Short Term Scientific Mission Report, COST Action ES1207

Total ozone column measurements with Phaethon MAX-DOAS system and comparison with Brewer retrievals

Applicant:
Theano Drosoglou
PhD Student
Aristotle University of Thessaloniki – AUTH
Laboratory of Atmospheric Physics
Thessaloniki, Greece
e-mail: tdroso@auth.gr

Host:
Dr. José Manuel Vilaplana Guerrero
National Institute for Aerospace Technology – INTA
Earth Observation, Remote Sensing and Atmosphere Department
Atmospheric Research and Instrumentation Area
Atmospheric Sounding Station "El Arenosillo"
Huelva, Spain
e-mail: vilaplanagjm@inta.es

Purpose of the STSM

The aim of this STSM was to assess the capabilities of the Phaethon system to provide measurements of the total ozone of quality comparable to Brewer spectrophotometers. Phaethon was installed besides the Brewer instruments participating in the COST ACTION ES1207 European Brewer Network (EUBREWNET) campaign / X Regional Brewer Calibration Center for Europe (RBCC-E) intercomparison held at El Arenosillo Atmospheric Sounding Station of the National Institute for Aerospace Technology (INTA), Huelva, Spain. The total ozone column retrieved from the direct sun spectra is compared with that derived by Brewer measurements. The accuracy of the methodology applied to Phaethon data for the ozone retrieval is investigated. Moreover, the possibility of transferring the calibration from the Phaethon system to Brewer spectrophotometers is explored, using collocated measurements of the two systems before, during and after the campaign.

Instrumentation

The Brewer spectrophotometer is capable of performing direct irradiance, global irradiance and sky radiance measurements at specific wavelengths in the UV and visible spectral region. The total column amount of atmospheric gases can be obtained by means of differential optical absorption spectroscopy (DOAS). The Brewer spectrophotometer has been approved as reliable high-quality instrument for the monitoring of the total ozone column (TOC) and its contribution to the understanding of the ozone layer and the dependence of surface UV radiation on stratospheric ozone is significant.

Two Brewer spectrophotometers operate on regular basis at the Laboratory of Atmospheric Physics (LAP), University of Thessaloniki, Greece, a single-monochromator (type MK II, with serial number 005) and a double-monochromator (type MK III, with serial number 086) (Bais et al., 1996). The single monochromator was installed in 1982 for the monitoring of total ozone and columnar sulfur dioxide. In late 1989, it was modified to conduct also spectral irradiance measurements. The operational wavelength range of Brewer #005 is 290–340 nm and the nominal step of the spectral irradiance measurements is 0.5 nm.

Phaethon is a recently developed mini MAX-DOAS instrument which consists of a cooled miniature CCD spectrograph (AvaSpec-ULS2048LTEC) and a 2-axes tracker and can be easily deployed at different locations (Kouremeti et al., 2013). It performs spectrally resolved measurements in the UV-visible region (300-450nm) of direct solar irradiance and sky radiance at several elevation viewing angles including the zenith direction. The total and tropospheric columns of trace gases (O_3, NO_2, HCHO, SO_2 etc.) are retrieved using the differential optical absorption technique. Particularly for the total ozone, the direct irradiance spectral measurements of Phaethon are analyzed using the QDOAS software to derive differential slant column densities relative to a selected reference spectrum. With the appropriate methodology and calibration the differential slant column densities are used to retrieve the total ozone column. The Phaethon system and both Brewers operate regularly side by side on the roof of the Physics Department building (latitude 40.634 N, longitude 22.956 E, altitude 60m above sea level) in the center of the city of Thessaloniki.

Description of the work carried out

The Phaethon system was installed besides the Brewer #005 during the inter-comparison campaign at INTA, Huelva and had been performing both direct sun irradiance and sky radiance measurements. According to the measurements' schedule (table 1) the system was performing continuously direct sun measurements for 50 minutes and sky radiance measurements pointing at an azimuth angle of 50^o away from the sun for 10 minutes maximum once every hour. The time needed for an elevation sequence to be completed was ~5 min in average, depending on the solar zenith angle (SZA) and the azimuth direction of the system's telescope relative to the sun. For 85^o<SZA<95^o the system was performing twilight zenith sky measurements. The internal temperature of the CCD spectrometer was stabilized to 5^{o}C. The TOC was retrieved from the measured direct sun spectra, while the sky radiance spectra were used for the retrieval of tropospheric ozone column.

