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RESEARCH ARTICLE

Comparison of Suomi-NPP OMPS total column ozone with Brewer and Dobson spectrophotometers measurements

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Abstract The objective of this study is to evaluate the accuracy of the daily nadir total column ozone products derived from the nadir mapper instrument on the Ozone Mapping and Profiler Suite (OMPS) flying onboard the Suomi National Polar-orbiting Partnership satellite (S-NPP) launched as a part of the Joint Polar Satellite System (JPSS) program between NOAA and NASA. Since NOAA is already operationally processing OMPS nadir total ozone products, evaluations were made in this study on the total column ozone research products generated by NASA's science team, utilizing the latest version of their Backscatter Ultraviolet (BUV) retrieval algorithms, to provide insight into the performance of the operation system. Comparisons were made with globally distributed ground-based Brewer and Dobson spectrophotometer total column ozone measurements. Linear regressions show fair agreement between OMPS and ground-based total column ozone measurements with a root-mean-square error (RMSE) of approximately 3% (10 DU). The comparison results indicate that the OMPS total column ozone data are 0.59% higher than the Brewer measurements with a standard deviation of 2.82% while 1.09% higher than the Dobson measurements with a standard deviation of 3.27%. Additionally, the variability of relative differences between OMPS and ground total column ozone were analyzed as a function of latitude, time, viewing geometry, and total column ozone value. Results show a 2% bias over most latitudes and viewing conditions when total column ozone value varies between 220 DU and 450 DU.

Keywords ozone mapping and profiler suite, total column ozone, Brewer, Dobson

1 Introduction

Even though the total amount of ozone comprises only 0.6 parts per million (ppm) of the Earth's atmospheric composition, it plays an important role in protecting life by blocking much of the potentially harmful high frequency ultraviolet (UV) radiation from the sun (Varotsos et al., 1995; Antón et al., 2011). As a greenhouse gas, ozone absorbs the infrared energy emitted by the Earth and in turn, causes a radiative forcing change. Thus, ozone layer changes could be closely associated with regional and global climate changes and vice versa (World Meteorological Organization, 2007; Antón et al., 2010).

Since ozone depletion was observed in the early 1970s, with the first dramatic ozone decrease in the lower stratosphere observed in the 1980s (Crutzen and Arnold, 1986; Stolarski et al., 1986), many scientific research programs have been monitoring the ozone layer thickness and investigating the causes for its depletion. According to scientific research, this decrease can primarily be attributed to photochemical losses related to anthropogenic activities and dynamical factors (e.g., Farman et al., 1985; Cariolle and Déqué, 1986; Varotsos, 2002; Antón et al., 2011). Relevant consequences of ozone depletion are the increase in harmful UV radiation at the Earth's surface and global climate change; thus, monitoring the amount of ozone in the ozone layer and analyzing its variability with high accuracy have become major challenges that must be addressed to protect the ozone layer.

Traditional ground-based spectrophotometers that measure total ozone, such as Brewer and Dobson spectrophotometers, the primary instruments used by the Global Atmospheric Watch Program, can provide daily and continuous total column ozone measurements with high accuracy (Scarnato et al., 2010; Redondas et al., 2014); however, the spatial coverage is limited. In this context, the

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uses of satellite-based instruments that measure total column ozone with daily global coverage have proven to be an effective scientific research technique for global ozone layer monitoring. To date, many instruments specifically designed for total column ozone and ozone profile monitoring have been launched into space, such as the Solar Backscatter Ultraviolet (SBUV and SBUV/2) (Flynn et al., 2009; Bhartia et al., 2013), the Total Ozone Mapping Spectrometer (TOMS) (McPeters et al., 1996a, b, 1998) and the Ozone Monitoring Instrument (OMI) (Levelt et al., 2006). Additional European missions include the Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) (Bovensmann et al., 1999) and the Globe Ozone Monitoring Experiment (GOME and GOME-2) (Balis et al., 2007a; Van Roozendael et al., 2012). The Total Ozone Unit (TOU) on board the Chinese FY-3 series satellite is also designed to map global total column ozone on a daily basis (Wang et al., 2011; Bai et al., 2013).

For more than 30 years, satellite measurements have provided a very detailed and important long-term record of the global distribution of ozone. These ozone records have been widely used by ozone-assessment researchers and policy makers to track the state of the ozone layer. The Ozone Mapping and Profiler Suite (OMPS), the latest generation of Backscattered Ultraviolet (BUV) radiation sensors, flying on board the Suomi National Polar-orbiting Partnership (S-NPP) spacecraft, launched on October 2011 through the Joint Polar Satellite System (JPSS) program, a collaborative mission between NOAA and NASA, is the most advanced space-borne instrument specifically designed to continue the nearly 40-years of ozone-mapping records created by previous BUV sensors. Since NOAA is already operationally processing OMPS nadir total column ozone products, NASA's science team is responsible for evaluating the performance of the sensors and the operational algorithm and products to determine their capability for continuing the long-term climate records and for making any needed improvements (Suomi NPP, 2013)[1].

Here, the performance of NASA's latest total ozone column research products derived from the OMPS nadir total ozone mapper utilizing the latest version of NASA's BUV retrieval algorithms in its early 14-month operation was examined to provide insight into the operation system. Validation was conducted by comparing OMPS total column ozone data with the spatially co-located ground-based Brewer and Dobson spectrophotometer total column ozone measurements. Discrepancies between the OMPS total column ozone and spatially co-located ground-based measurements were analyzed as a function of latitude and viewing conditions, and possible reasons for these discrepancies were discussed.

2 Instruments and measurements

The OMPS instrument and NASA's latest BUV retrieval algorithm are introduced in Section 2.1, and the spatially co-located ground-based Brewer and Dobson measurements are described in Section 2.2.

