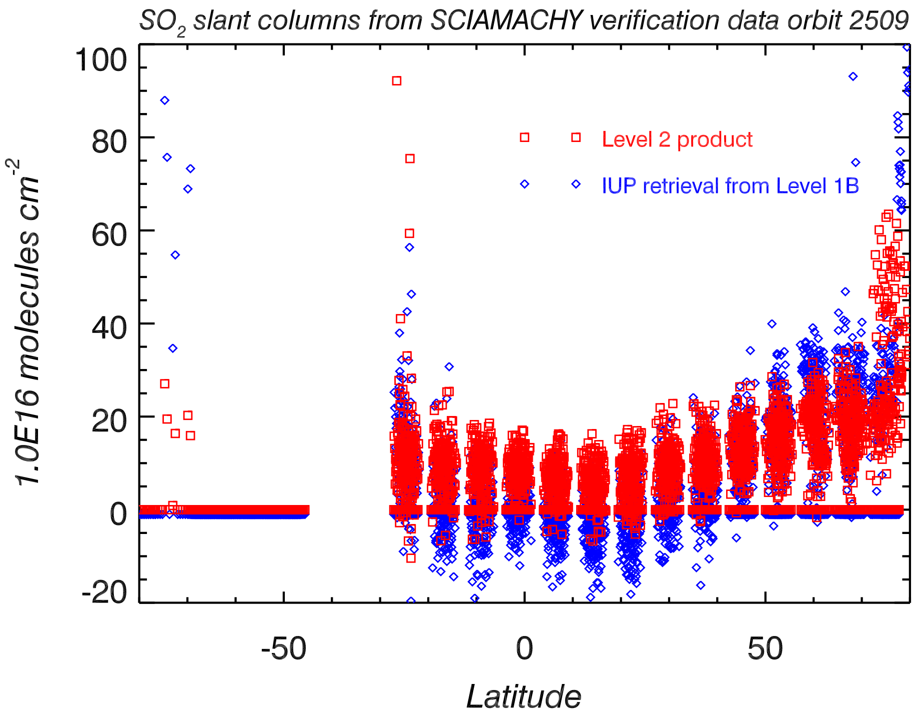

Figure 9: SCIAMACHY Level-2 and IUP SO_2 slant columns for verification Orbit 2509. Too large and negative values are obtained.

