IMPROVED SCIAMACHY WFDOAS TOTAL OZONE RETRIEVAL: STEPS TOWARDS HOMOGENISING LONG-TERM TOTAL OZONE DATASETS FROM GOME, SCIAMACHY, AND GOME2

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ABSTRACT

Currently three European satellite spectrometers, GOME1/ERS2 (1995-present), SCIAMACHY/ENVISAT (2002-present), and GOME2 (2006-present) provide a near global decadal data set of total ozone covering more than a decade. This data are very valuable for the detection of recovery in stratospheric ozone as expected from the levelling off of stratospheric chlorine. In order to detect such a signal beyond the level of the large inter-annual variability is challenging and requires high accuracy in retrieved ozone with a stability to within one percent (relative bias) over a decade and absolute accuracy to within a few percent. A particular challenge will be to homogenise data sets from different instruments. In this paper we discuss important retrieval issues that are deemed important in order to avoid excessive homogenisation of multiple data sets (if homogenisation is understood as bias removal). The relevant issues discussed here are the choice of ozone cross-sections, the use of a-priori O3 profile climatologies, and level-1 spectral calibration.

Key words: GOME; SCIAMACHY; ozone; retrieval.

1. WFDOAS V2 TO3 RETRIEVAL

The weighting-function DOAS algorithm in its first version (V1) has been summarised in Coldewey-Egbers et al. [1] and successfully applied and validated for GOME1 [2]. The agreement between WFDOAS V1 and ground-based Brewer and Dobson data is to within one percent globally, at high latitudes and high solar zenith angles the differences can reach a few percent. The major changes in V2 is the integration of the SCIATRAN radiative transfer [3] in the iterative retrieval replacing look-up tables (Fig. 1, [4]). In addition a simple parameterisation for the Ring effect has been introduced. The Ring spectrum r has been approximated as follows:

$$r = \frac{I_o^{rrs}}{I_o} \exp\big(\frac{\tau_{O3}^v}{\cos(\theta_o)}(1 - \frac{\sigma_{O3}^{rrs}}{\sigma_{O3}})\big), \qquad (1)$$

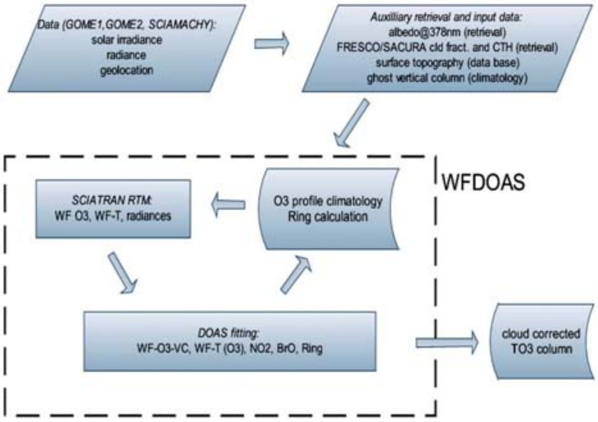

Figure 1. WFDOAS V2 scheme with SCIATRAN radiative transfer module.

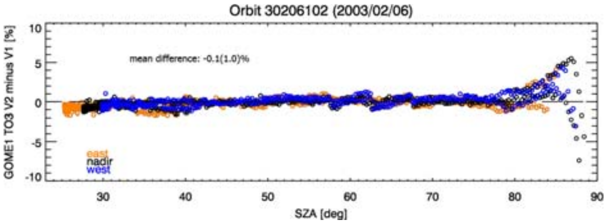

Figure 2. Comparison of new WFDOAS V2 with V1 [2] applied to one GOME1 orbit

where the index rrs indicates the Raman smoothed solar irradiance and ozone cross-section, respectively, θ_o, the solar zenith angle at the height of the ozone layer ($h \sim$ 20 km), τ_{O3}^v the vertical optical density. The difference between WFDOAS V2 and V1 is shown for one GOME1 orbit in Fig. 2. In the former version, the Ring spectra were determined with SCIATRAN [5] and stored in look-up-tables The new algorithm facilitates the flexible use of the same algorithm to different satellite instruments.

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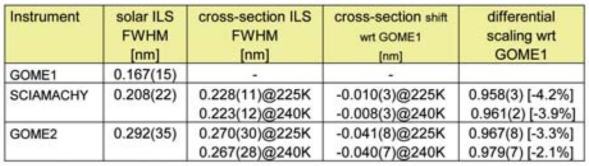
Table 1. Retrieved instrumental line shapes (Gaussian) in the WFDOAS fitting window 326.6-334.5 nm derived from solar data and cross-sections (the latter measured preflight with the flight model spectrometers). As reference the Kurucz Kitt Peak solar FTS data [9] and the GOME1 cross-sections have been used, respectively.