Table 1. Schedule of measurements performed with Phaethon during the campaign.

Dates (year 2015)	**Time (UTC)**	**Type of measurements**
May 26		Arrival – Instrument installation
May 27		Test measurements of Phaethon
May 27 – June 4	~06:00-19:00 (SZA< 85^o) ~05:00-06:00 & ~19:00-20:00 (85°<SZA<95°)	Direct solar irradiance (50min) and sky radiance (10min maximum) Twilight zenith sky measurements continuously
June 5		Packing – Departure

DOAS retrieval of TOC from Phaethon direct solar irradiance spectral measurements

The DOAS retrieval of total ozone column is based on differential slant column densities (dSCD) derived from the analysis of direct sun spectra measured with Phaethon. Before the spectra are analyzed, the contribution of the dark current and electronic offset is removed using spectra measured at the same temperature and integration time. For the analysis the QDOAS 2.108 software developed by BIRA-IASB and S[&]T is used. The wavelength window used for the ozone retrieval is 315 – 337 nm. The settings used for the DOAS analysis are presented in table 2.

Measured direct sun spectra are compared with a selected reference spectrum, obtained on a clear day under low tropospheric pollution conditions and for small solar zenith angle, for which the slant column density of ozone is SCD_{REF}.

Table 2. Main parameter settings used for the DOAS analysis applied to the measurements.

Spectral window		**315-337 nm**
Fit Parameters	Polynomial	order 3
	OrthoBase	order 2
	Linear offset	order 2
	Shift & Stretch	Shift fit
Cross sections		O_3 (Bass 228K, 1984) NO_2 (Vandaele 294K, 1998) SO_2 (Vandaele 294K, 1994) HCHO (Meller 297K, 1992)
Selected reference spectrum		May 31, 2015 (SZA=~15.18^o)

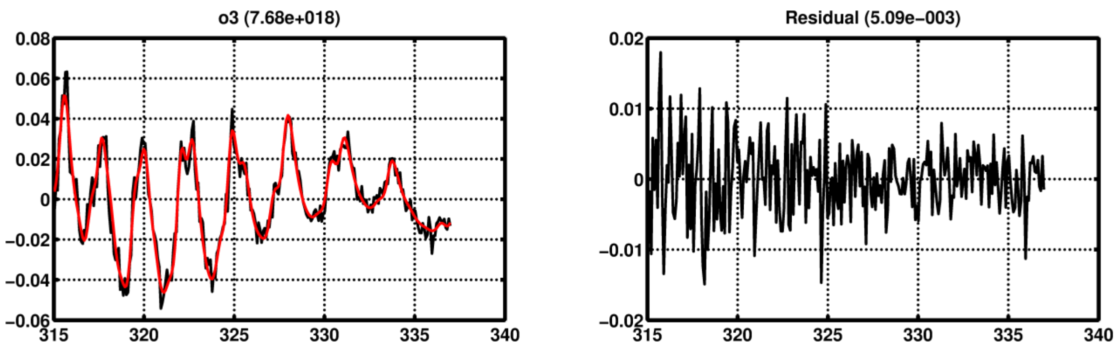

Figure 1. Example of differential slant column fit for O_3 obtained with Phaethon from direct sun irradiance measurements at SZA=58^o (May 31, 2015). The left panel shows the measured (black) and the fitted (red) values, and the right panel shows the residual from the DOAS fit.

For each spectrum (*i*) the differential slant column of ozone relative to the reference is derived, and can be expressed as:

$$dSCD_i = SCD_i - SCD_{REF} = VCD_i * AMF_i - SCD_{REF} \quad (1)$$

The air mass factor (AMF) for each case is the one corresponding to the stratospheric ozone layer where most of the ozone absorption occurs. For SZAs smaller than about 75° it is approximated with the sec(SZA) at the altitude of ~22 km (Bernhard et al., 2005).

