



LuftBlick Report 2014001

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

Network Intercalibration Procedure

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Document Change Record

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Acronyms and Abbreviations

H ₂ O	Water vapor
AEMET	Spanish Meteorological Service
AMF	Air mass factor
AOD	Aerosol optical depth
CIAI	Izaña Atmospheric Research Center of the National Meteorology Agency of Spain
DU	Dobson units
FOV	Field of view
FTIR	Fourier Transform Infrared Spectroscopy
FWHM	Full width at half maximum
GSFC	Goddard Space Flight Center
HCHO	Formaldehyde
MAXDOAS	Multi-Axes Differential Optical Absorption Spectroscopy
MLE	Modified Langley Extrapolation
MobREFI	Mobile reference instrument
MONI	Monitoring instrument
NO ₂	Nitrogen dioxide
O ₂ O ₂	Oxygen dimer
O ₃	Ozone
OMI	Ozone Monitoring Instrument
Pandonia	ESA Ground-Based Air-Quality Spectrometer Validation Network
Pandora	Pandora spectrometer system
Pandora-2S	Pandora dual spectrometer system
RBCC-E	Regional Brewer Calibration Center - Europe
RT	Radiative transfer
SO ₂	Sulfur dioxide
SpecAOD	Spectral aerosol optical depth over the entire range 300-900nm
StatREFI	Stationary reference instrument
StratNO ₂	Stratospheric nitrogen dioxide column
StratO ₃	Stratospheric ozone column
SZA	Solar zenith angle
TempNO ₂	Effective nitrogen dioxide temperature
TempO ₃	Effective ozone temperature
TotNO ₂	Total nitrogen dioxide column
TotO ₃	Total ozone column
TropNO ₂	Tropospheric nitrogen dioxide column
TropO ₃	Tropospheric ozone column
UV	Ultraviolet

1 Introduction

This report is deliverable D07 of the ESA Ground-Based Air-Quality Spectrometer Validation Network (Pandonia) project [2, 1]. It uses the general guidelines from 'Recommendations for Inter-Calibration of minispectrometer networks' [7] and adapts them to Pandonia. While *Cede and Tiefengraber* [7] is limited to total ozone column (TotO₃) and total nitrogen dioxide column (TotNO₂), this report discusses all planned main data products of Pandonia, i.e. TotO₃, tropospheric ozone column (TropO₃), stratospheric ozone column (StratO₃), TotNO₂, tropospheric nitrogen dioxide column (TropNO₂), stratospheric nitrogen dioxide column (StratNO₂), and spectral aerosol optical depth over the entire range 300-900nm (SpecAOD). Section 2 discusses general aspects of the Pandonia calibration, which are relevant to each data product. Sections 3 and 4 describe how we plan to maintain the accuracy of the stationary reference instruments (StatREFIs) and for the monitoring instruments (MONIs) respectively. Section 5 gives a tentative schedule for the algorithm development activities described in this report.

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.

1.2 Reference Documents

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2 General aspects

2.1 Uncertainty considerations

We can say that the uncertainty of a Pandonia data product will depend on:

- The uncertainty of the measurements
- The uncertainty of the algorithm

In this report we focus mainly on the uncertainty of the measurements since the primary goal of the network is 'homogeneity', which is explained in *Cede and Tiefengraber* [7]:

"In principle, accuracy reflects the difference between the measured value and the true value. One part of this 'difference to the truth' comes from measurement uncertainties like those listed above. Another part comes from 'algorithm deficiencies'. Assume we have several network instruments located at the same site. They will all retrieve somewhat different data, since the instrumental uncertainties are individual for each spectrometer. However, even if all were ideal instruments, free of uncertainties, and all gave basically the same value, it still does not mean that this is the true amount. Errors in the cross sections, effective gas temperature, etc. are still included and affect all units in approximately the same way. In order to produce homogeneous data in the network, we do not really have to focus on the algorithm deficiencies. What we want is that all network instruments measure in the same way, i.e. if they were installed at the same place, they should all produce the same data. We call this 'homogeneity'. Of course the closer the data are to the true value the better."

We can further subdivide the measurement uncertainty into the measurement uncertainty of the StatREFIs ('Reference uncertainty') and the measurement uncertainty of the MONIs ('Monitoring uncertainty'). To reduce the reference uncertainty, several steps will be taken (e.g. intercomparison with external instrumentation and/or models), which are described in details in section 3. The monitoring uncertainty will be larger than the reference uncertainty and should be minimized by the intercomparisons of the MONIs by a mobile reference instrument (MobREFI) as explained in section 4.

2.2 Data correction

All Pandonia data products are produced from the measured (ir)radiances, which are obtained from the raw data after applying several corrections. The current correction steps are:

- Dark correction
- Temperature correction
- Non-linearity correction
- Conversion to count rates
- Flat field correction
- Stray light correction
- Filter correction
- Conversion to (ir)radiances
- Wavelength correction

Systematic errors in the data correction will produce systematic errors in the final data products. To conserve the network homogeneity we will apply the corrections in a standardized way to all instruments. More details on the data correction process are given in *Cede and Tiefengraber* [10].

2.3 Principle of Pandonia calibration

Pandonia will be composed of three types of instruments:

- Stationary reference instruments (StatREFIs) determine the absolute calibration of the network. All network observations will be traceable to them.
- Monitoring instruments (MONIs) are distributed at different locations in order to obtain uninterrupted extended time series of atmospheric parameters.
- Mobile reference instruments (MobREFIs) transfer the calibration from the StatREFIs to the MONIs.

All Pandonia StatREFIs will be at the Izaña Atmospheric Research Center of the National Meteorology Agency of Spain (CIAI). This station was selected for the following reasons:

- It is a high-altitude, pristine site with many clear sky days (typically more than 180 a year), thus excellent conditions for instrument intercomparisons and for field calibration techniques such as Langley extrapolation.
- It disposes of laboratory calibration tools (FEL lamps, spectral lamps) and field calibration tools (halogen lamps to be used outside), which will be upgraded and adapted within this project to fit the needs of Pandonia.
- The staff is experienced in operating and maintaining remote sensing instrumentation, including the Pandora spectrometer system (Pandora). Part of the staff is continuously present and can prevent physical damage to the instruments from extreme weather.
- It is the host site for the Brewer triad from the Regional Brewer Calibration Center - Europe (RBCC-E), which will be the reference for Pandonia TotO₃.
- It has instrumentation measuring aerosol optical depth (AOD) at selected wavelengths [14, 15], which are overlapping with Pandora and Pandora dual spectrometer system (Pandora-2S) [9] and can be used to track the radiometric stability of the StatREFIs.
- The vertical distribution of ozone (O₃) and nitrogen dioxide (NO₂) is very stable, with rather constant O₃ concentrations and hardly any tropospheric NO₂. This makes it easy to estimate these profiles when needed.
- It has additional instrumentation, that can be used to define key input parameters for radiative transfer (RT) model calculations: zenith sky observations to get StratNO₂; in-situ measurements for surface concentrations of aerosols, O₃ and NO₂; an aerosol Lidar for aerosol profiles; daily radio-sondes and weekly ozone-sondes from a nearby location; ozone profile information from ground-based Fourier Transform Infrared Spectroscopy (FTIR)

Pandonia will initially have one StatREFI, which is the existing Pandora 101 at CIAI. Pandora 101 is a direct-sun-only standard Pandora system with wavelength range 280 to 500 nm. So it can be used as a reference for TotO₃, TotNO₂, and SpecAOD below 500 nm, but not for SpecAOD above 500 nm or other O₃ and NO₂ products. A second StatREFI will be installed at CIAI within this project. This one will be a Pandora-2S system and can be used as a reference for all data products. Ideally three Pandora-2S systems should be at CIAI in the future. Details on how to maintain the calibration of the StatREFIs are given in section 3.

