



LuftBlick Report 2017004

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

Methodologies for absolute calibration

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Document Change Record

Issue	Date	Section	Observations
1.0	31 Jul 2017	All	First draft version

Acronyms and Abbreviations

AERONET	Aerosol Robotic Network
AMF	air mass factor
AOD	aerosol optical depth
CCN	Contract Change Notice
CINDI2	Cabauw Intercomparison Campaign of Nitrogen Dioxide measuring Instruments
FCT	Field calibration tool
FOV	field of view
ND	neutral density filter
Pandonia	ESA Ground-Based Air-Quality Spectrometer Validation Network
SZA	solar zenith angle

1 Introduction

This report is deliverable D4 of CCN#1 [4, 3] to ESA's Pandonia project [2, 1]. This deliverable is the first part of WP3 of this CCN which concerns the determination of the aerosol optical depth (AOD) from Pandora instruments. The objective of this technical report is to describe the calibration methods suitable for the retrieval of the AOD and thus lay out a general strategy to achieve the goal of WP3. In deliverable D5, the resulting calibration of this report will be applied to measurements at selected wavelengths of two instruments during the CINDI2 campaign 2016 in Cabauw and compared to independent AOD data from the Aerosol Robotic Network (AERONET). The final assessment will allow a recommendation on operational AOD measurements within the Pandonia network (D6).

Traditionally, the AOD (referred to as τ_{aero} in the equations) is determined by filter radiometers, so called sun photometers, with a small FOV, pointing at the sun. While the detectors of sun photometers are photo diodes behind a narrow band filter as opposed to the grating and diode array sensor of the Pandora spectroradiometers, the measurement principle for the AOD of both instruments are identical. Here, we will transfer the methodology developed for filter radiometers to Pandora instruments and identify possible challenges.

The principle for determining the AOD is the Beer-Lambert-Bouguer law which describes the attenuation of the solar radiation on its path through the atmosphere:

$$V = V_0/r^2 \times \exp(-\tau_{\text{total}} \times m) \quad (1)$$

which, in more explicit terms, is written as

$$V = V_0/r^2 \times \exp(-\tau_{\text{aero}} \times m_{\text{aero}} - \sum_g \tau_g \times m_g) \quad (2)$$

The direct sun irradiance at the ground V (for sun photometers, the measured signal is a usually a voltage) is a result of the extraterrestrial irradiance V_0 being attenuated exponentially with the product of the total optical depth and the air mass factor (AMF) m . The AMF is the ratio of the slant to vertical optical path length and is a function of SZA. More specifically, it depends on the vertical profile and, for higher AMF, differs slightly for each atmospheric component. The total optical depth τ_{total} is the sum of the AOD τ_{aero} and the optical depth from Rayleigh scattering and absorption from other gases (τ_g), predominantly NO_2 and O_3 (and H_2O). The gas absorption optical depth is the product of the crosssection and the total column density. All expressions for AMF, crosssections etc. can be found in the Blick software suite manual [6]. Eventually, the AOD can be evaluated by rewriting equation 2:

$$\tau_{\text{aero}} = -1/m_{\text{aero}} \times (\log(V/V_0/r^2) + \sum_g \tau_g \times m_g) \quad (3)$$

In this CCN we will focus on selected wavelengths of 440 nm, 500 nm, 675 nm, 780 nm which are commonly used by sun photometers, including AERONET instruments, because they are only weakly affected by molecular absorption. Then, except for the significant but well known Rayleigh extinction, the term $\sum \tau_g \times m_g$ plays a minor role and uncertainties in the total columns of NO_2 and O_3 are negligible.

So here, the main challenge is to determine V/V_0 . Note that in order to determine τ_{aero} with an uncertainty of 0.01, which is the specification of well calibrated sun photometers, the ratio V/V_0 must be known to around 1%. This is a demanding requirement for radiometric quality. In principle, there are three complimentary methods for achieving this:

- absolute calibration of V in laboratory and taking V_0 from actual extraterrestrial measurements outside the atmosphere
- keeping relative units of V and determining V_0 by using the expected diurnal variation of the direct solar irradiance (field calibration)
- intercomparison with a reference instrument

In the following, we will apply the first two methods and explore its challenges in more detail. The study will be done using Pandoras 128 and 129 during the CINDI2 (Cabauw Intercomparison Campaign of Nitrogen Dioxide measuring Instruments) campaign in September 2016 as a test case.

1.1 Applicable Documents

- [1] Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study [Proposal], Luft-Blick 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. Cede. *Manual for Blick Software Suite 1.3, Version 7*, 2017. URL http://pandonia.net/media/documents/BlickSoftwareSuite_Manual_v7.pdf.
- [7] J. Herman, A. Cede, E. Spinei, G. Mount, M. Tzortziou, and N. Abuhassan. NO₂ column amounts from ground-based Pandora and MFDOAS spectrometers using the direct-sun DOAS technique: Intercomparisons and application to OMI validation. *Journal of Geophysical Research (Atmospheres)*, 114:D13307, July 2009. doi: 10.1029/2009JD011848.
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- [9] A. Kreuter, S. Wuttke, and M. Blumthaler. Improving langley calibrations by reducing diurnal variations of aerosol angstrom parameters. *Atmospheric Measurement Techniques*, 6(1):99–103, 2013. doi: 10.5194/amt-6-99-2013.
- [10] Robert L Kurucz. New atlases for solar flux, irradiance, central intensity, and limb intensity. *Memorie della Societa Astronomica Italiana Supplementi*, 8:189, 2005.

