Reviewer #1

AMTD Interactive comment Printer-friendly version Discussion paper Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2017-157-RC1, 2017 © Author(s) 2017. This work is distributed under the Creative Commons Attribution 3.0 License. Interactive comment on "Ozone Comparison between Pandora #34, Dobson #061, OMI, and OMPS at Boulder Colorado for the period December 2013–December 2016" by Jay Herman et al. R. Chatfield (Referee) Robert.B.Chatfield@nasa.gov Received and published: 30 June 2017 Review of Herman et al.

Response:

Since the manuscript was originally submitted, two significant changes have occurred. 1) NOAA updated the calibration of the Dobson#063 by applying the interim calibrations against the world standard Dobson#083. This changed all of the Dobson data slightly. 2) I investigated the influence of the endpoints on the percent difference time series and concluded that there was a significant effect on the slopes in some cases. Therefore, I de-seasonalized all of the percent difference time series as now described in the paper. All of the extensive changes in the paper are marked in green.

This is a good basic publication which just needs clarity and precision. Conclusions regarding trends in retrieved ozone need more modest standard error estimates, I believe The authors appear to make two assumptions:

(a) That "significance" means a 5% (? not stated) chance of Type 1 error (false acceptance) with a Gaussian distribution of errors.

The error estimates given are 1 standard deviation STD estimated from the least squares linear fit process. The error of the individual points was described in the previous paper as 1% with a precision of 0.1%. Most of the variation seen in the data is "natural" variation". It is clear that the error bars are large enough to make the statistical significance of some of the slopes marginal (see OMPS vs Pandora; 0.19 +/- 0.1). Some of the others are significant (see OMPS vs Dobson: -0.4 +/- 0.09) at the 2 STD level. P-values are now specified as are the number of points in each time series.

(b) That the "number of relevant samples" is the number of individual observations, apparently as averaged for 80 seconds for the PANDORA, the number of individual observations (averaged over 8 minutes, or once daily?) of observation recorded for the Dobson, and the number of days of observation (maximum once per day?) for OMI and OMPS.

Each Pandora data point is an average of 4000 measurements obtained during 30 seconds. All data for this study were clear-sky within the instrument's field of view based on the Dobson criteria for A-pair direct-sun clear sky. In addition, the Pandora data are averaged over a period of +/- 8 minutes surrounding the Dobson time of measurement (2 to 3 times per day). Pandora measurements are obtained every 80 seconds that means there were an additional 10 Pandora data points averaged together to compare to each Dobson measurement. The net averaging of Pandora is 40,000 (4x10⁴) measurements for each comparison. The same procedure was used for comparisons with OMI and OMPS, where they measure once or twice per day over Boulder, Colorado.

For some comparisons, "data were selected for scenes that are clear-sky conditions as determined from the Dobson A pair" For all?

All Dobson vs Pandora, OMI, or OMPS scenes were clear-sky A-pair using the Dobson criterion

All Pandora vs OMI and OMPS were clear-sky or light clouds using a Pandora criterion measuring the noise between adjacent groups of measurements within the 4000 individual measurements that make up one Pandora data point.

I added the following paragraph

Each clear-sky PSI data point is an average of 2000 (early morning to evening SZAs) to 4000 (mid-day SZAs) measurements obtained during 20 seconds. All data for this study were clear-sky within the instrument's field of view based on the Dobson criteria for A-D-pair direct-sun clear sky. In addition, the PSI data are averaged over a period of +/- 8 minutes surrounding the Dobson time of measurement (2 to 3 times per day). Since PSI measurements are obtained every 80 seconds, there were an additional 10 PSI data points averaged together to compare to each Dobson, OMI, or OMPS measurement. The result is high signal to noise values for Pandora and high precision (0.1%). The same procedure using cloud-screened PSI data was used for comparisons with OMI and OMPS, where they measure once or twice per day over Boulder, Colorado. Some of the variations in the day to day ozone values are driven by changes in the local weather over Boulder, Colorado (see Fig. 14 in Herman et al., 2015), with weekly averages having much smaller variation.

How many days?

Reply:

The maximum number of days would be 1096. Not every day had a clear-sky observation and Pandora was not operational for some short periods. There are a significant number of days when OMI does not have an observation near Boulder.

Each of these numbers should be stated in the relevant context .

I now list the number of points in each time series in the graphs and summarize in a table.

Table 1 Percent Difference Summary of Linear Fit Slopes and Mean Differences in Fig. 3					
Percent Diff(A,B)	Slope (% per Year)	Probability	Mean (%)	Points	Panel
Pan, Dob(BP)	-0.2 ± 0.04	P < 0.001	-2.1 ± 1.6	2020	А
Pan, Dob(BDM)	-0.2 ± 0.04	P < 0.001	-2.8 ± 1.6	2020	В
OMPS, Dob(BP)	-0.09 ± 0.08	P = 0.3	-1.4 ± 2.1	854	С
OMI, Dob(BP)	-0.18 ± 0.08	P = 0.03	-1.4 ± 1.9	654	D
OMPS, Pan	-0.18 ± 0.098	P = 0.06	0.96 ± 2.7	952	Е
OMI, Pan	+0.18 ± 0.096	P = 0.06	1.1 ± 2.1	624	F

There are many statistics quoted where the reviewer was confused. Please describe each. The appropriate statistic to quote is the p-value (0.05 ??) with the number of observations used in each statistic, and one- or two-sided calculation, where there could be confusion. For example, a p-value of 0.10 would suggest to the reviewer that there was something worth further investigation. The point of maximum confusion for the reviewer was the discussion of drift. What number of samples was used? The eye sees that "independent" observations seem to occur often due to some rapidly changing condition: experimental error in one or both instruments, or rapid weather variation?