To derive the VCD from (1) it is necessary to know the SCD_{REF}. For days, or part of a day, in which the total O_3 VCD can be assumed stable, the slant column density of ozone for the reference spectrum can be determined by applying a Langley extrapolation to the dSCDs derived during that period. Under such conditions (1) is linear and the Langley extrapolation should be valid. The intercept of the linear regression gives the -SCD_{REF}. Incidentally, the slope corresponds to the mean VCD of the reference day. Ideally the same value of SCD_{REF} should be derived if the analysis is repeated for more days.

As long as the SCD_{REF} is determined, (1) can be rewritten to get the VCD of ozone from each measured DS spectrum:

$$VCD_i = \frac{dSCD_i + SCD_{REF}}{AMF_i} \quad (2)$$

For the retrieval of total O_3 VCD from the campaign measurements, 3 minutes averaged spectra were used and a spectrum measured at local noon on May 31, 2015 was selected (SZA=~15.18^o) as a reference for the DOAS analysis. This day was selected because it was clear, except a short period of time right after the local noon when some cirrus clouds were observed, and the instrument operation was stable during the whole day. The Langley fit (figure 2) was applied on the dSCDs derived in the afternoon of the same day, during the period ~15:00-18:00 in which the O3 total VCD was quite stable. The calculated slant column of the reference spectrum is ~346 DU. The same reference spectrum was also used for the analysis of direct sun irradiance measurements taken before and after the campaign.

For the quality control of the total VCD retrieval the normal inverse cumulative distribution was used to calculate the 98%, 95% and 90% confidence intervals for the VCD error (figure 3). Retrievals with error greater than the 90% significance level were ignored.

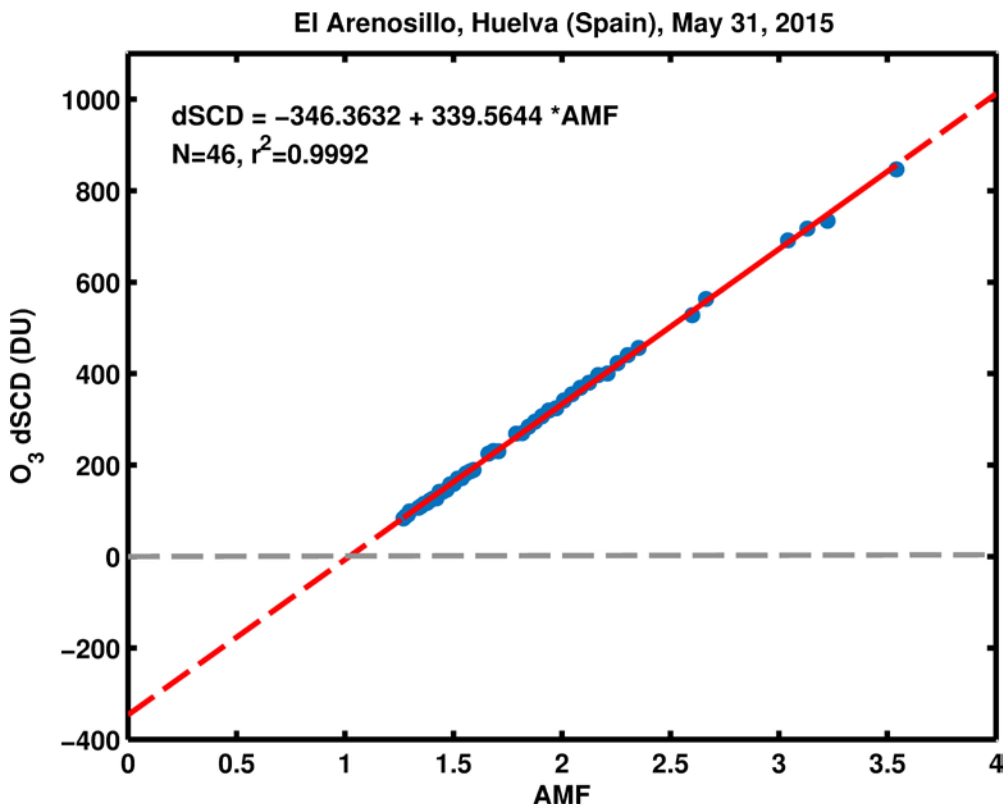

Figure 2. Langley extrapolation applied to the dSCDs derived from Phaethon measurements on May 31, 2015. The constant term of the linear regression gives the -SCD_{REF}, while the slope corresponds to the mean VCD of the reference day.