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- [11] Kwon H. Lee, Zhanqing Li, M. C. Cribb, Jianjun Liu, Lei Wang, Youfei Zheng, Xiangao Xia, Hongbin Chen, and Bai Li. Aerosol optical depth measurements in eastern china and a new calibration method. *Journal of Geophysical Research: Atmospheres*, 115(D7), 2010. ISSN 2156-2202. doi: 10.1029/2009JD012812. D00K11.
- [12] 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 Calibration Methods

2.1 Laboratory calibration

The absolute calibration in the laboratory is based on measuring a standard lamp with a known spectral irradiance. The desired result is the conversion factor from relative counts (cts) or measured signal in general, to absolute radiometric units of $\text{W/m}^2/\text{nm}$. This conversion is equivalent to the sensitivity of the sensor. In fact, several correction steps (e.g. correction of dark counts, non-linearity etc.) must first be applied in order to get 'true' relative counts. This process is well described in detail in the manual [6]. Furthermore, a quality filter is applied to all data which also serves as a cloud screen filter [12].

In the laboratory at the Innsbruck Medical University we keep the primary standard lamp, a 1000W FEL-type quartz-halogen lamp traceable to the German metrological institute, Physikalisch Technische Bundesanstalt (PTB). The calibration certificate has an uncertainty (1σ standard deviation) of the irradiance of about 3% and is defined for a measurement at a distance of 70 cm from the lamp. However, the exact reference point at which that distance is measured is influenced by the input optics, e.g. a diffusor plate. The determination of the reference point for each input optics is a critical step in the calibration process and may introduce an additional uncertainty. For the Pandora calibration, we apply the methodology adopted for the Brewer spectroradiometers [8].

The spectral range of the certificate is 250 nm - 1100 nm (step 10 nm) which has to be interpolated to the resolution of the spectrometer. Dividing the measured spectrum by the calibration certificate yields the desired sensitivity, the conversion factor in $\text{cts}/(\text{W/m}^2/\text{nm})$.

The sensitivity must be determined for each combination of filters in the two filter wheels of the Pandora instrument. The filter wheel allocation can be found in the instrument's operation file. With nine filters in each filter wheel there are 81 combinations. For the filter wheel allocation of Pandora 128 and 129 there are 42 unique combinations for which the sensitivity has to be determined. For the direct sun measurements used for the AOD retrieval, two combinations are typically used: 'open' in filter wheel 1 and 'diffusor' in filter wheel 2 for measurements at low solar elevations and 'ND1' and 'diffusor' (ND1 is a neutral density filter with an attenuation factor of 10). In addition, the combination 'ND1' and 'diffusor' + 'U340' may be used for short wavelengths to suppress stray light.

The measured sensitivities for Pandora 128 and 129 for the filter combination 'ND1' and 'diffusor' is shown in Fig. 1. S1 and S2 denote the two spectrometers (UV-VIS and VIS-NIR) in each instrument. The sensitivities are stored in the instrument's calibration file (rows sensitivity 1 - 42) and can then be applied in the conversion routines for L0 to L1 Pandora data formats. Calibrated L1 data (V) and extraterrestrial V_0 (from *Kurucz* [10], shown in Fig. 2) are the desired input for equation (3) to determine the AOD.

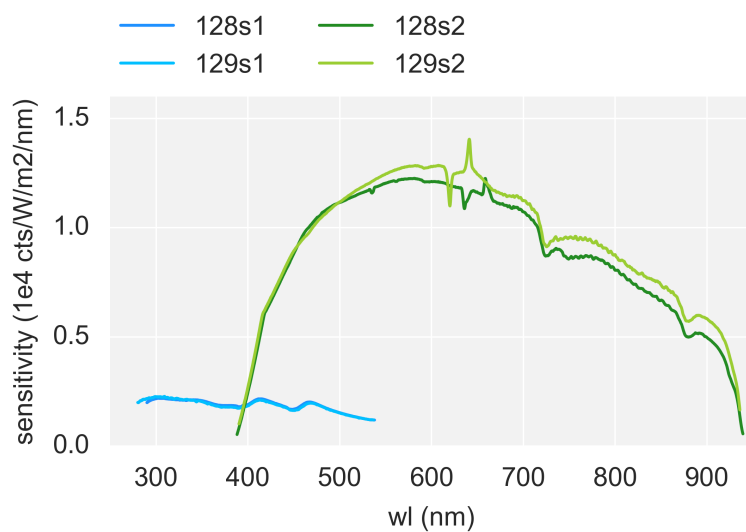


Figure 1: Sensitivities of Pandoras 128 and 129 (S1 and S2) for the filter combination ‘ND1’ and ‘diffusor’ typically used for direct sun measurements.