Reply:

P-value is now included in the graphs

Lowess(0.1), reference, explain "0.1)"?)

Reply:

Lowess(0.1) means that 10% of the total data were least squared averaged to form a smooth curve. It is the same as a "running average" except in the use of least squares instead of a linear average. Lowess(1) would give a tradition linear least squares. This was explained in the original referenced paper. Lowess(0.1) is roughly a 90-day low pass filter for this data set.

I added the sentence:

The Lowess(f) procedure is based on local least squares fitting using low order polynomials applied to a specified fraction f of the data (Cleveland, 1979).

The smoothed lines (which smoothing for Figure 3 as Figure 2. suggest that "weather" variation has a substantial impact on the smoothes and indeed the trends, especially in Figure 2. The smoothes for Figure 2 appear somewhat more convincing, but the uncertainty of 0.1% seems to be based on number of all samples rather than some partial contribution from "weather variability." One could guess a synoptic value of "five days per synoptic episode" and calculate a debatable approximate "number of samples" but the more appropriate value would be derived from a time series analysis which allowed for longer time-scales in that algorithm. In fact, there is enough excellent data here for most series to justify a more careful time-series analysis. For this publication, a disclaimer saying that "weather variability" could allow for a larger uncertainty in the apparent divergence is acceptable. In this case, "weather" is longer than one day but probably shorter than three years. Similar comments apply to the +/- 0.002 in Figure 1.

Reply There is weather variation in ozone – see the first paper on Boulder Colorado – that is mostly day to day variation. Averaging over a week would remove most of the weather variation. Deseasonalizing the percent difference time series removes any longer-term near periodic weather effects.

(minor points: explain acronym CCMI;

CCMI is Chemistry–Climate Modelling Initiative

The acronyms for OMI and OMPS are given in the opening paragraph

"Additional comparisons are made with satellite overpass data from OMI (Ozone Measuring Instrument on board the AURA spacecraft) and OMPS (Ozone Mapping Profiler on board the Suomi NPOESS satellite)."

perhaps OMI and OMPS are named on web pages, but could explained) This will be a nice addition to the description of stratospheric (and tropospheric) change and tropospheric change (TOAR). We may hope that the advent of many PANDORA instruments will add to a better discrimination of the variability and secular change of ozone as a function of altitude. Minimal re-review is expected. 1.

Does the paper address relevant scientific questions within the scope of AMT? Yes 2. Does the paper present novel concepts, ideas, tools, or data? Yes, Data 3.

Are substantial conclusions reached? Yes, sufficient when they are qualified as noted 4.

Are the scientific methods and assumptions valid and clearly outlined? Correctable. See notes above 5. Are the results sufficient to support the interpretations and conclusions? Ditto 6. Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)? Ditto 7. Do the authors give proper credit to related work and clearly indicate their own new/original contribution? Yes 8. Does the title clearly reflect the contents of the

paper? Yes 9. Does the abstract provide a concise and complete summary? Yes 10. Is the overall presentation well structured and clear? Yes 11. Is the language fluent and precise? Yes, but see 4. 12. Are mathematical formulae, symbols, abbreviations, and units correctly defined and used? Yes, minor additions needed for abbreviations, see above for e.g. "significant" and "Lowess(0.1)" 13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated? No 14. Are the number and quality of references appropriate? Yes 15. Is the amount and quality of supplementary material appropriate? Yes

Reply to Reviewer#2

This paper presents comparisons among column ozone measurements at Boulder Colorado from two ground-based instruments and two satellite instruments. Daily data are analyzed for three years, and the focus of this short paper is to evaluate absolute differences among the measurement systems and quantify possible drifts (or trends) over the three years. I suppose the analysis is especially focused on evaluating the (relatively new) Pandora ozone measurements, although this is not explicitly stated.

Response:

Since the manuscript was originally submitted, two significant changes have occurred. 1) NOAA updated the calibration of the Dobson#063 by applying the interim calibrations against the world standard Dobson#083. This changed all of the Dobson data slightly. 2) I investigated the influence of the endpoints on the percent difference time series and concluded that there was a significant effect on the slopes in some cases. Therefore, I de-seasonalized all of the percent difference time series as now described in the paper. All of the extensive changes in the paper are marked in green.

I have added the following to the Introduction:

The recalibration of the Dobson and the de-seasonalization of the percent difference time series suggests that it is accurate to say in the introduction:

The results demonstrate the accuracy and stability of both the Dobson and PSI for retrieval of total column ozone.

The results show small mean biases among the systems (+/- 1-2%), and excellent correlations for day-today and seasonal variability. The calculated difference trends show small drifts (0.2 to 0.6 %/year) among the various measurements, and these drifts turn out to be statistically significant based on the results shown (Fig. 3).