A MobREFI transfers the calibration from the StatREFIs to a MONI. In this way the time series of the MONIs is not interrupted. It was determined in *Cede and Tiefengraber* [7], that a MONI should be visited at least once every two years in order to maintain sufficient accuracy for TotO₃ and TotNO₂. This would mean

that the approximate number of MobREFIs needed for the entire network is $\text{ceil}(n/25)$, where n is the number of MONIs. No such numbers have been established yet for other data products. This will be a task of the current project. In this project we will have at most one MobREFI.

A MobREFI must be a 'good traveler', which means it should be a robust unit, possibly in a special packing that allows safe transportation to and from the network locations. The calibration transfer to a MONI is only valid, if the comparisons between the MobREFI and the StatREFIs before and after the visit at the MONI agree. The data of the MONI in between two calibration-visits by a MobREFI may have to be corrected retroactively. More details on how to maintain the calibration of the MONIs is given in section 4.

2.4 Operation and maintenance

Even the best network calibration procedure does not always give reliable data, if the Pandonia instruments are not well operated and maintained. E.g. if the Pandora entrance window is dirty, then the SpecAOD will be overestimated. As outlined in the proposal [1], LuftBlick plans to operate Pandonia using:

- Automatic data upload to a central server, which allows fast detection of data interruptions
- A central network operator, who checks the instruments periodically over the web
- Local operators, who physically check the instruments periodically and when contacted by the central network operator

More details on instrument operation and maintenance are given in *Cede and Tiefengraber* [10].

2.5 Alignment

The uncertainty of the Pandonia data products is also influenced by the pointing accuracy. A pointing error might have rather small consequences (e.g. when measuring sky radiance near the zenith direction), but can also have very substantial consequences (e.g. when measuring sky radiance near the horizon). The most drastic effects of a pointing error are seen for direct sun observations, when the incoming solar irradiance is outside the instrument's field of view (FOV), in which case the data are not usable at all.

Most Multi-Axes Differential Optical Absorption Spectroscopy (MAXDOAS) instruments measure sky radiance only. Their alignment is often done by placing a level on a flat surface at the body of the instrument and then adjusting the position of the instrument. This method has several deficiencies:

- It assumes that the optical axes of the unit is parallel to the respective surface, which is often not true.
- Even if the pointing is accurate for one position in the sky, it does not necessarily mean it is also valid for all other positions (see e.g. *Cede* [6], appendix I).
- It is not easy to ensure that the pointing (even if initially correct) does not change over time, since it is very difficult to notice a change in the alignment based on the sky observations themselves.

Therefore, one can often not give a reliable statement on the pointing accuracy of such instruments.

Pandora measures sky radiance AND direct sun irradiance, which is an enormous advantage with respect to the pointing. By comparing the theoretical position of the sun (based on astronomical formula) and the observed position of the sun, the Pandora software determines so-called leveling angles, which are used to calculate the correct pointing of the instrument [6, appendix I]. Thus we can state that for a properly maintained Pandora the pointing accuracy is $\pm 0.2^\circ$ (maximum deviation). More details on the alignment can be found in *Cede and Tiefengraber* [9].

2.6 Cloud screening

Since the calibration transfers from StatREFIs to MobREFIs and from MobREFIs to MONIs are done in the field, one has to decide which atmospheric conditions are valid for such intercomparisons. When using all data (i.e. also measurements at cloudy conditions), it can happen that a quickly changing atmosphere influences the results significantly, since the instruments do not necessarily measure at exactly the same time. Therefore it is typical to intercompare the units during relatively stable conditions, i.e. cloud free.

While it is relatively easy to screen clouds 'manually' by looking at data sequences, making an automated cloud screening algorithm is not so trivial. For direct sun observations clouds reduce the signal. For sky radiances both an increase and a decrease are possible. Therefore, a cloud screening algorithm will have to be developed for each Pandonia data product.

3 Calibration of StatREFIs

This section presents the calibration plan for the StatREFIs at CIAI for each Pandonia data product.

3.1 TotO₃

3.1.1 Introduction

The current Pandora TotO₃ retrieval is purely based on laboratory calibration, which means every instrument is 'self-calibrated' without the need of comparison to a reference. This method produces surprisingly good TotO₃, but there are still differences of $\pm 1.5\%$ on average, and up to 4% in extreme cases [23, figure 1]. This is due to small variations in the spectral sensitivity from instrument to instrument. Therefore calibration towards a common reference will be used for Pandonia. Nevertheless we will still produce results from the current method for comparison and also to understand its deficiencies and improve it.

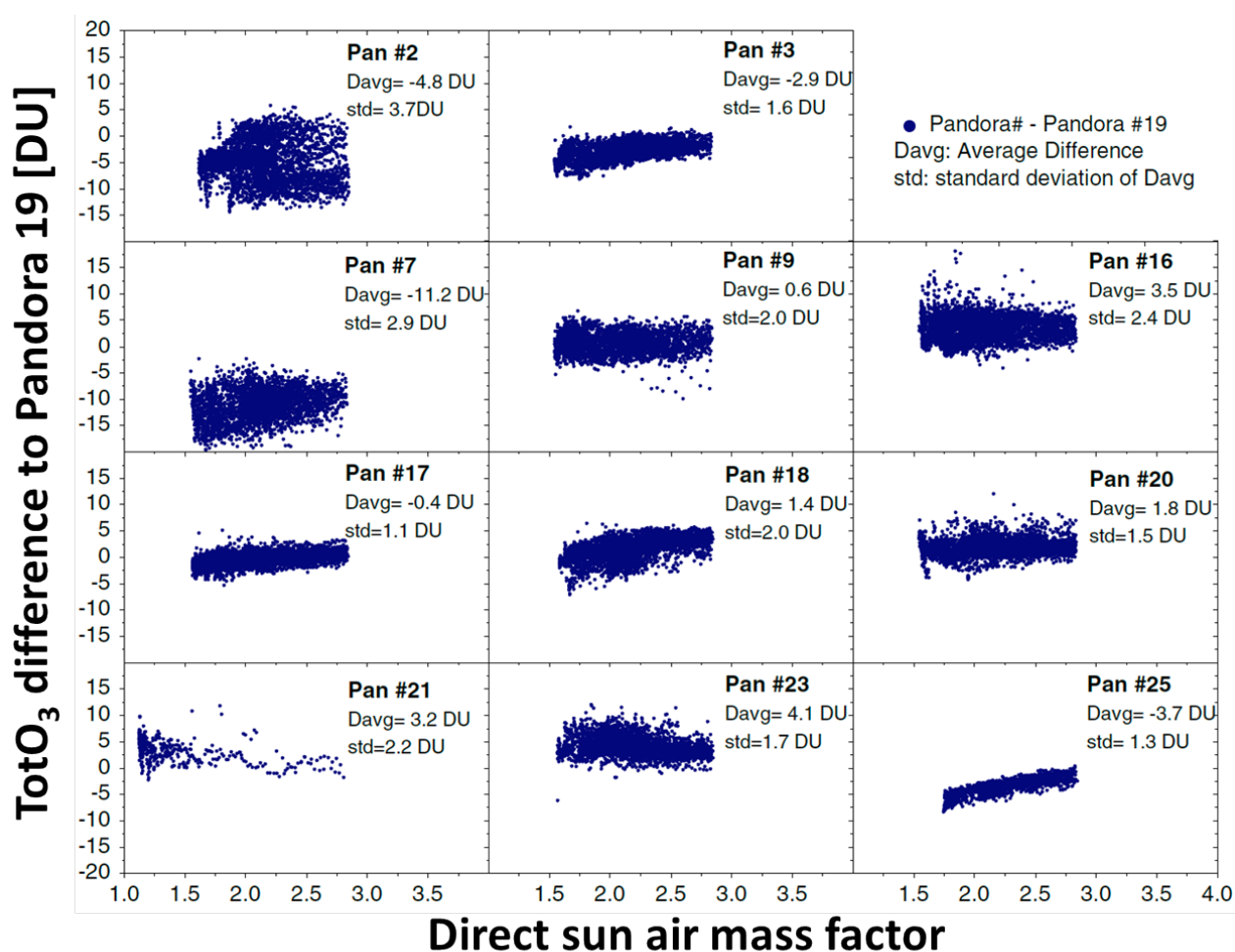


Figure 1: TotO₃ difference between 11 Pandoras and a reference unit (Pandora 19) as a function of the direct sun air mass factor (AMF). Taken from Tzortziou *et al.* [23].

