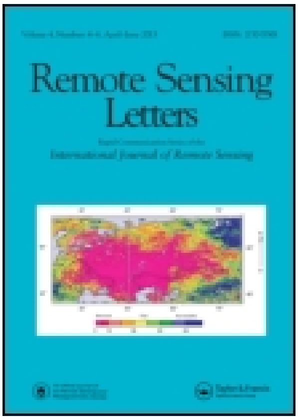

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Zuoqi Chen [a] , Bailang Yu [a] , Yan Huang [a] , Yingjie Hu [b] , Hao Lin [a] & Jianping Wu [a]

[a] Key Laboratory of Geographic Information Science , Ministry of Education, East China Normal University , Shanghai , 200241 , People's Republic of China

[b] Department of Geography , University of California , Santa Barbara , CA , 93106 , USA

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Validation of total ozone column derived from OMPS using ground-based spectroradiometer measurements

ZUOQI CHEN†, BAILANG YU*†, YAN HUANG†, YINGJIE HU‡, HAO LIN† and JIANPING WU†

†Key Laboratory of Geographic Information Science, Ministry of Education, East China Normal University, Shanghai 200241, People's Republic of China
‡Department of Geography, University of California, Santa Barbara 93106, CA, USA

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The total ozone column (TOC) observations derived from the Ozone Mapping and Profiler Suit (OMPS) on-board the Suomi National Polar-orbiting Partnership (Suomi NPP) spacecraft were recently released for monitoring ozone in the stratosphere. Two kinds of TOC data which are derived using the NPOESS algorithm (OMPS-NPOESS) and the TOMS Version 7 algorithm (OMPS-TOMS) are provided. So far, few studies have been conducted to validate the accuracy of the OMPS TOC data. In this letter, we validate a 1 year OMPS-derived TOC data set (from March 2012 to February 2013) by comparing them with ground-based spectroradiometer data. We also examine the difference of the data derived using OMPS-NPOESS and OMPS-TOMS algorithms. Our results show a moderate correlation between OMPS-derived TOC and ground-based data, and the average relative difference between the two data sets (OMPS data minus the ground-based data) is negative, which indicates an underestimation of the TOC in the OMPS data. Such relative difference is not globally consistent: smaller values (around –10% to 0%) are found in low latitudinal areas (from 30° S to 30° N), whereas comparatively larger differences (around –25% to –15%) are detected in data on the mid-high latitudinal areas. A comparison of the two different algorithms suggests that the OMPS-TOMS-derived data have a generally better accuracy than those from OMPS-NPOESS.

1. Introduction

Ozone, as a kind of greenhouse gas, is a key factor in climate change from regional to global scales. The Ozone Layer, though a small part of the atmosphere, contains about 90% of all the ozone present near the Earth's surface (Kiehl *et al.* 1999). Although the proportion of ozone in the atmosphere is low, it plays an important role in protecting humans from ultraviolet (UV) rays from the Sun, thereby reducing the incidences of skin cancer and eye cataracts (WMO 2007).

Since 1957, the total ozone column (TOC) has been measured systematically at the Halley Bay station (located at 72° S, 23° W) in Antarctica. Their measurement results show a decrease in the volume of the ozone during the mid-1980s (Farman *et al.* 1985). In addition, the stratospheric ozone depletion has been found in many

*Corresponding author. Email: blyu@geo.ecnu.edu.cn

areas throughout the world, including Hong Kong, Tibetan Plateau and other regions (Van Roozendael *et al.* 1998, Lam *et al.* 2002). To better understand the dynamic change of ozone concentration in the atmosphere, data from space-borne instruments, such as Atmospheric Infrared Sounder (AIRS) (Aumann *et al.* 2003), Total Ozone Mapping Spectrometer (TOMS) (Zou 1996, Anton *et al.* 2011, Lin *et al.* 2013), Ozone Monitoring Instrument (OMI) (Balis *et al.* 2007, McPeters *et al.* 2008, Anton *et al.* 2009) and Total Ozone Unit (TOU) (Wang *et al.* 2010, 2012, Bai *et al.* 2013), have been used in existing studies.