2.1 OMPS observations

2.1.1 OMPS system

OMPS, an important component of the National Polar-Orbiting Operational Environmental Satellite System (NPOESS) on S-NPP, is the latest generation of space-borne ozone-mapping instruments (Pan et al., 2012). OMPS is designed to measure the vertical, horizontal, and temporal distribution of ozone in the Earth's atmosphere on a daily basis and has the capability to determine whether the ozone layer is recovering as expected after the sharp decrease of ozone in the 1980s (Suomi NPP, 2013)[1].

OMPS is an advanced suite of three hyperspectral instruments that measure sunlight in the ultraviolet and the visible ranges backscattered from the Earth's atmosphere. The system consists of a nadir mapper that maps global ozone with an approximate ground resolution of 50 km, a nadir profiler that measures the vertical distribution of ozone in the stratosphere, and a limb profiler that measures ozone in the lower stratosphere and troposphere with high resolution (Dittman et al., 2002).

The OMPS radiation detectors are two-dimensional, charge-coupled devices (CCD), focal plane arrays (FPA), each arranged in one spectral and one spatial dimension. The nadir total column sensor uses a single grating spectrometer and a CCD array detector to measure backscattered radiance every 0.4 nm from 300 to 380 nm, with 1-nm full-width half maximum (FWHM) spectral resolution. It has a 110° cross-track field-of-view (FOV) and a 0.27° along-track slit width. The measurements from cross-track are combined into 35 bins as 3.35° (50 km) at nadir and 2.84° at ± 55°. The along-track resolution is 50 km at nadir for mapping TOC across a 2,800 km swath, with a 7.6 s reporting period (Flynn et al., 2004).

The nadir profiler employs a double monochromator and a CCD array detector to take measurements every 0.4 nm from 250 to 310 nm, with 1-nm FWHM resolution. The profiler has a 16° cross-track FOV and a 0.26° along-track slit width. The reporting period is 38 s, which forms a 250 km × 250 km cell size synchronized with the five center nadir TOC mapper cells (Flynn et al., 2004, 2012).

For the NPP mission, OMPS also contains a limb system with a focal plane operating from 290 to 1,000 nm for high vertical resolution ozone profile observations. The system

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[1] Suomi NPP http://npp.gsfc.nasa.gov/omps.html, last updated: August 7, 2013

has three vertical slits separated by 4.25° (across track) and a 19 s reporting period; these features result in a 125 km along-track motion. Each slit has a vertical FOV of 1.95° (112 km) equating to 0 to 60 km coverage at the limb and offsets for pointing uncertainty, orbital variation, and Earth oblateness (Flynn et al., 2004, 2012).

2.1.2 Nadir total column ozone measurements

OMPS-based total column ozone data were collected from the daily granules of nadir OMPS total column ozone products from January 2012 to February 2013 as generated by NASA's OMPS science team. This product was a beta released version which provides insight into the latest BUV retrieval algorithm. It can also be acquired from the ozone and air quality archive sets available from the NASA OMPS website (http://ozoneaq.gsfc.nasa.gov/beta/data/omps/); thus, only the algorithm utilized by NASA's science team to derive these total column ozone research products will be discussed here.

The nadir total column ozone product consists of the total ozone in a column of air from the surface to the top of the atmosphere (TOA) and is observed for all solar zenith angle (SZA) viewing conditions (Baker and Kilcoyne, 2011). The algorithm used by NASA's OMPS science team to derive this total column ozone research product is the latest version of NASA's BUV retrieval algorithm, which is a modified version of the version 8 (V8) algorithm (Bhartia and Wellemeyer, 2002) as is being utilized at NOAA to produce their operational ozone product (Bhartia et al., 2013). This algorithm estimates the total column ozone, based on the comparison of measured normalized radiance to calculated normalized radiance, by using a standard UV radiative transfer model for different ozone amounts, specific measurement geometry, and viewing and surface conditions. A detailed description of the scientific basis of ozone retrieval from SBUV irradiance can be found in literatures, such as Dave and Mateer (1967), McPeters et al. (1996a, 1998) and Rodriguez et al. (2003).

In comparison with the V8 algorithm, the current modified algorithm incorporates several changes, including updates to instrument calibration, use of new ozone absorption cross-sections, new ozone (McPeters and Labow, 2012), and cloud height climatologies (Bhartia et al., 2013). These can be summarized as follows: 1) The Malicet et al. (1995) ozone absorption cross-sections were applied to this algorithm rather than those of Bass and Paur (1985), which were commonly used in the Dobson and Brewer spectrophotometers. 2) This OMPS algorithm also uses a month and latitude climatology of temperatures developed using NOAA temperature data sets, in order to minimize biases due to the variation of the ozone cross-section with the temperature (Bhartia et al., 2013). 3) The cloud pressure climatology is based on optical centroid pressure (OCP) derived from rotational Raman scattering using OMI data (Vasilkov et al., 2008).

The forward model used in the current modified algorithm to compute the TOA radiance is based on the vector radiative transfer code developed by Dave (1964) with modifications to account for molecular anisotropy and rotational Raman scattering correction (Bhartia et al., 2013). As mentioned above, several modifications were conducted during the TOA radiance computation in the forward model for possible error minimization, which might be induced from the temperature dependence of ozone cross-section, aerosols and clouds contamination, and the difference between the standard profile and the retrieved profile (Bhartia et al., 2013).

The inverse model, as applied to this algorithm, is based on the optimum estimation formula of Rodgers (1976). The model is designed for retrievals for which the number of layers is greater than the number of wavelengths. According to Bhartia et al. (2013), the typical algorithmic errors are those in the ozone absorption cross-section or in various climatologies used in the forward model. Several sources of systematic errors can create time-independent (but month- and latitude-dependent) bias in the SBUV retrieved profiles, such as errors in a priori profiles for measured and calculated N-values.

