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Comparison of OMI-DOAS total ozone column with ground-based measurements in Argentina

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Abstract: Total ozone column (TOC) measurements through the Ozone Monitoring Instrument (OMI/NASA EOS-Aura) are compared with ground-based observations made using Dobson and SAOZ instruments for the period 2004–2019 and 2008–02/2020, respectively. The OMI data were inverted using the Differential Optical Absorption Spectroscopy algorithm (overpass OMI-DOAS). The four ground-based sites used for the analysis are located in subpolar and subtropical latitudes spanning from 34°S to 54°S in the Southern Hemisphere, in the Argentine cities of Buenos Aires (34.58°S, 58.36°W; 25 m a.s.l.), Comodoro Rivadavia (45.86°S, 67.50°W; 46 m a.s.l.), Río Gallegos (51.60°S, 69.30°W; 72 m a.s.l.) and Ushuaia (54.80°S, 68.30°W; 14 m a.s.l.). The linear regression analyzes showed correlation values greater than 0.90 for all sites. The OMI measurements revealed an overestimation of less than 4 % with respect to the Dobson instruments, while the comparison with the SAOZ instrument presented a very low underestimation of less than 1 %.

Key words: total ozone column, OMI, Dobson, SAOZ, Argentina.

Comparación de columna total de ozono OMI-DOAS con mediciones terrestres en Argentina

Resumen: En este trabajo se comparan mediciones de columna total de ozono (CTO) del *Ozone Monitoring Instrument* (OMI/NASA EOS-Aura), con observaciones terrestres de instrumentos Dobson y SAOZ para el periodo 2004–2019 y 2008–02/2020, respectivamente. Los datos del OMI analizados fueron los invertidos mediante el algoritmo *Differential Optical Absorption Spectroscopy* (*overpass* OMI-DOAS). Las 4 estaciones terrestres están ubicadas en latitudes subpolares y subtropicales del Hemisferio Sur, en las ciudades argentinas de Buenos Aires (34,58°S, 58,36°O; 25 m s.n.m.), Comodoro Rivadavia (45,86°S, 67,50°O; 46 m s.n.m.), Río Gallegos (51,60°S, 69,30°O; 72 m s.n.m.) y Ushuaia (54,80°S, 68,30°O; 14 m s.n.m.) cubriendo un rango latitudinal desde los 34°S hasta los 54°S. Los análisis de regresión lineal presentan valores de correlación superior a 0,90. Las mediciones OMI– DOAS muestran una sobrestimación menor al 4 % respecto de los instrumentos Dobson, mientras que la comparación respecto al instrumento SAOZ presenta una muy baja subestimación, menor al 1 %.

Palabras clave: columna total de ozono, OMI, Dobson, SAOZ, Argentina.

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1. Introduction

Ozone is a trace gas in the Earth's atmosphere. It reaches its maximum absolute concentration in the stratosphere, around 20 - 25 km high, forming what is known as the "ozone layer" (London et al., 1985). This ozone layer acts as a filter for UVB solar radiation. Therefore, the most direct impact that the total atmospheric ozone content has is the modification of the UVB solar radiation levels in the atmosphere and on the Earth's surface. Increases in UVB radiation have a variety of effects, generally harmful, on ecosystems and exposed materials (Zerefos, 1997).

The greatest production of ozone takes place in the equatorial region, where the highest levels of solar radiation occur during the year. Despite this, the maximum ozone concentration occurs towards polar regions. This latitudinal distribution is explained by the Brewer-Dobson circulation in the stratosphere (Brewer, 1949; Dobson, 1956), which transports ozone-rich air masses from the equator to the poles. However, since the 1970s, the concentration of ozone during the southern spring has strongly decreased within the Antarctic polar vortex, a phenomenon known as the Antarctic Ozone Hole (AOH), and defined as the area presenting TOC levels below the threshold of 220 Dobson Units (UD) (Chubachi, 1984; Farman et al., 1985). This phenomenon is a consequence of anthropogenic pollution due to the emission of ozone-depleting substances (ODS) into the atmosphere (WMO, 2011a). The decrease in the ozone layer over the Antarctic region has been related to changes in tropospheric circulation affecting the climate in the Southern Hemisphere (Son et al., 2010; Polvani et al., 2011; McLandress et al., 2011).

