



LuftBlick Report 2018003

ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study

Recommendations on operational AOD measurements for Pandonia

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Document Change Record

Issue	Date	Section	Observations
1.0	2 Feb 2018	All	First draft version

Acronyms and Abbreviations

AERONET	Aerosol Robotic Network
AOD	aerosol optical depth
CCN	Contract Change Notice
CINDI2	Cabauw Intercomparison Campaign of Nitrogen Dioxide measuring Instruments
FOV	field of view
GAW	Global Atmospheric Watch
mFCT	mobile field calibration tool
Pandonia	ESA Ground-Based Air-Quality Spectrometer Validation Network
PFR	Precision Filter Radiometer
PMOD/WRC	Physikalisch-Meteorologisches Observatorium Davos, World Radiation Center
rms	root mean square
s1	Pandora spectrometer 1, wavelength range 270 nm - 537 nm

1 Introduction

This report is deliverable D6 of CCN#1 [4, 3] to ESA's Pandonia project [2, 1]. The objective of this third and final part of WP3 of this CCN is to formulate recommendations for operational aerosol optical depth (AOD) measurements from Pandora instruments.

The basis for the recommendations are the preceding technical reports D4 [6] and D5 [7], where we introduced calibration methodologies (absolute radiometric calibration from the laboratory as well as multiple Langley type calibrations) to determine the AOD at three selected wavelengths of Pandora 128 and 129 during the CINDI2 campaign in September 2016 in Cabauw. The AOD was validated by independent AOD data from the Cimel sun photometer operated within the Aerosol Robotic Network (AERONET). The essential findings of these investigations on the CINDI2 dataset were:

- The AOD Langley calibration method [5] achieved the best results with a systematic error of the AOD at 440 nm, 675 nm and 870 nm between 0.02 and 0.06.
- The radiometric stability of the Pandora instruments during one month was 2-3%.

While these first results allowed reasonable optimism towards AOD retrieval they were not fully conclusive because, first, the atmospheric conditions were not ideal for Langley calibrations and second, the measurement period was rather short. So we looked at another dataset from Pandora 120s1, located in Davos, Switzerland.

1.1 Applicable Documents

- [1] Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study [Proposal], LuftBlick Proposal 201309A, Issue 2, 2013.
- [2] ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study [Statement of Work], ENVI-SPPA-EOPG-SW-13-0003, Issue 1, Revision 3, 2013.
- [3] CCN1 to ESA Ground-based Air-Quality Spectrometer Validation Network Uncertainties Study [Proposal, Proposal 201705A, Issue 2, 2017.
- [4] CCN1 to ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study [Statement of Work], ESA-EOPG- MOM-SOW-1, Issue 1, Revision 1, 2017.

1.2 Reference Documents

- [5] V. E. Cachorro, C. Toledano, A. Berjón, A. M. de Frutos, B. Torres, M. Sorribas, and N. S. Laulainen. An "in situ" calibration correction procedure (KCICLO) based on AOD diurnal cycle: Application to AERONET–El Arenosillo (Spain) AOD data series. *Journal of Geophysical Research: Atmospheres*, 113 (D12), 2008. ISSN 2156-2202. doi: 10.1029/2007JD009673. D12205.
- [6] A. Kreuter. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2017004: Methodologies for absolute calibration, 2017.
- [7] A. Kreuter. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2017006: AOD from Pandoras at selected wavelengths, 2017.
- [8] M. Müller and M. Tiefengraber. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2017005: Tracker prototype performance evaluation report, 2017.

- [9] D. Santana and M. Müller. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2017006: Report on mFCT design and performance, 2018.
- [10] M. Tiefengraber and A. Cede. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2017002: Network intercomparison campaign report, 2017.

2 Further Analysis: Pan120s1 in Davos

Pandora 120 is operated by the staff of the World Radiation Center PMOD/WRC in Davos since April 2016. This instrument is particularly suited for the extended analysis because

- it has a complete laboratory characterization including absolute calibration, has a fibre guide installed and runs on the newest version of the Blick operation and processing software
- is well maintained by experienced operators and runs continuously without mechanical problems at one location for more than 8 months
- Davos at an elevation of 1600 m typically has a low aerosol background and offers good Langley calibrations conditions especially in autumn
- Davos is a reference center for AOD measurements and operates several well calibrated sun photometers, including AERONET's Cimel (at 380 nm, 440 nm and 500 nm) and a Precision Filter Radiometer (PFR) at 368 nm, 412 nm and 500 nm operated within the GAW network.

In the following, we will analyse the dataset for Pandora 120s1 for an eight months period in 2017. The wavelength range of Pandora 120 spectrometer 1 (s1) coincides with all channels of the Cimel sun photometer and the AOD will be evaluated at 380 nm, 440 nm and 500 nm. The PFR will be used for additional quality control.