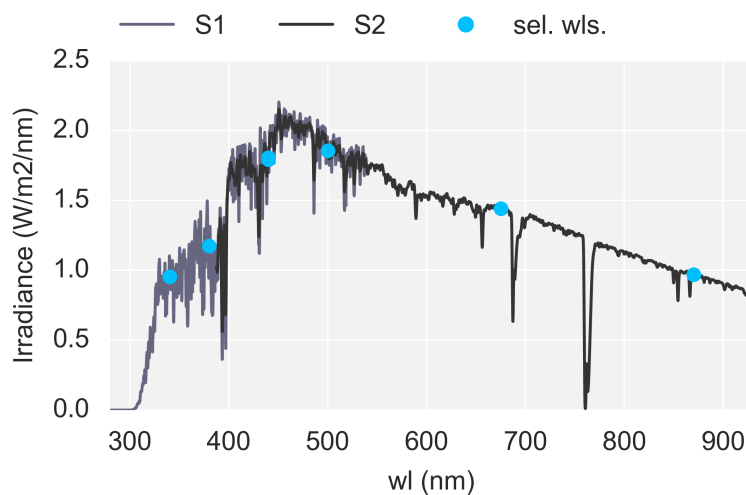


Figure 2: High resolution extraterrestrial irradiance spectrum from *Kurucz*. This is the relevant V_0 to determine the AOD with absolutely calibrated V . Selected AOD wavelengths are also shown.

2.2 Field calibrations

Field calibrations are all calibration methods that are done 'in situ', i.e. using only the data that an instrument acquires in the field. The most known example is the so called Langley extrapolation method. Many variations of this method have been proposed but essentially they are all based on the principle of using the air mass dependence of the measured signal from the direct sun (equation 2) to determine the extraterrestrial signal V_0 . In the following, we will discuss the most relevant versions of this technique.

2.2.1 Classical Langley extrapolation

The 'classical' Langley extrapolation is the simplest Langley calibration version. The principle here is to extrapolate the diurnal variation of V to air mass zero and hence determine the extraterrestrial V_0 . The principle becomes clear when rewriting equation 2:

$$\log V = \log(V_0/r^2) - \tau_{\text{total}} \times m \quad (4)$$

A linear least squares fit through $\log V$ as a function airmass m yields a slope τ_{total} and a y-intercept $\log(V_0/r^2)$ at $m = 0$. The underlying condition for a Langley calibration is that τ_{total} is constant over the course of the day. In particular, it has to be assumed that τ_{aero} is constant, since the contribution from Rayleigh scattering is constant and gas absorptions have a minor effect at the selected wavelengths. In practice, this assumption is not commonly fulfilled at typical stations at low altitude and Langley calibrations are usually performed at high altitude stations with low and constant aerosol background such as Izana (Tenerife) or Mauna Loa (Hawaii).

Although the variable aerosol conditions at the Cabauw station during the CINDI2 campaign are far from ideal and would not usually be considered suitable for Langley calibrations, we apply it here nonetheless to showcase the methodology and possibly estimate the quality of the calibration under more ideal conditions.

An example of classical Langley plots is shown in Fig. 3 for Pandora 128s2 for 12 selected days in September 2016. We plotted $\log V$ against air mass m where V are calibrated L1 data applying the results from section 2.1 which will allow us to directly compare the results to the expected V_0 from the extraterrestrial irradiance.

Note that, particularly for the days 31.8., 8.9. and 13.9., the AOD changes significantly from morning to afternoon which is noticeable as the $\log V$ vs m relationship is not adequately described by a straight line. These deviations may however be averaged out over the set of selected days. Also note that one day (15.9.) is a distinct outlier with a particularly steep slope and high y-intercept, the origin of this behaviour is not clear and will have to be investigated. So a critical part of Langley extrapolations is the selection of suitable subsets of data.