1) Note that the satellite comparisons suggest the largest drifts are associated with Dobson measurements. However, the authors downplay these significant trends and conclude that 'there is long-term stability in all four instruments'. In my opinion this summary statement needs to be better qualified in light of the significant trend results; I appreciate that the trends are derived from a short time record with arbitrary end points, with corresponding large uncertainties (the results look to be strongly influenced by the early 2014 data). But wouldn't drifts of magnitude ~6%/decade (as derived here) be troublesome if observed over a longer time record? I suggest that this detail needs some further discussion.

Response:

The paragraphs discussing the comparison now reads"

Calculations for Pandora#034 (Panels E and F in Fig. 3) show marginally significant (p = 0.06) trends for Pandora#034 compared to OMPS (Panel E, -0.18 ± 0.098 % per year) and OMI (Panel F, $+0.18 \pm 0.096$ % per year). If the Pandora#034 time series is extended into 2017 to minimize the effect of missing Pandora data in 2016, then the trends for Pandora compared to OMPS (-0.2 ± 0.08 % / Year p = 0.013) and OMI (0.15 ± 0.076 p=0.05) are significant, but not different from the shorter 2014 – 2016 period. The secular trends for the difference between Pandora#034 and Dobson#061 (-0.2% per year) are almost the same for both Dobson BP and BDM ozone absorption coefficients is small (0.042% per ^oC). This suggests that the stratospheric effective ozone temperature change is not a source for the small difference between Pandora#034 and Dobson#061.

Figure 4 shows that the TCO between Pandora#034 and Dobson#061 are highly correlated with 1:1 slope and the correlation coefficient $r^2 = 0.97$ for the 3-year period 2014 to 2016. Similar correlation plots (Fig. 5) for Pandora#034 and Dobson#061 with OMI and OMPS also show very high correlations. The correlations in TCO are obtained after only temperature corrections to Pandora#034 and Dobson#061 using T_E (TCO pairs similar to Fig. 2, panel A).

And changed the Summary to read:

Temperature corrected Pandora#034 and Dobson#061 differ by an average of 2.1% with Pandora using its standard retrieval BDM ozone absorption cross sections and Dobson using the recommended BP ozone absorption cross sections. Pandora compared to Dobson shows a small, but significant drift (-0.2 \pm 0.04 % per year. p < 0.001) for the 2014 – 2016 period. Comparisons of Pandora with OMI and OMPS are marginally significant drifts of 0.18 \pm 0.1 and -0.18 \pm 0.1 p=0.06 for 2014-2016, but are significant (0.15 \pm 0.076 % per year. p=0.05 and -0.2 \pm 0.08 % per vear. p = 0.013, respectively) if the period is extended to mid-2017 to minimize the effect of missing Pandora data during 2016. The small Pandora and Dobson trends compared to OMPS suggests that both instruments are stable. The conclusion is that the periodically calibrated Dobson#061 is able to detect smaller ozone trends than a Pandora instrument with no intermediate calibration during a 3-year period. The longer term trend for Dobson compared to OMPS for the 5.5-year period (2012 – June 2017) is -0.07 \pm 0.03 % per year, p = 0.047.

2) Aside from this, I believe this short paper is a useful contribution to evaluating the Pandora ozone measurements, and is appropriate for AMT.

Minor comment: In line 40, Ozone Measuring Instrument should be Ozone Monitoring Instrument. Corrected – Thank you

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2) Aside from this, I believe this short paper is a useful contribution to evaluating the Pandora ozone measurements, and is appropriate for AMT.

Minor comment: In line 40, Ozone Measuring Instrument should be Ozone Monitoring Instrument. Corrected – Thank you

Reply to Reviewer 3

Referee#3 Quad O3 Paper

General Comments: This paper gives a brief synopsis of comparisons for 3 years of Total Column Ozone (TCO) measurements from two ground-based (Dobson and Pandora) and two satellite-based (OMI and OMPS) platforms over Boulder, Colorado. The main objective is to analyze TCO differences between the instruments and find any trends (or drifts) over the short period. Since the Dobson instrument is usually a standard for TCO measurements,

 it would be worthwhile for the authors to mention this study as a validation effort of the Pandora, OMI and OMPS instruments (particularly those considered newer such as Pandora or OMPS).

Response:

Since the manuscript was originally submitted, two significant changes have occurred. 1) NOAA updated the calibration of the Dobson#063 by applying the interim calibrations against the world standard Dobson#083. This changed all of the Dobson data slightly. 2) I investigated the influence of the endpoints on the percent difference time series and concluded that there was a significant effect on the slopes in some cases. Therefore, I de-seasonalized all of the percent difference time series as now described in the paper. All of the extensive changes in the paper are marked in green.

I have added to the introduction

The results demonstrate the accuracy and stability of both the Dobson and PSI for retrieval of total column ozone, and serves as a validation demonstration at one location for both the fairly new PSI and for satellite ozone data from OMI and OMPS.

2) The comparisons presented give valuable information, but further detail in the methodology of the statistics would provide more support for the interpretations the authors make. In addition, the discussion of the drifts found in the TCO measurements was missing any explanation for the results despite the highly correlated datasets. Drifts of 0.6%/year (or for the long term of 6%/decade) are not trivial, but appear to be minimized in the text.