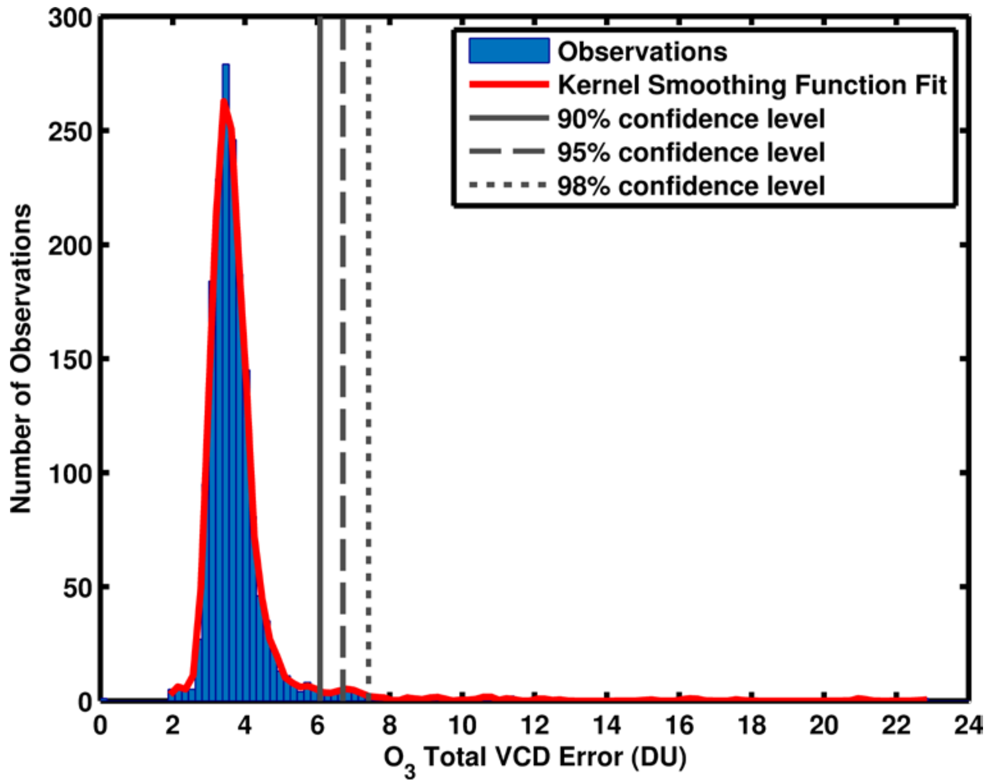

Figure 3. Frequency of total O_3 VCD error for all observations of Phaethon during the campaign. Retrievals with error greater than the 90% confidence level are ignored.

Description of the main results obtained

Comparison of Phaethon-derived TOC with Brewer measurements during the campaign at INTA, Huelva