As reported by Kramarova et al. (2013), the current modified SBUV algorithm showed mean biases and standard deviations are typically within 5% for monthly zonal mean ozone profiles in the stratosphere between 25 and 1 hPa, while the vertical resolution of the SBUV algorithm decreased above and below this layer. Meanwhile, a comparison of 40 years of SBUV measurements of column ozone with data from the Dobson/Brewer network was conducted by Labow et al. (2013) through comparisons between newly reprocessed SBUV total column ozone data with the current modified algorithm and corresponding ground based measurements. These time series comparisons showed an agreement within ± 1% over the past 40 years with the bias nearly zero over the last decade. In addition, the comparisons, as a function of a satellite SZA, showed consistent behavior for all instruments, while very little systematic offset was observed between the satellite and ground-based measurements as a function of latitude, with the Nimbus-4 BUV data (1970–1976) showing a larger offset. All these studies have generally indicated the high accuracy of the current modified algorithm as being utilized for NASA's total column ozone research products.

2.2 Ground-based measurements

To date, the worldwide, well-established ground-based network of Brewer and Dobson spectrophotometers has typically been considered the ground-truth of total ozone monitoring. Over past decades, total column ozone measured from these two spectrophotometers has been widely used to validate space-borne instruments due to its high accuracy (Fioletov, 2005; Fioletov et al., 2008). Both

Brewer and Dobson instruments measure total ozone in the atmosphere by observing direct sun (DS: measure the light directly from the sun's path) spectral irradiance of solar radiation at specific wavelengths, which mainly rely on the theory of differential absorption in the Huggins band in the UV part of the spectrum where ozone exhibits strong absorption features (e.g., Dobson, 1968; Brewer, 1973; Van Roozendael et al., 1998; Kerr, 2002; Bernhard, 2005). The Dobson instrument has a measurement principle which relies on the ratio of the DS intensities at two standard wavelengths (AD pair: 305.5 nm, 325.4 nm and 317.6 nm, 339.8 nm). Meanwhile, the working principle of the Brewer spectrophotometer is similar to that of the Dobson instrument with an improved optical design and full automation (Brewer, 1973). Total column ozone values are determined by taking the ratio of sunlight intensities at four wavelengths (306–320 nm) with a resolution of 0.6 nm overcoming the spectral interference of sulfur dioxide with ozone (Antón et al., 2009a).

A well-maintained and calibrated Dobson instrument measures total ozone with an estimated accuracy of 1% for direct sun and 2%–3% for zenith sky or for SZAs smaller than 75° (Basher, 1982). A well-calibrated Brewer instrument has an error level comparable to the Dobson instrument, with an estimated accuracy of 1% through DS measurements (Antón et al., 2009a). Despite the similarity in performance between the Brewer and Dobson instruments, small differences (within ± 0.6%) are still observed due to the use of different wavelengths and varying temperature dependencies for the ozone absorption coefficients (approx. keeping 0.13%/°C for Dobson while varying from 0.11–0.15%/°C for Brewer as temperatures range from −45°C to −70°C) (Van Roozendael et al., 1998; Scarnato et al., 2009, 2010).

In this study, total column ozone recorded by well-maintained 34 Brewer and 39 Dobson spectrophotometers during January 2012 to February 2013, from the World Ozone and Ultraviolet Data Centre (WOUDC) archive (http://www.woudc.org), were employed as the ground reference to compare with the total column ozone generated by the NASA's OMPS science team. The distribution of Brewer and Dobson sites is shown in Fig. 1.

3 Methodology

In this study, daily averages of the total column ozone measurements recorded from 34 Brewer and 39 Dobson spectrophotometers were used as ground references to validate the total column ozone research products retrieved from the OMPS nadir mapper utilizing the current modified BUV retrieval algorithms by NASA's OMPS science team. For each day, single total column ozone value of OMPS ground pixels that is most closely co-located with the ground stations was retrieved as the best match.

Due to different principles applied by Brewer and Dobson spectrophotometers, discrepancies between spatially co-located OMPS total column ozone records and ground-based total column ozone measurements were analyzed separately using Brewer and Dobson data sets. The bias dependence of total column ozone on latitude, SZA, cloud fraction, and total column ozone values were also examined. A global study of latitudinal dependence can only be analyzed from the Dobson measurements due to the lack of quality-assured total column ozone data measured from Brewer instruments in the Southern Hemisphere (Antón et al., 2010). To obtain a fair evaluation, only the ground-based total column ozone measurements under direct sun were included to compare

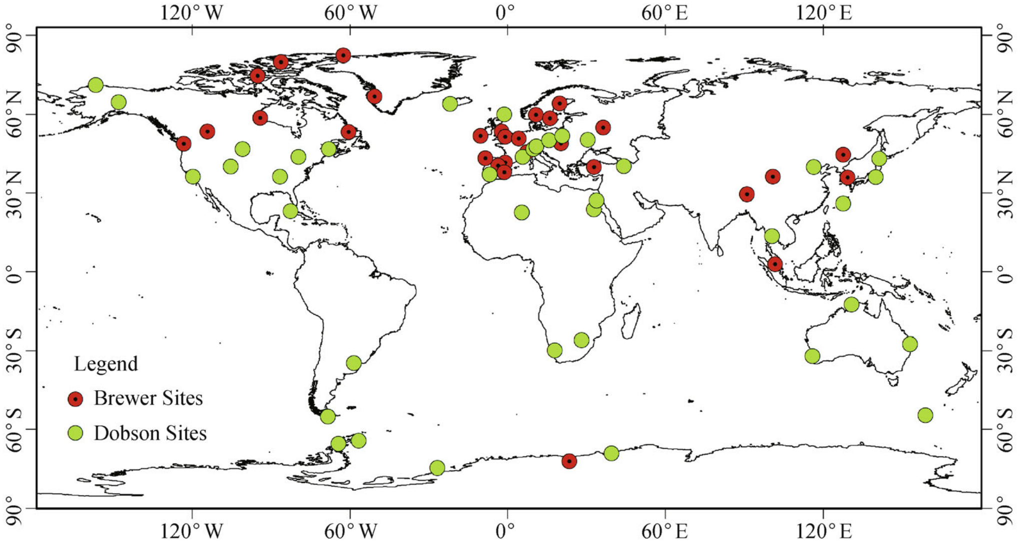

Fig. 1 Global distribution of 34 Brewer and 39 Dobson spectrophotometers used in this study.

with the spatially co-located OMPS total column ozone observations.