Response: The revised paper now has improved results due to the application of Dobson calibration and by the use of de-seasonalized percent difference (PD) time series. The drift of the Dobson relative to OMPS is now less than 1% per decade. The change was mostly an "end-point" effect of the PD time series.

3) Specific Comments: (1) Why was a Lowess fit (with 0.1) used versus another fit? If this analysis is related to what was presented in the Herman et al (2015) paper, this should be explicitly stated and any differences should also be pointed out. Is the fit used in Figure 2B the same as in Figure 3? If so, this should be stated. If not, an explanation is also needed.

Response: I used a Lowess fit since it is the least squares equivalent of a running average that minimizes the effect of outliers. This is not to be confused with Loess(0.1) - I now give a reference for the Lowess algorithm.

The Lowess(0.1) is roughly a 90-day average, and as such acts as a "low-pass" filter on the data that can be used to derive a zero trend function needed to de-seasonalize the percent difference time series. Other functions could be used, but using the Lowess fit is one of the simplest starting points for deriving a zero-trend low-pass filter function.

The caption to Figure 3 now reads

Comparisons of Pandora(BDM) with Dobson(BP) retrieved ozone for Boulder, Colorado in percent differences of retrieved ozone and comparisons with OMI and OMPS. Slope = value of the linear least square fit, $\pm N$ is 1 STD, and p is the probability (0 to 1) that the slope is statistically different from 0 relative to p = 0.05. The solid lines are a Lowess(0.1) fit and a linear least squares fit.

4) (2) The meaning of "significance" is not clear as written. What is used to test this? I think there is a level of assumption on the authors' part that we should know this, but some additional information would resolve any confusion.

Response: I have added two criteria for significance 1) agreement to better than 2 standard deviations, and 2) the use of the p-value (probability of significance > 0.05).

5) (3) After 2014, there is a noticeable separation between the TCO measurements between the Pandora and Dobson in Figure 2B. Do the authors have any explanation for this drift?

No explanation. However, the net drift in the percent difference is now reasonably small (about 2% per decade)

The last statement of the summary including "long term stability of the four instruments" seems presumptive without any explanation for the observed trends. In my opinion, these results need to be characterized further to support that statement.

Response: The revised time series analysis suggests that there is some drift in the OMI data, but that the other 3 instruments are stable (see Figure 3). OMI vs Dobson is statistically significant (p=0.03) at about -2% per decade while the drift with respect to OMPS (<1% per decade) is not statistically significant (p = 0.3). OMI vs Pan is about 2% per decade (marginally significant p=0.06) and OMPS vs Pan is about -2% per decade (p=0.06). If one assumes that the recalibrated Dobson is stable, then Pandora drifted downwards relative to the Dobson by a small amount, 2% per decade. 6) Minor comments: Line 40 – OMI and OMPS acronyms need to be corrected to Ozone Monitoring Instrument and Ozone Mapping Profiler Suite respectively.

Response: Done

7) Line 88 – 'archived at WOUDC', missing "at". Line 102 – missing ";" to separate listed references.

Response: Fixed -

After addressing the above concerns and clearing up some confusion in the results, I believe this paper would be appropriate for publication with AMT and provides useful evaluation of TCO observations over an extended time period. 1. Does the paper address relevant scientific questions within the scope of AMT? Yes 2. Does the paper present novel concepts, ideas, tools, or data? Yes - data 3. Are substantial conclusions reached? For the most part with some additional support suggested in point 3 above. 4. Are the scientific methods and assumptions valid and clearly outlined? Yes except for the specific points 1 & 2 mentioned. 5. Are the results sufficient to support the interpretations and conclusions? Yes after point 3 is resolved. 6. Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)? After specific points 1 & 2 are addressed. 7. Do the authors give proper credit to related work and clearly indicate their own new/original contribution? Yes 8. Does the title clearly reflect the contents of the paper? Yes 9. Does the abstract provide a concise and complete summary? Yes 10. Is the overall presentation well-structured and clear? Yes 11. Is the language fluent and precise? Yes 12. Are mathematical formulae, symbols, abbreviations, and units correctly defined and used? Same as 4. 13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated? No 14. Are the number and quality of references appropriate? Yes Interactive comment on Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2017-157, 2017.

Marked Changes

- 1 Ozone Comparison between Pandora #34, Dobson #061, OMI, and OMPS at Boulder
- 2 Colorado for the period December 2013 December 2016.
- 3
- 4 Jay. Herman¹, Robert Evans⁴, Alexander Cede³, Nader Abuhassan¹, Irina.
- 5 Petropavlovskikh², Glenn McConville², Koji Miyagawa⁵, and Brandon Noirot²
- 6
- ¹ University of Maryland Baltimore County (JCET) at Goddard Space Flight Center, Greenbelt,
 MD
- 9 ² NOAA Earth System Research Laboratory, Boulder, CO. Cooperative Institute for Research in
- 10 Environmental Sciences (CIRES), University of Colorado, Boulder, CO
- ³ LuftBlick, Austria and Goddard Space Flight Center, Greenbelt, MD
- ⁴Former scientist at NOAA/ESRL/GMD, Boulder, CO: Retired
- ⁵Guest Scientist at NOAA/ESRL/GMD, Boulder, CO
- 14

