VALIDATION OF DIFFERENT CONFIGURATIONS OF THE GODFIT/GDP5 ALGORITHM USING GROUND-BASED TOTAL OZONE DATA

MariLiza Koukouli[(1)], Jean-Christopher Lambert[(2)], Dimitris Balis[(1)], Diego Loyola[(3)], Walter Zimmer[(3)], Michel Van Roozendael[(2)], Christophe Lerot[(2)] and Jose Granville[(2)]

(1) Laboratory of Atmospheric Physics, Aristotle University of Thessaloniki, Thessaloniki, Greece. Email: mariliza@auth.gr

(2) Belgian Institute for Space Aeronomy, Brussels, Belgium

(3) German Aerospace Centre (DLR), Wessling, Germany

ABSTRACT

In the frame of the ESA-funded project "GDP 5.0 - Upgrade of the GOME Data Processor for Improved Total Ozone Columns", total ozone estimates from different GODFIT/GDP5 configurations were compared with the current operational GOME GDP4.x data products (including the latest algorithm improvements) and with ground based total ozone data from quality controlled Brewer, Dobson and SAOZ measurements available at WOUDC and NDACC. The different configurations of the total ozone retrieval algorithms include the use of different input temperatures (ECMWF analyses or TOMS v8 climatological database with a retrieved temperature shift), different a priori ozone profile databases (TOMS v8, and various modes of NNORSY) and different schemes for the cloud treatment (OCRA/ROCINN, FRESCO+). GOME retrievals using all possible combinations were also compared with GDP4.x data products. The use of different combinations of the above a priori choices in the retrievals introduce marked deviations in the amplitude of the seasonal dependence of the differences between satellite and ground-based data, in the solar zenith angle dependence of the satellite retrievals, and in their offset and latitudinal dependence. Irrespective of said differences in retrieval configuration, all GDP5 products are in better agreement with the ground-based measurements for extreme cases such as high solar zenith angles, low stratospheric temperatures, low total ozone conditions, etc. than the respective GDP4.x total ozone data products.

1. INTRODUCTION

GOME on ERS-2 is an across-track nadir-viewing spectrometer with four linear photodiode array detectors covering the spectral range 240-793 nm, at 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 (GDP) [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 fourteen years. The length and the long-term stability of this data record make it desirable for use in long-term ozone trend monitoring [3].

The main aim of this work is to assess a new algorithm for the analysis of GOME total ozone measurements using correlative ground-based observations as a validation tool, and to suggest the optimal retrieval settings for the new operational GOME total ozone data product.

1.1. The operational GDOAS GDP4.x and future GODFIT GPD5 algorithms

Following ESA's call in summer of 2002 for improved GOME total ozone algorithms to meet trend analysis accuracy and stability requirements, the GDOAS algorithm was selected to be implemented in the operational environment of D-PAF at DLR, as 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 [4]. A proposal to ESA for further GDP improvement was accepted in summer 2007, and this project is based on the implementation of GODFIT into the GDP at DLR and its installation therein. This phase also includes delta validations of different retrieval settings to verify the improvement with respect to GDP 4.x, the thorough validation of the resulting GDP 5.0, and the complete reprocessing of the entire GOME total ozone record.

Within the framework of this project a new direct fitting algorithm called GODFIT (GOme Direct FITting) was developed. Compared to the DOAS approach used in GDP up to version 4.x, the GODFIT algorithm determines the vertical ozone column without the need for a separation between slant column fitting and AMF-based conversion to vertical column. The main product is the vertical column itself and the main error diagnostic is the solution variance of this retrieved parameter. The inversion is a straightforward non-linear least-squares minimization based on an iterative series of linearized forward model steps. It is a property of GODFIT that the total column error emerges naturally from the chi-square minimization; this property depends on the ability of the forward model to deliver the appropriate Jacobian with respect to the total column. The final data product is thus simpler to characterize than that for DOAS-type retrievals; there are no intermediate quantities such as slant column density and AMF values.

Two different ozone profile climatologies have been implemented as a priori for radiative transfer calculations, both in GDOAS/GDP4.x and GODFIT/GDP5:

a) The column-classified ozone profile climatology that was created for the **TOMS Version 8** (V8) total ozone retrieval algorithms [*Bhartia*, 2003]. Profiles are specified for 18 latitude bands from pole to pole (10° intervals), and for each month of the year. Latitude and time variations are treated using a bilinear interpolation scheme.
b) A complete ozone climatology has been developed from a multi-year record of ozone profiles retrieved from GOME using the neural network NNORSY.. This is the **NNORSY** climatology [*Muller et al*., 2003; *Kaifel et al*., 2007]available in four modes taking different input parameters. For this work we use the mode that takes as input the latitude, longitude, time, and total column amount; the climatology output is a ozone profile.