With the aim of mitigating the stratospheric ozone depletion and the effects that this phenomenon entails, in 1987 the Montreal protocol was signed, whose main objective is to reduce ODS emissions (WMO, 2014). Evidence that the ozone layer has begun to recover over the Antarctic region has been reported as a consequence of the success of the Montreal Protocol (Kuttippurat and Nair, 2017; Solomon et al. 2016) and analyses carried out using model ensemble have suggested that recovery of stratospheric ozone to 1980s levels would occur around 2060-2065 in the Antarctic region (Dhomse et al., 2018; WMO, 2018), depending on the ODS emission levels (Dhomse et al., 2019).

On the other hand, recent studies indicate that the changes in the tropospheric circulation trend due to the AOH have stopped around the year 2000, a fact that is attributed to the recovery of the stratospheric ozone as result of the Montreal Protocol (Banerjee et al. 2020).

Surface monitoring of TOC in southern Argentina and Chile is particularly important as they constitute the southernmost continental regions of the world (excluding Antarctica) and the closest to the Antarctic polar vortex. The scarce coverage of ground-based observations along the Southern Hemisphere compared to the Northern Hemisphere highlights their importance.

Ozone studies carried out using different ground-based and satellite monitoring techniques have reported extremely low TOC values due to the passage of the AOH through subpolar latitudes (Wolfram et al., 2012; Orte et al., 2019). Likewise, measurements of ozone vertical profiles have been performed at the Observatorio Atmosférico de la Patagonia Austral [Atmospheric Observatory of Southern Patagonia] (OAPA) (CITEDEF (UNIDEF – CONICET)) to study the variability of ozone levels at different altitudes and the intrusion of the AOH over the continental region of South America (Wolfram et al., 2008; Salvador, 2011; Orte et al., 2011).

Historically, Dobson instruments have played an important global role in TOC monitoring since their development in 1927 (Dobson and Harrison, 1926; Dobson, 1931). Farman et al. (1985) used a Dobson to observe the AOH for the first time, which was later confirmed by TOMS satellite instrument measurements (Stolarski et al., 1986).

Since the OMI instrument entered in orbit in 2004, several comparisons have been made with ground-based measurements to validate the TOC measurements (Balis et al., 2007; McPeters et al., 2008; Antón et al., 2009; Kim et al., 2017; Vaz Peres et al., 2017; Kuttippurath et al., 2018)

This work compares the OMI TOC using the Differential Optical Absorption Spectroscopy technique (OMI-DOAS) with four ground-based TOC databases at subpolar and subtropical latitudes in the Southern Hemisphere obtained using three Dobson instruments operated and maintained by Servicio Meteorológico Nacional [Argentina Meteorological Service] (SMN), and a SAOZ instrument, which belongs to LATMOS /CNRS (Laboratoire Atmosphères, Milieux, Observations Spatiales/Centre National de la Recherche Scientifique) and is operated by the OAPA.

It is organized as follows: in Section 2 a brief description of the principle of operation of the measuring instruments is presented, together with the databases analyzed at each site and their location. Section 3 describes the methodology used for comparing satellite versus ground-based databases. Section 4 describes the results of the OMI – ground-based comparisons and their discussion. Finally, the conclusions are presented in section 5.

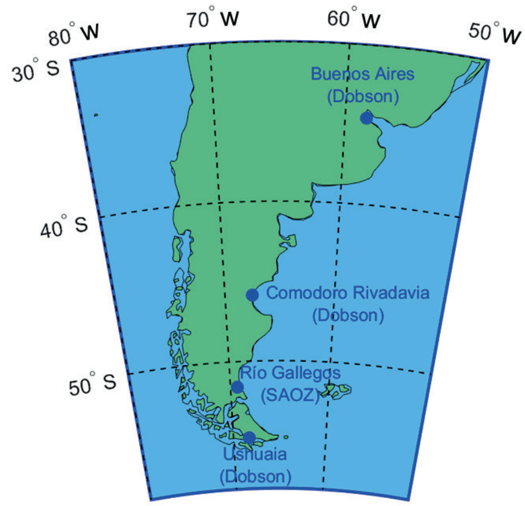

Figure 1. Location of Argentine land stations with TOC measurement instruments whose data are used in this work.