The Pandonia reference for TotO₃ will be the Brewer triad of the RBCC-E located at CIAI (see <http://www.iberonesia.net/index.php/RBCC-E>). This means that TotO₃ of the StatREFIs will be 'bound' to the values of the Brewer triad and possible drifts in the StatREFIs can be detected easily. In order to reference

to the Brewer triad, the TotO₃ algorithms of the two instrument types should be homogenized to some extent. Several aspects of this homogenizations are discussed in the following sections.

3.1.2 O₃ cross sections

The standard Pandora TotO₃ spectral fitting algorithm uses the 'Brion' cross sections [5] at a fixed effective ozone temperature (TempO₃) of -48°C, while the official data product of the Brewer triad uses the 'Bass and Paur' cross sections [3] at a fixed TempO₃ of -45°C. A recent study [16] has shown that the newly measured 'Harmonics' cross sections [18] give the most consistent results for Brewer spectrometers with no dependence of the retrieved TotO₃ on the TempO₃. This means that using this source of cross sections, the TempO₃ in the atmosphere and also the TempO₃ used in the retrieval do not matter and the Brewer spectrometer always derives the correct TotO₃. Based on this study we suggest to change the Pandonia O₃ algorithm to use the Harmonics cross sections and bind them to an unofficial data product of the Brewer triad data, which uses the Harmonics cross sections and is provided to us by RBCC-E.

3.1.3 TempO₃

In contrast to the Brewer, Pandora is sensitive to TempO₃. This is expected and can be seen in comparisons with a Brewer spectrometer (figure 2) and also with the Ozone Monitoring Instrument (OMI) data (figure 3). When the atmospheric TempO₃ is above -48°C (summer time), then Pandora underestimates TotO₃. In the winter time it overestimates. The approximate TempO₃-sensitivity of Pandora TotO₃ is 1% per 3°C.

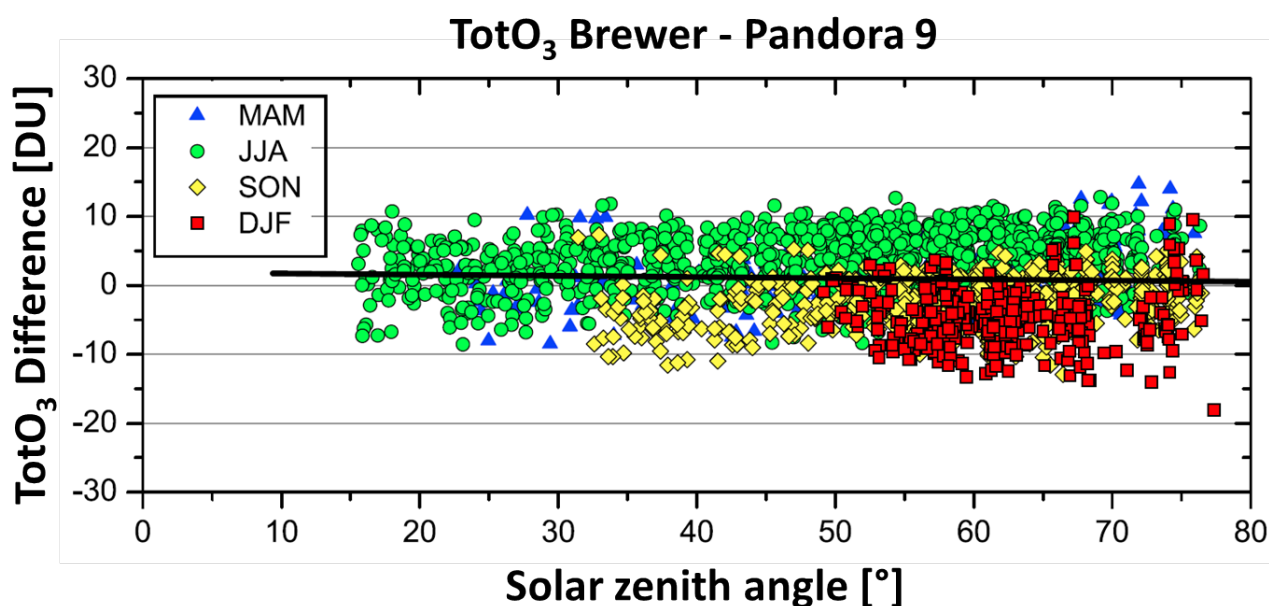


Figure 2: TotO₃ difference between a Brewer spectrometer and Pandora 9 as a function of solar zenith angle (SZA), separated into different seasons (spring=MAM, summer=JJA, fall=SON, winter=DJF). Taken from Tzortziou et al. [22].

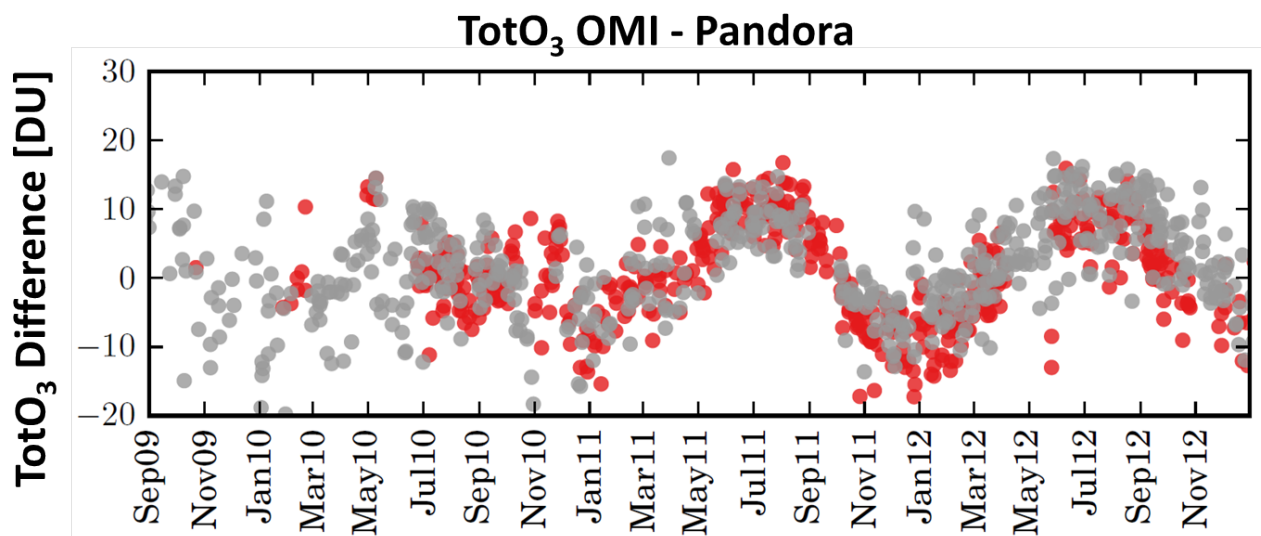


Figure 3: TotO₃ difference between OMI and two Pandoras (grey and red dots) as a function of time. Taken from Tiefengraber and Cede [21].