Two different cloud treatments have been tested in GODFIT/GDP5:

a) **FRESCO+** (Fast Retrieval Scheme for Clouds from the Oxygen A-band) is a fast and robust algorithm providing cloud information from the O_2 A-band for cloud correction of ozone retrieval [11]. FRESCO provides a consistent set of cloud parameters by retrieving simultaneously the effective cloud fraction and the effective cloud top pressure.
b) ROCINN (Retrieval of Cloud Information using Neural Networks) [12] is based on O_2 *A* band reflectances from GOME. It delivers cloud-top pressure and cloud-top albedo. The independent pixel approximation is used; the cloud fraction derived from the OCRA (Optical Cloud Recognition Algorithm) [12] algorithm is taken as a fixed input to the ROCINN algorithm. This dual treatment will be referred to as **OCRA/ROCINN** hereafter. OCRA/ROCINN are the cloud algorithms currently used operationally for GOME/ERS-2 and GOME-2/MetOp-A.

Both cloud treatment algorithms use the Lambertian Equivalent Reflectivity cloud model (LER), also called clouds as reflecting boundaries model, and hence share a common and known problem. The total ozone column below the cloud top height is in reality the sum of the intra-cloud ozone column plus the column below the cloud itself. Backscatter measurements are sensitive to the intra-cloud ozone column which is improperly modelled in the LER approach and total column errors could be large [13]. A simple correction called Semi-transparent Lambertian cloud (STLC) model has been developed for GDP4.x and provides an initial empirical characterization of the intra-cloud total ozone column as a function of the ozone column below cloud top (ghost column, estimated from a climatology), the cloud albedo, and the solar zenith angle (SZA).

1.2. The ground based datasets

The present study is based on archived total ozone measurements provided by two major contributors to WMO's Global Atmosphere Watch (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 Network for the Detection of Atmospheric Composition Change (NDACC, formerly NDSC; (public archive available via http://www.ndacc.org). Total ozone data from a large number of the WOUDC and NDACC stations have already been used extensively both for trend studies as well as for validation of satellite total ozone data [3, 5-9]. To prepare ground-based data sets for the GOME validation, we investigated the quality of the total ozone data of each station and instrument that deposited data at NDACC and WOUDC for any periods during 1995-2008 [3] and finally about 42 Brewer, 62 Dobson and 27 UV-visible DOAS instruments were considered for this work. A complete listing of all instruments used in the validation may be found in the GDP 4.0 Delta-Validation Report [10].

For the Dobson and Brewer instruments, coincidences are considered for a maximum of 150 km between GOME footprint centre 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 ground-based air mass estimated with a ray tracing model [5, 3].

2. VALIDATION RESULTS

Four different GODFIT/GDP5 and one GDOAS/GDP4.x scenarios were validated against the ground-based measurement records. The five scenarios differed in the following parameters, which have been mentioned in the previous section:

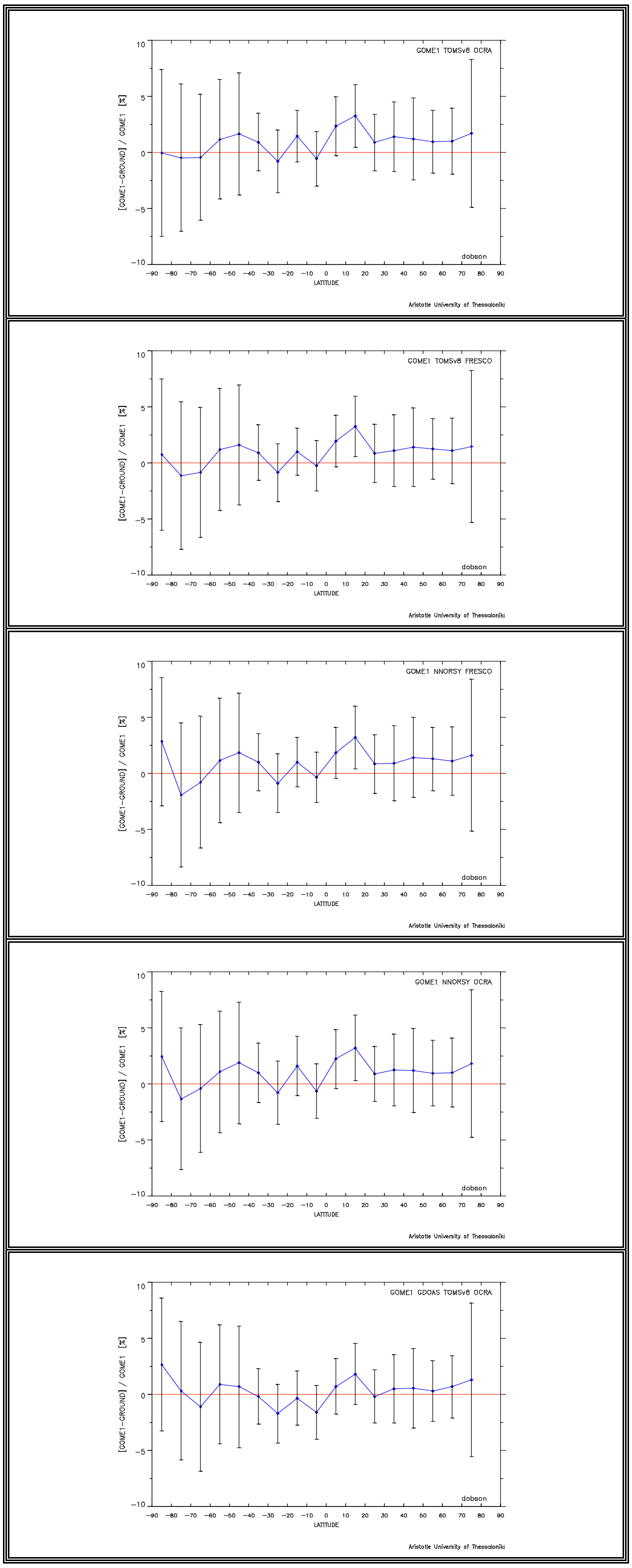

Figure 1. The latitudinal dependence of the percent difference between GOME and Dobson total ozone. From top to bottom: scenarios I to V.

I. GODFIT/GDP5, with TOMSv8 ozone climatology, OCRA/ROCINN for cloud treatment.
II. GODFIT/GDP5, with TOMSv8 ozone climatology, FRESCO+ for cloud treatment.
III. GODFIT/GDP5, with NNORSY ozone climatology, FRESCO+ for cloud treatment.
IV. GODFIT/GDP5, with NNORSY ozone climatology, OCRA/ROCINN for cloud treatment
V. GDOAS/GDP4.x, with TOMSv8 ozone climatology, OCRA/ROCINN for cloud treatment and intra-cloud correction.

The latitudinal dependence of the percentage differences between ground-based and GOME total ozone estimates for the five scenarios are shown in Fig. 1. The mean differences for all stations have been gridded in bins of 10° to generate these plots. The bars represent the standard deviation of the difference within a bin. Scenarios I to V are shown from top to bottom,. For the Northern Hemisphere, the first four scenarios show a constant satellite overestimation of approximately 1.0% compared to Dobson instruments, whereas for scenario V no such overestimation exists. For the tropical and equatorial region, the same pattern but with different magnitude is followed by all scenarios. This pattern is attributed to issues with ground-based measurements in these regions. For the Southern Hemisphere, the following can be said: an overestimation of around 2% is observed for all scenarios at mid-latitudes. The Antarctic polar region is represented the same for all scenarios, but for scenario I which shows an excellent agreement southwards of 60° and scenario II which follows second. The reason for this is attributed to the better representation of the southern polar total ozone conditions in the TOMS v8 climatology used in these two scenarios compared to the NNORSY climatology used in scenarios III and IV.

The SZA dependence of the percentage differences between ground-based and GOME total ozone estimates for the five scenarios is shown in Fig. 2. The mean differences for all stations have been gridded in bins of 1° to generate these plots. The bars represent the standard deviation of the differences within the bin. Scenarios I to V are shown from top to bottom. For scenario I [Fig 2, upper, left] the GOME overestimation is almost stable at all SZA values. The difference introduced in scenario II by using the FRESCO cloud retrieval instead of the OCRA-ROCINN can only be observed at very high SZAs of above 80°, where the picture is turned into an underestimation, an effect of the different cloud treatment algorithms used. For scenarios III and IV, which share the NNORSY ozone climatology and differ in the cloud retrieval, the comparison shows a complex structure: a slight overestimation at low SZA, followed by a near zero deviation up to 40° and the known overestimation up to high SZA. A slightly better comparison at very high SZA is seen in scenario IV, again pointing to the fact that the OCRA/ROCINN cloud treatment behaves better at the extremes.