2. Materials and methodology

2.1. Satellite Data

The OMI instrument, on board of the Aura satellite, was launched in July 2004 within the framework of the Earth Observing System (EOS) Project with the aim of continuing the TOMS satellite measurements. OMI retrieves the total content of O_3, NO_2, SO_2 and aerosols, among other components, from the reflected and backscattered solar irradiance in UV–VIS range with a spectral resolution from ~0.45 nm to ~0.63 nm, in nadir view. It has a daily nearly global coverage, with a spatial resolution of 13 km×24 km (Levelt et al., 2006).

There are two OMI TOC databases depending on the retrieval algorithm used: OMI-TOMS and OMI-DOAS. OMI-TOMS is obtained by using the algorithm used for the ancestor instrument TOMS (Bhartia and Wellemeyer, 2002), while OMI-DOAS is retrieved using the DOAS (Differential Optical Absorption Spectroscopy) technique, as mentioned above. In this work, the OMI-DOAS database (OMDOAO3 L2 overpass data) is used (Veefkinf et al., 2006). These data can be downloaded from https://avdc.gsfc.nasa.gov/index.php?site=1882082496&id=46.

2.2. Ground-based measurements

Figure 1 presents the geographical location of the four ground-based measurement sites used in the comparison with the OMI retrievals, covering a latitudinal extension from subtropical latitudes (~34°S) to subpolar latitudes (~54°S).

The ground-based TOCs were measured using three Dobson instruments located in Buenos Aires, Comodoro Rivadavia and Ushuaia, and a SAOZ instrument at OAPA, Río Gallegos, Argentina.

The Dobson spectrophotometers used here are based on the observation on direct sunlight (DS) of two pairs of wavelengths: 305.5/325.4 nm (pair A) and 317.6/339.8 nm (pair D) (Carbajal et al. 2014). As detailed in Table 1, three different Dobson instruments have operated in Buenos Aires since the first ozone measurement in October 1966. For this satellite – ground-based comparison, the data of Dobson #097 and #070 were used, which were operating in the period 1966-2014 (except for the period 1992-1993, where instrument # 099 was operative) and 2014-present, respectively. A detailed description about the history of Dobson observations in Buenos Aires can be found in Cañellas (2017).

The Dobson instruments participated in calibration and maintenance campaigns in 1977, 1980, 1985, 1993, 1994, 1998, 1999, 2003, 2006, 2010, 2014 and 2019 (WMO/GAW report, 2019) and were compared with reference instruments following the WMO/GAW quality control standards.

Table 1. Ground-based TOC measurement sites. Location, type of instrument, serial number and operating period of each instrument.

Site	Geographical Location; altitude	Instrument	SN	Measurement period
Buenos Aires	34.6°S, 58.4°W; 25 m. asl.	Dobson	#097 #099 #070	1966 – 1992 / 1993 – 2014 1992 – 1993 2014 – 2019
Comodoro Rivadavia	45.9°S, 67.5°W; 46 m. asl.	Dobson	#133	09/1995 – 02/2019
Río Gallegos	51.6°S, 69.3°W; 72 m. asl.	SAOZ	#26	03/2008 – 02/2020
Ushuaia	54.8°S, 68.3°W; 14 m. asl.	Dobson	#131	09/1994 – 12/2018

Typical uncertainty of individual ozone measurements using the standard Dobson AD-pair is about 5% (Evans, 2009, Basher, 1982). Even though successive improvements have been achieved during the last decades in many subjects including instrument's technology, measurement algorithm, atmospheric parameters entering the calculations, among others (Moeini et al, 2019; Basher, 1985), we sustain this conservative value of the uncertainty for the Dobson TOC measurements given the long-time character of the analyzed data series.