The relative differences (RDs) and mean bias error (MBE) between ground-based total ozone measurements and co-located OMPS total column ozone were calculated as:

$$\mathrm{RDs} = 100\frac{\mathrm{OMPS}-\mathrm{Ground}}{\mathrm{OMPS}}, \tag{1}$$

$$\mathrm{MBE} = \frac{1}{N}\sum \mathrm{RD}_i, \tag{2}$$

where OMPS denotes nadir OMPS total column ozone, Ground denotes ground-based total column ozone measurements, and N is the total number of data pairs applied. Uncertainties regarding MBE are characterized by the standard deviation of the RDs.

4 Results and discussion

Linear regressions were performed to analyze the consistency of OMPS total column ozone and ground station measurements (Fig. 2). Statistical parameters were also presented (Table 1). Results indicate fair agreements between OMPS and both types of ground-based total column ozone measurements with an R^2 value of 0.96 and the root mean square error (RMSE) values of 2.88% (9.5 DU) for Brewer and 3.44% (10.2 DU) for Dobson since the OMPS system accuracy requirement is of 9.5 DU. These values reveal a high degree of proportionality with a small spread. The MBE values are + 0.59% with a standard deviation of 2.82% (OMPS – Brewer) and + 1.09% with a standard deviation of 3.27% (OMPS – Dobson), indicating that the OMPS total column ozone tends to estimate Dobson measurements higher than Brewer measurements. These discrepancies can possibly be ascribed to the different measuring principles and station distributions of the two types of ground-based spectrophotometers (Kerr et al., 1988). Additionally, the frequency count of RDs, as shown in Fig. 3, demonstrates fair agreement (i.e., most of the RDs vary within ± 2%).

Figure 4 shows the distribution of the relative differences between OMPS total column ozone and ground-based total column ozone measurements as a function of latitude. The mean bias error for each station (Fig. 3(a)) has a value within 2% for most latitudes compared by using both types of ground-based measurements. Compared with the Brewer measurements, OMPS shows a positive bias near the equator to mid-latitudes in the northern hemisphere, whereas negative bias is observed over high latitudes in both hemispheres. Compared with Dobson measurements, OMPS nearly overestimates the Dobson total column ozone measurements with a mean bias error within 2% over all latitudes. Comparison results from the high latitude stations in the southern hemisphere show a large spread; this effect can be partially attributed to fewer observations in this region throughout the year due to viewing limitations. The latitudinal variability of mean bias between OMPS and ground-based total column ozone measurements is shown as binned at 10° latitude intervals in Fig. 4. The results suggest a sizeable latitudinal dependent error (< 2%) due to the large bias shown in the boreal mid-latitudes and the austral high latitudes.

The time series of the monthly mean relative differences were analyzed to evaluate data consistency in the OMPS early 14-month operation (Fig. 5). Similarly, the mean bias error varies within 2% when comparing with both the Brewer and Dobson measurements. The time series of both comparisons do not exhibit significant mean bias error drift

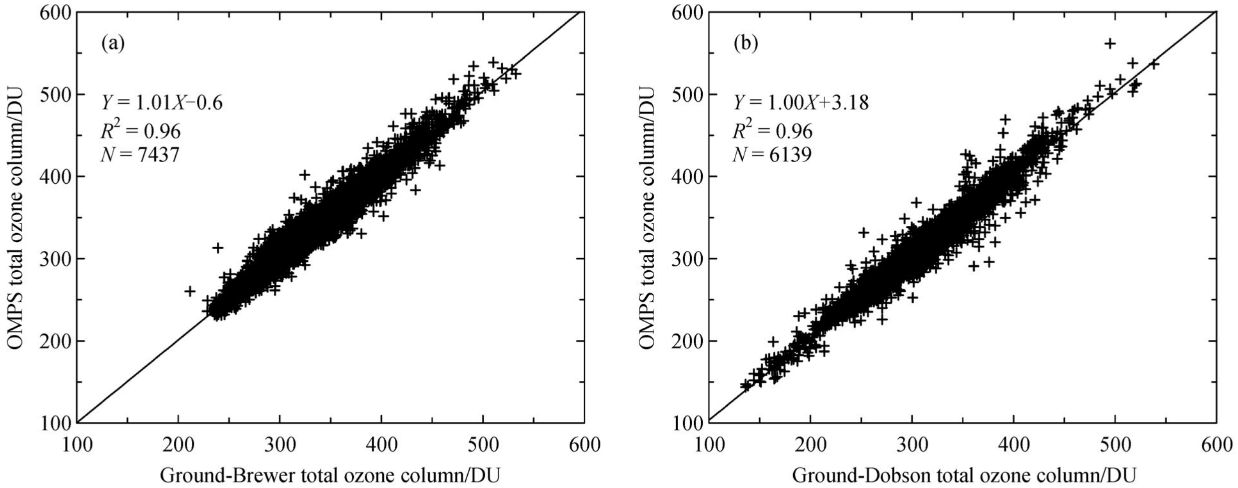

Fig. 2 Scatterplots of OMPS total column ozone against ground-based observations for Brewer (a) and Dobson (b) measurements. The daily average of ground-based Brewer and Dobson total column ozone measurements was applied to compare with co-located OMPS total column ozone.