A different way to visualise the validation efforts is to examine which of the four GODFIT/GDP5 scenarios yields the lowest standard deviation of the differences (STDV) for the largest amount of ground-based stations, as shown in Fig. 3. In the upper graph, the latitudinal dependence of the STDV with respect to the Brewers is shown, in the middle the same for the Dobsons, and in the lower, the same for the UV-Vis. Inspecting all three comparisons, at the majority of stations, the standard deviation between GODFIT and ground-based data does not vary by more than 0.2-1% from one scenario to another. The first four scenarios, i.e. using either the TOMS V8 or the NNORSY ozone climatologies with either the OCRA/ROCINN or FRESCO cloud treatment, show the same picture. In all three STDV plots shown in Fig.3, two groups of behaviour appear: scenarios I and IV, which were all calculated with OCRA/ROCINN, and scenarios II and III, which use the FRESCO+ algorithm. Apparently, the choice of the cloud algorithm controls the standard deviation results. It also appears that scenario III (NNORSY & FRESCO+) offers the lowest standard deviation for all three ground-based networks for about 80% of the stations.

3. CONCLUSIONS

Complementary validation studies were performed which aimed to check the sensitivity of GOME total ozone accuracy to the a priori ozone profile climatology, i.e. NNORSY versus TOMSv8, its sensitivity to the cloud retrieval, i.e. FRESCO+ versus OCRA/ROCINN, and its sensitivity to the ozone column retrieval approach, i.e. GDOAS versus GODFIT. The findings are as follows:

I. *For the effect of the a priori ozone climatology:* Comparing scenario I to scenario IV & scenario II to scenario III, it was shown that the NNORSY climatology behaves equally well as the TOMSv8 one for all latitudes and SZAs up to 75°. However, for larger SZAs and from 70° to 90° South in latitude TOMSv8 applies better

II. *For the effect of the cloud treatment:* Comparing scenario I to scenario II & scenario III to scenario IV, it was shown that OCRA/ROCINN behaves equally well as FRESCO+ at all latitudes and SZAs up to 75°. Slight deviations above 75° in SZA and 70° South in latitude vindicate in favour of OCRA/ROCINN.