2.1 Langley Calibration

Screening the dataset, we found eight days in the period from end of September to end of October 2017 with low and constant AOD, particularly well suited for Langley calibrations. Fig. 1 shows the fit results for the AOD Langley routine for 500 nm. The 1σ standard deviation of fitted slopes, corresponding to the precision of the resulting V_0 is below 1% for all considered wavelengths, 380 nm, 440 nm and 500 nm.

The resulting AOD at 500 nm using the fitted V_0 calibration constants for the selected days are shown in Fig. 2. Note the extremely low AOD of 0.02-0.04. The agreement to the Cimel AOD is mostly within 0.01 which is close to the cited uncertainty of the Cimel. The AOD variation during the selected days have a 1σ standard deviation ranging from 0.002 for October 15 to 0.008 for September 21. These numbers should be considered as guidelines for the selection of Langley days. Higher AOD variations could be tolerable if the variations do not feature a diurnal trend from morning to afternoon. In general, higher variations require a larger selection of days for improved statistics in the Langley calibration.

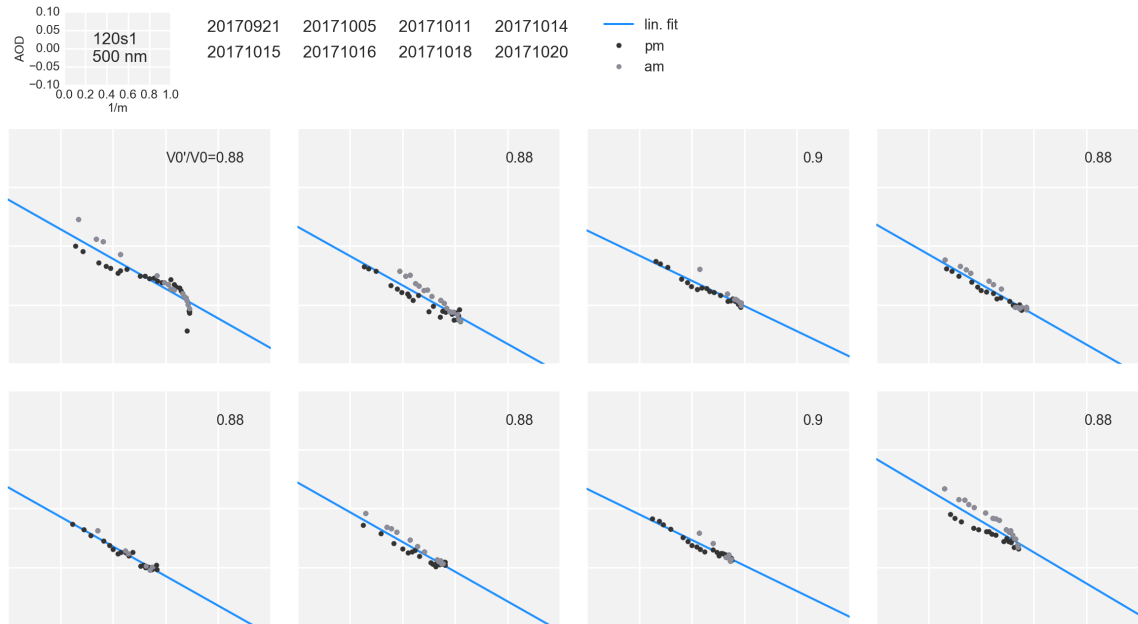


Figure 1: AOD Langley calibration at 500 nm for eight selected days in September / October 2017. The variation of the fitted V_0 between the days is 1%.