Dobson datasets (Buenos Aires, Comodoro Rivadavia and Ushuaia) were downloaded from the World Ozone and Ultraviolet Radiation Data Center (https://woudc.org/home.php; last access: March 2020).

The SAOZ spectrometer has been in operation at OAPA, Río Gallegos, since March 11, 2008. In 2009, it was incorporated to the NDACC (Network for the Detection of Atmospheric Composition). It performs spectral diffuse solar irradiance measurements at zenith twice a day (at sunrise and sunset), for solar zenith angles (SZA) between 86° and 91° (Pazmiño, 2010). The wavelength range covers part of the UV and visible bands (300-650 nm) with an approximate spectral resolution of 0.9 nm. This instrument also measures the total NO_2 column applying the DOAS technique. TOC measurements are retrieved in the visible Chappuis band (450-550 nm), where the dependence of the ozone cross section on temperature can be neglected. In addition, synthetic tables of air mass factor obtained from the UVSPEC/DISORT radiative transfer model using TOMS ozone and temperature climatologies are used. A detailed description of the SAOZ measurements and their associated error analysis (~6%) can be found in Hendrick et al. (2011). The SAOZ database was downloaded from http://saoz.obs.uvsq.fr/ (last access: March 2020).

Figure 2 presents the ground-based (blue) and OMI (red) TOC time series since 1994, where the annual cycle at each site and the increase of the amplitude with the latitude are observed, showing a wider range of ozone values for high-latitude sites. It is observed that Río Gallegos and Ushuaia present TOC values below 220 DU during late winter and spring, related to Antarctic ozone hole overpass events.

The TOC data comparison was performed within the time overlap period, where both instruments, ground-based and satellite, measured simultaneously (OMI – Dobson: October 2004 - March 2019; OMI – SAOZ: March 2008 - February 2020).

2.3. Comparison methodology

The OMI-DOAS (OMI hereinafter) and ground-based TOC observations are compared, including a seasonal analysis. The temporal criteria considered for the comparisons differ for the Dobson and SAOZ instruments due to the time frequency of the measurements of each ground-based instrument. The closest OMI – Dobson data pairs are selected within a time window of ±3 hours.

On the other hand, given that SAOZ measurements are retrieved at sunrise and sunset and taking into account the OMI overpass time (~19:00±1.5 UTC), the comparison between these instruments is performed in two ways: 1) comparing each SAOZ measurement (sunrise and sunset) with the closest-in-time OMI data, and 2) comparing the daily average of OMI and SAOZ measurements.