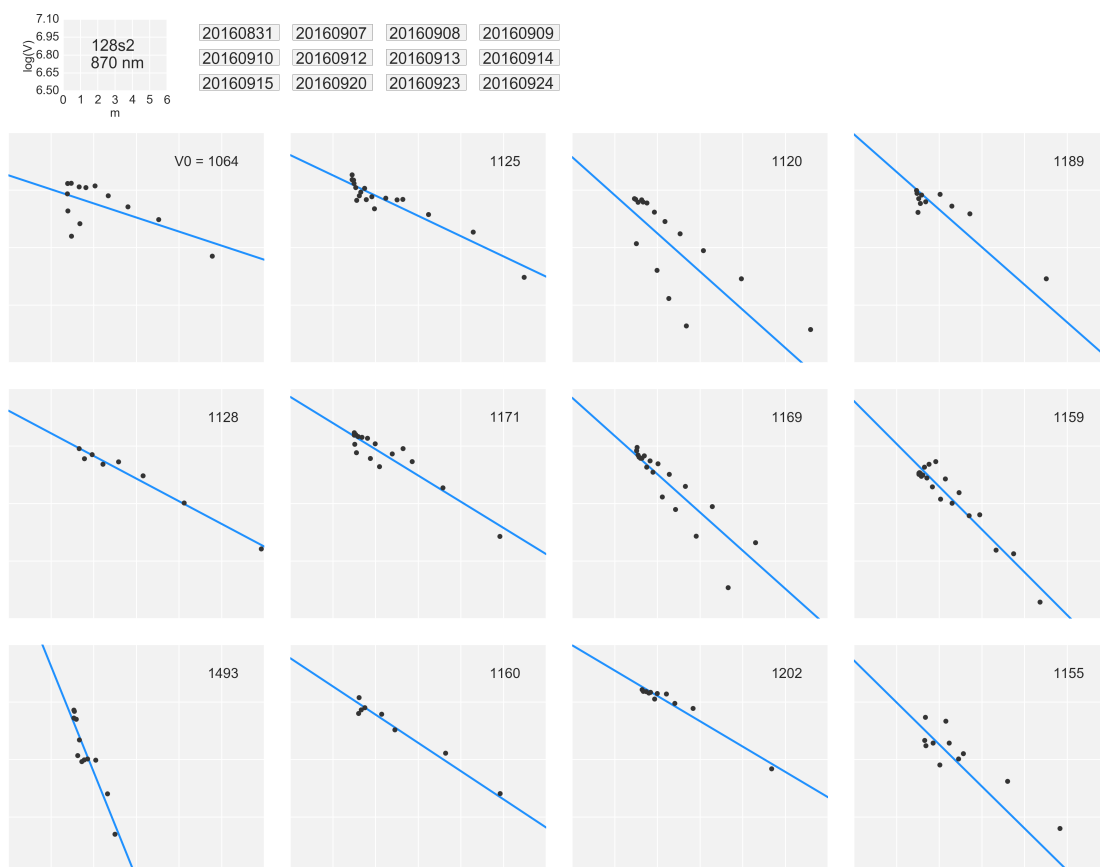


Figure 3: Classical Langley extrapolation plots for Pandora 128s2 for 870 nm for relevant days during CINDI2. Scale and labelling of axes and corresponding dates of each subplot are shown in the legend above. The evaluated V_0 s are given in mW/m²/nm.

2.2.2 Minimum Langley extrapolation

Addressing the impact of AOD variations on the classical Langley method, the 'minimum Langley extrapolation' has been proposed independently by *Herman et al.* [7] with respect to gas retrievals and *Lee et al.* [11] specifically for AOD. In these proposals the data of multiple days are binned with respect to air mass and a linear least squares fit is performed through a certain percentile of each bin. As for the classical Langley extrapolation, V_0 is determined from the y-intercept. The idea behind this method is the assumption that a similarly low AOD (high V) will occur for each air mass range (bin), and only these AOD values contribute to the fitted slope, minimizing the effect of diurnal AOD variations for individual days.

In Fig. 4, we show the minimum Langley extrapolation method for the relevant days during CINDI2 for Pandora 128s2 for 870 nm. We used 20 air mass bins and fitted the 95 percentile of data in the bins. Note how only the highest $\log V$ values contribute to the linear fit which in turn also increases the statistical uncertainty. Furthermore, the choice of these fit parameters have a slight impact on the resulting V_0 and the optimal choice, which also depends on the selection of data points, will have to be evaluated by the accuracy of V_0 when compared to a reference.

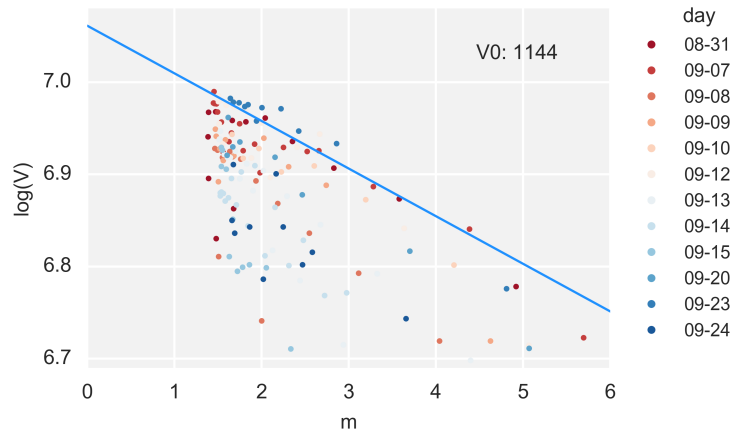


Figure 4: Minimum Langley extrapolation plot for Pandora 128s2 for 870 nm. Linear fit through the 95 percentile of the data of all previously selected days in 20 air mass bins. Only the highest $\log V$ values contribute to the fitted slope minimizing the effect of diurnal AOD variations of individual days.

