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Atmospheric Measurement Techniques
Discussions

Interactive comment on "Comparison of ozone retrievals from the Pandora spectrometer system and Dobson spectrophotometer in Boulder, Colorado" *by* J. Herman et al.

J. Herman et al.

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A nicely formatted reply is given in the pdf attachment

Reviewer #2 AMTD

Discussions

Interactive comment on "Comparison of ozone retrievals from the Pandora spectrometer system and Dobson spectrophotometer in Boulder, Colorado" by J. Herman et al. Anonymous Referee #2 Received and published: 24 April 2015

This paper presents mainly a comparison of the total ozone data derived from the DOAS-based Pandora system and the standard Dobson spectrophotometer that operates in Boulder CO. Such DOAS-based systems may have the potential to be included in the global total ozone observing network, following a thorough investigation of their quality and comparability with the existing standard Dobson and Brewer instruments. The Pandora systems can supplement the existing network of the standard Dobson and Brewer total ozone instruments, and is essential to have thorough analyses of their performance. In this context this paper could be an essential contribution towards this goal. In addition, the paper presents comparisons among total ozone data derived from satellite-borne instruments, but these are discussed only briefly. Although interesting results are presented showing, generally, a good comparison between the Pandora and the Dobson, parts of the paper would need further work in order to prove the quality of the Pandora data.

My major concern for this paper is the use of different absorption cross section data when comparing the two systems. Despite the general agreement that the Bass and Paur (BP) data are outdated and would be probably be replaced in the near future, still the official total ozone data reported by the standard Dobson and Brewer instruments are based on BP. Since the aim of the paper is to compare the total ozone retrieved by the two instruments, the comparison should be based on the same spectroscopic data.

The goal was to compare Pandora results with Dobson data as the instruments are currently operated. We have now done the work using common cross sections. This material has been added to the paper in an appendix.

While the paper has started very nicely with adequate discussion of the Pandora and Dobson comparison, later on, a lot of figures are included addressing very briefly different topics, not all relevant with the title and aims of the paper. For instance, the cross comparisons of the satellite data cannot be considered a significant contribution to the paper. Similarly, Figures 10-12 show some examples of daily variations of radiance under clear and cloudy conditions and of total ozone. I don't think that are necessary. I am sure that some of the figures could be omitted to the benefit of the paper.

The figures showing the effects of clear and cloudy conditions are quite useful in that the Pandora O3 values retrieved are quite good even if there is additional noise. Unlike the Dobson, the nearly continuous data record makes it possible to assess the cloud induced effects when compared to a clear day. Part of the purpose of this paper was to demonstrate the quality and limitations of the Pandora data under more general conditions, other than just clear sky used for the Dobson comparison.

Finally, the discussion of the 2 last paragraphs of section 4 is rather simple and I do not consider it as a significant contribution to the paper. If the diurnal pattern of total ozone were to be discussed, I would expect a more thorough statistical analysis, where uncertainties in the measurements are taken into account, at least, quantitatively. To conclude, I think that although the paper is a good contribution to the emerging network of Pandora spectrometers, I believe that the authors should improve the dis- cussion of the weak sections, and possibly reduce the number of figures.

I have removed the figures on diurnal variation at Boulder Colorado. The reviewer is correct, in that this discussion is not part of the paper's main topic.

Specific comments by page and line number

3054 3: Please include the units for the resolution (500000!). Resolution R is dimensionless. R = ïĄňïĂŕïĄĎïĄň

How the normalization was done? The radiometric normalization procedure is given in the quoted references, Thuillier et al., 2004; Bernhard et al., 2004. Basically, the high spectral resolution of the Kurutz spectrum is reduced to that of the Atlas-3 SUSIM. Then the reduced resolution Kurutz spectrum and the Atlas-3 spectrum are fit with a low order polynomial over a small spectral range, 10 – 20 nm. Finally, the difference in the polynomials is determined and the Kurutz spectrum is shifted by that amount. We then return to the newly normalized high resolution Kurutz spectrum and work with the Pandora measured slit function. This slit function is measured in the laboratory throughout the entire Pandora spectral range, 280 – 525 nm. The error in measuring the core slit function is less than 1%, which propagates into an ozone error of less than 1%.

5: Why the Malicet cross sections have been used, considering that the Dobson is based on BP? The effect from the different cross sections should be discussed.

This paper is not about comparing cross sections, but rather about comparing standard Pandora TCO using BDM cross sections with standard Dobson TCO using B&P. I have added an appendix with a figure showing the effect of using DBM cross sections for Dobson #061 data.