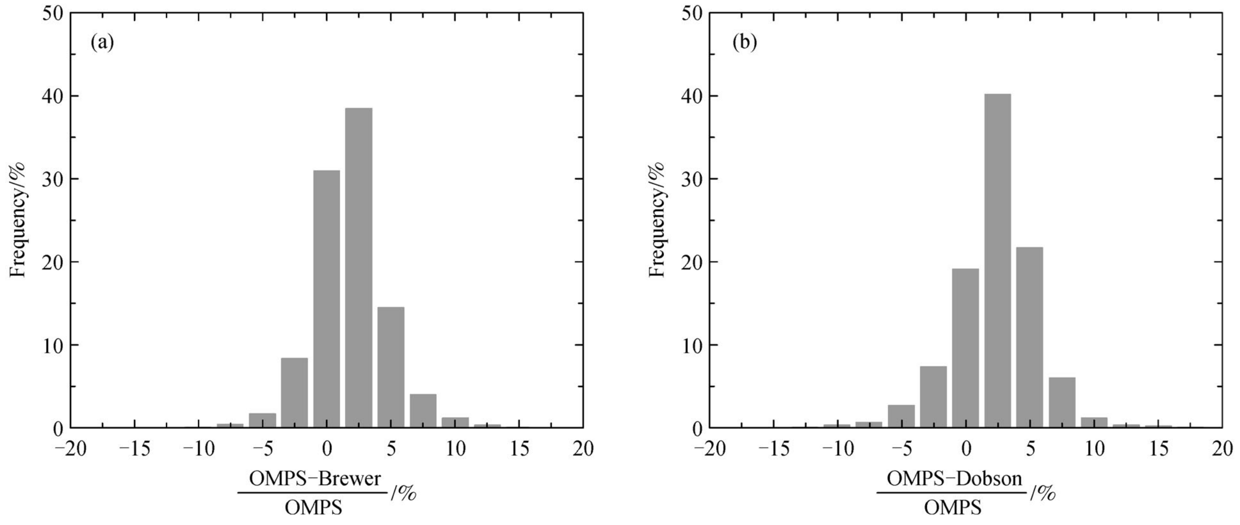

Fig. 3 Frequency statistics of the relative differences between OMPS and Brewer (a) and Dobson (b) total column ozone measurements.

Table 1 The number of correlative data points (N), the slope of regression, the coefficient of regression (R^2), the root mean square error (RMSE), and the mean bias error (MBE) with standard deviation collected from the comparisons

	N	Slope	R^2	RMSE		MBE/%
				%	DU	
Brewer	7437	1.01	0.96	2.88	9.54	+ 0.59 ± 2.82
Dobson	6139	1.00	0.96	3.44	10.24	+ 1.09 ± 3.27

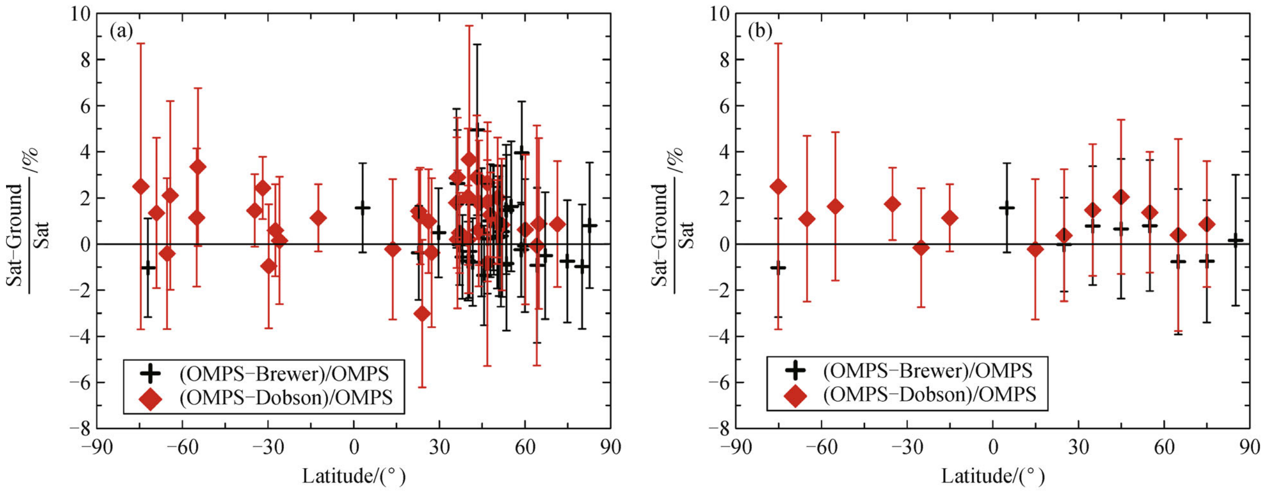

Fig. 4 Mean relative differences between OMPS and ground total column ozone measurements as a function of each ground-based stations' latitude (a) and 10° latitude bins (b).

through these periods, which indicates a relatively stable performance of the OMPS in its early 14-month operation. Due to limited time series, seasonal variability of bias error is not observed.