Therefore TempO₃ must be included in the Pandonia TotO₃ algorithm in some form. Our plan is to develop a spectral fitting algorithm that retrieves both TotO₃ and TempO₃ at the same time. Recent tests have shown that this is possible, but will probably require combined data from several observations. If only TotO₃ is fitted, then the Pandora data show very little noise, but are potentially biased due to the temperature dependence. If both TotO₃ and TempO₃ are fitted, then the retrieved data are noisier, but unbiased. So the best results are obtained when smoothing the obtained TempO₃ over a certain time period (e.g. one hour) and using these values in a spectral fitting process that only retrieves TotO₃.

3.1.4 Stray light

Pandora is a single monochromator, which means it suffers from spectral stray light, which causes underestimation of TotO₃ at high SZA. Depending on the unit, this effect starts between SZA 70° and 80° [8, figure 4]. The Brewers of the triad are all double monochromators, which means they do not have a stray light error. When using the Brewer triad as a reference this has to be taken into account. Without a good stray light correction for Pandora one may have to reduce the SZA-range for the comparisons. We are currently working on an improved Pandora stray light correction algorithm, which is based on the instrument's slit functions. Our goal is to extend to range of useful Pandora measurements of TotO₃ beyond a SZA of 80°.

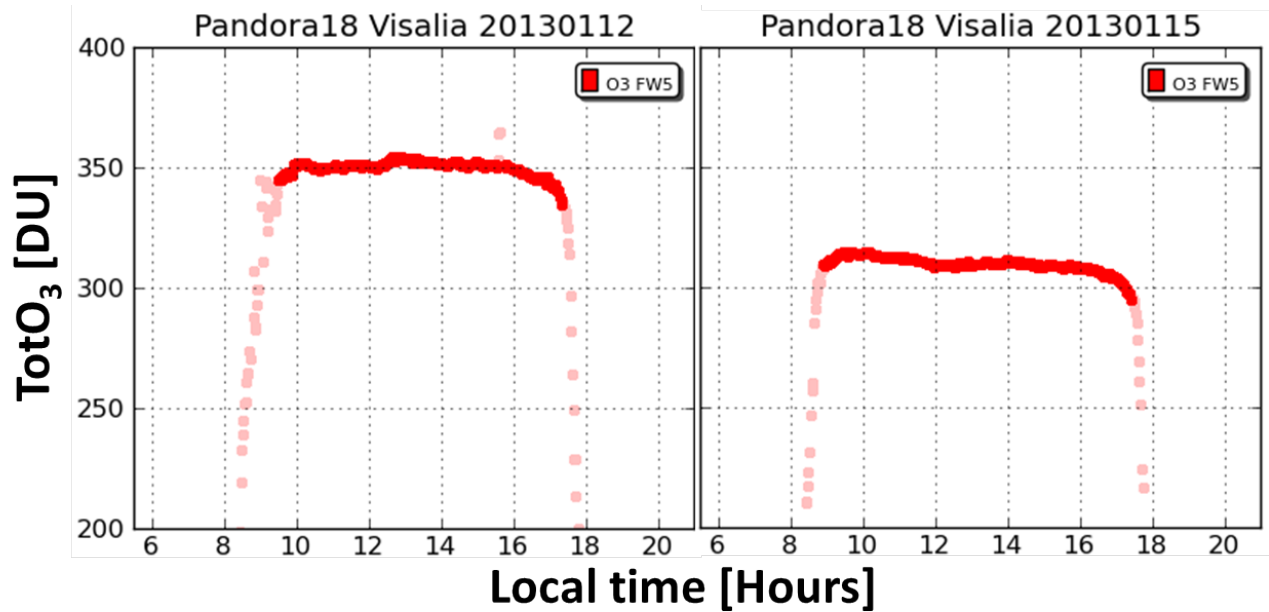


Figure 4: TotO₃ of Pandora 18 for two clear sky days at Visalia, California, USA. Light red data at the beginning and the end of the day have SZA>80° and show data reduction due to spectral stray light. The effect starts for SZA<80°. Taken from *Cede and Tiefengraber* [8].

3.1.5 Optimization of direct sun spectral fitting in the O₃ wavelength range

In addition to the changes mentioned in the previous sections, i.e.

- New cross sections
- Inclusion of TempO₃
- Improved stray light correction

We also plan to optimize the remaining parameters in the Pandora direct sun spectral fitting algorithm. The current algorithm uses a fitting window from 310 to 330nm, a 4th order smoothing polynomial, allows for a wavelength shift and a constant offset. In addition to O₃, it also fits NO₂, formaldehyde (HCHO) and sulfur dioxide (SO₂). These settings have thus far not been optimized, therefore we are currently working on such an optimization using simulated retrievals.

3.2 TropO₃ and StratO₃

3.2.1 Introduction

Splitting TotO₃ into TropO₃ and StratO₃ is a very difficult task. The principle idea is to make so-called 'Elevation scans', i.e. measuring sky radiance at a fixed azimuth for a set of elevation angles. From these measurements one derives the ozone profile by comparing the measurements with RT calculations. One varies the input parameters of the RT calculations (especially the O₃ profile) until the model output agrees sufficiently with the measurements. This is called an inversion algorithm.

3.2.2 Options for inversion algorithm

There are basically two options for the inversion algorithm:

- Compare the measured and modeled sky radiances directly: this is the most direct way of comparison, where no information of the measurements is lost. However it is very sensitive to possible instrumental errors and also requires an inversion algorithm, that is more flexible and time consuming.
- Compare the measured and modeled O_3 slant columns and other auxiliary slant columns (e.g. oxygen dimer (O_2O_2) slant columns as an indicator of the aerosol profile): here it is possible that some information content in the measurements is lost, but this method is less sensitive to possible instrumental errors and allows a faster and simpler inversion algorithm.

An inversion algorithm for O_3 still has to be developed as part of this project. At this stage we assume it will be based on slant columns, i.e. the 2nd method.

3.2.3 Optimization of sky radiance spectral fitting in the O_3 wavelength range

We also plan to optimize the Pandora sky radiance spectral fitting algorithm. For consistency we would prefer to stay as close as possible to the settings for the direct sun spectral fitting (see section 3.1.5), just adding the Ring effect [12], but small adaptations may be needed. We will also test fitting of Temp O_3 in the sky radiances.

3.2.4 Calibration of StatREFI O_3 slant columns

Since no external instrumentation measures absolute O_3 slant columns, we cannot ensure the StatREFIs measure the correct slant columns in a direct way by intercomparison. Instead we will make use of the auxiliary measurements available at CIAI. We will make RT calculations with accurately defined input parameters:

- Temperature profile based on the radio-sondes and surface temperature data
- Ozone profile based on the ozone-sondes, FTIR data, surface O_3 concentrations from in-situ sensors Tot O_3 from Pandora and the Brewer triad
- Aerosol profile based on the Lidar data, aerosol surface concentrations from in-situ sensors, and SpecAOD from Pandora and other sun photometers

We expect the error in the calculated slant columns to be small, especially since the AOD at CIAI is in general very low, which means that uncertainties in the sun photometer or Lidar measurements have a very small effect. Differences between the data and the calculations can of course also be attributed to the RT model. In this sense this comparison is an interesting closure experiment by itself.

3.3 Tot NO_2

3.3.1 Introduction

The Pandora standard technique for the calibration of Tot NO_2 is the Modified Langley Extrapolation (MLE) [11, 13]. So-called 'relative slant columns' are derived by spectral fitting, with one measurement (or the average of several measurements) used as reference spectrum. The slant columns are plotted as a function of the direct sun AMF and a straight line is fitted into the lower envelope of the data (see figure 5).