15 Abstract

- 16 A one-time calibrated (in December 2013) Pandora Spectrometer Instrument (Pan #034) has
- been compared to a periodically calibrated Dobson spectroradiometer (Dobson #061) co-located
- in Boulder, Colorado, and compared with two satellite instruments over a 3-year period. The
- results show good agreement between Pan#034 and Dobson#061 within their statistical
- 20 uncertainties. Both records are corrected for ozone retrieval sensitivity to stratospheric
- 21 temperature variability obtained from the Global Modeling Initiative (GMI) and Modern-Era
- 22 Retrospective analysis for Research and Applications (MERRA-2) model calculations.
- Pandora#034 and Dobson#061 differ by an average of $2.1 \pm 3.2 \%$ when both instruments use
- their standard ozone absorption cross sections in the retrievals algorithms. The results show a
- relative drift ($0.2 \pm 0.08\%$ per year) between Pandora observations against NOAA Dobson in
- 26 Boulder, CO over a three-year period of continuous operation. Pandora drifts relative to the
- satellite Ozone Monitoring Instrument OMI and the Ozone Mapping Profiler OMPS are +0.18 \pm
- 28 0.2 % per year and -0.18 \pm 0.2 % per year, respectively, where the uncertainties are 2 standard
- 29 deviations. The drift between Dobson #061 and OMPS for a 5.5-year period (January 2012 –
- 30 June 2017) is -0.07 ± 0.06 % per year.
- 31
- 32 Author(s): Jay Herman et al.
- 33 MS No.: amt-2017-157
- 34 MS Type: Research article
- 35 Iteration: Revised
- 36 Special Issue: Quadrennial Ozone Symposium 2016 Status and trends of atmospheric ozone
- 37 (ACP/AMT inter-journal SI)
- 38

39 Introduction

A Pandora Spectrometer Instrument #034 (PSI) located on top of the NOAA building in 40 Boulder, Colorado has been operating since December 2013 with little maintenance and using 41 the original calibration. The purpose of this paper is to present a comparison between two co-42 43 located ozone measuring instruments, Pandora #034 and Dobson #061 for the period December 2013 to December 2016. Additional comparisons are made with satellite overpass data from 44 OMI (Ozone Monitoring Instrument on board the AURA spacecraft) and OMPS (Ozone 45 Mapping Profiler Suite on board the Suomi NPOESS satellite). This paper is an extension of a 46 previously published paper (Herman et al., 2015) that presented just 1 year of data. The results 47 demonstrate the accuracy and stability of both the Dobson and PSI for retrieval of total column 48 ozone, and serves as a validation demonstration at one location for both the fairly new PSI and 49 for satellite ozone data from OMI and OMPS. Part of the experiment comparing Pandora #034 to 50 51 Dobson #061 was to see if Pandora #034 would perform well over a long period without 52 additional calibration or adjustments. The only change made during the period 2014 to the present (August 2017) was to replace a broken motor on the suntracker that caused a data gap in 53 early 2016. 54

55

56 The characteristics of both the PSI and the Dobson Spectroradiometer are described in Herman et al. (2015). Briefly, the PSI consists of a small Avantes low stray light spectrometer 57 (280 - 525 nm with 0.6 nm spectral resolution with 5 times oversampling) connected to an 58 optical head by a 400 micron core diameter single strand fiber optic cable. The spectrometer is 59 temperature stabilized at 20^oC inside of a weather resistant container. The optical head consists 60 of a collimator and lens giving rise to a 2.5^o FOV (field of view) FWHM (Full Width Half 61 Maximum) with light passing through two filter wheels containing diffusers, open hole, a UV340 62 filter (blocks visible light), neutral density filters, and an opaque position (dark current 63 measurement). The optical head is connected to a small suntracker capable of accurately 64 65 following the sun's center using a small computer-data logger contained in a weatherproof box along with the spectrometer. Pandora#034 is capable of obtaining NO₂ and Total Column Ozone 66 TCO amounts sequentially over a period of 80 seconds. The integration time in bright sun is 67 about 4 milli-seconds that is repeated and averaged for 30 seconds to obtain very high signal to 68 noise and an ozone precision of less than 1 DU or 0.2% (1 DU = 2.69×10^{16} molecules/cm²). 69

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The Dobson record in Boulder started in **1966** based on an improved design from the instrument first deployed in the 1920's (Dobson, 1931). Dobson instrument is using differential absorption method to derive total column ozone from direct–sun measurements using two UV wavelength pairs in the 300 – 340 nm range (see Herman et al., 2015). The extensive Dobson network uses the Bass-Paur (BP) ozone absorption cross sections (Bass and Paur, 1985) for operational data processing (Komhyr et al., 1993).

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- 78

All NOAA Dobson instruments are periodically calibrated against WMO world standard Dobson #083, which in turn uses Langley method calibrations at the Mauna Loa Observatory station (Komhyr et al., 1989). Standard lamps are used to check Dobson spectral registration stability. Recently, July 2017, intermediate calibrations were applied to the Dobson #061 ozone data record that improved its comparison with satellite data (the calibration updates were processed by one of the co-authors, Koji Miyagawa).

85

The main sources of noise in the PSI measurement comes from the presence of clouds or haze in the FOV, which increases the exposure time needed to fill the CCD wells to 80% and reduces the number of measurements in 20 seconds. For this comparison study, data were selected for scenes that are clear-sky conditions as determined from the Dobson A-D pair directsun data record.