2.2.3 Weighted Langley

One weakness of the classical and minimum Langley methods is that they ignore the slight differences in air masses for the different attenuators (m in equation 4 is a mean of all air masses). As a refinement, one can modify equation 4:

$$\log V_a = \log(V_0/r^2) - \tau_{\text{aero}} \times m_{\text{aero}} \quad (5)$$

where V_a is defined as the signal if aerosols were the only contributors to τ_{total}

$$V_a = V \times \exp\left(\sum_g \tau_g \times m_g\right) \quad (6)$$

and extrapolate the linear V_a versus m_{aero} dependence as above. However, there remains another general weakness of these extrapolation methods regarding the weights of the linear fit of $\log V$. Random AOD fluctuations of $\Delta\tau_{\text{total}}$ causes $\Delta\log V = m \times \Delta\tau_{\text{total}}$, so fluctuations at larger air masses have a larger weight towards the fit than fluctuations around noon. This issue can be eliminated by multiplying equation 4 by $1/m$ and plotting $\log V/m$ against $1/m$:

$$\log V/m = \log(V_0/r^2)/m - \tau_{\text{total}} \quad (7)$$

Now V_0 is a result of the fitted slope where all measurements contribute equally which increases the statistical robustness. The result of this Langley variation is depicted in Fig. 5. Note how the $1/m$ scaling reduce the apparent scatter around the linear dependence. However, this does not necessarily imply a reduced standard deviation of the resulting V_0 between the selected days and hence an increased precision of the method.

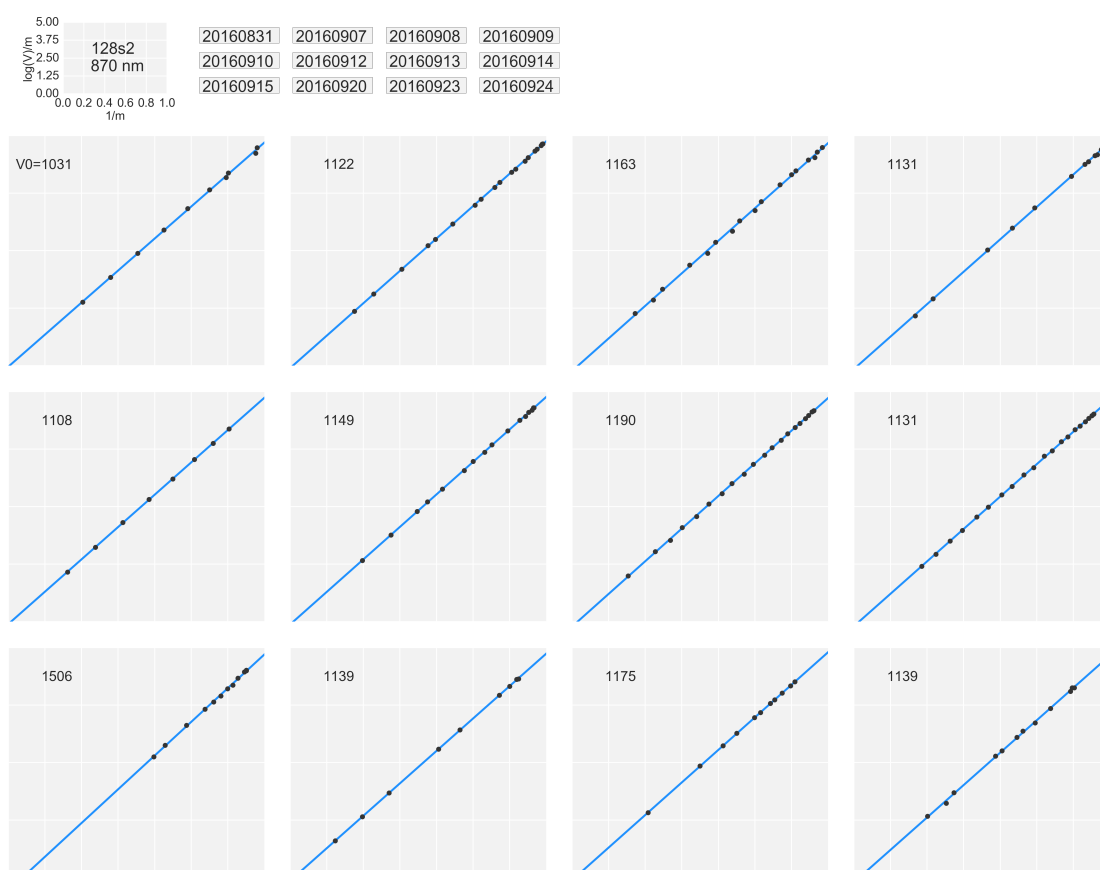


Figure 5: Weighted Langley plots for Pandora 128s2 for 870 nm where $\log V/m$ is plotted against $1/m$ and V_0 is determined from the slope instead of the y-intercept.