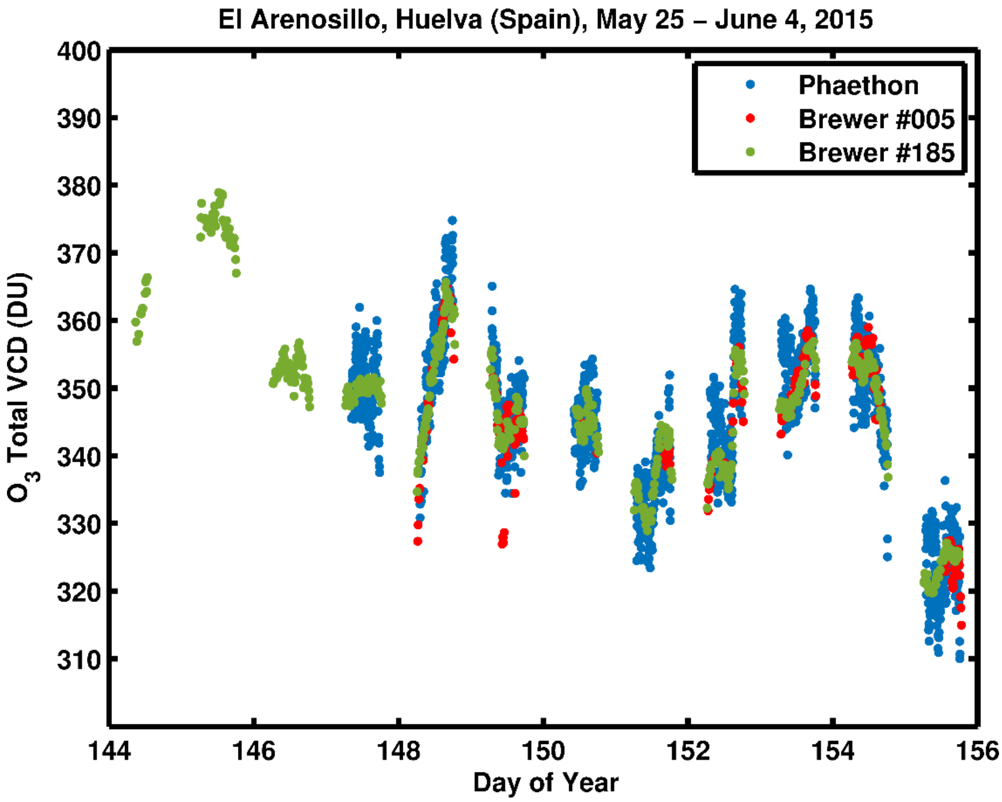

Figure 4. Total O_3 VCD time series obtained from Phaethon system during the campaign. Brewer #005 and #185 measurements are also presented.

The Phaethon system was installed besides the Brewer #005 during the inter-comparison campaign at INTA with the aim to compare the O3 column derived from the two instruments. The total column of O_3 obtained from Phaethon measurements is also compared with retrievals from the Brewer #185 which is one of the Triad operating at Izana Atmospheric Research Center, AEMET, in Tenerife (Spain) and is used as the reference instrument for the calibration of all the other Brewer spectrophotometers. For the O_3 data derived from the measurements of Brewer #005 during the campaign and presented in this report, the new configuration was used.

Phaethon retrievals catch quite well both day to day and daily variations compared with the Brewer O_3 data (figures 4 and 5). However, the Phaethon columns are noisier during the day, while some jumps are also observed. Part of this behavior could be explained by problems in tracking the Sun, which were occasionally observed. This behavior has not been fully explained yet and further investigation is needed. Even when measurements performed with the telescope not pointing accurately to the sun and/or under overcast or partly cloudy sky conditions are excluded from the analysis, the problem partially remains.