91

92 Accuracy in the PSI spectral fitting retrieval is obtained using careful measurements of the spectrometer's slit function, wavelength calibration, and knowledge of the solar spectrum at the 93 top of the atmosphere. The current operational PSI ozone retrieval algorithm used in this study is 94 based on extraterrestrial solar flux from a combination of the Kurucz spectrum (wavelength 95 96 resolution $\lambda/1\lambda = 500\ 000$) radiometrically normalized to the lower-resolution shuttle Atlas-3 SUSIM spectrum (Van Hoosier, 1996; Bernhard et al., 2004, 2005), BDM ozone cross sections 97 (Brion et al. (1993, 1998) and Malicet et al. (1995)), corrections for stray light, and an effective 98 ozone weighted temperature. 99

100

101 The Dobson data used in this study contain the individual measurements (more than 1 per 102 day between 09:00 and 15:00 local time with almost all of the data between 10:00 and 14:00) for 103 clear-sky direct-sun observations using the quartz plate and A-D wavelength pairs for ozone 104 retrieval. These were made available by one of the co-authors (I. Petropavlovskikh, private 105 communication, Table 2). The NOAA Dobson total ozone data are typically archived at 106 WOUDC (World Ozone and Ultraviolet Radiation Data Centre) or NDACC (Network for the 107 Detection of Atmospheric Composition Change) with one representative ozone value per day. 108

- 109 **1. Temperature Sensitivity**
- 110

The PSI ozone retrieval algorithm is more sensitive to the effective ozone weighted
average temperature than is the 4 wavelength Dobson retrieval (Redondas et al., 2014).
Neglecting the temperature sensitivity creates a seasonal difference between the two instruments.
To correct for this, we use an effective ozone temperature T_E based on daily ozone weighted
altitude temperature averages (Redondas et al., 2014). The temperature and ozone profile data

116 were obtained from the GMI (Global Modeling Initiative) model calculation for 2012 to 2016.

117 (https://gmi.gsfc.nasa.gov/merra2hindcast/). The GMI model provides atmospheric composition

118 hindcasts using MERRA-2 (Modern-Era Retrospective analysis for Research and Applications,

- 119 Version 2, meteorology (Strahan et al., 2013; Wargan and Coy, 2012)
- 120 <u>https://gmao.gsfc.nasa.gov/reanalysis/MERRA-2/</u>). The simulation with 2 x 2.5 degree resolution
- uses the CCMI (Chemistry–Climate Modelling Initiative, Morgenstern et al., 2017) emissions
- and boundary conditions. MERRA-2 uses assimilation schemes based on hyperspectral radiation,
- 123 microwave observations and ozone satellite measurements. The resulting seasonal cycle for T_E
- shows variations over the four year period, while day-to-day variability is enhanced during
- winter and spring season (Fig. 1). An estimated 5th year (2017) has been added (Fig. 1) by
- 126 forming the average of the daily temperatures from the 2013 to 2016 period.
- 127

128 The T_E time series data are used for an ozone retrieval temperature correction TCO_{cor} 129 coefficient per ^OK given in the form $TCO_{corr} = TCO (1 + C(T))$ and $O_3(corr) = O_3 TCO_{corr}$ 130 (Herman et al., 2015), where $C(T_E)$ is given by eqns. 1 and 2.

$C_{Pandora-BDM}(T_E) = 0.00333(T_E - 225)$	(Herman et al., 2015)	(1)
$C_{\text{Dobson-BP}}(T_{\text{E}}) = -0.0013(T_{\text{E}} - 226.7)$	(Redondas et al., 2014)	(2)
$C_{\text{Dobson-BDM}}(T_{\text{E}}) = 0.00042(T_{\text{E}}-226.7)$	(Redondas et al., 2014)	(3)

132	As mentioned earlier, the Dobson TCO retrieval normally uses the Bass and Paur (BP)
133	ozone absorption coefficients, while Pandora uses the Brion-Daumont-Malicet (BDM)
134	coefficients. A change in T_E of $+1^{\circ}$ change leads to TCO changes for the Pandora(BDM),
135	Dobson(BP), and Dobson(BDM) instruments of +0.33%, -0.13%, and 0.042%, respectively.
136	For a nominal TCO value of 325 DU, the change would be +1.1 and -0.4 DU, a net relative
137	change of 1.5 DU for a 1 ⁰ K change between Pandora(BDM) and Dobson(BP).
138	
139	While BDM cross sections are not currently recommended for use in standard Dobson
140	processing, their use yields slightly different values of TCO and a smaller sensitivity to
141	temperature. The basic Dobson algorithm, based on pairs of wavelengths, is intrinsically less
142	sensitive to T_E than Pandora's spectral fitting retrieval.
143	
144	2. TCO Comparisons between Pandora, Dobson, OMI and OMPS
145	
146	Comparing retrieved TCO from the PSI, Dobson, OMI and OMPS instruments show that
147	there are small, but significant differences between the PSI and Dobson instruments and between
148	the ground-based instruments and satellite derived values of TCO. The difference is calculated
149	using three-year estimates of secular change based on a linear least squares fit to the percent
150	differences between the instruments. The cloud-free direct-sun A-D pair Dobson ozone data are
151	selected for comparison with time-matched Pandora#034 retrieved ozone data (Herman et al.,
152	2015). The Pandora#034 retrieved ozone (every 80 seconds) are matched to the less frequent
153	Dobson#061 retrieval times that are obtained for mid-day solar zenith angles (SZAs) and