8: What is the uncertainty of the applied slit function, which usually is wavelength dependent? What is the resultant uncertainty in the ozone retrieval? As mentioned above, the core slit function (not the extreme tails) is determined for all pixels (wavelengths) to within 1%. A 1% error in the slit function would produce less than a 1% error in O3 retrieval. The measured wavelength dependence of the slit function is small for this symmetric Czerny Turner spectrometer.

How much is the stray light reduced? How much remains and what is the effect on ozone retrieval? Does the UV340 filter block wavelengths above 525 nm (e.g. in the solar infrared) that can be also a source of stray light? If one compares the open hole measurements with the UV340 filter measurements, the percent difference is 95% at 305 nm and 20% at 320 nm caused by stray light. The UV340 filter transmission is essentially zero for wavelengths greater than 380 nm until the NIR at about 720 nm. A typical transmission curve is shown below, with about 5% leakage near 720 nm. Most of the light from 720 nm will completely miss the detector (wrong diffraction angle) except for a very small fraction that bounces off of the edges of the matte black interior baffles. What stray light is present can be measured at 280 to 290 nm, which is normally dark from O3 absorption in the atmosphere, and subtracted from the measurements at 305 – 320 nm. The answer is that the stray light has little effect on the retrieved O3.

An empirical measure of stray light is obtained by examining the retrieved O3 as a function of airmass. If there is residual uncorrected stray light, then the retrieved vertical column O3 will be curved downward from noon (inverted u-shape) with increasing airmass. This is especially evident on days when O3 is nearly constant throughout the day. It is also evident at very large airmasses, when the signal is almost all stray light (no UV), and the retrieved O3 decreases rapidly near sunrise and sunset. For spectrometers that happen to have an unexpectedly large amount of stray light, a stray light correction as a function of airmass is applied so that days with nearly constant O3 have no retrieved curvature.

For the particular Pandora used at Boulder Colorado Pandora 34, the spectrometer was one of the older models that had more stray light than the newer models. Part of the reason is in the way the baffles were mounted as part of the spectrometer cover instead of being fixed to the spectrometer bench. This resulted in the observed curvature of O3 vs time of day centered about noon as mentioned above. To correct this, we used the following empirical stray light correction equation applicable to this specific older spectrometer.

O3(Corrected) = O3(Measured) [1 + 0.066 AMF0.4 - 19.0] Where the AMF is approximately equal to 1/cos(SZA) for direct sun measurements.

This completely removed the noon centered O3 curvature vs time of day. I have added a discussion of this in the text.

14: What is meant by “weighting system”? The “weighting system” is a method of estimating noise as a function of wavelength for increasing airmass factors. On a clear day, the direct sun exposures can be as little as approximately 5 ms. The 4000 measurements are broken up into smaller groups and averaged for each wavelength (pixel). If the ensemble average measurement is noisy (large standard deviation), then the counts from that wavelength are weighted inversely to its standard deviation from the mean. The practical effect is to shift the retrieval emphasis toward longer wavelengths as a function of ozone airmass where a high signal to noise ratio can be maintained.

16-17: If I understand correctly, 4000 spectra in 20s correspond to an integration time of 5 milliseconds. Have you tested the linearity of the system at such low integration time? We have tested the linearity. The spectrometer is linear in this range. The shortest integration time is 4 ms.

Is the signal to noise ratio sufficiently large? Text added to the paper: The exposure times to sun or sky photons are adjusted so that the readout pixel with the highest intensity is never in excess of 80% of the CCD readout well depth of 200,000 electrons. This means that each pixel in the 64 rows for each wavelength is limited to less than 2500 electrons

The effective signal to noise ratio is composed of a combination of electron noise and readout noise. For pixels having the maximum intensity, the exposure time is adjusted automatically to 80% readout well depth filling (80% of 200,000 electrons, or an electron signal to noise greater than 400:1). The electron signal to noise at the O3 absorption wavelengths is less (about 40,000 electrons) or about 200:1. Averaging 4000 measurements gives an increase of a factor of 60, or a SNR of 12000. In addition the spectrometer is better than 4 times over sampled, which gives another factor of 2. Finally, we use a 20 nm band for the spectral fitting, which further increases the signal to noise. Other noise signals in the Pandora system and in the changing atmosphere are larger. On days when O3 is nearly constant, the low instrument noise is evident in the very low retrieved ozone scatter between successively retrieved O3 values. For all conditions, the optimum exposure time is determined using a test exposure just prior to the 20 second measuring period, which can range from 4 ms to 4 seconds. The linearity of the spectrometer system has been determined over the entire range of exposure times used in the measurements.