To evaluate the quality of the TOC data acquired from the space-borne instruments, TOC data from ground stations have been used. For example, Wang *et al.* (2010) used ground-based measurements to examine the first-year data of Total Ozone Unit (TOU) on FY-3A and found a 4.2% Root Mean Square (RMS) relative error. Anton *et al.* (2009) compared the data from five Brewer spectroradiometers with the data from OMI Total Ozone Mapping Spectrometer (OMI-TOMS) and OMI Differential Optical Absorption Spectroscopy (OMI-DOAS) on the Iberian Peninsula, and discovered a significant correlation between the two data sets.

The Ozone Mapping and Profiler Suit (OMPS) is a new ozone sensor carried by the Suomi National Polar-orbiting Partnership (Suomi NPP) spacecraft which was launched on 28 October 2011. It is one of the five instruments on the spacecraft, and is configured to monitor the global ozone concentration. OMPS is the first instrument of the next generation of US ozone monitoring instruments, which is inherited and improved on the current operational atmospheric ozone products. It will play a significant role in monitoring ozone dynamics (Flynn *et al.* 2004). However, as OMPS is a new member of the space-borne measurements, few papers have reported its performance as well as its data quality. Therefore, an evaluation and validation of the OMPS-derived TOC data would provide a better understanding of the data quality, as well as support error and uncertainty analysis in future research.

In this letter, we compare a 1 year OMPS-derived TOC data (from March 2012 to February 2013) with the data obtained from the ground stations. Specifically, we use the ground-based TOC data from the Brewer and Dobson spectroradiometers installed at different locations around the world. The correlation between the OMPS-derived data and the ground-based data is analysed, and the latitudinal dependence of the relative difference between the two data sets is discussed. We have also examined the accuracy difference between the data acquired from the two algorithms (NPOESS and TOMS).

The rest of this letter is organized as follows. Section 2 describes the two data sets used in this research, respectively: the OMPS-derived TOC data and the ground-based measurements. Section 3 presents the methods for data comparison and correlation analysis. Then, we discuss the analysis results and their indications. Finally, we summarize our work and draw some conclusions.

2. Data

2.1 *OMPS-derived data*

The OMPS consists of three components, two for nadir measurements (the Nadir Mapper and the Nadir Profile) and one for limb measurements (Flynn *et al.* 2004). The TOC data, examined in this study, are acquired by the Nadir Mapper. The daily and global total ozone estimates generated from the Nadir Mapper are continuing heritage products from the Total Ozone Mapping Spectrometer (TOMS) (Flynn *et al.*

2009). The Nadir Mapper has a cross-track wide Field of View (FOV) of about 110°. The Nadir Mapper provides a 0.45 nm spectral sampling across the wavelength range of 300 nm to 380 nm with a 1 nm full-width half maximum (FWHM) spectral resolution (Flynn *et al.* 2004). The OMPS TOC data can be downloaded from the NOAA Comprehensive Large Array-Data Stewardship System (http://www.class.noaa.gov/).† Each data file (organized by the Hierarchical Data Format) contains OMPS-NPOESS and OMPS-TOMS which are computed with the NPOESS and the TOMS Version 7 algorithms, respectively.

The NPOESS algorithm (Flynn *et al.* 2011) extends the TOMS Version 7 algorithm with improvement of using the increased spectral coverage (McPeters and Labow 1996, Flynn *et al.* 2004). Multiple triplets of wavelengths are utilized in this algorithm. The first and second triplets are selected to be pairs for ozone sensitivity. The pairs have one weak and one strong ozone absorption channel, which are placed at 321.0, 329.0, 332.0, or 336.0 nm and 308.5, 310.5, 312.0, 312.5, 314.0, 315.0, 316.0, 317.0, 318.0, 320.0, 322.5, 325.0, 328.0, or 331.0 nm, respectively. The third triplet is chosen for ozone insensitivity (at 364, 367, 372 or 377 nm), including the evaluation of the cloud fraction and surface reflectivity, as well as the variation of the reflectivity with wavelength. Finally, the TOC are estimated using radiative transfer look-up tables (Flynn *et al.* 2011). The reason why the algorithm needs multiple sets of triplets is to balance the ozone sensitivity for various but expected range of ozone column amounts and solar zenith angles (SZA) (Flynn *et al.* 2004).