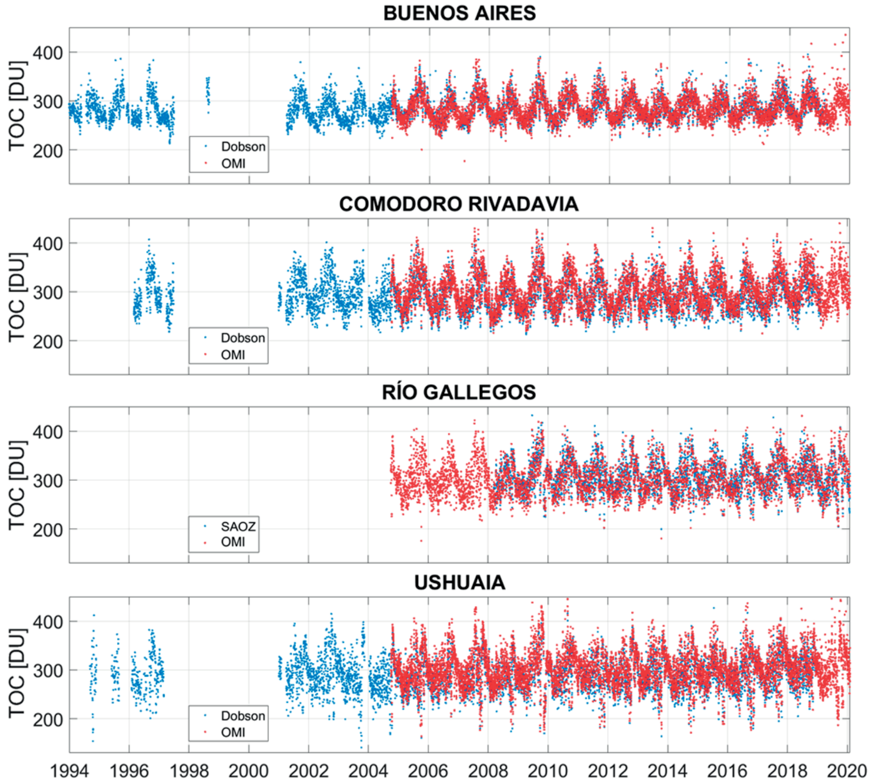

Figure 2. Time series of OMI (OMI - DOAS) (red) and ground-based (blue) TOC measurements in Argentina.

The distance between ground-based and satellite measurement pairs (distance between the site locations and the OMI Cross Track Position) are within a maximum radius of 150 km. The mean and maximum median distances are presented at the Comodoro Rivadavia site, with ~27 km and ~18 km, respectively. This indicates that the vast majority of data is much closer than the maximum radius of 150 km and that half of the OMI – ground-based measurement pairs is within a distance closer than 18 km.

The correspondence between the OMI and ground-based databases was evaluated by means of a linear regression analysis. The correlation coefficient (R) and the relative root mean squared error (rRMSE) were analyzed. The rRMSE was calculated by means of the following expression:

$$rRMSE = \frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(TOC_{OMI_i} - TOC_{ground_i})^2}}{\overline{TOC}_{ground}} x\,100 = \frac{RMSE}{\overline{TOC}_{ground}}$$

Where N is the total number of compared pairs, while, TOC_{OMI_i}, TOC_{ground_i} and $\overline{TOC}_{ground}$ are the TOC of each satellite and ground-based measurement and the average of ground-based TOCs, respectively.

In addition, the mean bias error (MBE) was analyzed using the following expression:

$$MBE = \frac{100}{N}\sum_{i=1}^{N}\frac{TOC_{OMI_i} - TOC_{ground_i}}{TOC_{ground_i}}$$

The uncertainties of the MBE are obtained from the standard deviation of the relative difference.

3. Results and discussion

Figure 3 shows the scatterplot between OMI and ground-based TOC observations for the whole period at each site and the corresponding linear regression analyses. The comparison between OMI and SAOZ at sunrise and sunset is presented