Figure 6 presents the mean relative difference variation as a function of SZAs. The comparison reveals different variation behaviors between OMPS – Brewer and OMPS – Dobson measurements. The relative differences for the OMPS – Brewer comparisons exhibit some significant changes under large SZAs, whereas the MBE varies from 0.26% to 1.39% as SZAs increase from 65° to 85°. In contrast, the values for the OMPS – Dobson comparisons

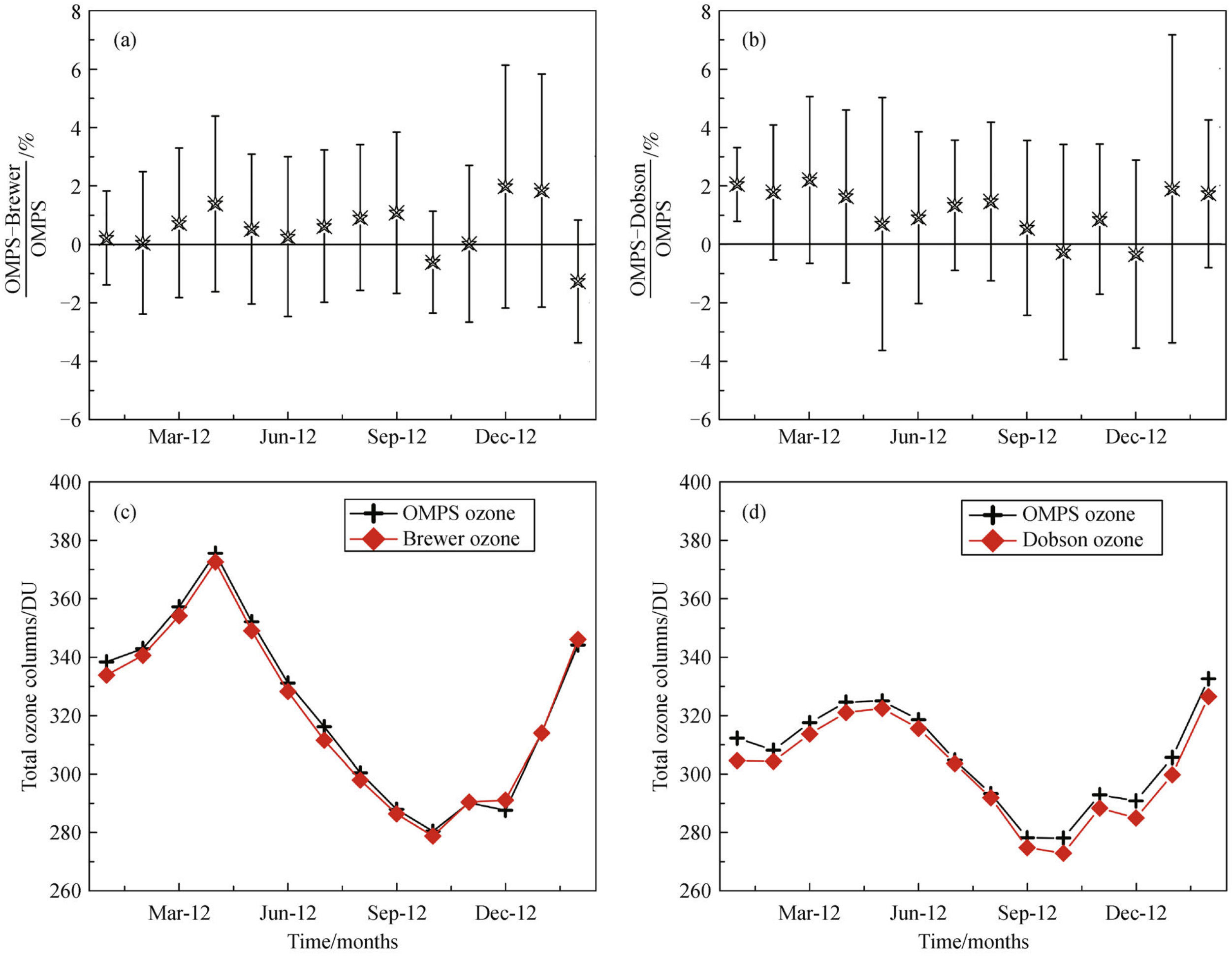

Fig. 5 Monthly variability of mean relative differences (top) and total column ozone values (bottom) between OMPS and ground measurements.

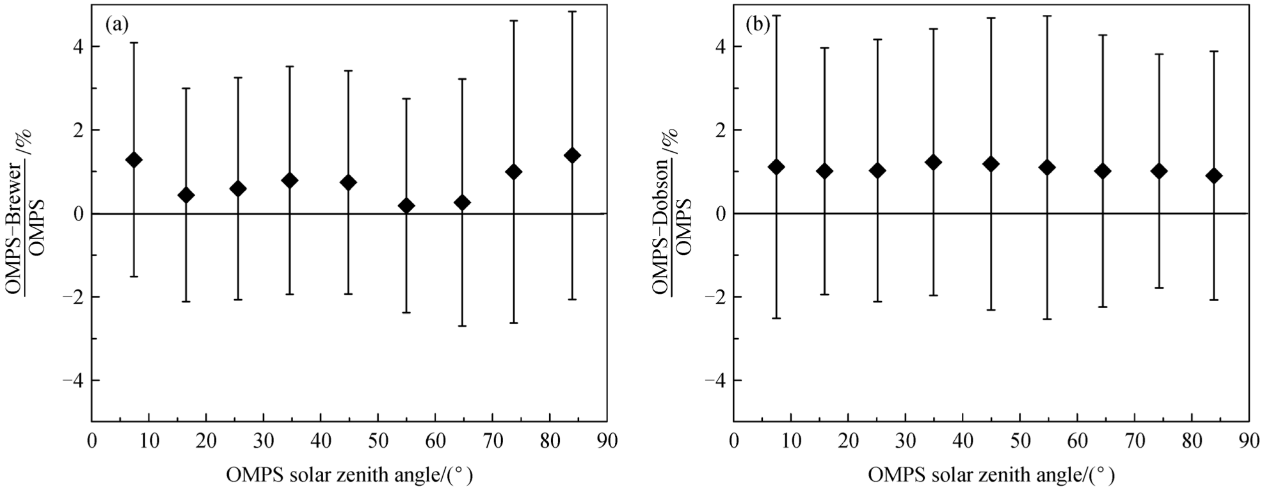

Fig. 6 Investigation of the relative difference dependence on OMPS SZA (bins of 10°).