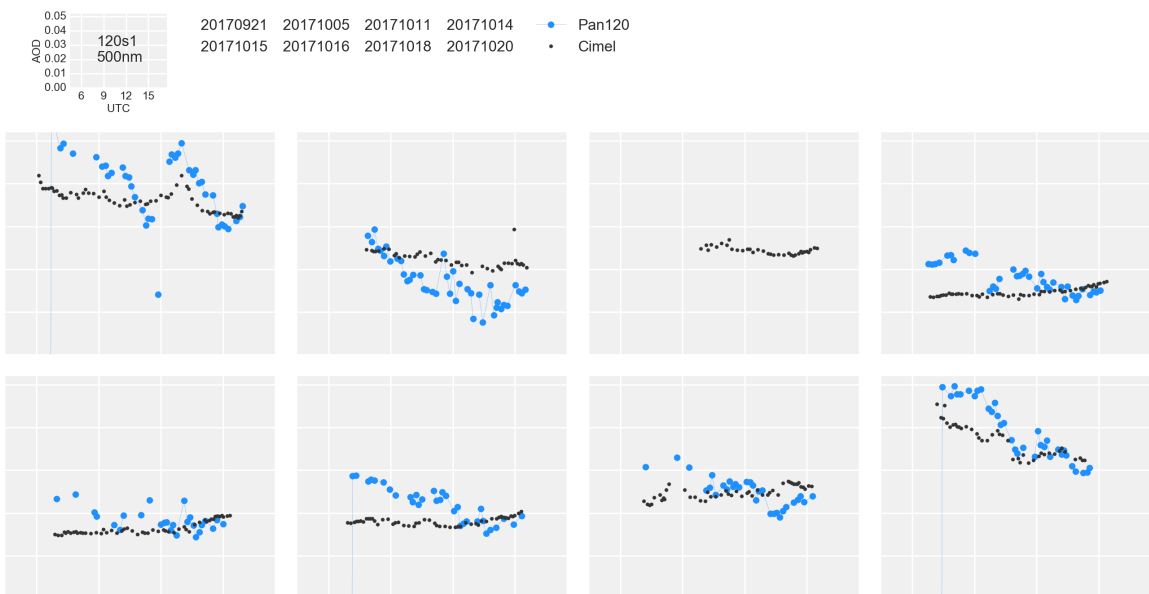


Figure 2: AOD at 500 nm for the V_0 from the Langley calibration compared to the AOD of the Cimel sun photometer. Note that one division of the y-scale is 0.01.

2.2 AOD comparison to the sun photometer

The AOD has been determined for 24 days from April to November 2017 using the Langley calibration from above. The days have been selected on the criteria that both the Pandora and the Cimel have more than 35 data points in the raw data files. The comparison of the AOD from Pandora and the Cimel at 500 nm is shown in Fig. 3, the AOD differences are visualized in Fig. 4. The differences were computed with a time tolerance of 5 minutes between Pandora and Cimel measurements.