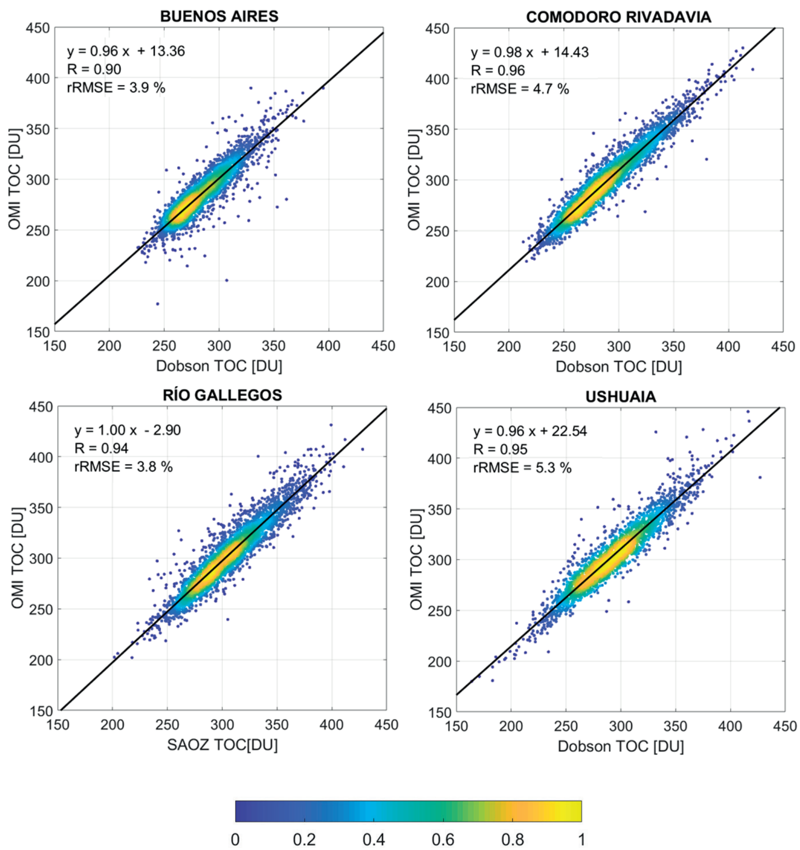

Figure 3. TOC data measured by the OMI satellite instrument as a function of ground-based measurements for the 4 sites analyzed and linear regression line of the comparisons. The color bar indicates the normalized dot density.

in Figure 4. Table 2 summarizes the parameters of all intercomparison. Finally, Figure 5 and Table 3 present a seasonal analysis of the comparison between OMI and ground-based TOC.

3.1. OMI – Dobson comparison

The correlation analyses present values of 0.90, 0.96 and 0.95 for Buenos Aires, Comodoro Rivadavia and Ushuaia, respectively. Bian et al.

Table 2. Parameters of the OMI – ground-based linear regression. The rows that refer to all OMI –SAOZ intercomparisons in Río Gallegos are slightly shaded to differentiate from OMI – Dobson ones. N: number of pairs compared. S: slope of the linear regression; I: Intercept; R / R2: correlation coefficient / determination coefficient. rRMSE: relative root mean squared error; MBE: mean bias error; SE: Standard error of the slope and the intercept.

Site	N	S±SE	I±SE	R / R^2	rRMSE (%)	MBE (%)
Buenos Aires	2758	0.96±0,01	13.4±2.5	0.90 / 0.81	3.9	0.6±3.9
Comodoro Rivadavia	3240	0.98±0.01	14.4±1.4	0.96 / 0.92	4.7	3.5±3.3
Río Gallegos	3235	1.00±0.01	-2.9±1.9	0.94 / 0.88	3.8	-0.9±3.8
Río Gallegos-SR	3289	0.90±0.01	28.9±2.6	0.88 / 0.77	5.4	-0.5±5.4
Río Gallegos-SS	3406	0.94±0.01	13.6±2.2	0.92 / 0.85	4.9	-1.1±4.9
Ushuaia	2440	0.96±0.01	22.5±1.9	0.95 / 0.90	5.3	3.9±3.9

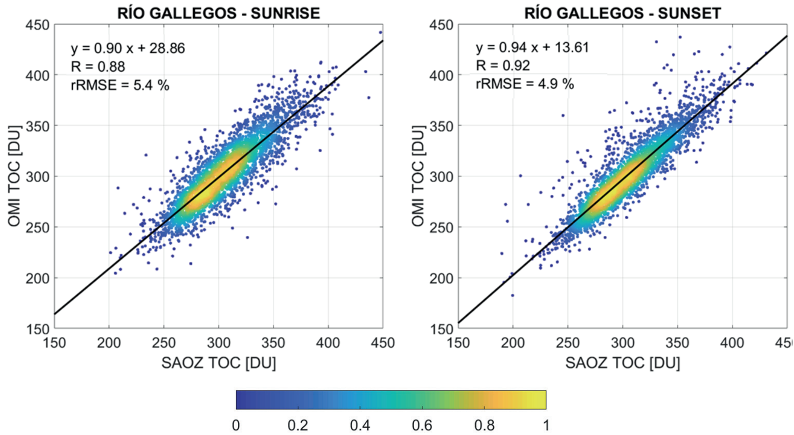

Figure 4. Individual TOC OMI measurements as a function of SAOZ-sunrise and SAOZ-sunset for Río Gallegos. The color bar indicates the normalized dot density.