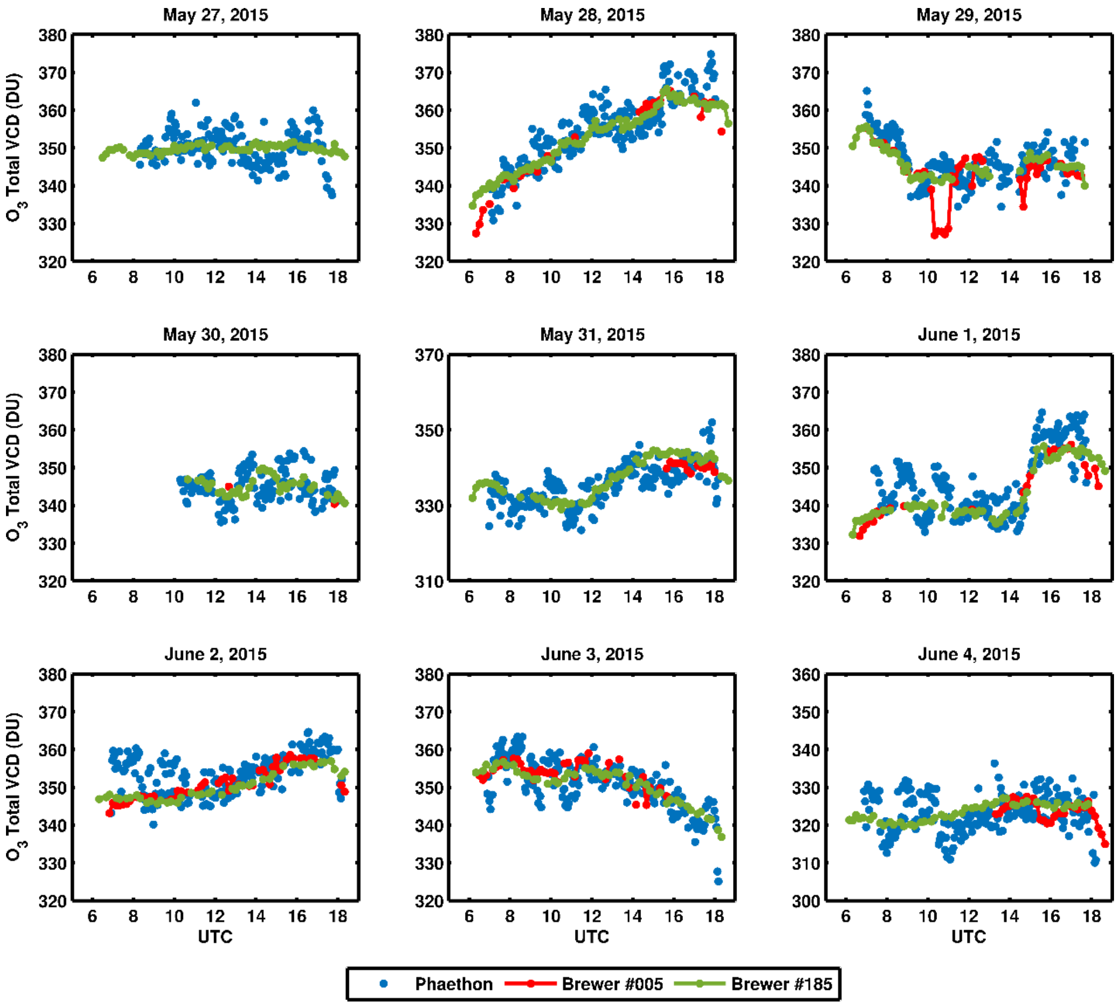

Figure 5. Comparison of total O_3 VCD measured by Phaethon system and Brewers #005 and #185 during the campaign.

Comparison of Phaethon-derived TOC with Brewer #005 at Thessaloniki before and after the campaign

The Phaethon measurements before and after the campaign are also noisy. Better agreement is observed in the retrievals performed after the campaign than the ones before it, probably due to the modifications made to the Brewer #005 within its maintenance during the campaign at the INTA station. It should be noted that for consistency, the Brewer TOC before and after the campaign was calculated with the old configuration, i.e. without applying the new calibration constants that were derived during the campaign.