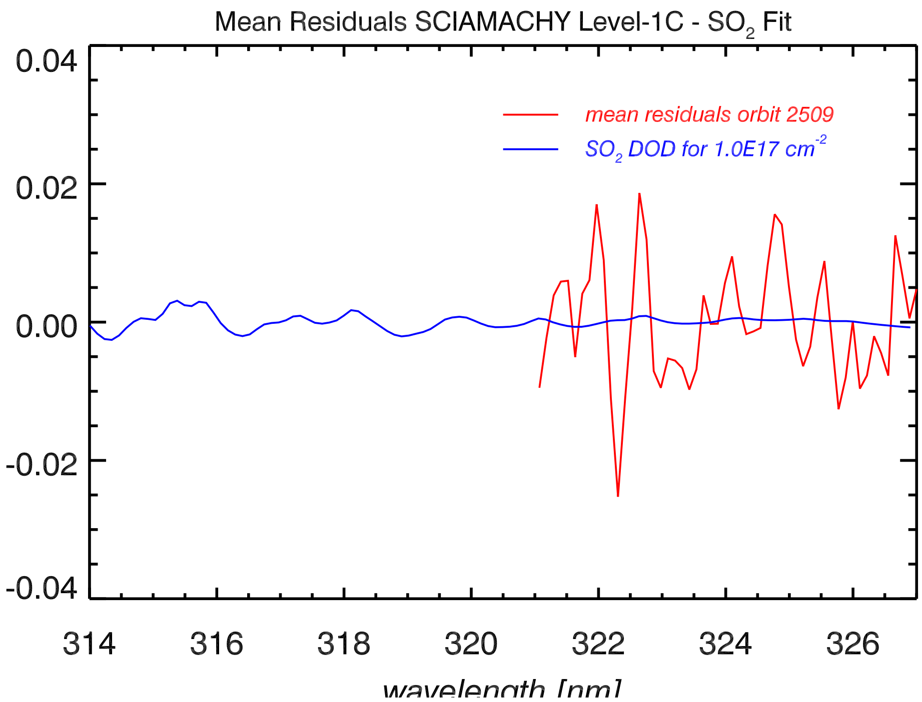

Figure 10: Spectral error pattern revealed after averaging all residuals obtained from Orbit 2509 spectral fittings. Residuals are expected to deminish when averaged as such. If the structure is systematic it should reduce the residuals when included in the fittings. It can be seen that the fit-window of choice is in-appropriate for accurate retrieval, as most of the SO_2 absorption information is located in the left half of the spectral window recommended.

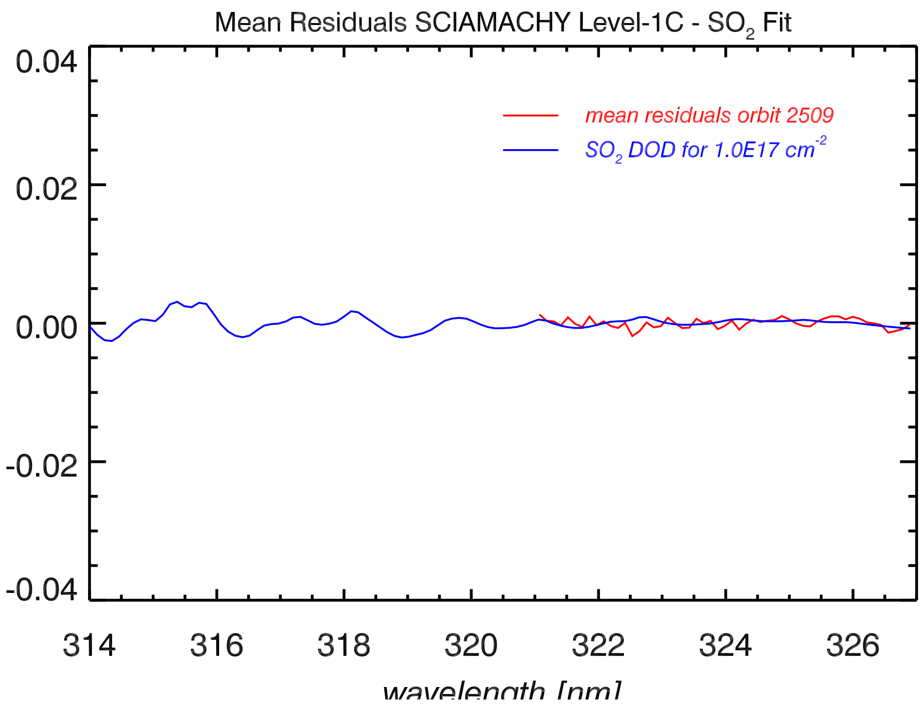

Figure 11: Spectral error pattern after averaging all residuals obtained from Orbit 2509 when error pattern from Fig. 10 is included in the fittings. Structure turns out to be systematic. It reduces residuals significantly when fitted!