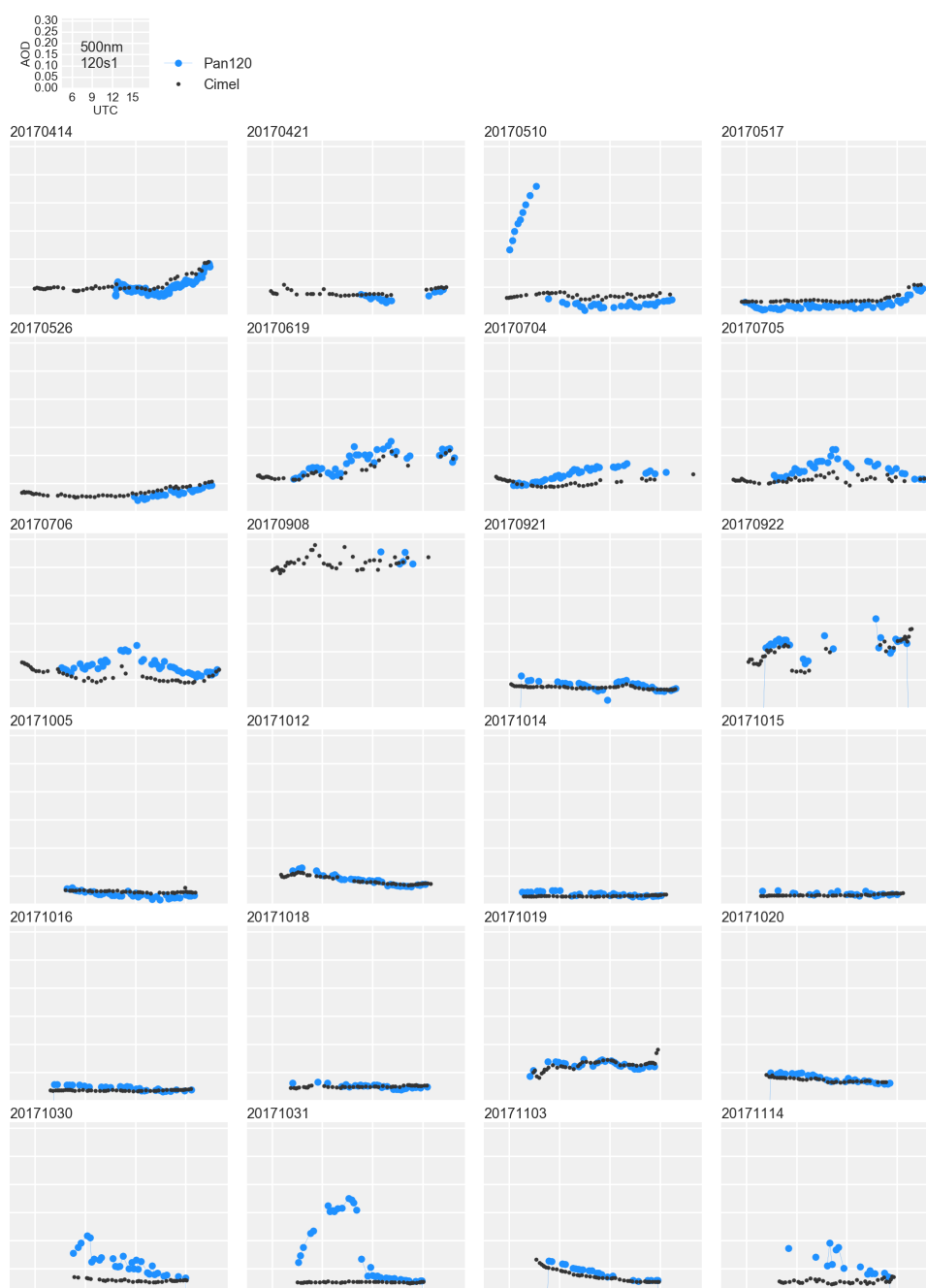


Figure 3: AOD at 500 nm for Pandora 120s1 and Cimel. The result from one Langley calibration is applied to the whole period.

The median difference of the AOD at 500 nm between the Pandora and Cimel is below 0.001 and the full width at half maximum of the histogram is about 0.03. For 67% of the 832 data points, the difference to the Cimel is below 0.02 and 46% of the differences are below 0.01. The AOD differences during the calibration days are of the same order as the differences between the PFR and the Cimel, shown in the inset of Fig. 4.

While these observations are satisfactory and a promising step towards operationally measuring AOD at these wavelengths, we also note a number of brief periods with significant deviations compared to the Cimel, e.g. in the mornings of May 10 and October 31. Also, some AOD values are negative and are not shown within the scales of figures 3 and 4.

Possible reasons for these outliers include pointing inaccuracies of the tracker and spectrometer temperature effects. These issues will be investigated separately in the appendix.

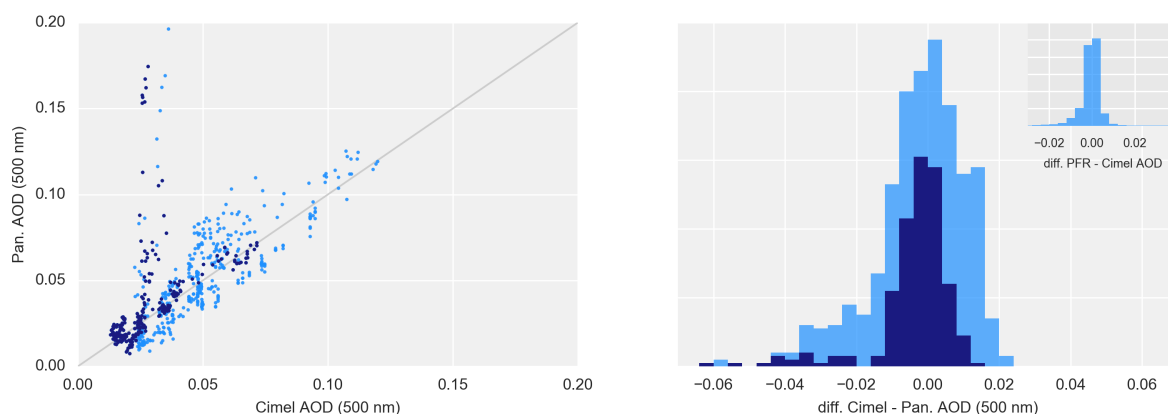


Figure 4: Correlation plot of the AOD at 500 nm for Pandora 120s1 and Cimel and a histogram of the AOD differences. Dark blue denotes the calibration period. The inset shows the difference between the Cimel and the PFR sun photometers.

2.3 Radiometric stability

Next, we compare the radiometric stability of Pandora 120s1 in terms of the measured irradiance, rather than the resulting AOD, which allows a more sensitive analysis. As done in report D5 [7], we multiply the AOD differences $\Delta\tau_{\text{aero}}$ with the air mass m , to determine the ratio of the measurement or calibration error, $R(V/V_0)$, of the Pandoras with respect to the Cimel:

$$R(V/V_0) = \exp(\Delta\tau_{\text{aero}} \times m) \quad (1)$$

These ratios of $R(V/V_0)$ of Pandora 120 to the Cimel are shown in Fig. 5 for all three compared wavelengths 380 nm, 440 nm and 500 nm for the 24 selected days. The overall radiometric stability of the median ratios is better than 3% for all three wavelengths over the period of seven months. However, the intra day variation often reaches 5% and even exceeds 10% on rare occasions. This variation looks systematic with different patterns. From end of May until July, the ratios show a minimum around local noon. In October, the ratios for 440 nm and 500 nm show a monotonous increase over the day. Probable causes such as pointing errors and spectrometer temperature effects are investigated in the appendix, however, without conclusive answers.