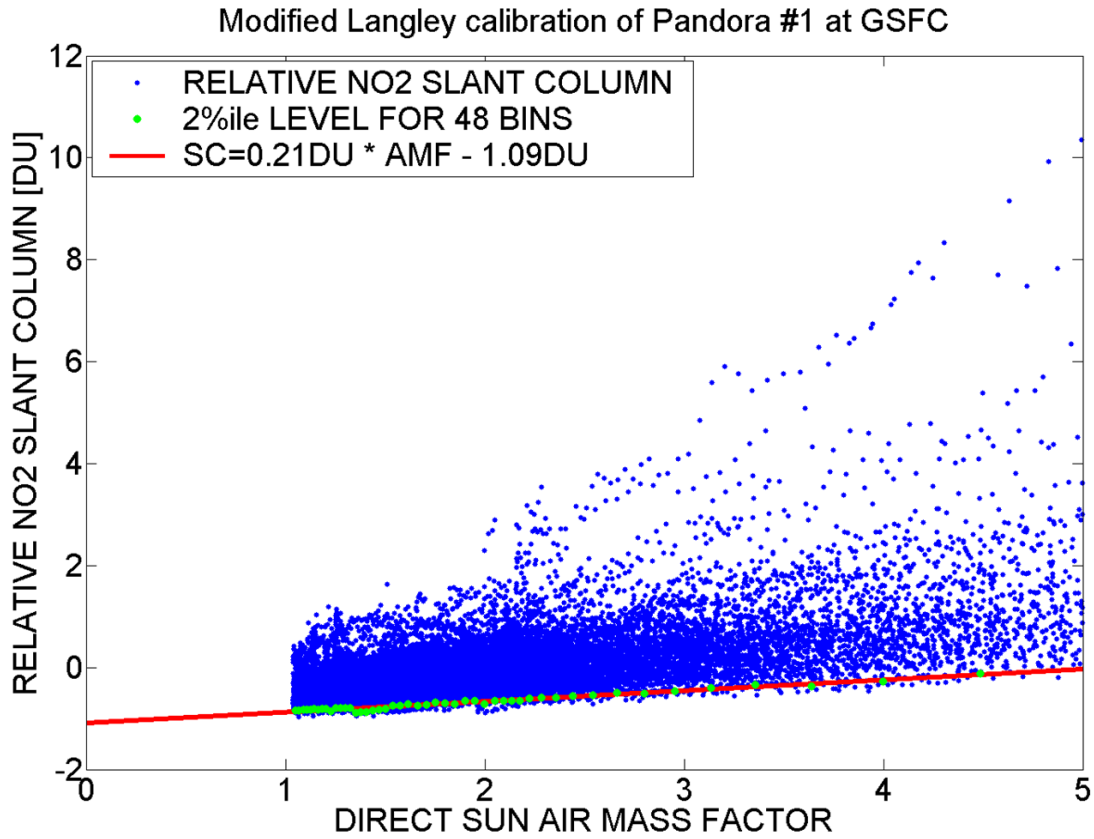


Figure 5: Example of Modified Langley Extrapolation for NO₂ at Goddard Space Flight Center (GSFC). Taken from *Herman et al.* [13].

The assumption of this technique is that even at polluted sites there will be days with hardly any TropNO₂, where the slant columns are determined by the approximately constant StratNO₂. The intercept of the fitted line equals the (negative value) of the initially unknown absolute NO₂ slant column in the reference spectrum and the slope equals the StratNO₂ on these unpolluted days. The major shortcomings of MLE are:

- There may be a lack of days without TropNO₂ over the calibration period. This should not be a problem at CIAI.
- StratNO₂ is not exactly constant and has a seasonal and diurnal cycle [e.g. 19, 25]. This also affects measurements at CIAI.
- A database has to be established before reliable data can be obtained. Depending on the location, this might be a rather long period (>1 month).

In an effort to minimize these shortcomings, we will use a different calibration to get TotNO₂ from the Pandonia StatREFIs.

3.3.2 Langley extrapolation at CIAI

For this project we plan to replace the standard MLE method and adjust for the varying amount of StratNO₂. The daytime StratNO₂ can be approximated by equation 1:

$$\text{StratNO}_2(\text{dd}, t) = \text{StratNO}_2(\text{dd}, 0) + k_{\text{StratNO}_2} \cdot t \quad (1)$$

dd is a given day of the year, t is the time since sunrise, and k_{StratNO_2} is the 'StratNO₂ daytime increasing rate'. StratNO₂(dd,0) varies from about 0.04 Dobson units (DU) in winter to 0.19 DU in summer and k_{StratNO_2} ranges from about 0.001 DU/h to 0.007 DU/h [19]. Assume we would make an MLE with days from an entire year, then the lower envelope of the data as in figure 5 would be only be driven by unpolluted winter data before noon, since those have the smallest StratNO₂. Therefore we make the following two adjustments to the calibration technique:

- Instead of applying MLE for a group of days, we plan to make two Langley extrapolations (morning and afternoon) at each single day. This way the summer data are not neglected and it also allows us to track possible changes in calibration of the StatREFIs.
- We will adjust for the diurnal variation in StratNO₂ in the Langley extrapolations. Neglecting it would lead to an overestimation of the extrapolated intercept (i.e. an underestimation of the NO₂ slant column amount in the reference) of about 0.03 DU. This offset will be reduced by including k_{StratNO_2} , either taking the average value of 0.004 DU/h [19] or even using data from the zenith sky observations at CIAI.

3.3.3 Optimization of direct sun spectral fitting in the NO₂ wavelength range

As for O₃, we plan to optimize the parameters in the Pandora spectral fitting algorithm. The current algorithm uses a fitting window from 400 to 440 nm, the 'Vandaele' NO₂ cross sections [25], a 4th order smoothing polynomial, allows for a wavelength shift and a constant offset. Besides NO₂, it also fits O₃. These settings have never been optimized, but we are currently working on such an optimization using simulated retrievals. We will also test the inclusion of the effective nitrogen dioxide temperature (TempNO₂) in the fitting. No change is planned for the NO₂ cross sections.

3.4 TropNO₂ and StratNO₂

3.4.1 Introduction

Many principles already discussed in section 3.2 also apply here:

- The basic technique is to make sky radiance measurements at different elevations and compare them to RT calculations.
- An inversion algorithm for NO₂ still has to be developed as part of this project and at this stage we assume it will be based on slant columns.
- We plan to optimize the Pandora sky radiance spectral fitting algorithm for NO₂ in a way that it is most consistent with the direct sun spectral fitting, but also considering the recommendations given by *van Roozendaal and Hendrick* [24].
- To ensure the StatREFIs measure the correct NO₂ and O₂O₂ slant columns we will make use of the auxiliary measurements available at CIAI.

The main difference to the principles of section 3.2 is that there are no external measurements (such as NO₂-sondes), which could directly provide the vertical NO₂ profile for the RT calculations.

3.4.2 Calibration of StatREFI NO₂ slant columns

To ensure the StatREFIs measure the correct NO₂ and O₂O₂ slant columns we will make RT calculations using the auxiliary measurements listed in section 3.2.4 plus the following:

- NO₂ profile based on surface NO₂ concentrations from in-situ sensors, TotNO₂ from Pandora, and StratNO₂ from zenith sky observations during twilight

We will compose the NO₂ profile using a technique similar to the one described in *Tiefengraber and Cede* [20]. We count again on the assumption that on most days, there will not be any significant TropNO₂ in the atmosphere at CIAI, which will result in a rather small uncertainty for the composed profile.

