10-YEARS OPERATIONAL GOME/ERS-2 TOTAL COLUMN PRODUCTS: THE GDP 4.0 VALIDATION

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ABSTRACT

Results of a geophysical validation exercise regarding the new operational GOME data processor (GDP 4.0) are presented. This exercise involves comparisons with NDSC and WMO/GAW ground-based networks as well as with the TOMS version 8 total ozone products. For GOME ozone total column, RMS values have improved by a factor of two compared with GDP 3.0; seasonal dependency is reduced by the same amount. For GOME NO_2 total column the overall accuracy is estimated to fall within the 5% to 10% range , depending on the contribution of tropospheric NO_2. On a global basis, GDP 4.0 total ozone results lie between -1% and +1.5% of ground-based values for solar zenith angles less than 70°; accuracy is now comparable to that obtainable from ground based stations. At higher solar zenith angles in Polar Regions, larger discrepancies of up to +4% are found; in these regimes, errors on both satellite and ground-based measurements are higher. Up to 2003, total column products have not suffered from any long-term drift of quality, even with expected instrument degradation. The validation results demonstrate that the re-processed GOME total ozone record is now sufficiently accurate for trend analysis (detection of 1% change in total ozone over 10 years).

1. INTRODUCTION

GOME on ERS-2 is an across-track nadir-viewing spectrometer with four linear array detectors covering the spectral range 240-793 nm and with resolutions from 0.2 to 0.4 nm [1]. The satellite has a sun-synchronous polar orbit at height ~790 km, and the instrument swath is 960 km, with three forward scans (footprint 320x40 km^2) in nominal viewing mode. Since August 1996, GOME total O_3 and NO_2 column data have been processed operationally with the GOME Data Processor [2] at the German Processing and Archiving Facility (D-PAF) established at the German Aerospace Centre (DLR) on behalf of the European Space Agency (ESA). GOME has now been producing global distributions of total ozone and NO_2 for over ten years. The length and the long-term stability of this data record make it desirable for use in long-term ozone trend monitoring. Following the ESA's call in summer 2002 for improved GOME total ozone algorithms to meet trend analysis accuracy and stability requirements the GDOAS algorithm was selected to be implemented operationally in the D-PAF at DLR. This GDOAS implementation has become GDP 4.0 (Version 4.0 of the GOME Data Processor). A description of the GDP 4.0 GDOAS algorithm is given in detail by van Roozendael et al [3]. The complete reprocessing of the entire GOME total ozone record was finished in December 2004, and the reprocessed GOME data record, including historical data, is available to the public via the ERS Help & Order Desk.

2. SUMMARY OF THE GDP 4.0 ALGORITHM

GDP 4.0 is a DOAS retrieval algorithm, comprising a least squares fitting for the slant column of ozone followed by an AMF (Air Mass Factor) computation to derive the corresponding vertical column amount. In addition to the ozone slant column, the DOAS part of the algorithm also retrieves an effective temperature to characterize the Huggins-bands ozone absorption temperature dependence, and two fitting amplitudes corresponding to additive reference spectra for undersampling and Fraunhofer filling-in (Ring) effect [3]. There is also an explicit shift and squeeze fitting to improve the wavelength registration of the earthshine radiance spectrum, plus an additional cross-correlation for the Level 1b irradiance spectrum in the region of the DOAS fitting window (325-335 nm). GDP 4.0 uses an iterative computation for the AMF and vertical column density VCD, with the radiative transfer calculations based on the use of a column classified ozone profile climatology. This method was first used in GDP 3.0 [4], where neural network functions were employed to deliver the AMFs at 325.0 nm. In GDP 4.0, AMFs are calculated directly with calls to a radiative transfer model. Also in GDP 4.0, the improved TOMS Version 8 ozone profile climatology [5] was used and the AMFs were calculated at 325.5 nm. A new cloud pre-processing step has been introduced in GDP 4.0 for the treatment of clouds in the independent pixel approximation (IPA) including two new algorithms; OCRA, which uses data fusion techniques to derive the cloud fraction from the sub-pixel PMD measurements and ROCINN which derives the required cloud-top information from the spectral fitting of reflectivity in and around the Oxygen A band [3]. The most important change from GDP 3.0 to GDP 4.0 has been the introduction of the completely new algorithm which deals with the "molecular Ring correction". It has resulted in a dramatic improvement in accuracy [3].