(2012) reported similar values for comparisons made between OMI-DOAS and Dobson (0.955) and OMI-DOAS and Brewer (0.931) at the Syowa Antarctic base. Kim et al. (2017) compared the OMI and ground-based measurements observed with Pandora, Brewer and Dobson instruments in Korea. In particular, the intercomparisons with the Dobson instrument presented a high correlation, reporting coefficients of determination of 0.93 and 0.94 for OMI-DOAS and OMI-TOMS (correlation coefficients of 0.96 and 0.97, respectively).

On the other hand, the OMI–Dobson MBE presents positive values in all the cases, showing overestimation of OMI with respect to Dobson TOC, in agreement with results reported by Balis et al. (2007) and McPeters et al. (2008). MBE values of 0.6±3.9% in Buenos Aires (lat.: 34.58°S), 3.5±3.3 in Comodoro Rivadavia (lat.: 45.86°S) and 3.9±3.9% in Ushuaia (lat.: 54.80°S) are obtained, which reflect an increase with latitude. A similar increase was reported by Balis et al. (2007) for OMI – Dobson intercomparisons between 2005 and 2006, taking the averaged over 10° latitude bins.

The rRMSE is calculated to analyze the differences between satellite and ground-based measurements, obtaining values below 5.5% at all sites.

3.2. OMI – SAOZ comparison

The intercomparison between OMI and SAOZ daily average TOC in Río Gallegos presents a correlation coefficient of 0.94, while for SAOZ sunrise and SAOZ sunset comparisons it takes values of 0.88 and 0.92, respectively.

The MBE of the OMI – SAOZ daily average TOC intercomparison is -0.9±3.8%, indicating a slight underestimation of OMI with respect to SAOZ. Comparisons made by Hendrick et al. (2011) in

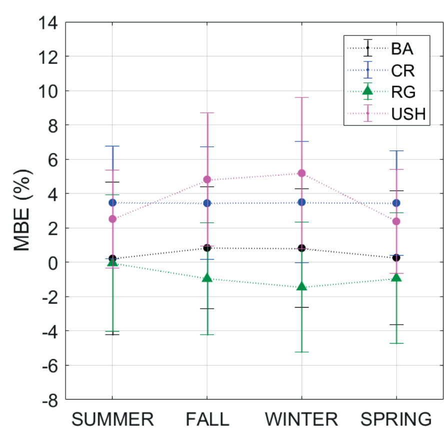

Figure 5. Seasonality of the MBE for each site. Dots indicate OMI – Dobson comparison while triangles indicate daily average OMI – SAOZ comparison. BA: Buenos Aires; CR: Comodoro Rivadavia; RG: Río Gallegos; USH: Ushuaia.

Table 3. MBE (%) between OMI-DOAS and ground-based TOC for each season. The error bars depict the standard deviation of the mean relative difference.

	SUMMER	FALL	WINTER	SPRING
Buenos Aires	0.2±4.5	0.84±3.56	0.83±3.46	0.26±3.91
Comodoro Rivadavia	3.5±3.3	3.44±3.28	3.50±3.53	3.45±3.05
Río Gallegos	0.0±4.0	-0.96±3.28	-1.45±3.79	-0.93±3.81
Ushuaia	2.5±2.9	4.82±3.87	5.19±4.42	2.38±3.01

subpolar latitudes (Kergelen, 49°S, 70°E) between OMI-DOAS and SAOZ also obtained MBE values close to zero but positive (0.6±4.2%). Negative MBE values were reported by Antón et al. (2009) in comparisons performed in the Iberian Peninsula with Brewer instruments, although with greater biases than the present in Río Gallegos. Kuttippurat et al. (2018) reported an overestimation in the OMI – SAOZ comparison for a particular condition, within the polar vortex, but for values inferred with the OMI-TOMS algorithm.