exhibit a smoother behavior with an MBE of 1% as the SZAs increase from 0° to 90°. This effect is consistent with former studies, which have shown little to no significant dependence on SZAs in comparisons between OMI-TOMS total column ozone and ground measurements under all sky conditions (Balis et al., 2007b; Antón et al., 2009b). The relative differences between the viewing zenith angles (VZAs) are also analyzed (Fig. 7). Both comparison results present smooth variation behaviors as the VZAs increase from 0° to 70°; no VZA-dependent error is observed for the OMPS total column ozone.

The relative differences varying with the radiative cloud fraction are shown in Fig. 8. Results indicate that no cloud-dependent error is observed (i.e., the bias is approximately 0.6% for Brewer and 1.2% for Dobson). Due to cloud contamination, the satellite sensor can only confidently derive the ozone amount above clouds. The ozone below the cloud top must be inferred from climatological tables (McPeters et al., 2008). Thus, the cloud height should be estimated with high accuracy for total column ozone derived under cloudy conditions. It suggests that the new cloud height climatologies used in the current modified algorithm are feasible and reliable based on the smooth variation behavior of the results. Figure 9 exhibits the variability of the relative differences as a function of reflectivity. In this study, the reflectivity derived from 311 nm measurements of OMPS is employed. Reflectivity-dependent errors are not observed for any comparisons. The MBE is 0.6% for the OMPS – Brewer comparisons and 1.1% for the OMPS – Dobson comparisons.

The variability of the mean relative differences as a function of the OMPS and ground-based total column

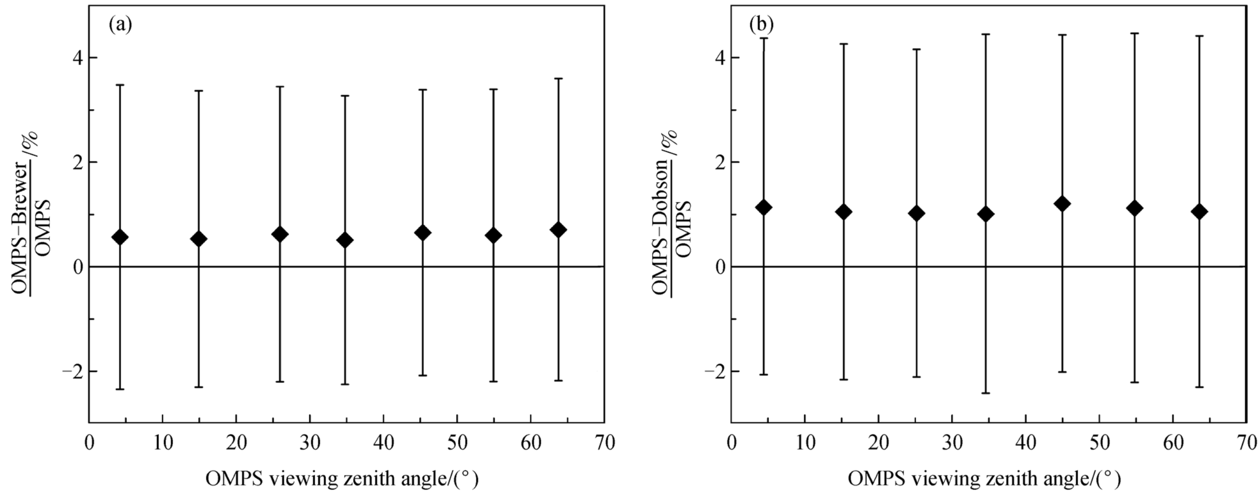

Fig. 7 Same as Fig. 6, but for OMPS VZA.

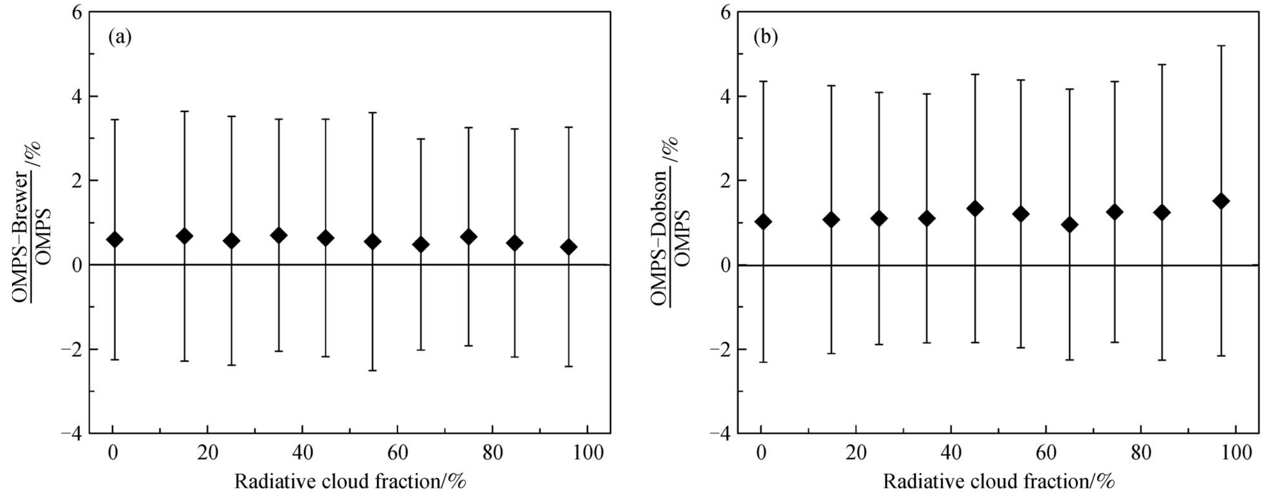

Fig. 8 Investigation of the relative difference dependence on radiative cloud fraction (bins of 10%).