3.5 SpecAOD

3.5.1 Introduction

While a change of the Pandora radiometric sensitivity, that is smooth as a function of wavelength, does not have any effect on the O₃ and NO₂ data products, it does affect the SpecAOD retrievals. On the other hand, small spectral signals raising from instrument deficiencies [20] can affect O₃ and NO₂, but have negligible influence on SpecAOD. In this sense SpecAOD sets rather different requirements to Pandonia than the other data products. SpecAOD is a new data product for Pandora instruments and will be developed within the Pandonia project. The following sections discuss important aspects for the calibration of SpecAOD.

3.5.2 Field of view

Figure 6 shows the FOV for Pandoras 2 and 3 with open hole in the filter wheels. It has a full width at half maximum (FWHM) of about 1.5°. The FOV of Pandora 3 has a flat top and varies for less than 1% within $\pm 0.2^\circ$ around the center (as stated in section 2.5, the Pandora pointing accuracy is $\pm 0.2^\circ$). This means that when pointing at the sun the signal varies less than 1% due to small pointing variations. This translates into a variation in SpecAOD of < 0.01 , which is below the uncertainty goal.

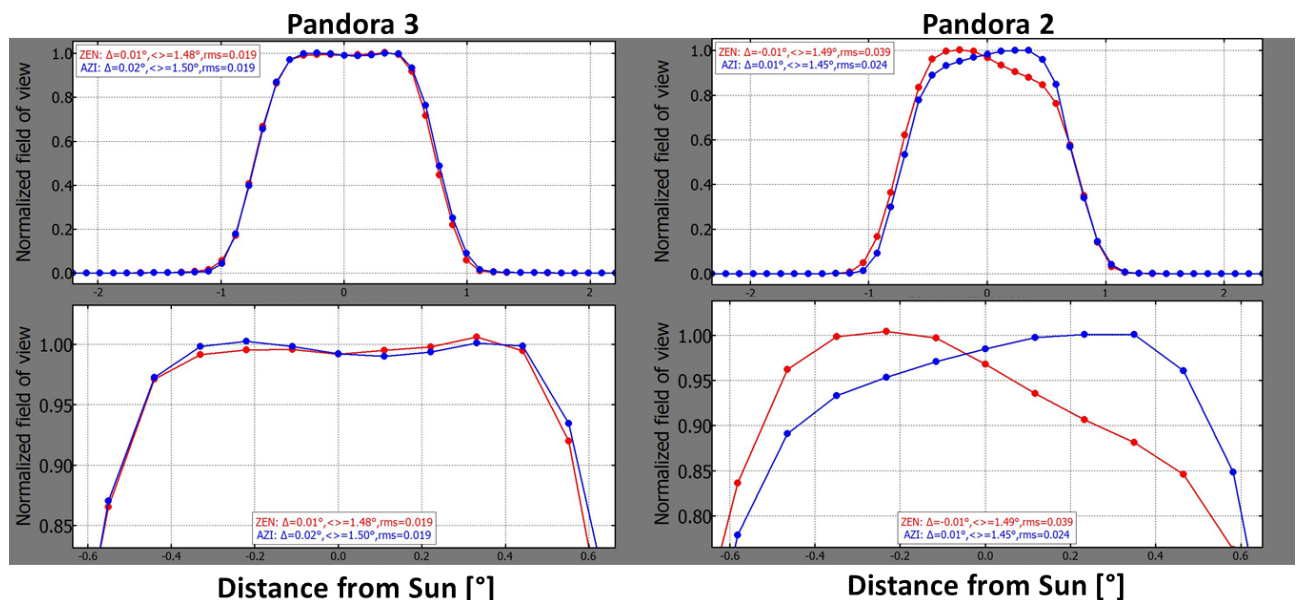


Figure 6: Field of view for Pandora 3 (left) and Pandora 2 (right) measured in zenith (red) and azimuth (blue) directions. Bottom panels are zooms of top panels. No diffuser is placed in the filter wheel.

However the open hole FOV does not always have a totally flat top due to imperfections in the fiber front surface and the fiber connection. The FOV of Pandora 2 e.g. varies for $\pm 4\%$ within $\pm 0.2^\circ$ around the center (figure 6). This translates into a variation in SpecAOD of up to ± 0.04 , which is above the uncertainty goal and is the reason we noticed unsatisfactory results in first tests of AOD retrievals.

Therefore we introduced a change to the Pandora optics adding a ground quartz diffuser in one filter wheel. The aim of this change was to produce a flat top of the FOV, that is not as sensitive to the fiber connection. With the diffuser, the FWHM of the FOV is around 2° (figure 7) and the FOV varies for less than 1% within $\pm 0.2^\circ$ around the center for basically all instruments. We think that this was a key hardware change to allow SpecAOD retrievals with Pandora. Note that the diffuser will only be in used for direct sun observations. When looking at the sky (or the moon) the FWHM of the FOV is still 1.5° .

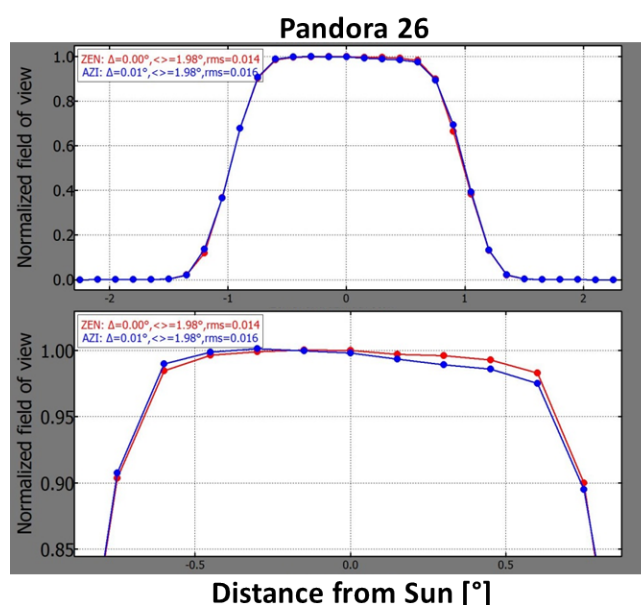


Figure 7: Field of view for Pandora 26 (with diffuser) measured in zenith (red) and azimuth (blue) directions. Bottom panel is zoom of top panel.

3.5.3 Laboratory calibration

One step in the Pandora data correction (see section 2.2) is the 'Conversion to (ir)radiances'. This step is only really needed for SpecAOD and is new to the data correction sequence. We plan to develop a technique to make absolute radiometric calibration in the laboratory using 1000 W FEL lamps. Two laboratories (at CIAI and at the University of Innsbruck) are being upgraded to do such calibration. We are confident being able to do an accurate absolute calibration in the laboratory in that way, but have no experience on how this calibration might transfer to the field as of yet. It is possible that by moving the instrument from the laboratory to the field location, the calibration is not maintained, since there is a very different fiber layout and a fiber disconnection and reconnection involved. Nevertheless, based on our experience using different setups in the laboratory, we expect that this calibration change is affecting the whole spectral range for approximately the same amount at first order. Thus if the calibration changes for 10% at 500 nm, it should also change for about 10% at any other wavelength. This assumption still has to be verified, but if it holds, it would mean that the 'relative radiometric calibration' is invariant. This is nearly more important than the exact absolute calibration, since we can detect a common bias to all wavelengths when we compare Pandora to other instrumentation (see next section).