2.2.4 AOD Langley

The principle of deriving V_0 from the slope has also been proposed by *Cachorro et al.* [5] in a slightly different form, explicitly involving the AOD. They emphasize the fact that a calibration error manifests itself in an artificial diurnal variation (air mass dependence) of the derived AOD. It follows from equation 3, that applying a wrong V_0' causes an erroneously derived τ'_{aero} :

$$\tau'_{\text{aero}} = \tau_{\text{aero}} + \log(V_0'/V_0)/m_{\text{aero}} \quad (8)$$

So the error $\tau'_{\text{aero}} - \tau_{\text{aero}}$ is maximal at (and symmetric around) local noon and decreases with air mass. More specifically, from equation 8, it can be understood that the slope of a straight line fit through the dependence of τ'_{aero} against m_{aero} is $\log(V_0'/V_0)$ which yields the factor to derive the correct V_0 . A plot of the application of this method is shown in Fig. 6. Here τ'_{aero} has been evaluated using equation 3 and the extraterrestrial V_0 from Fig. 2. The correction factors V_0'/V_0 are also depicted.

As a refinement of this method, *Kreuter et al.* [9] have proposed the minimization of artificial diurnal variations of the Angstrom exponent α and its curvature which are even more sensitive to calibration errors.

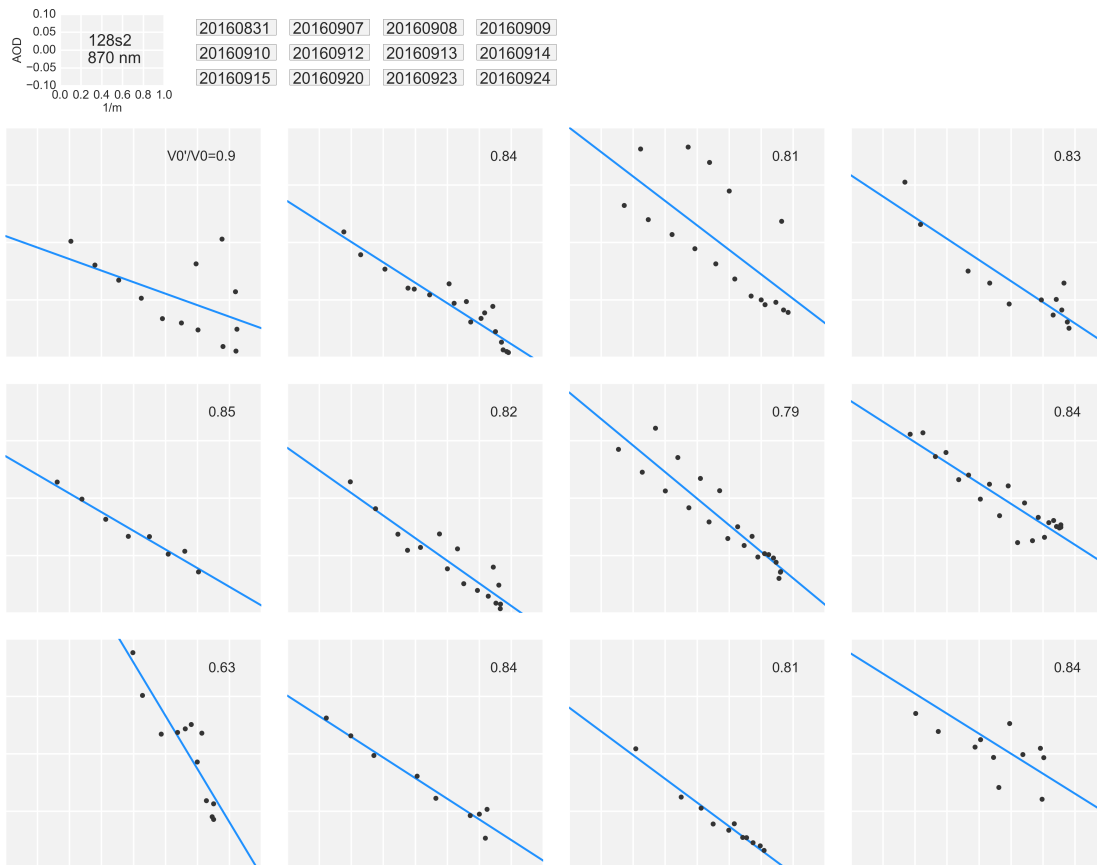


Figure 6: AOD vs $1/m$ for Pandora 128s2 for 870 nm. From the slope of the plots correction factors for the extraterrestrial V_0 have been derived.

2.3 Calibration by intercomparison

The last method mentioned in section 1 is the calibration by intercomparison with a well-calibrated reference instrument and will only be briefly discussed in this report. Sun photometer networks such as AERONET maintain a set of reference, so called 'master' instruments which have the best possible calibration (from high quality Langley calibrations at a high mountain site). The field instruments are regularly sent to a reference site and set up next to the reference instrument for a period of simultaneous measurements and by intercomparison, the calibration is transferred.