3. VALIDATION OF GDP 4.0

3.1 Selection of validation data sets, coincidence criteria and errors

The present study is based on archived total ozone measurements provided by two major contributors to WMO/GAW: Dobson and Brewer total ozone data records, as deposited at the WOUDC in Toronto, Canada (http://www.woudc.org); and UV-visible DOAS, Dobson and Brewer total ozone data records acquired as part of the NDSC (public archive available via http://www.ndsc.ws). The WOUDC contains total ozone data mainly from Dobson and Brewer UV spectrophotometers and from M-124 UV filter radiometers. The NDSC database contains total ozone data from DOAS UV-visible and Fourier Transform infrared spectrometers, plus Dobson and Brewer instruments at selected stations. Total ozone data from a large number of the WOUDC and NDSC stations have already been used extensively both for trend studies as well as for validation of satellite total ozone data [6,7,8,9,10]. To prepare ground-based data sets for GOME and TOMS validation, we investigated the quality of the total ozone data of each station and instrument that deposited data at NDSC and WOUDC for any periods during 1995-2004 [11] and finally some 41 Brewer, 61 Dobson and 27 UV-visible DOAS instruments were considered for the comparisons with GDP 3.0, GDP 4.0, and TOMS V8. A complete listing of all instruments used in the validation may be found in the GDP 4.0 Delta-Validation Report [12]. For Dobsons and Brewers coincidences are considered for a maximum of 150 km between GOME footprint center and the stations, and within a temporal window of three hours. For UV-visible zenith-sky observations of the same day, the GOME footprint must intercept the air mass estimated with a ray tracing model.

There are several sources of uncertainty in the ground-based data that are known to interfere with GDP validation. The work of Roozendael et al [13] has shown that mutual agreements between Dobson, Brewer and UV-visible data can reach the "percent" level when the major sources of discrepancy are properly accounted for. For Dobson instruments, the temperature dependence of the ozone absorption coefficients used in the retrievals might account for a seasonal variation in the error of 1% to 2%. The effect is smaller for Brewer instruments because of their use of wavelengths with reduced ozone absorption temperature dependency. For zenith-sky UV-visible spectrometers measuring ozone in the Chappuis band, the use of DOAS minimises uncertainties associated with the temperature dependence of the absorption cross-sections and major uncertainties on the vertical column are associated with the AMF conversion from spectrally derived slant columns to vertical columns. Accounting for these errors Dobson, Brewer and SAOZ effects, apparent seasonalities between Dobson/Brewer and SAOZ ozone column measurements vanish and the mutual consistency can reach the "1% level" on average. However, we do not include these corrections in the standard NDSC and WOUDC ozone data products as used in this GDP 4.0 validation. Consequently, ground-based uncertainties can be larger than differences between improved satellite ozone column data and the ground-based results.

In the GOME and TOMS ozone validation literature, collocation criteria are based on spatial windowing varying from 100 to 600 km and temporal windows from 1 hour to 1 day. Dobson and Brewer air masses are located between the measuring station and a maximum distance of 80 km in the direction of the sun. Zenith-sky air masses extend over several hundred kilometers in the azimuth of the rising and setting sun. Selection criteria based on simple time/space window limits can lead to comparisons based on very different perceptions of the atmospheric ozone burdens.

Figure 1 illustrates this issue for a GOME/SAOZ total ozone comparison at Jungfraujoch on a day with large spatial gradients and high variability typical of the fall season over the European Alps. These horizontal smoothing uncertainties due to air mass extensions are in part be responsible for differences in the scatter patterns observed between GOME/SAOZ, and GOME/Dobson More generally, inappropriate selection of collocated data can dramatically increase the dispersion of the comparison results, from a few percent at middle latitudes to values approaching 60% percent at Antarctic stations located at the edge of the polar vortex and situated sometimes inside and sometimes outside the ozone hole. At stations experiencing stationary gradients, e.g. those near high mountain ranges with a North-South orientation or close to the vicinity of a stationary weather pattern, poor selection can even result in fictitious systematic biases up to 10% and beyond.