Longer time series also from a growing number of instruments will allow an increasing level of understanding and control of the multiple, often subtle, factors affecting the determination of the AOD.

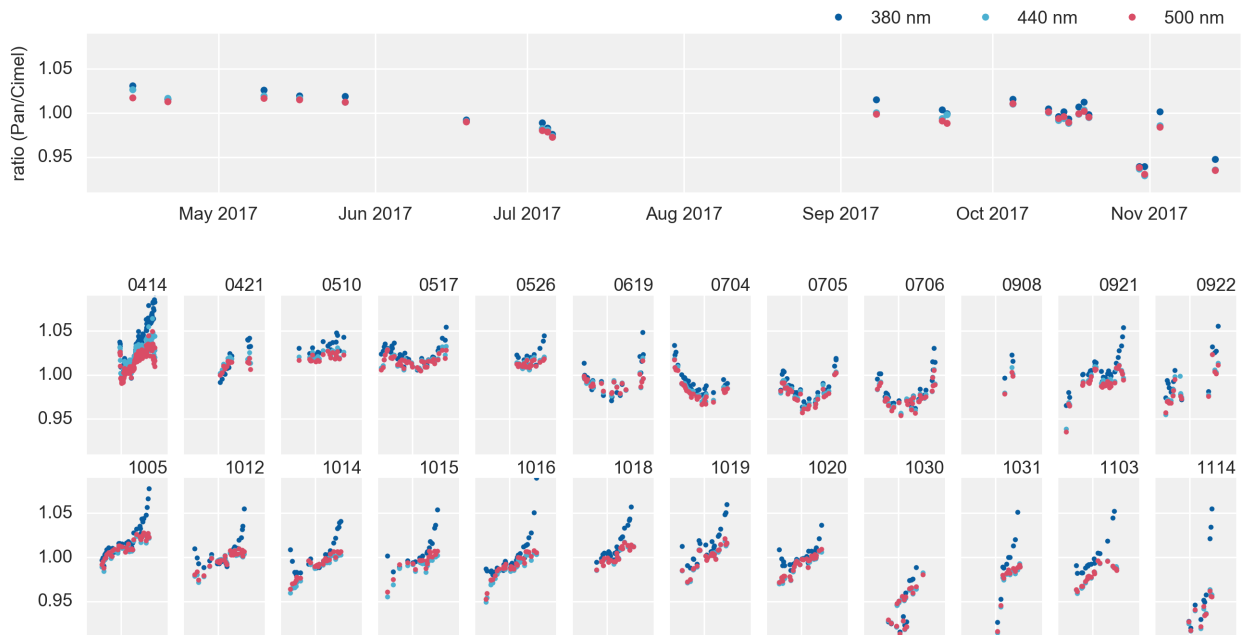


Figure 5: Ratios of V/V_0 Pandora 120 to Cimel. The upper panel shown the daily medians for all three compared wavelengths 380 nm, 440 nm and 500 nm for the 24 selected days. The lower panels show each day in detail. The time scale of the x-axis is identical to Fig. 3 and 4.

3 Recommendations

We summarize our findings from this and the previous investigations on AOD measurements from Pandora instruments in the following recommendations on operational practices. First, for the calibration procedures, we recommend:

- a **Langley calibration** should be performed at least once a year. The ideal selection features a few cloud free days with a diurnal AOD variability of less than 0.01
- in addition, a calibration period with a co-located **mobile sun photometer** is recommended. Using a well calibrated reference instrument is the basis for the calibration of the sun photometers within networks such as AERONET and GAW. It should be kept in mind that for many locations, Langley conditions similar to Davos are rare, in which case, a reference sun photometer may be the only way to ensure the accuracy of an operationally measured AOD
- a field calibration with the **mobile field calibration tool** (mFCT) should be performed every 3 months. The mFCT calibration should always be performed before and after relocation or any modification on the instrument, e.g. disconnecting a fibre connector. Details about the mFCT can be found in report D3 [9]

Second, for the routine operational procedures the following recommendations are given:

- the instrument should have a **fibre guide** installed. The fibre guide is designed to minimize radiometric variability due to movement of the fibre. The fibre guide may be one reason for the improved radiometric stability of the instrument in Davos compared to e.g. the instruments during the CINDI campaign
- the **sun tracking accuracy** is of critical importance for AOD measurements. The new sun tracker with increased mechanical robustness which has been developed for the future instrument set ups is a valuable contribution towards this issue [8]. Furthermore, an adequate sun tracking accuracy should be ensured by, either more frequent sun search routines (quick sun searches before each AOD measurement) or by an independent sun tracking monitoring device (a CCD camera or 4-quadrant detector as typically used for sun photometers). This would allow the definition of an additional pointing quality flag.
- **daily maintenance and checks** of the instrument is an important aspect of AOD quality control. This includes regular checks of instrument parameters such as spectrometer temperature and cleaning of the entrance window. Especially in the initial phase of operational AOD measurements, the retrieved AOD values should be regularly assessed to detect unreasonable high AOD or variations correlating with air mass, in which case a radiometric check with the mFCT should be performed

A Appendix

In the retrieved AOD time series from Davos there are two remaining issues which are highlighted in Fig. 6, which is an expanded scale version of Fig. 3 ranging from -0.3 to 0.3.