3.5.4 Radiometric stability

A fundamental part of the SpecAOD calibration is to track the radiometric stability of the StatREFIs at CIAI. We plan to do this in the following way:

- We will do automated Langley extrapolations every day (morning and afternoon). We will do them in the standard way and also in a modified version applying correction terms for changing trace gas amounts and SpecAOD over the day.
- We will check the StatREFIs periodically (at least once a month) using a field calibration tool (see figure 8). This tool contains a 200 W tungsten halogen lamp and will be adapted for use with Pandora within this project.
- The retrieved SpecAOD will be compared with the existing sun photometer data at CIAI at the overlapping wavelengths.

The combination of all three methods listed above should give us excellent information on the stability of the StatREFIs.

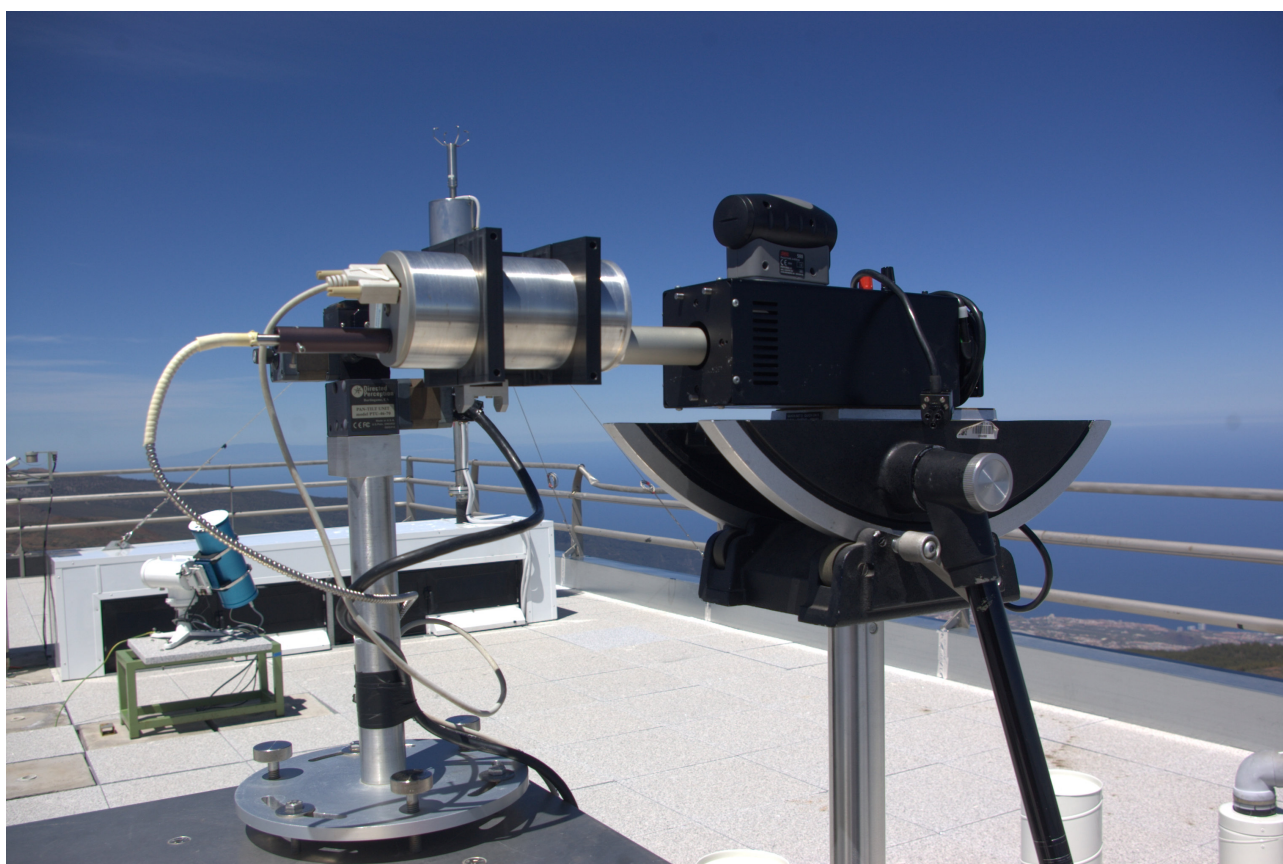


Figure 8: Field calibration tool at CIAI to be adapted for Pandonia. The Pandora head sensor sticks into the black box, which contains a 200 W tungsten halogen lamp.

3.5.5 Stray light

Stray light was already discussed in section 3.1.4 with respect to TotO₃. While only the near field stray light (approximately ± 10 nm around the center) is important for TotO₃ retrievals, the entire stray light, including the far field has influence on SpecAOD. In principle we can fully characterize each instrument for spectral stray

light in the laboratory. However, a deficiency in the Pandora readout electronics does not allow determination of the far field stray light level [9]. This creates a problem for SpecAOD in the ultraviolet (UV), which we plan to address in the following way:

- We have a 'U340 filter' in the filter wheel, which has a peak transmission at 340 nm and cuts off all signal above 380 nm. By placing this filter the stray light is significantly reduced and SpecAOD at 340 nm has a negligible stray light error until SZA=85°.
- We develop a stray light correction based on the near field stray light and use the atmospheric cut-off to estimate the far field stray light level. This means we vary the far field stray light level until the average signal below 290 nm is zero.

3.5.6 SpecAOD algorithm

Developing an algorithm for SpecAOD is an important part of this project. Just like AOD-algorithms for regular filter-sun photometers, the Pandora algorithm will do a Rayleigh correction, for which we will use the formula from *Bodhaine et al.* [4]. Filter instruments do in general not need to correct the measurements for trace gas absorption, since their channels are (on purpose) placed outside of the absorption regions of major absorbers. For the Pandonia SpecAOD algorithm trace gas absorption cannot be neglected and we plan to do a correction for all gases potentially exceeding an optical depth of 0.001 anywhere in the Pandora-2S wavelength range (figure 9).

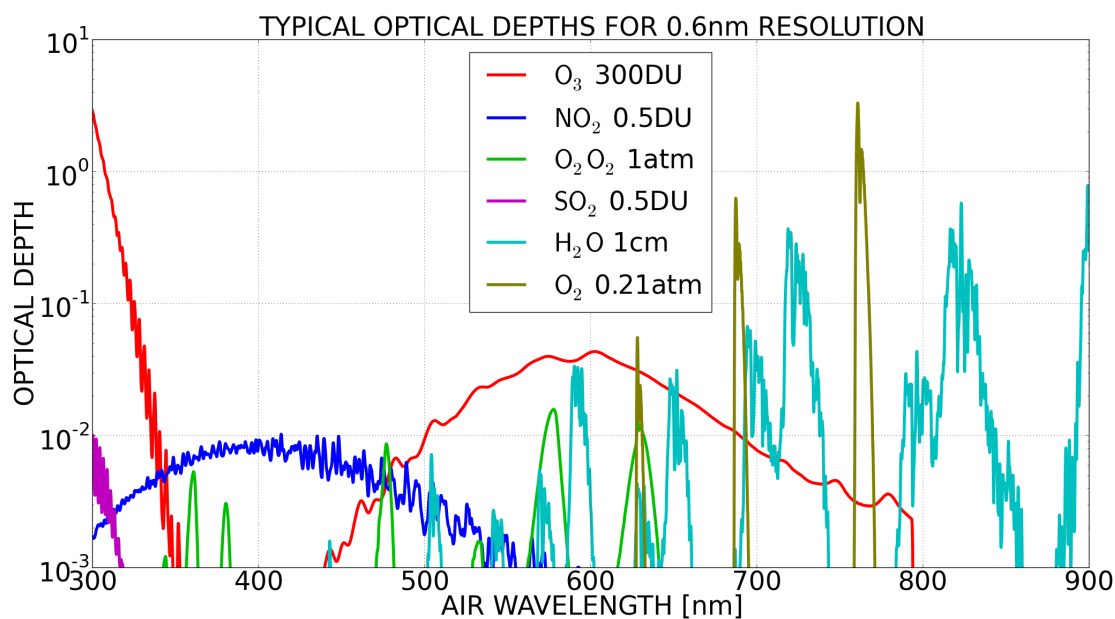


Figure 9: Optical depth for typical trace gas amounts in the Pandora-2S wavelength range. A fixed resolution of 0.6 nm is assumed. Note that the 'cut-off' for O₃ at 800 nm is seen because our cross section database has not been updated above 800 nm yet.