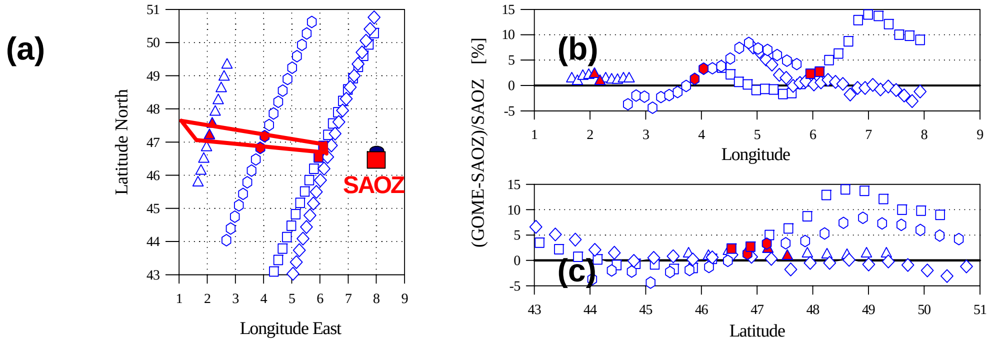


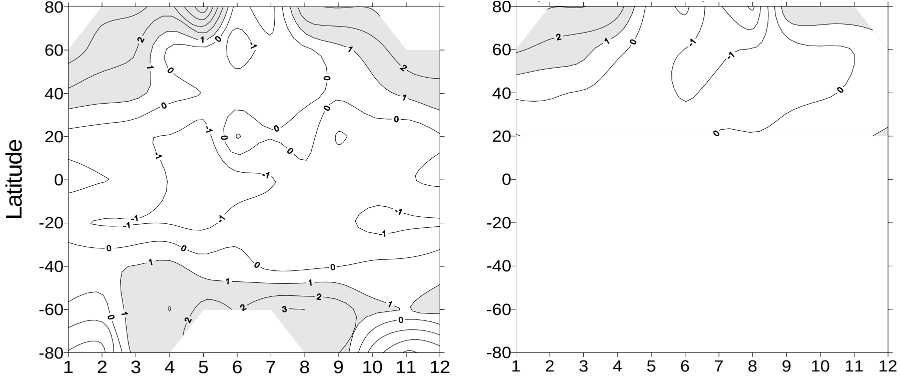
Fig. 1. Effect of air mass differences on the GOME/SAOZ comparisons, illustrated at Jungfraujoch (Switzerland) on 4 September 1995. Differences corresponding to the GOME footprints overlapping the SAOZ air mass are highlighted in red [11].

3.2 Ozone column validation

GDP 2.7 overestimated ground-based total ozone during winter-spring by 2%, while during summer-autumn it underestimated ground-based ozone values by as much as 4%, the resulting amplitude is about 3%. In the tropics there was no significant seasonal dependence in the differences but in general, ozone was underestimated with GDP 2.7 by 1-2%. With GDP 3.0 the amplitude of the seasonal dependence over the middle and high latitudes was reduced by almost 50%. The remaining dependence was found to have almost the same phase with its counterpart in GDP2.7 [14]. The change was mainly reflected in the winter-spring season where overestimation by GOME was minimised. In addition, GOME underestimated ground-based total ozone by 2% to 4% over desert areas. In the tropics, GDP 3.0 showed again a negative bias of about 2%, similar to that observed with GDP 2.7. The algorithm upgrades introduced in GDP 4.0 (see section 1.2) have generated a different picture of the month-latitude cross sections of the differences between GOME and ground-based stations. The comparison results are shown in Figures 2a and 2b separately for the Dobson and the Brewer, and they are based on the selection of validation orbits as described in section 2.2. Figures 2c and 2d show the same month-latitude cross-sections, but here direct-sun Dobson (left panel) and Brewer (right panel) data are compared to TOMS V8 overpass data records. TOMS V8 has almost no bias against the Dobson total ozone observations and shows no seasonality in nearly all latitudes. The systematic TOMS V7 overestimation of Southern Hemisphere total ozone values has disappeared. Both GDP 4.0 and TOMS V8 results show substantial improvements compared to total ozone from previous operational versions. Remaining structures in time and latitude will be discussed below in sections 4.3 and 4.4 respectively. Systematic offsets of GDP 3.0 vs. Brewer (-1.89%) and Dobson (-2.06%) data have all but vanished with GDP 4.0: to -0.17% for Brewer and 0.11% for Dobson comparisons. Zonal mean agreement varies within ±1-2%, with no marked meridian structure. Over the polar latitudes of both hemispheres, GDP 4.0 results are based on few measurements, especially at large SZA, and therefore they do not have the same significance with results at other latitudes. Studies relevant to high latitude and large SZA are detailed in section 4.5. TOMS has improved performance in all latitudes no meridian dependence of the differences. TOMS V8 data, when compared with Dobson instruments, have almost no offset (-0.3%), but they show a negative bias of about 1.5% compared with Brewer instruments.