First, the occasional negative AODs (dark yellow dots) correspond to measurements where filterwheel 1 is in position 2 (open) as opposed to position 5 (ND1 filter). Filter wheel 2 is always in position 2 (diffusor). This points to a problem in the absolute calibration, which has to be checked in the laboratory. The absolute calibration of the Pandora instruments is one of the challenges on the roadmap to AOD measurements, especially

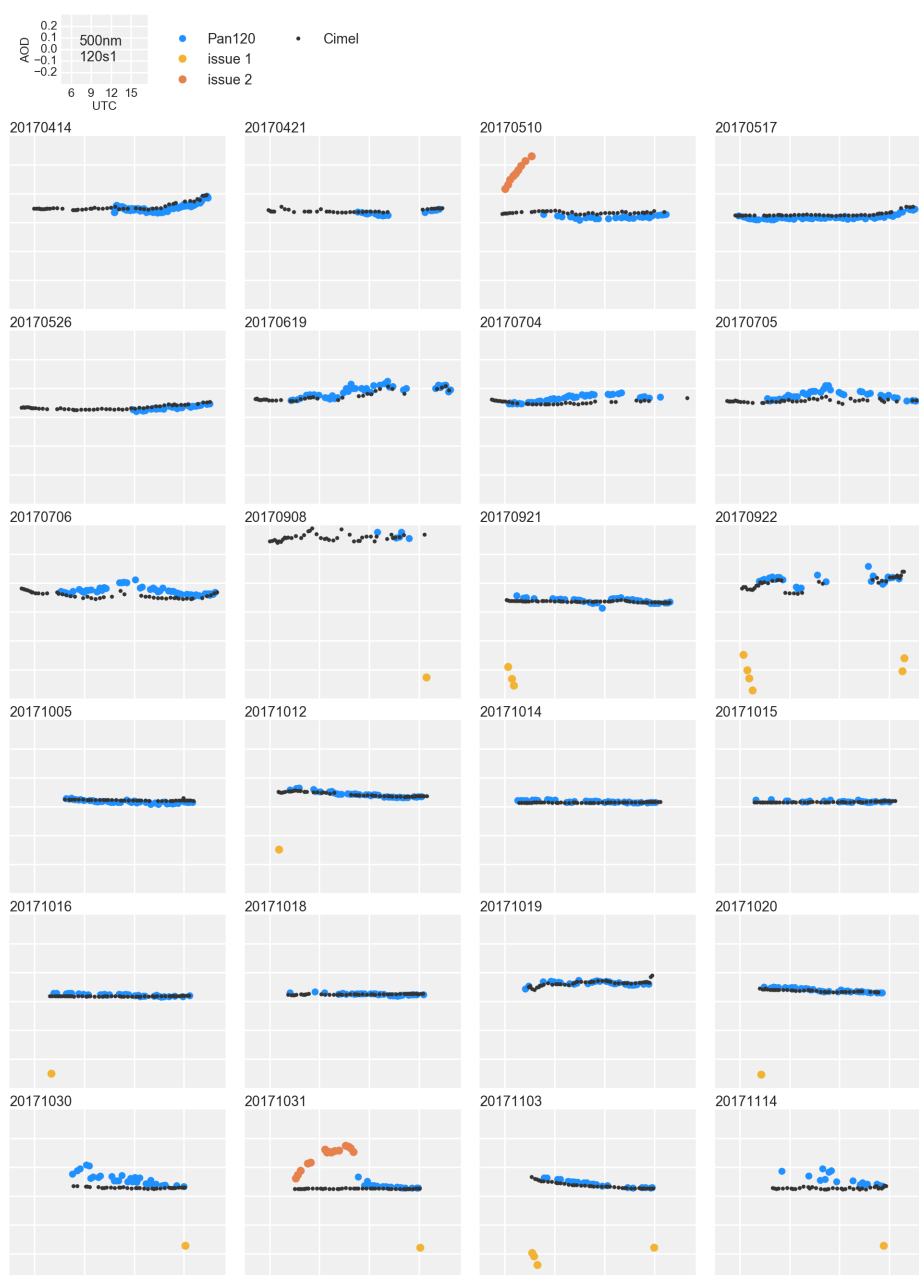


Figure 6: Expanded scale of Fig. 3. Two classes of outliers are highlighted.

because there are a possible 81 combinations of filter wheel positions that have to be characterized.