The rRMSE of the OMI – SAOZ daily average TOC comparison is 3.82%. These values are higher than those obtained by Antón et al. (2009), who reported a 3% of rRMSE between OMI-DOAS and Brewer. Vaz Peres et al. (2017) reported rRMSE of less than 2% for a daily average TOC comparison between OMI-TOMS and Brewer.

The correspondence between individual OMI measurements was also analyzed against individual SAOZ measurements at sunrise and sunset (SAOZ-SR and SAOZ-SS hereinafter) (Figure 4). Both comparisons present good correspondence although OMI – SAOZ-SS shows a better agreement. Table 2 summarizes the parameters obtained from the linear regression analysis, where a higher correlation and a lower rRMSE are observed for OMI-SAOZ-SS respect to OMI-SAOZ-SR. This slightly better correspondence for the OMI-SAOZ-SS comparison is expected, since the OMI instrument takes measurements closer in time to sunset than to sunrise (mean time difference of ~3 hours and ~8 hours, respectively).

The comparisons between OMI and SAOZ TOC (daily average, sunrise and sunset) show a slight underestimation of OMI with MBE close to -1%, while those made with respect to Dobson instruments showed overestimation. Despite this opposite behavior, the differences are small enough to be within the uncertainties of each instrument. In addition, Hendrick et al. (2011) reported a negative mean bias of SAOZ compared to Dobson which is consistent with the results obtained here.

3.3. Seasonal comparison

The SZA dependency of a nadir-viewing satellite instrument over the covered ground swath and the larger uncertainties that the radiative transfer calculations present at higher SZA induce seasonal and latitudinal biases in the satellite TOC retrievals (Kuttippurath et al. 2018). Thus, the seasonal dependence of MBE between the OMI and ground-based instruments was also analyzed (Figure 5). The seasonal MBE for OMI – Dobson intercomparisons present negative values for all the sites. Buenos Aires and Ushuaia show a similar behavior accounting with the lowest MBE values during summer and spring and increasing during fall and winter, while Comodoro Rivadavia shows a rather constant value along all seasons. In agreement with the behavior for the whole dataset analysis, the MBE increases for higher latitudes, except in summer, where the MBE in Comodoro Rivadavia is higher than in Ushuaia, although these values are within the uncertainty of the MBE.

On the other hand, the MBE for daily average OMI – SAOZ comparison present a negative bias for all seasons. The minimum and maximum are found in summer and winter, respectively.

Given that MBE values are smaller than 4% at the four stations, and all of them overlap and include the zero value at two standard deviations level, it can be considered that OMI-DOAS TOC retrievals are statistically reliable in these Southern Hemisphere low-altitude regions.

4. Conclusions

Total ozone column retrievals from the OMI satellite instrument with the DOAS technique were compared with ground-based measurements at three Dobson sites and one SAOZ site in Argentina, enhancing the knowledge of satellite measurements performance in the Southern Hemisphere, where scarce monitoring stations exist.

Within a close agreement on average, OMI TOC measurements are slightly higher at Dobson sites, from 0.6% at Buenos Aires up to 3.9 % at Ushuaia. The daily average OMI TOC presents a slight underestimation (-0.9 %) with respect to SAOZ TOC measurements. These values are in agreement with the literature. The comparison between individual OMI and SAOZ measurements made at sunrise and sunset presents higher differences than the comparison with daily average SAOZ measurements, as expected. rRMSE of the OMI – ground-based TOC comparison at all sites presents values smaller than 5 %.

The seasonal comparison between OMI and ground-based measurements shows larger MBE during fall and winter (higher SZA), except at Comodoro Rivadavia where MBE shows a strong seasonal stability.

Even though these four stations are placed in subpolar and subtropical latitudes, the agreement between OMI TOC and ground-based measurements for the larger and the smaller TOC values, some of them over 430 DU and also below the ozone hole threshold of 220 DU, particularly at Ushuaia and Río Gallegos, shows that OMI TOC retrievals are reliable for both the crucial monitoring of the Antarctic ozone hole overpasses along South American continental areas, as well as for very high TOC content which are within the largest worldwide.

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