Instrument	solar ILS FWHM [nm]	cross-section ILS FWHM [nm]	cross-section shift wrt GOME1 [nm]	differential scaling wrt GOME1
GOME1	0.167(15)	-	-	
SCIAMACHY	0.208(22)	0.228(11)@225K 0.223(12)@240K	-0.010(3)@225K -0.008(3)@240K	0.958(3) [-4.2%] 0.961(2) [-3.9%]
GOME2	0.292(35)	0.270(30)@225K 0.267(28)@240K	-0.041(8)@225K -0.040(7)@240K	0.967(8) [-3.3%] 0.979(7) [-2.1%]

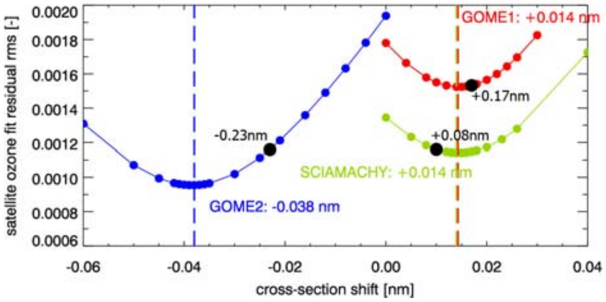


Figure 3. Ozone fit residual RMS for GOME1, SCIAMACHY, and GOME2 as a function of cross-section shifts. Black dots indicate optimum shifts from direct comparisons between cross-sections with respect to a shift of 0.017nm in GOME1 as used in WFDOAS V1.

2. OZONE CROSS-SECTIONS

All three instruments (GOME1, SCIAMACHY, and GOME2) slightly differ in their spectral resolution. As GOME1 is undersampled (sampling is about 0.11nm and with a spectral resolution of 0.17 nm the sampling is below the Nyquist limit), the GOME2 design was slightly altered to get a sufficient oversampling (see Table 1). For each instrument, the ozone cross-sections have been measured using the same satellite spectrometers during preflight calibrations [6, 7, 8]. Their use avoids the need to know the exact instrumental line shape of each instrument. As Table 1 shows there are differences in the scaling of each cross-section after subtracting a polynomial. A reduction of 4% in the scaling therefore introduces a bias of +4% in the retrieved ozone column (as is the case for SCIAMACHY with respect to GOME1 if cross-sections are unadjusted).

SCIAMACHY WFDOAS V2 uses the SCIAMACHY FM ozone cross-sections (Bogumil et al. 2003), differentially scaled by 3.9% and shifted by 0.009 nm (see Table 1 and Fig. 3). A comparison between SCIAMACHY (V2) and GOME (V1) is shown in Fig. 4. As expected the agreement is very good except for high solar zenith angles ($> 87°$), where differences are getting larger. A more detailed validation with other algorithms and satellites are shown by Bracher et al. (this issue).

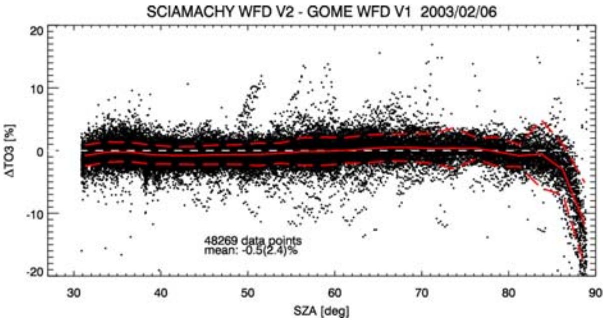


Figure 4. Differences between SCIAMACHY V2 and GOME V1 on 6th February 2003. All GOME results within a distance of 300 km to the SCIAMACHY ground pixel have been averaged. GOME and SCIA follow each other in the same orbit. For the SCIAMACHY retrieval spectral data (level 1 data) Version 5 have been used.

3. CLOUD CORRECTION: SACURA VS. FRESCO

For SCIAMACHY an alternative cloud algorithm SACURA/OCRA [10] is available that retrieves cloud fraction (cf), cloud-top-height (cth), and other cloud parameters from the oxygen A-band (760 nm). The cloud parameters as retrieved from FRESCO in the same oxygen band assumes that the cloud is a reflecting surface [11]. SACURA accounts for the penetration of radiation in the clouds using analytical expressions. In WFDOAS the clouds are treated as Lambertian reflecting surfaces like in FRESCO. Figure 5 shows the difference in O3 columns due to the use of the different cloud algorithms. On average total columns retrieved with SACURA are 0.7% ($\pm 1.8\%$, 1σ) higher. In selected cases differences can reach several percent.