Second, we have to investigate the origin of the distinctly high AOD retrievals on May 10 and October 31 in Fig. 6 (orange dots). Possible causes of this issue include sun tracking inaccuracies and temperature dependence of the spectrometer which will be discussed in the following.

A.1 Sun tracking accuracy

Imperfections in the optical field of view (FOV) of the input optics in combination with inaccurate sun pointing may lead to a lower measurement signal and a higher retrieved AOD. Ideally, the transmission function of the input optics should be constant when the sun is fully within the FOV. The shape of the FOV of the Pandoras is measured intensively during the initial alignment phase for the first days after instrument set up. The data is saved in the L0 data files (FS, FD, FN or FA) and an example of the FOV shape from such a sun search routine (FD), measured on April 14, is shown in Fig. 7.

These measurements show that for sun tracking inaccuracies of $\pm 0.2^\circ$, the signal varies by 1%. During the CINDI2 campaign, the pointing accuracy was determined to be better than 0.1° [10]. In routine operation, sun searches are performed once per hour and the solar position is determined, so the error in the measured irradiance is not expected to exceed 1%.

The quality of the sun search results is quantified by fitting a trapezoid to the FOV shape and a threshold criterion is used to discard data with e.g. cloud covered sun. The root mean square (rms) errors of the fitted sun search routines are shown in Fig. 8. Note that no data are shown before beginning of September because the controlling computer was replaced and a new datafile for the sun searches was created. So while the origin of issue 2 on May 10 remains unclear, sun tracking inaccuracies on October 31 can be excluded.

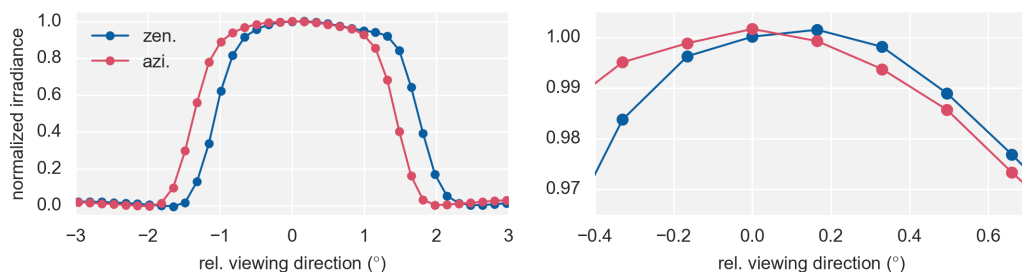


Figure 7: Sun search routine on April 14, 2017. The measured irradiance when scanning the tracker over the solar position reveals the shape of the FOV. The irradiance has been averaged over the whole wavelength range.

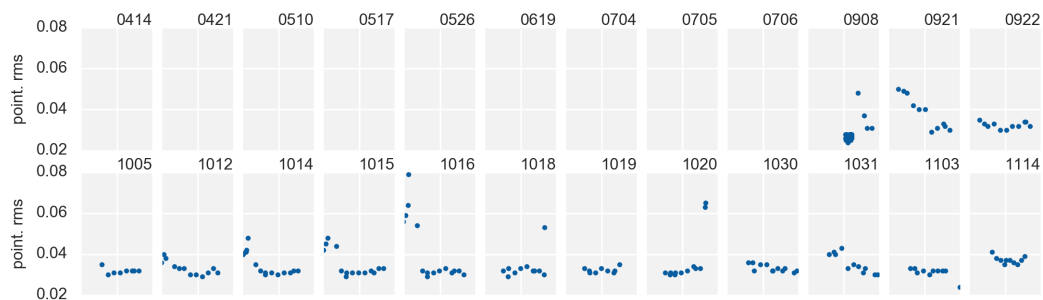


Figure 8: Quality of the sun search routines: RMS error of fitting a trapezoid to the FOV shape.

A.2 Spectrometer temperature

Next, we investigate the temperature log of the Pandora during the seven months period. The instrument logs four temperatures and the two important ones, the spectrometer control temperature and the temperature of the electronics board are shown in Fig. 9. AOD correlation plots for temperature and air mass are shown in Fig. 10. The significant deviations corresponding to May 10 and October 31 correlate with low temperature and high air mass, which could be misleading because they occurred in the morning. It is shown that low temperature and high air mass does not systematically cause a higher AOD retrieval.