The corrections for O₃, NO₂, and SO₂ will be based on Pandora retrievals. The corrections for O₂O₂ and O₂ will be based on the surface pressure or on Pandora retrievals. The correction for water vapor should be based on Pandora retrievals, but such an algorithm has yet to be determined. Uncertainties in the trace gas correction will in general have a small effect on SpecAOD. E.g. if the column amount of NO₂ is 0.5 DU and

TotNO₂ has an error of 10%, then the maximum error in SpecAOD (at 400 nm) is only about 0.002. There are, however, three exceptions:

- The O₂ optical depth at 760 nm is about 3. So a 1% error causes 0.03 error in the AOD. If this turns out to be a problem one could eventually interpolate the SpecAOD in the 758 to 772 nm range.
- The water vapor (H₂O) optical depth can exceed 1 in some wavelength regions. In these cases a 10% uncertainty in the H₂O correction translates to >0.1 error in the AOD. Therefore an accurate estimation of the total H₂O column is important.
- The O₃ optical depth increases rapidly towards shorter wavelengths. Consequently, the uncertainty in TotO₃ in combination with stray light will also cause the uncertainty in the retrieved SpecAOD to grow rapidly towards shorter UV wavelengths.

4 Calibration of MONIs

4.1 Introduction

It was determined that calibration transfers from the StatREFIs to a MobREFI and from a MobREFI to a MONI shall include at least five clear sky days [7]. Therefore, we recommend an average time for the intercomparison between a MobREFI and a MONI of two weeks. Weather conditions can increase or reduce the number of days needed. MONIs will only be transported if laboratory calibration is required and no proper laboratory is present at the operation site. If the personnel at the monitoring site are well trained, a MobREFI can be sent by mail to the monitoring site, installed, operated by local operators, and then returned by mail. If the local operators are not adequately trained, the MobREFI shall be brought, installed, operated, and returned by network operators.

4.2 Calibration sequence

This is the suggested calibration sequence for Pandonia:

1. The MobREFI is intercompared with the StatREFIs at CIAI for at least 5 clear sky days.
2. The MobREFI is transferred to the MONI location.
3. The MobREFI is intercompared to the MONI for at least 5 clear sky days. Note that the MONI should not be 'treated in a special way' because of the intercomparison. E.g. it should not be 'cleaned more' than during regular monitoring. If maintenance has to be done on the MONI (e.g. tightening the tracker screws), then this maintenance should be done on a 'not-clear sky day' in the middle of the intercomparison, i.e. first 2-3 clear sky days measuring, then maintenance work, then again 2-3 clear sky days measuring.
4. The MobREFI is transferred back to CIAI or to another MONI location. Visiting another MONI location is somewhat risky, since it involves more transportation of the MobREFI, but it may be needed due to logistical reasons.
5. The MobREFI is intercompared with the StatREFIs at CIAI for at least 5 clear sky days.
6. The intercomparisons between the MobREFI and the StatREFIs before (=step 1) and after (=step 5) the visit at the MONI location are analyzed. The MONI calibration is only valid if these intercomparisons agree. Otherwise the whole cycle has to be repeated.
7. The intercomparison between the MobREFI and the MONI is analyzed.

In the case a difference to the previous MONI-calibration is detected, then a new calibration file for the MONI has to be built, and used for future measurements. The MONIs data base should then be analyzed to see whether one can detect a specific moment for the calibrations change. If such a 'sudden calibration change' can be found, one should reprocess the prior data after the applicable date using the new calibration file. If no such sudden calibration change can be found, previous data should be reprocessed with both calibrations (the new and the previous versions) and a weighted average should be applied to the official data product.

The experience accumulated within this project will show, whether one needs to bring a field calibration tool as shown in figure 8 along with the MobREFIs for their trips to the MONI locations. In the case the MobREFI does not agree with the StatREFIs after the calibration cycle, then measurements with the field calibration tool would help to investigate when the change of the MobREFI occurred.

5 Algorithm development

This section gives the current status and an outlook of the algorithm development described in section 3.

5.1 Optimization of fitting windows

Goal: Fitting parameters (starting wavelength, ending wavelength, polynomial order, etc.) shall be optimized for O₃ and NO₂ slant columns.

Affects: TotO₃, TropO₃, StratO₃, TotNO₂, TropNO₂, StratNO₂

Development team: Martin Tiefengraber, Alexander Cede

Technique used: A Pandora (ir)radiance simulator, which includes all instrument characteristics (resolution, optical transmission, noise, stray light, etc.), is used to determine the fitting setup, which produces the smallest uncertainty for each data product.

Current status: The simulator is finished and we are currently running simulations to optimize the retrieval of O₃ and TempO₃.

Plans for 2014: Finish simulations for O₃ and TempO₃.

Plans for 2015: Apply optimized fitting setup for O₃ and TempO₃ to the existing Pandora database and validate results with other data sources. Make simulations for NO₂, apply optimized fitting setup for NO₂ to the existing Pandora database and validate results to other data sources.

5.2 NO₂ profiling algorithm

Goal: The NO₂ vertical profile shall be approximated.

Affects: TropNO₂, StratNO₂

Development team: Elena Spinei (from GSFC), Alexander Cede, Martin Tiefengraber

Technique used: NO₂ and O₂O₂ slant columns from sky observations at different SZAs plus TotNO₂ from direct sun measurements are compared to tabulated results from RT calculations.

Current status: A first version of the algorithm is finished as a separate tool (i.e. not automated and incorporated in the Pandora software).

Plans for 2014: Start incorporating the algorithm in the Pandora software.

Plans for 2015: Finish incorporating the algorithm in the Pandora software, apply it to the existing Pandora database and validate results to other data sources.

5.3 O₃ profiling algorithm

Goal: The O₃ vertical profile shall be approximated.

Affects: TropO₃, StratO₃

Development team: Elena Spinei (from GSFC), Alexander Cede, Martin Tiefengraber

Technique used: O_3 and O_2O_2 slant columns from sky observations at different SZAs plus $TotO_3$ from direct sun measurements are compared to RT calculations in an iterative way using an optimal estimation technique as described by *Rodgers* [17].

Current status: A first version of the algorithm is under development.

Plans for 2014: Finish a first version of the algorithm as an offline tool (i.e. not automated and incorporated in the Pandora software).

Plans for 2015: Incorporate the algorithms in the Pandora software, apply it to the existing Pandora database, and validate results to other data sources.

5.4 SpecAOD algorithm

Goal: Retrieve SpecAOD from measured Pandora direct sun data.

Affects: SpecAOD

Development team: Alexander Cede, Martin Tiefengraber

Technique used: Retrieved optical depths are corrected for molecular scattering and trace gas absorption to obtain SpecAOD.

Current status: The algorithm development has not started yet. The SpecAOD algorithm is straight forward, i.e. there are no mathematical options to be tested, and therefore the development will not take much time. If the instrument is radiometrically stable, SpecAOD will be reliable.

Plans for 2014: Produce AOD at selected wavelengths for some Pandora units and compare them to external data to test the stability of the instruments.

Plans for 2015: Make a operational SpecAOD algorithm, apply it to the existing Pandora database, and validate results to other data sources.