The TOMS Version 7 algorithm (McPeters *et al.* 1996) only uses a single triplet of wavelengths at 317, 331 and 364 nm. It is similar to the traditional algorithm used by the TOMS instruments launched by NASA (McPeters *et al.* 1996).

2.2 *Ground-based data*

The TOC data from ground stations can be downloaded from the World Ozone and Ultraviolet Radiation Data Centre (WOUDC) in Toronto, Canada.‡ Such data were mainly acquired by the Brewer and Dobson spectrophotometers. The data from the Dobson spectrophotometer are well maintained and calibrated with an estimated error of 1% under direct sunlight (DS) and 2–3% for zenith sky or for SZA less than 75° (Basher 1985). The Brewer spectrophotometer has a similar working mechanism, but has an improved optical design and is fully automated (Brewer 1973).

In this work, we select 16 Brewer instruments and 26 Dobson instruments based on the OMPS TOC data to be examined with a restriction: the measurements must be under DS. These instruments are listed in table 1 and table 2. Due to the restriction of DS observation data, all of the selected Brewer instruments are only located in the Northern Hemisphere, with 13 in Europe, 1 in Africa and 2 in Asia. The selected Dobson instruments deployed in our research are installed throughout the world.

3. Methodology

The OMPS measures the TOC several times in one day, and saves each measurement in a separate file. Therefore, our first step towards validating the OMPS data is to extract locations and TOC values from the files in the same day and calculate the daily average value. The calculated results are then converted into a grid data with a spatial resolution of $1^\circ \times 1^\circ$. Since the ozone in the stratosphere has a well-known

†The OMPS-derived data, used in our study, were downloaded in March 2013.

‡http://www.woudc.org

Table 1. List of Brewer stations selected for validating OMPS TOC products.

ID[1]	Country	Station name	Lat (°)	Lon (°)	Elevation (m)
090	MYS	Petaling Jaya	3.10	101.65	86
201	DZA	Tamanrasset	22.78	5.52	1384
161	KOR	Pohang	36.03	129.38	6
070	ESP	Madrid	40.45	−3.72	680
151	ESP	La Coruna	43.33	−8.41	65
066	ITA	Aosta	45.74	7.36	570
010	DEU	Hohenpeissenberg	47.81	11.01	975
097	SVK	Poprad-Ganovce	49.03	20.32	706
184	CZE	Hradec Kralove	50.18	15.83	285
098	CZE	Hradec Kralove	50.18	15.83	285
016	BEL	UCCLE	50.80	4.35	100
178	BEL	UCCLE	50.80	4.35	100
075	GBR	Reading	51.44	−0.94	66
088	IRL	Valentia Observatory	51.93	−10.25	14
172	GBR	Manchester	53.47	−2.23	76
128	SWE	Norrköping	58.58	16.15	43

Note: [1]ID: Instrument ID.

Table 2. List of Dobson stations selected for validating OMPS TOC products.

ID[1]	Country	Station name	Lat (°)	Lon (°)	Elevation (m)
122	JPN	SYOWA	−69.01	39.58	22
131	ARG	Ushuaia	−54.85	−68.31	17
006	AUS	Macquarie Island	−54.50	158.95	10
111	AUS	Melbourne	−37.68	144.84	132
134	URY	Salto	−31.43	−57.97	41
132	ZAF	Springbok	−29.67	17.90	1006
012	AUS	Brisbane	−27.39	153.13	4
089	ZAF	Irene	−25.92	28.22	1523
078	AUS	Darwin	−12.42	130.89	30.4
090	THA	BANGKOK	13.67	100.61	53
011	DZA	Tamanrasset	22.78	5.52	1382
067	CUB	Havana	23.14	−82.34	50
127	JPN	NAHA	26.21	127.69	28
125	JPN	TSUKUBA	36.06	140.13	31
120	ESP	El Arenosillo	37.10	−6.73	41
118	GRC	Athens	37.98	23.73	280
075	CHN	Xianghe	39.98	116.37	80
044	ARM	Amberd	40.38	44.25	2070
126	JPN	SAPPORO	43.06	141.33	26
101	CHE	Arosa	46.78	9.68	1840
104	DEU	Hohenpeissenberg	47.81	11.01	975
074	CZE	Hradec Kralove	50.18	15.83	285
040	UKR	Kyiv-Goloseyev	50.36	30.50	206
084	POL	BELSK	51.84	20.79	180
032	GBR	Lerwick	60.13	−1.18	82
050	ISL	Reykjavik	64.13	−21.90	64