An estimate of TCO retrieval precision and standard deviation can be obtained from a similar Pandora located at Mauna Loa Observatory where the geophysical ozone variability is at a minimum compared to other sites. On a quiet cloud-free day (1 February 2015) the ozone value was 236.27 ± 0.35 DU for 77 values between 11:00 and 13:00 hours. Some of this variation, 0.15%, is natural TCO variability and some from instrument noise. If we assume that the entire variability is instrument noise, the signal to noise ratio would be 650:1. From a spectral fitting viewpoint, the Mauna Loa estimated ozone error is 0.069 ± 0.0016 DU, or about 0.029%, which gives a SNR of about 3500:1. This estimate includes both total instrument noise and spectral fitting errors. The estimated SNR will decrease with increasing AMF and with cloud cover. The conclusion is that the Pandora spectrometer system is not noise limited for clear-sky conditions.

23: What is the degree of the polynomial used in practice? Is it the same for all solar zenith angles? A fourth order polynomial is used for all zenith angles to remove spectrally smooth aerosol and Rayleigh scattering effects.

24: How much the total ozone is overestimated under such conditions? Is that a problem for locations with significant aerosol loads? Ozone is not significantly overestimated under moderate aerosol loading or in the presence of light cloud cover. However, the noise level is increased as shown in the paper. An example is given for light to moderate cloud cover and the ozone daily time dependence is given for a series if successive days regardless of cloud or aerosol effects. There are no jumps in TCO retrieval for light to moderate cloud cover or aerosols.

3055 10: When Pandora TCO is compared with the Brewer, what absorption cross-section dataset is used? Here again the Brewer TOC is based on BP, while the Pandora TOC is based on Malicet. I would expect an additional effect, even seasonal. The GSFC Brewer that was compared with Pandora used BDM cross sections, not BP.

There was a seasonal effect based on temperature that can easily be removed with a temperature correction. This is discussed in the paper by Tzortziou et al. referenced in the current paper.

3056 18: The systematic difference between the two systems cannot be attributed solely to differences from the effective temperature, since differences should appear also due to the use of different absorption cross sections. Although the differences in the measurements match those calculated from the change in the stratospheric temperature, there is an almost 2-month shift in the maximum of the annual patterns between figures 1 and 2. In addition, after the temperature correction (Fig 3), there is still a residual seasonal pattern.

The residual pattern is less than the standard deviation of the differences as indicated in the figures. From a statistical viewpoint, the differences are negligible. It is possible that if we used measured temperatures instead of climatology, the small difference would disappear. Figure 3 shows that same 2 month shift as a small second order effect. What is important here is that the Pandora and Dobson show the same day-to-day variation with very little bias. Either data record would yield the same average O3 amount. Only further studies will show if the long-term TCO trend is the same. Measurements of Pandora #34 vs Dobson #061 are continuing.

20: “The seasonal difference is significant at the level of 1 standard deviation 5DU of the observed data about the Loess(0.5) curve (Fig. 1b).” I don’t understand this statement. To my understanding, the seasonal difference is described by the loess curve which spans between -5 and +10 DU. On top of this there is day-to-day variability (noise ?) which is the order of ±5DU. Please clarify. The scatter of the difference data about the Loess curve is +/- 5 DU (1 standard deviation). The Lowess curve in Figure 1 shows systematic differences that are larger than +/-5DU before temperature correction. As stated in the paper, -5DU in the winter and +10 DU in the summer. The Lowess curve is intended as a guide to seeing the seasonal difference. The measurement scatter is not Pandora noise, but rather representative of the physical differences between the two instruments and their respective retrieval algorithms. It is very difficult to quantify the Dobson scatter, since the Dobson does not obtain many measurements per hour (usually 1) compared to Pandora (45). I am not sure about the effective Dobson signal to noise ratio of a single measurement. However, a comparison of Dobson #061 with the standard Dobson #083 yielded a small difference with a significant standard deviation, 0.5% ±1% , or about 1.5 ± 3 DU.

24-25: I do not understand why in Table 1 the effective temperature for each month is given as a function of total ozone. The effective temperature is usually calculated by weighting the temperature profile with the ozone profile. The total ozone does not enter into this calculation. Please explain in more detail the procedure for the calculation of the ozone weighted effective temperature. The effective temperature was obtained as described in the references. Namely, by using an ozone profile climatology that is a function of total ozone amount and a temperature profile climatology. The effective temperature was obtained by weighting the temperature profile with the ozone profile. Since the profiles were specified by ozone amount, the effective temperature became a function of total ozone. The location of the temperature table is ftp://toms.gsfc.nasa.gov/pub/ML_climatology/ The temperature is given as a function of Month, latitude and Umkehr layer (altitude) in the file Temperature_climo.xlsx and the ozone profiles in ML_du_table.dat. These profiles have a total ozone amount associated with them (see Wellemeyer et al., 1997). The effective weighting changes with total ozone amount, since the stratosphere contains most of the O3. For a given latitude, the effective temperature can be estimated as a function of the measured total ozone amount and month.