4. OZONE PROFILE CLIMATOLOGY

In the SCIATRAN RTM various a-priori profile climatologies are available. For satellite column retrievals, the TOMS V7 [12], IUP Bremen [13], and TOMS V8 [14] are particularly suited since the profile shapes are defined as a function of total column and, therefore, better represent the natural variability in profile shapes related to tropopause changes. As discussed in Lamsal et al. [4], the profile effect can lead to differences of up to 5% or more under high solar zenith angle conditions that occur mainly in the polar regions (Fig. 6).

5. SCIAMACHY LEVEL 1 CALIBRATION ISSUES

In 2005 a new spectral data version with updated calibration key parameters (V6) were introduced. Fig. 6 shows

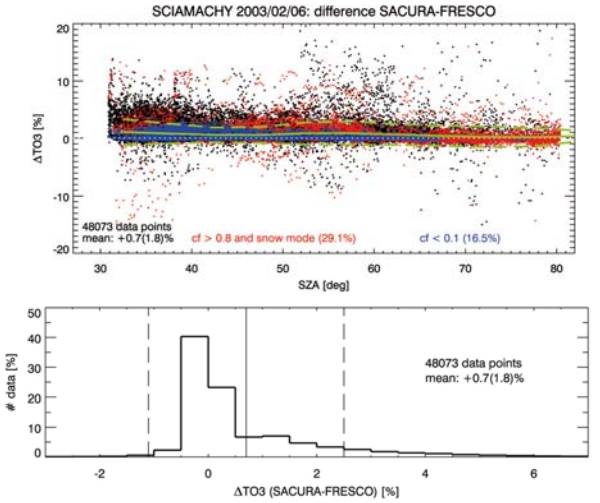


Figure 5. Top: The effect of different cloud retrievals on the retrieved SCIAMACHY columns for all data from 6th February 2003 as a function of SZA (top). The green lines show the mean and 1σ variance of the calculated mean. Bottom: The frequency distribution of the differences is asymmetric, nevertheless, about 72% of the data are within 1%. All SCIAMACHY retrievals were done with the spectral data version 5.

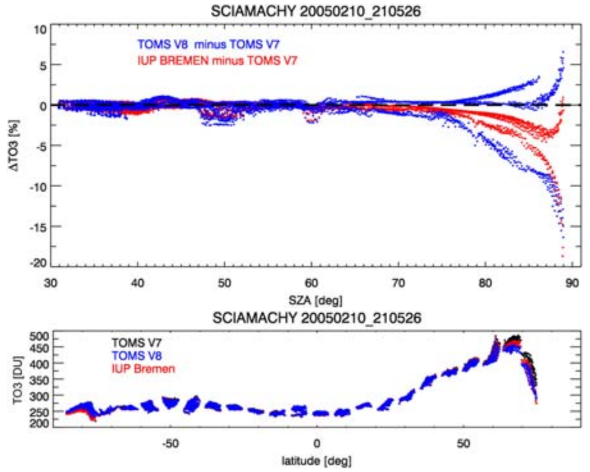


Figure 6. Differences in TO3 retrieved using different a-priori O3 profile climatologies: TOMS V7 [12], IUP Bremen [13], and TOMS V8 [14]. Top: Differences in percent as a function of SZA. Bottom: TO3 as a function of geographic latitude.

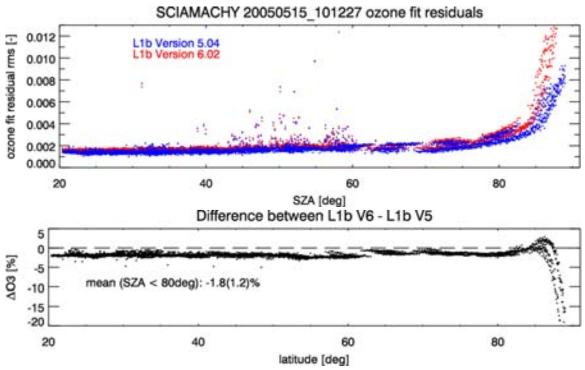


Figure 7. Ozone fit residual rms (top) and retrieved total ozone (bottom) for a selected SCIAMACHY orbit using different calibration versions of level 1 spectra, V5 and V6.

the difference in the ozone fit residual (top panel) and total ozone (bottom) between V6 and V5 for a selected orbit in May 2005. Below 80° SZA the diffences in ozone is 2% and larger beyond 85° SZA. The fit residuals with level V6 slightly increased and get particularly worse at high SZA. The key parameters for calibration are now determined on a finer wavelength grid, that may produce spurious noise in the spectra that is picked up by the sensitive DOAS retrieval.