Note: [1]ID: Instrument ID.

long-term chemical stability, daily average of OMPS-NPOESS and OMPS-TOMS are calculated during the pre-process of the data. As discussed in section 2, we select the ground-based data, which are during the same period (from March 2012 to February

2013) and are under DS, for comparison. It is worth to note that some deficiencies, such as missing data and no DS measurements, exist in the ground-based data set due to the presence of clouds (Anton *et al.* 2009).

According to McPeters *et al.* (2008), a more reliable result can be acquired by treating the ground-based data as an entire data set than conducting a station-by-station analysis. Therefore, we classify all the ground-based data into two groups (the Brewer and the Dobson data sets), and perform linear regression on the OMPS-derived TOC data and the two groups of ground-based data, respectively. The coefficients of determination (R^2) can be calculated by estimating the proportion and similarity between the ground-based and OMPS-derived TOC.

The relative difference (RD) and Root Mean Square Error (RMSE) between the daily OMPS-derived TOC and ground-based TOC for the whole data set are used to describe relation between the two data sets. RD and RMSE can be calculated using the equations (1) and (2).

$$\mathrm{RD}_i = \frac{\mathrm{OMPS}_i - \mathrm{Ground}_i}{\mathrm{OMPS}_i} \times 100\%, \tag{1}$$

$$\mathrm{RMSE} = \sqrt{\sum_{i=1}^{N} \mathrm{RD}_i^2 / N}, \tag{2}$$

where OMPS_i denotes the OMPS-NPOESS or OMPS-TOMS TOC products of *i*th pairs, and Ground_i represents the Brewer or Dobson measurements of *i*th pairs, RD_i is the relative difference of *i*th pair and N is the number of the pairs.

We also count the frequency of different RD values from the entire data set to quantify the difference between the OMPS-derived and ground-based TOC. To analyse the latitudinal dependence of the RD, we also calculate its average value for each station and sort these values using the latitudes of their corresponding stations.

4. Results and discussion

4.1 *General comparison*

Figure 1 shows a general comparison between the OMPS data and the ground-based data. The statistical parameters calculated from the four linear regressions are contained in table 3. From table 3, we can see the value range of R^2 is between 0.4845 and 0.6632 and all the slopes of trend line are higher than 0.75. This result indicates a relatively strong correlation between OMPS-derived and ground-based data sets. The maximum and minimum values of RMSE are 19.12% and 11.35%, which suggest that OMPS-derived TOC has a certain degree of similarity with a spread.

The regression analysis also shows a slightly higher R^2 value between OMPS and Brewer TOC than the value between OMPS and Dobson TOC. This result may be caused by the difference of the wavelength selected by the two instruments: the wavelength of Brewer is much more similar to OMPS's than Dobson's.

Figure 2 displays the frequency count of relative difference (RD), which indicates that around 80% of the RD are within the range of –10% to 10%. This result confirms that there is a great consistency between the OMPS-derived and ground-based TOC product.