26-27: “The tables are given as a function of latitude, ozone amount, and height for each month”. Please make clear if these are the tables from Labow (2011) and Wellemeyer et al. (1997). The following has been added to the paper: A compiled climatology of ozone and temperature (Table 1) was used to generate the ozone weighted effective temperature TE for the location of Boulder, Colorado at 40ON latitude. The tables are given as a function of latitude and ozone amount for each month (see ftp://toms.gsfc.nasa.gov/pub/ML_climatology for climatology data files, and discussions by Wellemeyer et al., 1997; McPeters et al., 2007; McPeters and Labow (2011)). For this study, only the monthly data for latitudes of 30O-40ON and 40O-50ON are used to form an average suitable for 40ON.

3057 24: It is not clear how the Dobson data were corrected; using the constant temperature coefficient as mentioned in line 13, or using Table 3?

The Dobson data were corrected using Table 3, which is based on -0.13%/OK from the reference temperature of 226.7OK

3058 4: I suggest redrawing figures 4a and 4b, with axes of equal length. (Same for Figure 7) I have now made the plots square

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5: In this case the high correlation arises from the seasonal variation of TOC. The high correlation arises from the tracking of daily values and the seasonal variation (see Fig 3)

The scatter is more important for establishing the level of agreement between the two systems. The tracking of daily values and the small scatter is what is important. If this level of correlation continues, the two systems would report the same long-term trend, if any.

24: I assume that the satellite TOC is based also on the Malicet absorption cross section, and this removes the seasonal dependence that was seen in the Dobson comparison. I think this should be discussed.

The OMI data are processed with temperature corrected Bass and Paur. The Pandora comparison uses the BDMt temperature corrected data for comparison. The next version of OMI will use BDM cross sections. I have added a comment that OMI uses BP. NPP, on the other hand, uses BDM cross sections. Even so, the OMI and NPP temperature corrected data agree as do the comparison of Pandora with OMI and NPP except for a known offset between OMI and NPP.

3059 1: Comparison of the TCO data from the 2 satellites is shown but results are discussed very briefly, without any background information, even in the Introduction. I do not see strong relevance with the aims and title of the paper. Generally, this section (3) of the paper is very short with a lot of figures.

I have added a small amount of discussion to the introduction concerning the satellite comparison. The purpose is to show that Pandora and Dobson are equivalent and that both agree with the satellite data. The figures do not need a lot of discussion. We are only showing that all the data sets are essentially equivalent over Boulder, Colorado.

3060 21: It would be good to provide some more details on the method that tis used to weight the different wavelengths according to their noise. Two lines later it is said that the retrieval range is shifted. Which of the two methods is actually used?

I will correct the wording. The only method used is to weight the different wavelengths inversely to their noise. The effect of this weighting is to shift the retrievals to longer wavelengths where the noise is less. In the paper there are two sections mentioning the weighting The algorithm for deriving ozone amounts differs from Dobson or Brewer instruments in that spectral fitting is used to cover the entire 310 to 330 nm range with a weighting system that measures the noise as a function of wavelength for each single pixel and inversely weights the significance of the fitting to the amount of noise. On a typical clear-sky day, about 4000 direct-sun measurements are taken in 20 seconds at low to moderate solar zenith angles (SZA). The 4000 measurements are broken into small groups, which are averaged together and their standard deviation is determined. Averaging improves the single measurement signal to noise ratio by a factor of 60, and the standard deviation from the mean provides the inverse weighting. The Pandora ozone spectral fitting retrieval algorithm inversely weights the contribution of each wavelength by its increased standard deviation from the mean caused by reduced count rate with increasing AMF. The effect of the effectively shifted wavelength retrievals is taken into account in the temperature corrections shown in Table 2 and Figure 3.

27: It would be interesting to plot on fig 14 the data from the Dobson. How many Dobson measurements are taken on average every day? The Dobson data frequency is very variable depending on whether there is clear sky or not. At best there are just a few points per day. Figures 1, 2, 3 have every Dobson clear sky AD pair plotted compared to the corresponding Pandora data – sometimes 3 or 4 per day. Since the Pandora data is obtained every 80 seconds, temporal data matching is easy to do. For Pandora, Figure 14 contains all data, clear and cloudy.

3061 1-24: The last paragraphs of section 4 are very brief, again with lot of figures, addressing different topics, not very much related to the aims of the paper.

These figures have now been removed. They add nothing to the comparison of Dobson vs Pandora as the referee has noted.

Please also note the supplement to this comment:
http://www.atmos-meas-tech-discuss.net/8/C1503/2015/amtd-8-C1503-2015-supplement.pdf

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