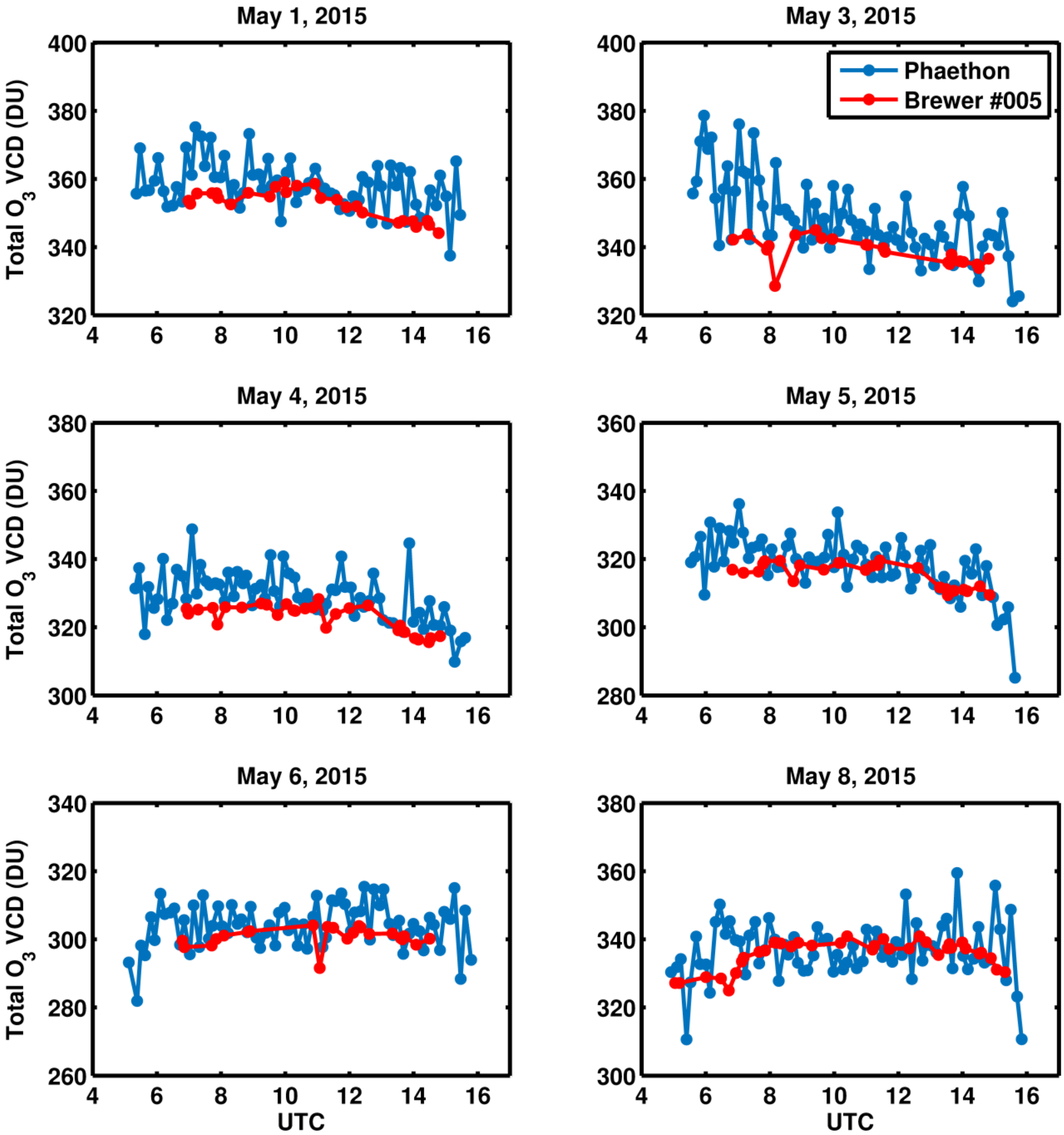

Figure 6. Total O_3 VCD derived from both the Phaethon system and Brewer #005 at LAP in Thessaloniki in May 2015, before the campaign period.