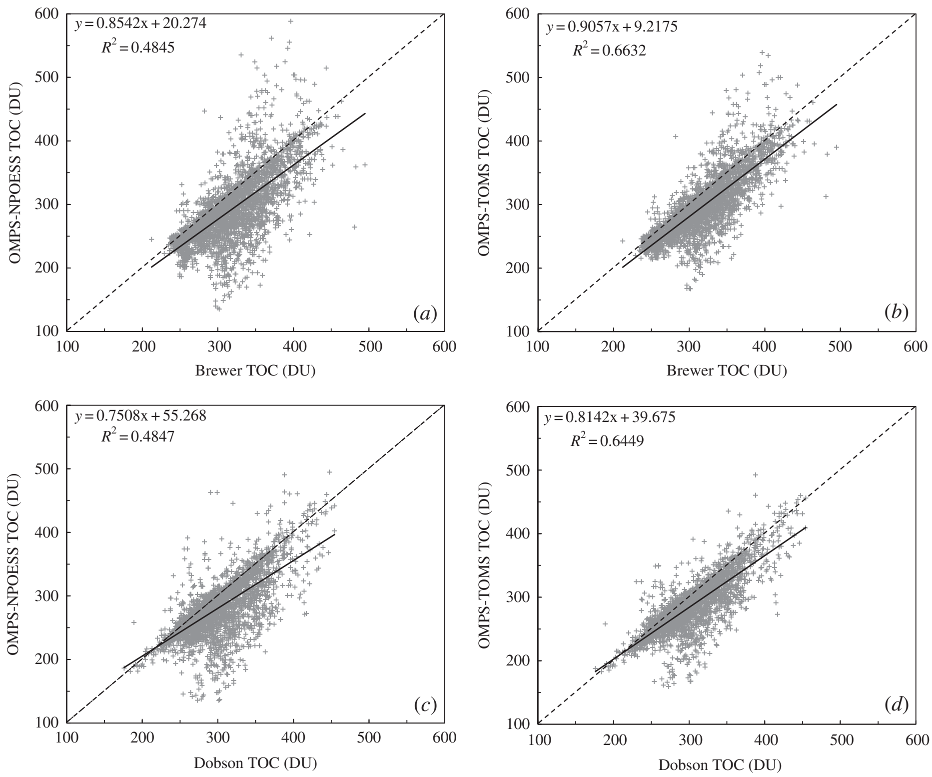

Figure 1. Scatter plots between daily OMPS and Ground-based TOC. (*a*) OMPS-NPOESS compared with Brewer; (*b*) OMPS-TOMS compared with Brewer; (*c*) OMPS-NPOESS compared with Dobson; (*d*) OMPS-TOMS compared with Dobson. The dashed line denotes the non-bias line and solid line denotes the trend line.

Table 3. Statistical parameters calculated from the line regressions between satellite measurements and ground-based observations during March 2012–February 2013.

Satellite measurements	Ground-based observations	Number of the pairs	R^2	Equation of the trend line	RMSE (%)
OMPS-NPOESS	Brewer	3525	0.4845	$0.8542x + 20.274 + \varepsilon$	19.12
	Dobson	3524	0.4847	$0.7508x + 55.268 + \varepsilon$	17.53
OMPS-TOMS	Brewer	3955	0.6632	$0.9057x + 9.2175 + \varepsilon$	13.12
	Dobson	3966	0.6449	$0.8142x + 39.675 + \varepsilon$	11.35

4.2 *Latitudinal dependence*

To understand the variation of the RD between the OMPS and ground-based measurements with regard to the change of the latitude, we create two line charts using the mean RD value of each station and its corresponding latitude (figure 3). It can be seen that the OMPS underestimates TOC for all latitudes.

For Brewer instruments, values obtained in low latitudes at the Northern Hemisphere (Brewer-NH) are greater than –10% (i.e. the absolute value is smaller than 10%), and the major bias appears in the range of 40° N and 50° N. The data

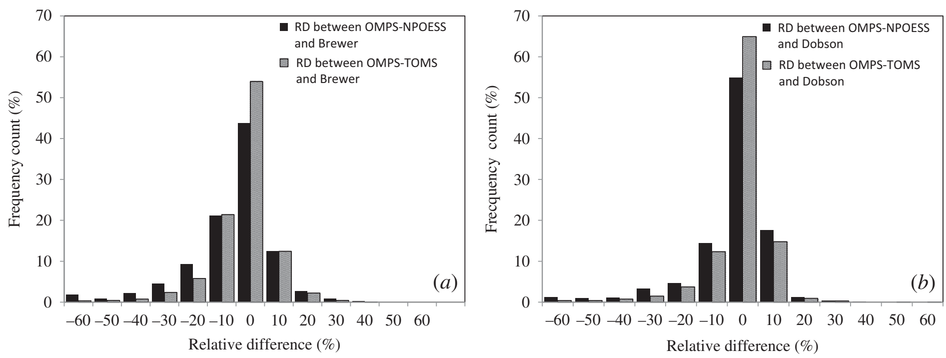

Figure 2. Frequency of relative difference between OMPS-derived TOC and two type of ground-based measurements in 10% bins: (*a*) Brewer and (*b*) Dobson.