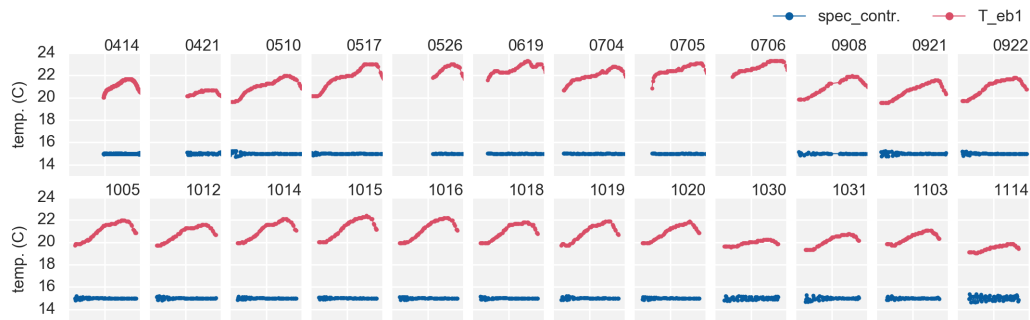


Figure 9: Pandora temperature log: Spectrometer control temperature and temperature of the electronics board.

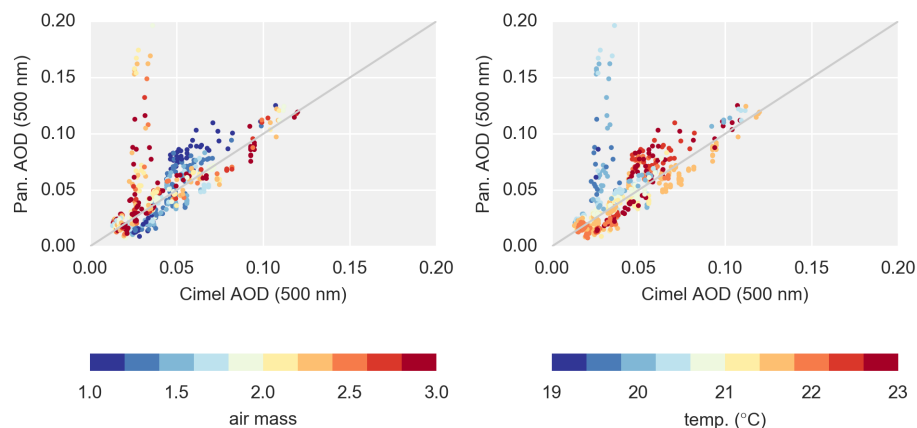


Figure 10: AOD correlation plots, air mass and temperature of the electronics board.

A.3 Further discussion

Another possible cause of uncertainty includes stray light. Both spectral and spatial stray light causes the measured irradiance to increase and the effect is more pronounced for short wavelengths, low solar elevations and is symmetric around noon. Note how in Fig. 5 on some days the ratios are roughly symmetric around noon (e.g. May 5) while the symmetry is absent on others days (e.g. October 16). Furthermore, the ratios do not show a significant wavelength dependence which would be expected for stray light contributions. So for the wavelengths considered here, stray light is a negligible factor in the AOD retrieval.

Finally, we consider the spectral accuracy of the absolute calibration which is important for the concept of transferring the Langley calibration at one wavelength to an arbitrary wavelength and eventually retrieving the AOD over the continuous spectral range of the spectrometer. Fig. 11 shows the ratio of the theoretical

extraterrestrial irradiance to the V0 of the Langley calibration for all Cimel and PFR wavelength channels. The spectral dependence of the ratio is about 20% between 368 nm and 500 nm. This spectral feature is much higher than the requirement for a spectral calibration transfer and should be investigated. It is also surprising and not necessarily a universal problem, because the analysis of the CINDI2 data revealed a spectral dependence of less than 4% and for Pandora 128s2 [7]. In the laboratory, a spectral dependence of the reference lamp measurements has been documented. The measured irradiance has a spectral variability of up to 2% resulting from varying the relative pointing angle to the lamp by 0.2° .

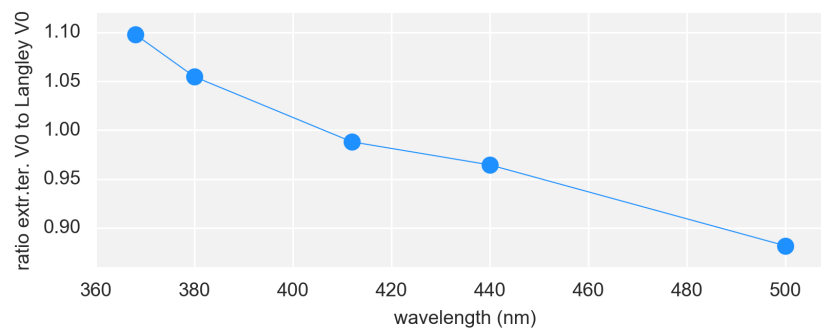


Figure 11: Ratio of the expected extraterrestrial V0 to the V0 from the Langley calibration.