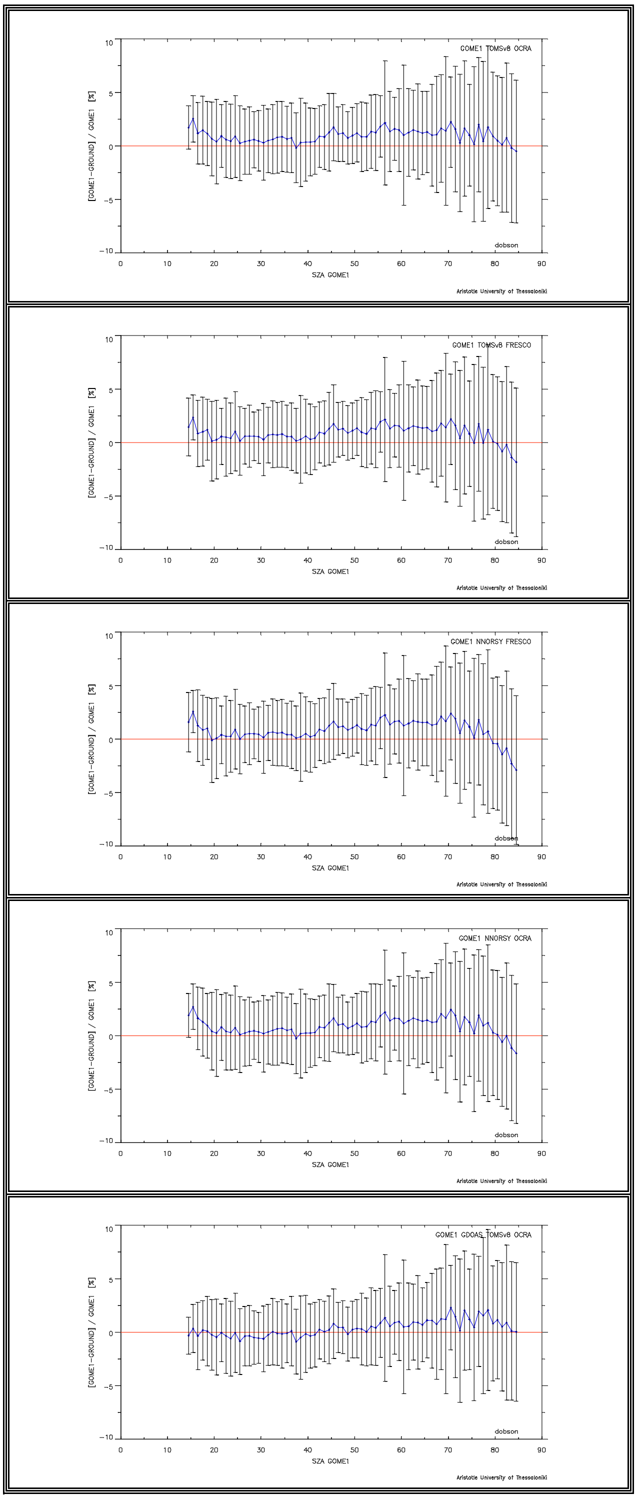

Figure 2. The solar zenith angle dependence of the percent difference between GOME and Dobson total ozone. From top to bottom: scenarios I to V.

III. *For the effect of the retrieval approach:* Comparing scenario I to scenario V it was shown that using GDOAS with TOMSv8 and OCRA/ROCINN with the Vic correction, provides results in excellent overall agreement with ground-based data. However, as already pointed out in past validation exercises, GDOAS differences to ground-based data display a larger SZA dependence than corresponding GODFIT results [3].

Considering the statistical estimates that can be derived from the comparisons, for the first four scenarios, the mean global differences were around 0.5±1.0% for the Brewers and 1.0±1.0% for the Dobson comparison. The fifth scenario gave comparisons with differences of the order of -0.0±1.0% for the Brewers and 0.3±1.0% for the Dobsons. Even though in absolute numbers the GDOAS analysis technique provides smaller mean deviations, the fact that the GODFIT offsets are constant with changing SZA and latitude band, leads us to suggest that, after this validation exercise and the ones preceding it, the GODFIT analysis using the TOMSv8 ozone climatology, and OCRA/ROCINN for cloud treatment is the most appropriate to be used for the generation of the future GPD5.0 GOME Ozone Column Data Product.

REFERENCES

[1] Burrows, J., et al., The Global Ozone Monitoring Experiment (GOME): mission concept and first scientific results, *J. Atmos. Sci*, *56*, 151-175, 1999.

[2] Loyola, D., et al., Ground Segment for ERS-2 GOME Data Processor, *3rd Symposium on Space in the Service of our Environment,* Florence, Italy, *ESA SP-414*, 591-597, 1997.

[3] Balis, D., et al., Ten years of GOME/ERS2 total ozone data—The new GOME data processor (GDP) version 4: 2. Ground-based validation and comparisons with TOMS V7/V8, *J. Geophys. Res.*, 112, D07307, doi:10.1029/2005JD006376, 2007.

[4] Van Roozendeal M., et al., Reprocessing the 10-year GOME/ERS-2 total ozone record for trend analysis: the new GOME Data Processor Version 4.0, Algorithm Description, *J. Geophys. Res.*, 111, D14311, doi:10.1029/2005JD006375, 2006.

[5] Lambert, J.-C., et al., Investigation of pole-to-pole performances of spaceborne atmospheric chemistry sensors with the NDSC, *Journal of the Atmospheric Sciences*, Vol. 56, pp. 176-193, 1999.

[6] Fioletov, V., et al., An assessment of the world ground-based total ozone network performance from the comparison with satellite data, *J. Geophys. Res.*, 104, 1,737-1,747, 1999.

[7] Lambert, J.-C., et al., Combined characterization of GOME and TOMS total ozone measurements from space using ground-based observations from the NDSC, Advances in Space Research, Vol. 26, 1931-1940, 2000.

[8] Bramstedt, K., et al., Comparison of total ozone from the satellite instruments GOME and TOMS with measurements from the Dobson network 1996–2000, *Atmos. Chem. Phys., 3,* 1409-1419, 2003.

[9] Labow, G. J., et al., A Comparison of TOMS, SBUV and SBUV/2 Version 8 Total Column Ozone Data with Data from Ground Stations, *Proceedings of QOS2004*, Kos, 1-8 June, Kos, Greece, 2004.

[10] Lambert, J-C., and D. Balis, Delta validation report for ERS-2 GOME Data Processor upgrade to 4.0, ESA Report ERSE-CLVL-EOPG-TN-04-0001, 15 December 2004, 2004.