154	averaged over ±8 minutes (l	Fig.	2A).
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156	Each clear-sky PSI data point is an average of 2000 (early morning to evening SZAs) to
157	4000 (mid-day SZAs) measurements obtained during 20 seconds. All data for this study were
158	clear-sky within the instrument's field of view based on the Dobson criteria for A-D-pair direct-
159	sun clear sky. In addition, the PSI data are averaged over a period of +/- 8 minutes surrounding
160	the Dobson time of measurement (2 to 3 times per day). Since PSI measurements are obtained
161	every 80 seconds, there were an additional 10 PSI data points averaged together to compare to
162	each Dobson, OMI, or OMPS measurement. The result is high signal to noise values for Pandora
163	and high precision (0.1%) . The same procedure using cloud-screened PSI data was used for
164	comparisons with OMI and OMPS, where they measure once or twice per day over Boulder,
165	Colorado. Some of the variations in the day to day ozone values are driven by changes in the
166	local weather over Boulder, Colorado (see Fig. 14 in Herman et al., 2015), with weekly averages
167	having much smaller variation.
168	
169	Figure 2B shows a Lowess(0.1) fits to the two time series in Fig. 2A that is approximately
170	equivalent to a 3-month running average. The Lowess(f) procedure is based on local least
171	squares fitting using low order polynomials applied to a specified fraction f of the data
172	(Cleveland, 1979) that reduces the effect of outlier points from the mean. The smooth curves
173	show a small variable difference between the Dobson and Pandora time series. Fig. 2C shows the
174	percent difference PD between the time series in Fig. 2A and the residual seasonal variation in
175	PD. Estimating the slope of the least squares fit to the percent difference is sensitive to the
176	selection of the end points of the time series. This effect can be minimized by removing the
177	seasonal time dependence (Fig. 2C) using a low-pass filter function with zero slope derived from
178	the Lowess(0.1) fit. The result is shown in Fig. 3A.
179	
180	Figure 3 shows the de-seasonalized percent differences PD(A,B) for six pairs between
181	Pandora #034, Dobson #061, OMI, and OMPS for the 3-year period 2014 – 2016 (summarized in
182	Table 1). The slightly curvy Lowess (0.1) lines about each linear fit show the residual seasonal
183	cycles, which are too small to have an effect on slope determination. Error estimates (Fig. 3 and
184	Table 1) for the linear least squares slopes and averages are one standard deviation (1-STD).
185	Some of the error estimates are large enough to make the statistical significance of the slopes
186	marginal (see Panel E OMPS vs Pandora; 0.18 ± 0.098 , p = 0.06), while others are significant
187	(see Panel D OMI vs Dobson: -0.18 ± 0.08 , p = 0.03) at the 2-STD level. The significance
188	probability parameter p is given, where p is the probability (0 to 1) that the slope is statistically
189	different from 0 relative to $p = 0.05$. Also shown are the numbers of data points in each time
190	series.
191	
192	After removal of the residual seasonal variation in the calculated percent differences,
193	there still is a statistically significant drift of 0.2% per year ($p < 0.001$) between the Pandora#034

194	and Dobson#061 (Panels A and B in Fig. 3) using either BP or BDM ozone cross sections for the
195	Dobson. The differences in the mean values (-2.1 and -2.8%) are not significant at the 2-STD
196	level.
197	
198	The linear trend (Panel C, -0.09 ± 0.08 % per year, p = 0.3) between the Dobson and
199	OMPS is not significantly different from zero, while the drift with OMI (Panel D,-0.18 \pm 0.08 %
200	per year, $p = 0.03$) is significant. This suggests that OMI ozone retrievals are drifting with
201	respect to OMPS and the Dobson. Extending the period from 2012 to June 2017 gives a very
202	small, but significant trend, -0.07 ± 0.03 % per year, p = 0.047 for PD(OMPS,Dobson).
203	
204	Calculations for Pandora#034 (Panels E and F in Fig. 3) show marginally significant (p =
205	0.06) trends for Pandora#034 compared to OMPS (Panel E, -0.18 \pm 0.098 % per year) and OMI
206	(Panel F, $+0.18 \pm 0.096$ % per year). If the Pandora#034 time series is extended into 2017 to
207	minimize the effect of missing Pandora data in 2016, then the trends for Pandora compared to
208	OMPS (-0.2 \pm 0.08 % / Year p = 0.013) and OMI (0.15 \pm 0.076 p=0.05) are significant, but not
209	different from the shorter 2014 – 2016 period. The secular trends for the difference between
210	Pandora#034 and Dobson#061 (-0.2% per year) are almost the same for both Dobson BP and
211	BDM ozone absorption coefficients even though the temperature sensitivity using the Dobson
212	BDM ozone absorption coefficients is small (0.042% per 0 C). This suggests that the
213	stratospheric effective ozone temperature change is not a source for the small difference between
214	Pandora#034 and Dobson#061.
215	
216	Figure 4 shows that the TCO between Pandora#034 and Dobson#061 are highly
217	correlated with 1:1 slope and the correlation coefficient $r^2 = 0.97$ for the 3-year period 2014 to
218	2016. Similar correlation plots (Fig. 5) for Pandora#034 and Dobson#061 with OMI and OMPS
219	also show very high correlations. The correlations in TCO are obtained after only temperature
220	corrections to Pandora#034 and Dobson#061 using T_E (TCO pairs similar to Fig. 2, panel A).
221	
222	The Pandora, OMI, and OMPS data used in this study are from the overpass files located
223	on the public websites (Table 2).
224	
225	Summary
226	Temperature corrected Pandora#034 and Dobson#061 differ by an average of 2.1% with
227	Pandora using its standard retrieval BDM ozone absorption cross sections and Dobson using the
228	recommended BP ozone absorption cross sections. Pandora compared to Dobson shows a small,
229	but significant drift (-0.2 \pm 0.04 % per year, p < 0.001) for the 2014 – 2016 period. Comparisons
230	of Pandora with OMI and OMPS are marginally significant drifts of 0.18±0.1 and -0.18±0.1
231	p=0.06 for 2014-2016, but are significant (0.15 \pm 0.076 % per year, p=0.05 and -0.2 \pm 0.08 % per
232	year, $p = 0.013$, respectively) if the period is extended to mid-2017 to minimize the effect of
233	missing Pandora data during 2016. The small Pandora and Dobson trends compared to OMPS
234	suggests that both instruments are stable. The conclusion is that the periodically calibrated