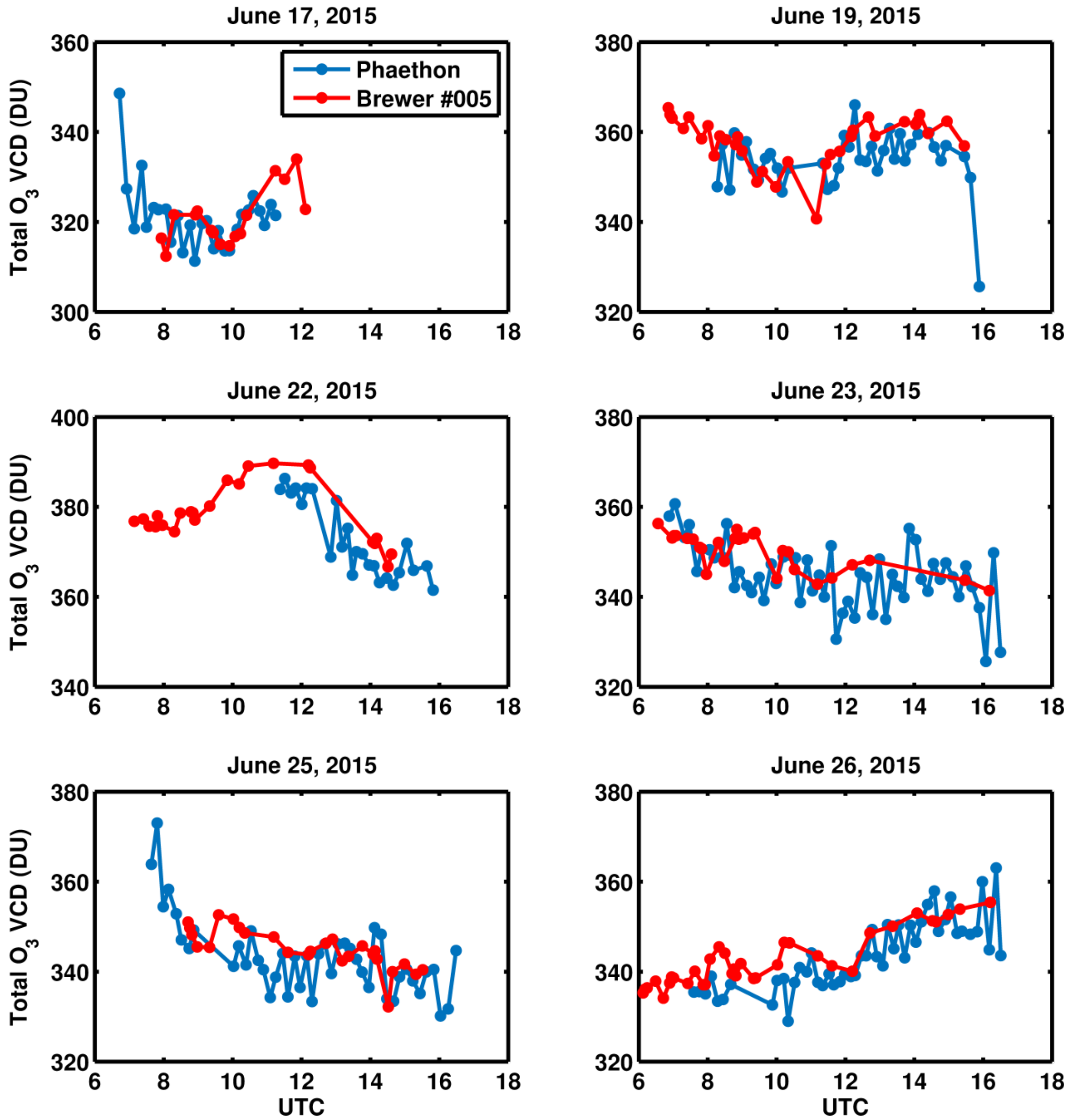

Figure 7. Total O_3 VCD obtained from both the Phaethon system and Brewer #005 at LAP in Thessaloniki after the campaign period.

Conclusions

The method used for the retrieval of total O_3 VCD from Phaethon measurements is sensitive to different factors. Hence, the reference spectrum used for the DOAS analysis of the spectra as well as the measurements in which the Langley extrapolation method is applied should be carefully selected. Otherwise, an offset could be introduced to the O_3 results. Although the Phaethon total O_3 column results are promising and the comparison with Brewer retrievals is quite good, the noise in the data of Phaethon should be further investigated. Among the tasks that are scheduled is a sensitivity analysis of the effect of the spectral range of the DOAS retrieval, the inclusion of additional absorbers in the analysis, and testing of different reference spectra.

References

Bais, A. F., Zerefos, C. S., and McElroy, C. T.: Solar UVB measurements with the double- and single- monochromator Brewer Ozone Spectrophotometers, Geophys. Res. Lett., 23, 833–836, 1996.

Bernhard, G., Evans, R. D., Labow, G. J., and Oltmans, S. J.: Bias in Dobson total ozone measurements at high latitudes due to approximations in calculations of ozone absorption coefficients and air mass, J. Geophys. Res., 110, D10305, doi:10.1029/2004JD005559, 2005.

Dackaert Th., Fayt C. & van Roozendael M., QDOAS software, http://uv-vis.aeronomie.be/software/QDOAS/.

Kouremeti, N., Bais, A. F., Balis, D., and Zyrichidou, I.: Phaethon: A System for the Validation of Satellite Derived Atmospheric Columns of Trace Gases, in: Advances in Meteorology, Climatology and Atmospheric Physics, edited by: Helmis, C. G., and Nastos, P. T., Springer Atmospheric Sciences, Springer, 1081-1088, 2013.