[11] Koelemeijer, R. B. A., et al., A fast method for retrieval of cloud parameters using oxygen A-band measurements from the Global Ozone Monitoring Instrument, *J. Geophys. Res.*, D, 106, 3475–3490, 2001.

[12] Loyola, D., Automatic Cloud Analysis from Polar-Orbiting Satellites using Neural Network and Data Fusion Techniques, *IEEE International Geoscience and Remote Sensing Symposium*, **4**, 2530-2534, Alaska, 2004.

[13] Liu, X., M. Newchurch, R. Loughman, and P.K. Bhartia, Errors resulting from assuming opaque Lambertian clouds in TOMS ozone retrieval, *Journal of Quantitative Spectroscopy and Radiative Transfer,* 85, 337-365, 2004.

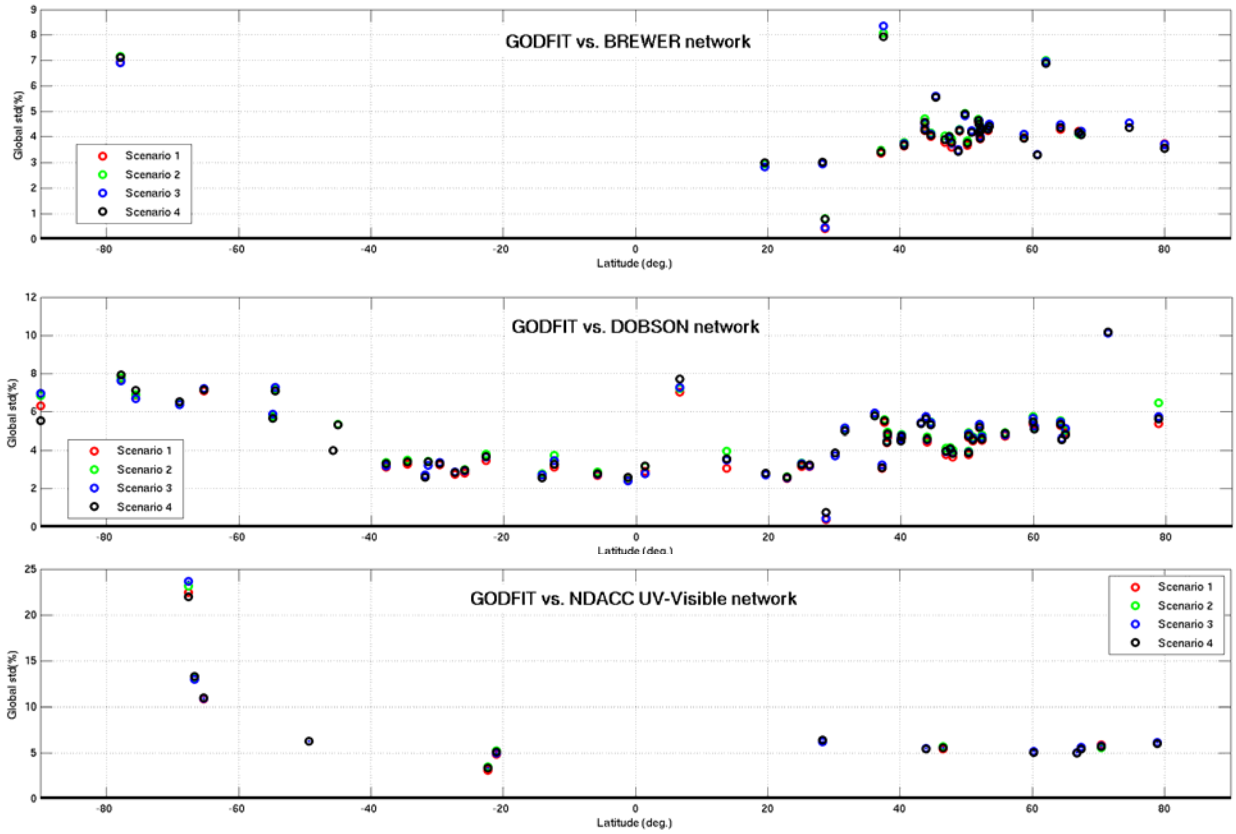

Figure 3. The latitudinal dependence of the standard deviation between GOME (first four scenarios) and ground-based total ozone. From top to bottom: the comparisons with the Brewer, Dobson and NDACC/UV-Visible networks.