235	Dobson#061 is able to detect smaller ozone trends than a Pandora instrument with no
236	intermediate calibration during a 3-year period. The longer term trend for Dobson compared to
237	OMPS for a 5.5-year period (2012 – June 2017) is -0.07 ± 0.03 % per year, p = 0.047.
238	
239	Acknowledgement: The authors would like to thank Dr. Susan Strahan and the MERRA-2 team
240	for supplying the atmospheric temperature data for Boulder, Colorado.
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314 Tables

315

Percent Diff(A,B)	Slope (% per Year)	Probability	Mean (%)	<mark>Points</mark>	Pane
Pan, Dob(BP)	-0.2 ± 0.04	P < 0.001	<mark>-2.1 ± 1.6</mark>	<mark>2020</mark>	A
Pan, Dob(BDM)	-0.2 ± 0.04	P < 0.001	<mark>-2.8 ± 1.6</mark>	<mark>2020</mark>	B
OMPS, Dob(BP)	-0.09 ± 0.08	P = 0.3	<mark>-1.4 ± 2.1</mark>	<mark>854</mark>	C
DMI, Dob(BP)	-0.18 ± 0.08	P = 0.03	<mark>-1.4 ± 1.9</mark>	<mark>654</mark>	D
OMPS, Pan	-0.18 ± 0.098	<mark>P = 0.06</mark>	0.96 ± 2.7	<mark>952</mark>	E
OMI, Pan	+0.18 ± 0.096	<mark>P = 0.06</mark>	1.1 ± 2.1	<mark>624</mark>	F

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Table 2 Data Availability

<u>OMI</u>:

https://avdc.gsfc.nasa.gov/index.php?site=1593048672&id=28/aura omi l2ovp omto3 v8.5 boulder.co 067.txt

<u>OMPS</u>:

<u>ftp://toms.gsfc.nasa.gov/pub/omps_tc/overpass/suomi_npp_omps_l2ovp_nmto3_v02_boulder.co_067.txt</u> Pandora34:

https://avdc.gsfc.nasa.gov/pub/DSCOVR/Pandora/DATA/Boulder/Pandora34/L3c/

Dobson061:

<u>ftp://aftp.cmdl.noaa.gov/data/ozwv/Dobson/WinDobson/Pandora%20comparisons/Dobson61%20Bould</u> <u>er%20Ad-dsgqp%20120213-032717_w_Header.txt</u>

Figure Captions

321	Fig. 1 Calculated T _E using model estimates of O ₃ and temperature profiles. The Trend is
322	calculated from the difference of T_E from its 4-year daily mean that is also used for year 2017
323	labelled Avg.
324	
325	Fig. 2 Panel A shows the retrieved ozone time series (December 2013 – June 2017) for Pandora
326	(red) and Dobson (Black). Panel B shows Lowess(0.1) fit to the each time series. Panel C shows
327	the percent difference, a linear least squares fit, and a Lowess(0.1) fit showing seasonal residuals.
328	
329	Fig. 3 Comparisons of Pandora(BDM) with Dobson(BP) retrieved ozone for Boulder, Colorado
330	in percent differences of retrieved ozone and comparisons with OMI and OMPS. Slope = value
331	of the linear least square fit, ±N is 1 STD, and p is the probability (0 to 1) that the slope is
332	statistically different from 0 relative to $p = 0.05$. The solid lines are a Lowess(0.1) fit and a linear
333	least squares fit.
334	
335	Fig. 4 Correlation between Pandora #034 and Dobson #061: 2014 – 2016
336	
337	Fig. 5 Correlation of Pandora#034 and Dobson#061 with OMI and OMPS: 2014 - 2016

338 Figures339







342 F2



346 F3











355 F5