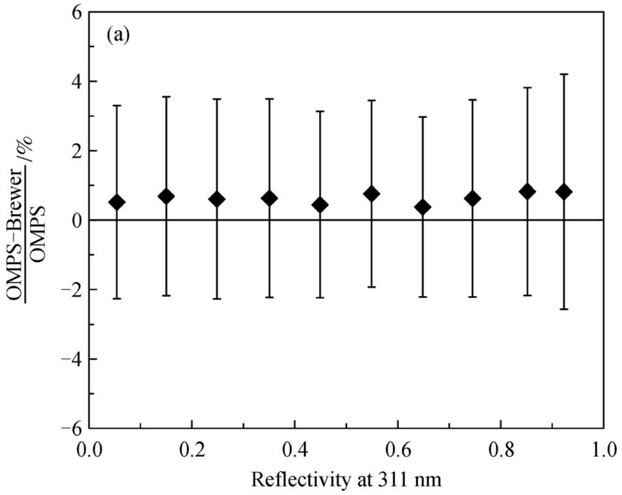

Fig. 9 Mean relative differences versus reflectivity at 311 nm (bins of 0.1).

ozone measurements is shown in Fig. 10. Comparative analysis suggests fair agreement as total column ozone values vary between 220 DU and 450 DU. Negative bias (about −2% from Dobson data set) is observed as total column ozone values less than 220 DU (the level of the ozone hole), which always occur near the polar night. In this situation, ground measurements are recorded under large SZAs, and many other errors (i.e., more aerosol absorption, scattering effects, etc.) will be introduced into the long viewing limb. In contrast, large positive bias error (~ 4%) is observed as the total column ozone increases to 450 DU. This effect can be explained by a decrease in ground-measurable UV radiation penetration in the atmosphere to the ground due to significant ozone absorption of UV radiation (Antón et al., 2010). The dependency of relative differences on total column ozone itself can change under different total column ozone values compared with satellite and ground-based total column ozone (Fioletov et al., 2006; Kravchenko et al., 2009). Kravchenko et al. (2009) indicated that total ozone measurements over polar regions, especially in Antarctica, remain influenced by total ozone dependence. This effect was probably more significant for a total column ozone value less than 220 DU or larger than 220 DU for Dobson and EP-TOMS. Similar methods will be applied to the OMPS ground-based comparisons to investigate individual contributions to the relative differences in total column ozone dependence.

5 Conclusions

Based on 14 months of total ozone column records, the

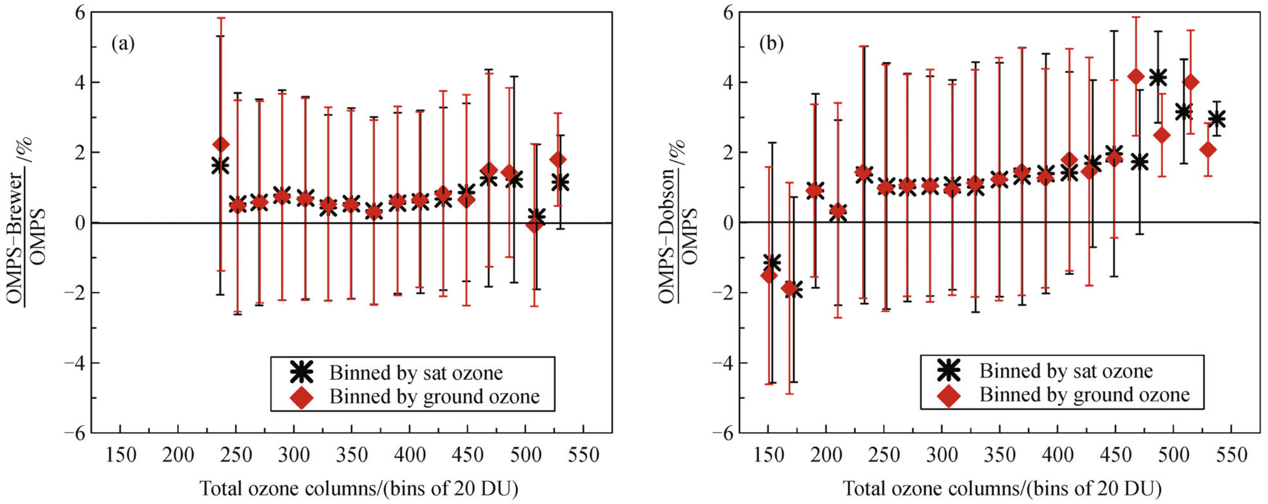

Fig. 10 The relative differences of OMPS and ground-based total column ozone measurements as a function of the Brewer data set (a) and Dobson data set (b) for total ozone column value.

performance of OMPS total ozone column research products generated by the NASA's OMPS science team utilizing the latest version of their BUV retrieval algorithms was evaluated. OMPS total ozone column compares very well with co-located ground-based measurements from the network of worldwide, well-maintained Brewer and Dobson spectrophotometers. A bias of about 2% was observed due to varying latitudinal- and viewing geometries. In addition, fair agreements were suggested as total ozone column values varied between 220 DU and 450 DU.

Overall, the OMPS total ozone column product generated by the NASA's OMPS science team performs well with a mean bias error of approximately 2%. The product can be used with confidence for global ozone monitoring and other atmospheric applications over most regions of the world.

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