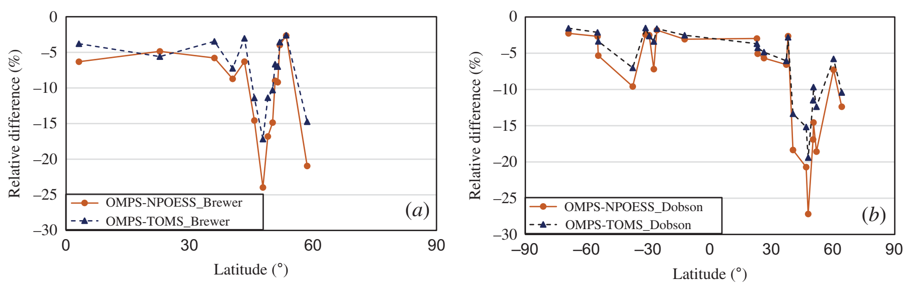

Figure 3. Relative difference between OMPS-derived TOC and two types of ground-based measurements as a function of the ground station latitude: (*a*) Brewer and (*b*) Dobson.

from the Dobson instruments show a result similar to that of the Brewer-NH at the Southern Hemisphere (Dobson-SH), whereas the values at the Northern Hemisphere (Dobson-NH) are much larger than those at the Dobson-SH, especially on the mid-high latitudes where random fluctuations are detected. The maximum absolute RD reached 27.17% at #104 Dobson Spectroradiometers (at Hohenpeissenberg, 47.81° N, 11.01° E)

4.3 *Comparison between OMPS-NPOESS and OMPS-TOMS*

To examine the difference between the OMPS-NPOESS and the OMPS-TOMS algorithms, we compare the TOC data derived from the two algorithms with the ground-based data set from the same instruments during the same period. As shown in table 3, $R^2_{\mathrm{OT-Brewer}}$ (the R^2 between OMPS-TOMS and Brewer TOC) is about 0.179 larger than $R^2_{\mathrm{ON-Brewer}}$ (the R^2 between OMPS-NPOESS and Brewer TOC), and the $R^2_{\mathrm{OT-Dobson}}$ (the R^2 between OMPS-TOMS and Dobson TOC) is about 0.160 larger than $R^2_{\mathrm{ON-Dobson}}$ (the R^2 between OMPS-NPOESS and Dobson TOC). The situation of the RMSE is similar to R^2, with $\mathrm{RMSE_{ON-Brewer}}$ (the RMSE between OMPS-NPOESS and Brewer TOC) and $\mathrm{RMSE_{ON-Dobson}}$ (the RMSE between OMPS-NPOESS and Dobson TOC) are both about 6% higher than $\mathrm{RMSE_{OT-Brewer}}$ (the RMSE between OMPS-TOMS and Brewer TOC) and $\mathrm{RMSE_{OT-Dobson}}$ (the RMSE between OMPS-TOMS and Dobson TOC) respectively. To sum up, the accuracy of OMPS-TOMS is generally higher than that of OMPS-NPOESS, even though OMPS-NPOESS is an extension of the TOMS Version 7 algorithm and has a wider spectral coverage.

5. Conclusion

In this study, we evaluated the accuracy of TOC data derived from the OMPS by comparing it with the data measured by ground stations. The comparison results indicate a moderate correlation between the OMPS-derived TOC data and the ground-based measurements. In terms of the latitudinal dependence of the RD, the TOC data from OMPS show a low RD (the absolute value is smaller than 10%) compared with the ground-based data in the low latitudinal region (–30° –30°). However, in the mid-high latitude, the RD becomes larger and shows a random fluctuation. The OMPS data generated by the two algorithms have difference accuracies, and our analysis indicates a higher accuracy in the TOMS Version 7. In conclusion, the TOC products from OMPS are generally consistent with the ground-based data, and therefore can be applied to atmospheric research, such as global ozone monitoring. However, the data derived from the NPOESS algorithm still need some rectifications to improve its accuracy.

Acknowledgements
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