6. FIRST WFDOAS RESULTS FROM GOME2

In 2006 GOME2 was successfully launched aboard METOP1. Two more GOME2s about five years apart are to be launched, extending the ozone observations well into the next decade. Fig. 8 shows GOME2 ozone from April 2nd, 2007. Here the WFDOAS V2 has been applied (using resolution adjusted GOME1 FM spectra and TOMS V7 climatology). These results are preliminary, since GOME2 is still in the commissioning phase.

Collocated SCIAMACHY data are shown for one GOME2 orbit (Fig. 8) indicating excellent agreement to within 0.5%. GOME2 has a larger across scan width (∼1900 km) that has doubled with respect to SCIAMACHY and GOME1. As discussed in de Beek et al. [15], the viewing geometry at the ozone layer height (or ground) should be used in the RTM in order to minimise the error in the pseudo-spherical approximation at large line-of-sight angles.

7. CONCLUSIONS

The following conclusions can be drawn:

- WFDOAS V2 has been successfully applied to satellite instruments with varying spectral resolutions

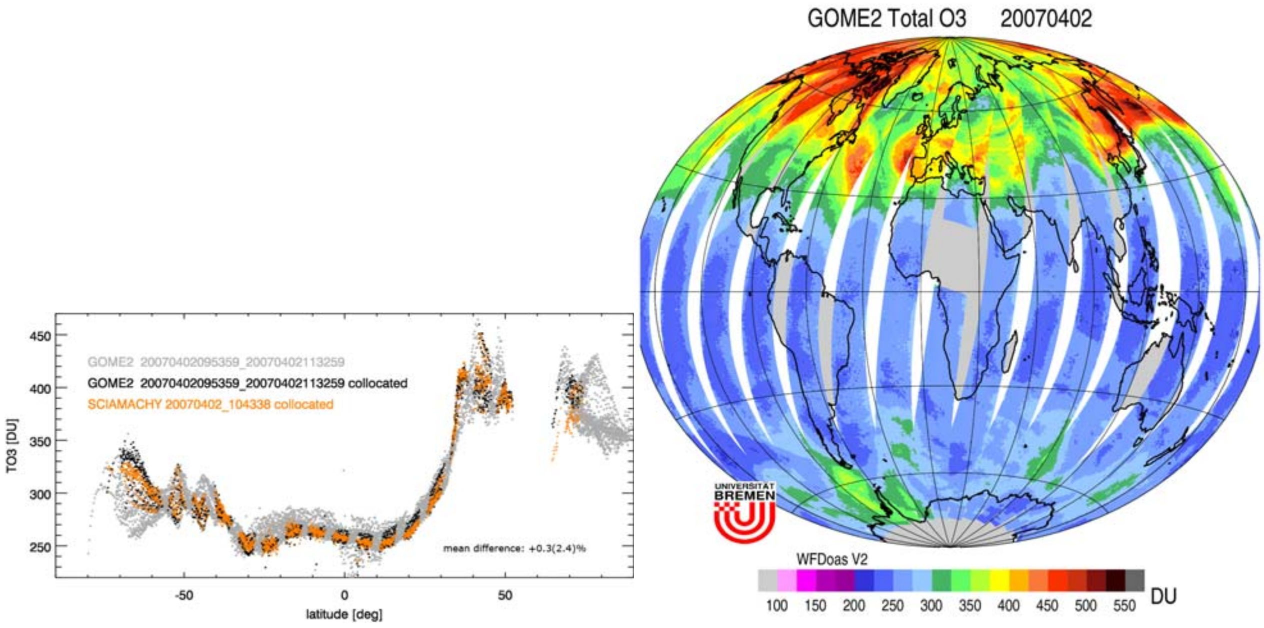


Figure 8. Left: One GOME2 orbit from April 2nd, 2007, collocated with SCIAMACHY (to within 80 km). The SCIAMACHY retrieval was applied to V6 spectral data. Right: Global TO3 map from GOME2 from the same day.

(GOME1, SCIAMACHY, and GOME2) after careful adjustments to ozone cross-sections.

- For good agreement between different satellite instruments, proper adjustements in the spectral resolution, scaling, and wavelength shifts of the used ozone cross-sections have to be applied.
- Largest differences in ozone, when using different climatologies and L1 calibrations (SCIAMACHY), are found under high SZA conditions, where errors of 5% percent or more can be reached. One should note here that high SZA conditions are challenging for ground instruments measuring in the UV as well (see for instance, discussion in Weber et al. [2].
- All three instruments (GOME1, SCIAMACHY, and GOME2) will provide an excellent TO3 long-term data record covering possibly more than two decades

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