From Figures 2a-d it can be concluded that there is still a small mean seasonal dependence remaining in the comparisons with the ground-based measurements north of 40°N and south of 40°S. The amplitude of this seasonality does not exceed 1%-1.5% for the Dobson comparisons and is even less for the Brewer comparisons. Over the tropics, the comparisons show results between 0 and 1% with nearly no seasonal variation. The GDP 4.0 seasonality is not in phase with the one observed in GDP 3.0, but it is rather in phase with the variation of the stratospheric temperatures (see 25°N-65°N zonal mean temperatures estimated by NOAA at 50 hPa (http://www.cpc.ncep.noaa.gov/products/stratosphere)): there is almost no bias to date during the warm period, while a positive bias of about 2% occurs during the cold period (including ozone hole conditions). The use of absorption coefficients at a fixed temperature for both Dobson and Brewer total ozone measurements results in ozone column values dependent on stratospheric temperature variations. On the other hand, GDP 4.0 includes the spectral fitting of the effective temperature at which cross-sections are calculated. Therefore GDP 4.0 should not depend significantly on the variability of stratospheric temperatures. A seasonal signature with similar phase and amplitude is found when comparing co-located Brewer and Dobson measurements from well-calibrated instruments for a long period [15]. This indicates that a large part of the observed differences between GDP 4.0 and ground-based measurements can be attributed to characteristics of the ground-based retrieval algorithms rather than to aspects of the GDP 4.0 algorithm.. Further confirmation is provided by the comparisons between Dobson, Brewer and TOMS V8 total ozone displayed in Figure 2c and 2d which indicate that TOMS has almost no bias against the Dobson total ozone observations and shows no seasonality almost in every latitude belt. On the other hand the Brewer comparisons over middle latitudes show a small negative bias of -1% and a seasonal behaviour with an amplitude of 0.5% in phase with the one found in GDP 4.0. Given that: (a) the forward model of TOMS V8 uses a single temperature profile for calculating radiances, and (b) the TOMS wavelengths are closer to those for the Dobson instruments, we can infer that TOMS V8 and Dobson measurements have similar dependence on the lower stratospheric temperature. In consequence, their temperature-related errors are likely to cancel out when calculating their differences. This is also partly valid in the Brewer comparisons.

(a) (GDP 4.0 - Dobson)/Dobson [%]   (b) (GDP 4.0 - Brewer)/Brewer [%]



(c) (TOMS V8 - Dobson)/Dobson [%]   (d) (TOMS V8 - Brewer)/Brewer [%]

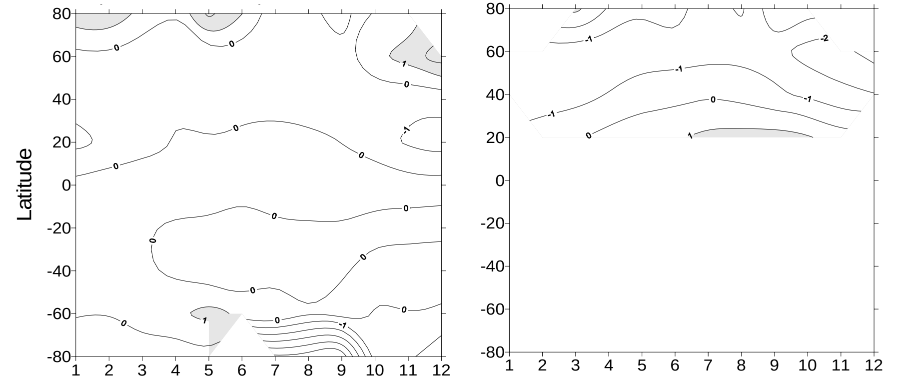


Fig. 2. Month-latitude cross-section of the relative difference between GOME and TOMS ground-based total ozone. GOME total ozone data are taken from the 4900 validation orbits processed with GDP 4.0, and the results obtained by comparison with Dobsons (a) and Brewers (b) are presented separately (note that nearly no Brewers operate in the Southern Hemisphere). TOMS Version 8 total ozone overpass data are also compared separately with Dobsons (c) and Brewers (d) [11].

GDP 4.0 ozone record shows a weak sensitivity not only to instrumental degradation but also to trends in atmospheric parameters other than ozone [6]. In order to examine and compare the long-term stability of GDP 3.0, GDP 4.0 and TOMS V8 on a global basis, we averaged the individual station comparisons (based on all available orbits) separately over the Northern and Southern Hemisphere [11]. In this paper we only show the Brewer N.H. comparisons. It is evident from Figure 3 that until June 2003, both GDP 3.0 and GDP 4.0 total ozone data do not show any drift with respect to the ground-based data. [Because of technical problems on ERS-2, GOME data lack global coverage from June 2003 onwards]. However, sampling issues (less ground-based data available during 2003-2004 and fewer validation orbits) might increase the noise at the end of the time series