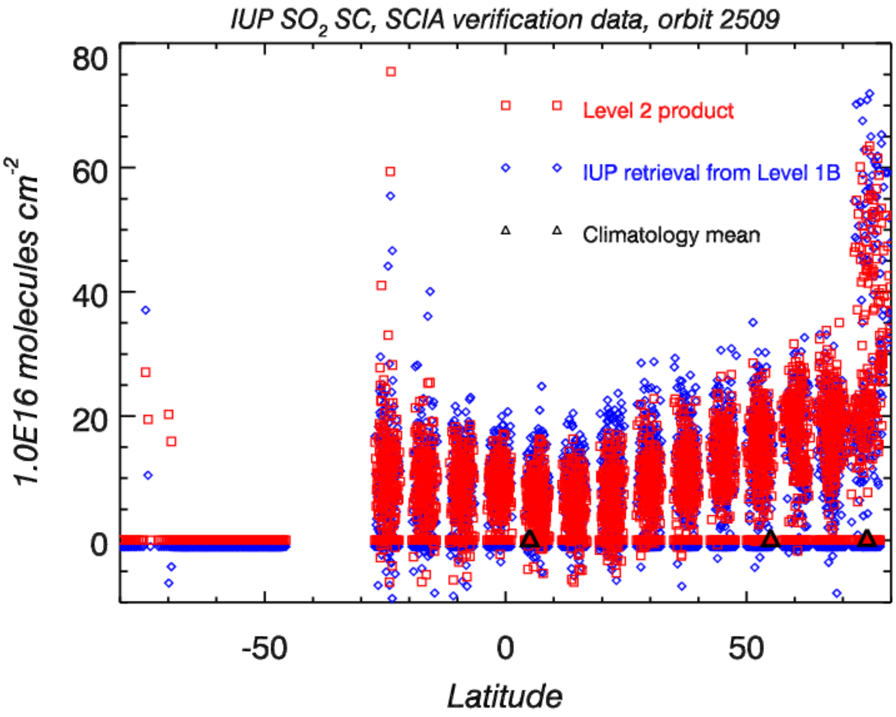

Figure 12: IUP $SO_2$2 is more similar to Level-2, when systematic spectral residual pattern is included in the fitting. Results are still erroneous, when compared to climatological mean background.

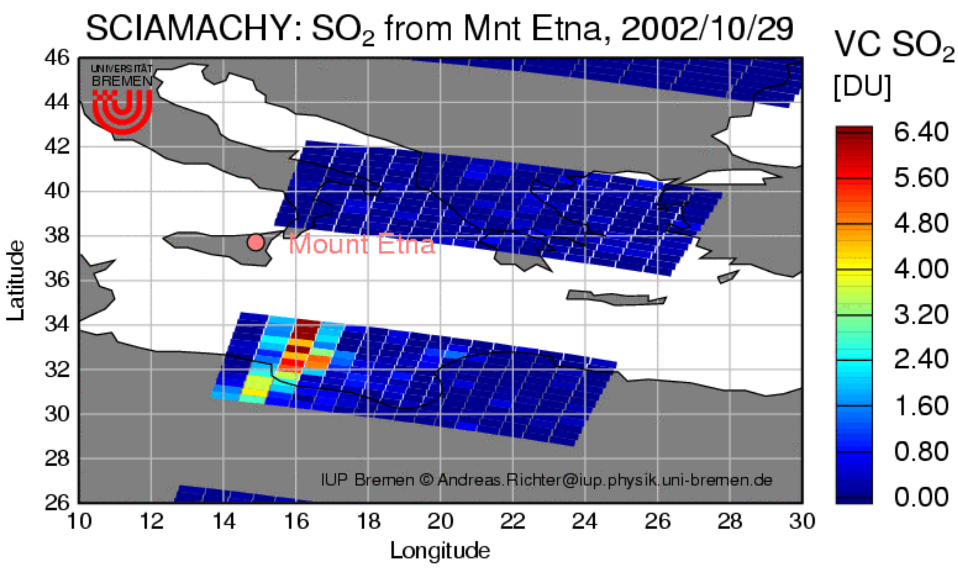

Figure 13: SO_2 slant columns retrieved by Andreas Richter (IFE
using SCIAMACHY Level-0 data obtained near Sicily two days after the 2002 Ätna erruption. Clearly the plume of enhanced SO_2 concentrations shows up as expected.

4 CONCLUSIONS

Unexpectedly large slant columns are observed from both SCIAMACHY Level-2 and independent retrievals of BrO and SO_2. Large systematic residual structures have been observed after fitting, which source is unclear and under investigation. However, these are indications for errors.

Zonal variations observed vary, as expected, with solar zenith angle. Good agreement with GOME BrO when using earth-shine reference could be achieved after adding an off-set of 2E14cm-2. Using an earth-shine radiance spectrum as reference, also plausible SO_2 is observed from SCIAMACHY.

Main possible reasons for errors observed:

- in-accurate polarization correction,
- in-accurate wavelength calibration,
- as a result, incorrect undersampling correction (not applied yet in operational processing anyway),
- structures in solar irradiance due to diffuser plate.

Facit: the minor trace gas products available are not yet in shape for further validation.

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