This method is not feasible as a general method for the Pandora since the instruments are much more delicate than mechanically robust filter radiometers with no moving parts and the high standard for an absolute calibration cannot be ensured during shipping. In addition, using a calibrated sun photometer as reference for the Pandora calibration has the draw back that only few wavelengths bands are available and the wealth of spectral information from the Pandora instrument is not fully explored.

However, the intercomparison with a sun photometer at selected wavelengths will be used as a validation and quality assessment of the above field and laboratory calibrations. In deliverable D5 we will compare the AOD from the Pandoras at CINDI2 with the AOD from the Cimel sun photometer in Cabauw operated within AERONET.

3 Discussion and Conclusions

Now we compare all calibration results from the previous sections, evaluate their precision and discuss possible issues relevant for a strategy for determining the AOD within Pandonia.

First, we note that in this report, the absolute calibration from the laboratory cannot be validated directly. A validation will be performed by comparison of the resulting AOD with the AERONET sun photometer. However, since we performed all Langley calibration methods in section 2.2 using absolutely calibrated data from 2.1, we can already draw some conclusions from comparing the resulting V_0 s amongst each other and with the expected extraterrestrial V_0 . The comparison of all Langley variations for Pandora 128s2 and 129s2 for 870 nm is shown in Fig.7, together with the extraterrestrial V_0 from *Kurucz*. Here we can observe the following:

- The medians of all Langley methods for both instruments and 870 nm agree to better than 3%. Note that values outside 1.5 times the interquartile range have been treated as outliers and are not considered in the median.
- All Langley calibrations at 870 nm have an estimated precision of around 3% from the interquartile range for Pandora 128s2 and slightly higher for Pandora 129s2. This is quite remarkable considering the suitability of conditions. For a larger data set with more favourable conditions, an achievable standard deviation of 1% for the Langley calibration does not seem unreasonable.
- All Langley calibrations are about 15% and 10% higher than the extraterrestrial V_0 , for Pandora 128s2 and 129s2, respectively. This is the systematic error of the absolute calibration, which is substantial. However, considering that between the laboratory calibration and measurements in Cabauw, the instruments were packed and unpacked, including the optical fibres being mounted and unmounted, this is very reasonable and not surprising. This issue will be addressed by a mobile field calibration tool that is currently being developed.
- This systematic error in the absolute calibration is different for each instrument and explains the discrepancy of the Langley calibrations at 870 nm between Pandoras 128s2 and 129s2.

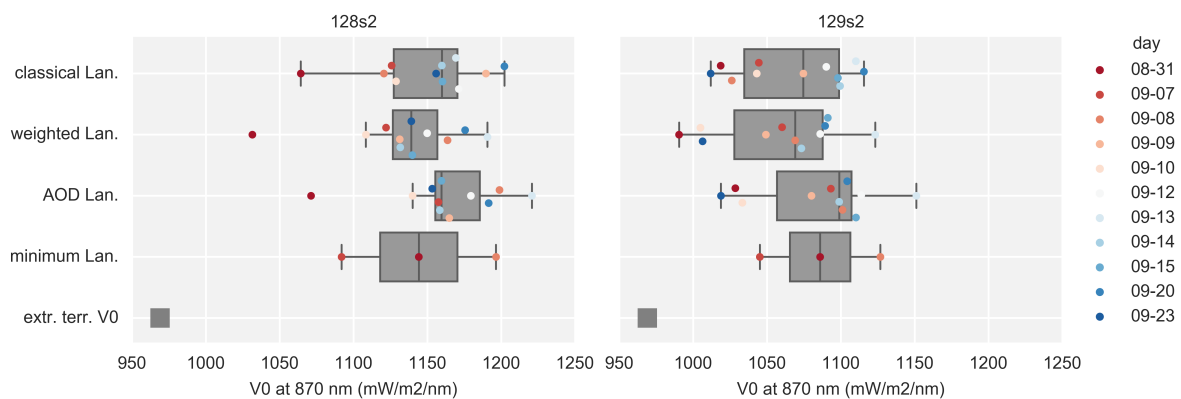


Figure 7: Comparison of different field calibration methods for Pandoras 128 and 129 for 870 nm and the extraterrestrial V_0 from *Kurucz*. The box plots indicate median and 25 and 75 quartiles. For the minimum Langley method, the box width has been scaled to correspond to the V_0 uncertainty from the fitted slope. The color coded dots indicate the results from each individual day with no apparent systematic change over the month. The x-grid spacing corresponds to about 5% relative change in V_0 .

One preliminary conclusion from this is that the accuracy of the laboratory calibration is not sufficient. So on its own, it is not suitable for AOD retrievals. Actually, this should come as no surprise as no other AOD retrieving network relies solely on the laboratory and Langley calibrations under pristine conditions are considered superior for evaluating V_0 . Nonetheless, although the accuracy of the absolute laboratory calibration is poor as a result of transport and issues of the optical fibre, the relative spectral sensitivity should remain accurate, i.e. if the calibration error can be described by a wavelength independent factor, the relation of V_0 between wavelengths is not affected. So the absolute calibration may still hold important information which will be revisited further below.