To detect and quantify possible improvements in the SZA dependences in GDP 4.0, we have first compared GOME data acquired during polar day at different solar elevations, to ground-based data acquired at fixed SZA values and therefore free from any air mass or SZA dependence. During polar summer, when the poles are illuminated permanently, GOME acquires measurements over the same high latitude stations at least two times a day under different solar elevations. This multiple daily overpass allows for the detection of the SZA dependence between GOME data acquired in the mid-morning (medium SZA) and GOME data typical of midnight sun conditions (large SZA). Figure 4 shows comparisons with the FMI Brewer at Sodankylä (67°N) and demonstrates that the average bias of about 6% observed between mid-morning (moderate SZA) and midnight sun (large SZA) data with GDP 3.0 has reduced to a value of 1.5% with GDP 4.0.

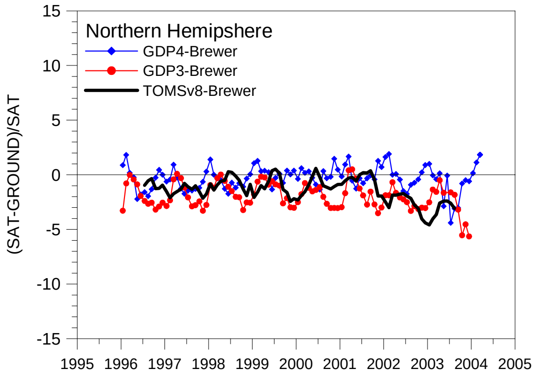


Figure 3. Time-series of the percent relative differences between satellite (GDP 3.0, GDP 4.0 and TOMS V8) and ground-based Brewer ozone data for the period 1996-2004, averaged over the Northern Hemisphere (updated from [11])

The column dependence of the difference between GOME (GDP 3.0 and GDP 4.0) and ground-based total ozone was also studied for three different instruments (two Dobson and one SAOZ) operating in the Antarctic with comparisons are limited to the ozone-hole period (from September 1 to November 1) in order to avoid interferences with possible SZA and seasonal dependencies. At all stations, the upgrade to GDP 4.0 generates an increase of the ozone column value by about 3% over the entire ozone column range; there is thus no perceptible change in the ozone column dependence..

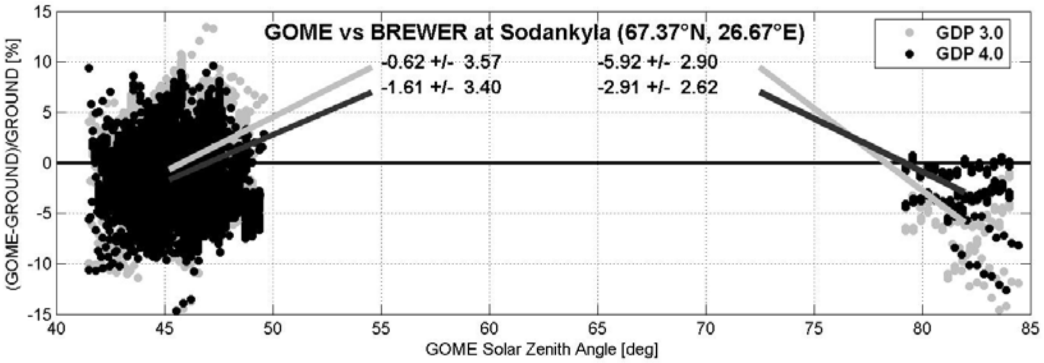


Figure 4. Comparison of the polar day SZA dependence of GDP 3.0 and GDP 4.0 total ozone at Sodankylä (Arctic Finland) (updated from [11])

3.3 NO_2 column validation

The GOME GDP total nitrogen dioxide product has also been validated from pole to pole, with comparisons to ground-based measurements of the NDSC network of SAOZ/DOAS UV-visible spectrometers and Fourier Transform Infrared spectrometers, and to global data from the HALOE and POAM satellite sensors and tropospheric and stratospheric modelling tools. GOME total nitrogen dioxide is in reasonable agreement with ground-based and other satellite measurements: within ±5 10^{14} molec.cm^{-2} in areas of low tropospheric NO_2 and within ±8 10^{14} molec.cm^{-2} in areas of very low slant column of NO_2. Although it is difficult to make a precise evaluation of the NO_2 total column accuracy (due to various problems such as the photochemical diurnal cycle of NO_2), the overall accuracy is estimated to fall within the 5% to 10% range, provided that the contribution of tropospheric NO_2 to the vertical column remains low.

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