Regarding the field calibration methods presented here, the analysis is not fully conclusive yet as to which flavour of Langley variation qualifies first. The AOD Langley method (section 2.2.3) might seem like a preferable choice because it adequately addresses both weight and air mass issues mentioned in section 2.2.3 and most directly aims at eliminating the artificial diurnal AOD variation, the most suspicious manifestation of a calibration error. It also has one of the smallest interquartile ranges in Fig. 7. It should be noted, that there is no convincing consensus in the literature either and that the application of Langley methods depend on the specific atmospheric conditions and the selection of data subsets used for the fitting procedure. So it will be essential to define clear criteria and limits for the selection of suitable data and outliers to implement automatic Langley calibrations on an operational basis.

Furthermore, we have to discuss the ability to extend the calibration to arbitrary wavelengths. The analysis shown above has been restricted to 870 nm since it can be expected that the accuracy and precision of all Langley type methods improve with increasing wavelength. The reason for this is that natural AOD variations (which impair the methods) increase nonlinearly with decreasing wavelength as the Angstrom exponent α is typically bigger than 1. In addition, the Angstrom exponent itself may vary, increasing the sensitivity to AOD variations at shorter wavelengths.

The analysis for Langley calibrations at 440 nm is shown in the comparative plot in Fig. 8. The interquartile ranges for all Langley methods are larger than for 870 nm corresponding to about 5% relative uncertainty, confirming the above assumption.

The decreasing precision with wavelength now points to a more holistic calibration methodology involving

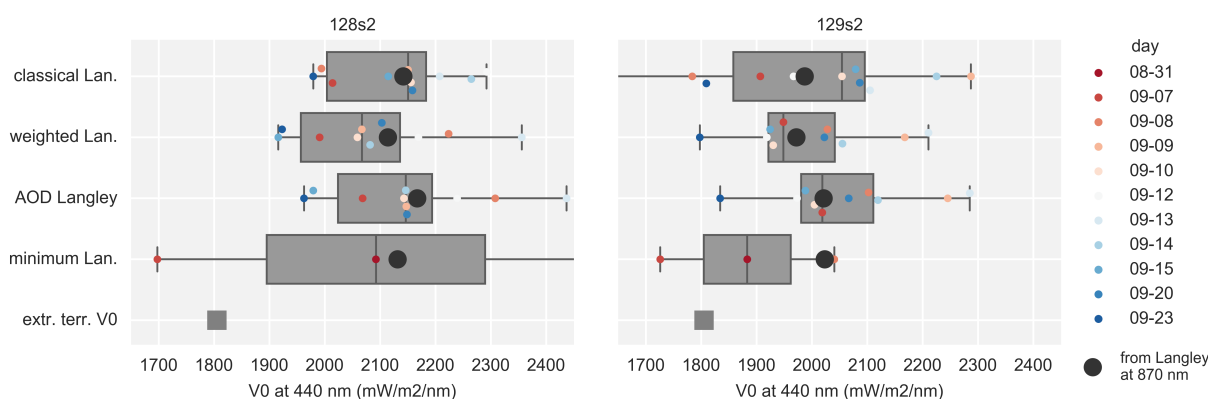


Figure 8: Comparison of different field calibration methods for 440 nm (boxplots with median and 25 and 75 quartiles). Using the ratio of each Langley method at 870 nm to the extraterrestrial V_0 at 870 nm as a pivot, V_0 at 440 nm has been deduced which are shown as dark dots. This allows to transfer the superior Langley calibration at long wavelengths to the rest of the spectrum.

the combination of both Langley and spectral sensitivity from the absolute laboratory calibration. The Langley calibration at a long wavelength, e.g. 870 nm, can be used as a pivot to determine a correction factor for the spectral sensitivity which then allows the transfer of the calibration to lower wavelengths.

This combination method has been assessed by taking the ratio of each Langley method at 870 nm (Fig. 7) to the extraterrestrial V_0 at 870 nm and using that factor to correct the V_0 at 440 nm. These spectrally corrected V_0 are shown in Fig. 8 as dark dots for each method. The agreement with the Langley results is good, but what is more relevant is that these V_0 at 440 nm agree with each other within about 3%, much better than the medians for the Langley derived V_0 . This finding generates reasonable confidence in the chances of success of the combined method and emphasizes the importance of a careful laboratory calibration.

As mentioned before, the final assessment of all Langley methods including the combination of Langley and spectral sensitivity from the laboratory will be performed in deliverable D5 using the intercomparison with AERONET data at selected wavelengths of 440 nm, 675 nm and 870 nm.

Finally, we note that radiometric stability between calibration periods is another important and delicate prerequisite for operational AOD retrieval and a foreseen issue. To address this concern we are in the process of developing a field calibration tool (FCT) as a portable standard lamp to be able to regularly monitor the relative stability of Pandora instruments within the growing Pandonia network.