LuftBlick Report 2014004

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

Pandora-2S Design and Evolution Document

	Name	Company	Date
prepared by	Alexander Cede	LuftBlick	9 Sep 2014
	Martin Tiefengraber	LuftBlick	9 Sep 2014
checked by	Katherine Cede	LuftBlick	9 Sep 2014
approved by			

Contents

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1.0	28 Jul 2014	All	Minor changes; correct typos
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Acronyms and Abbreviations

NO_2	Nitrogen dioxide
O_3	Ozone
BP300	Interference bandpass filter with maximum transmission at 300 nm
CCD	Charge coupled device
DIFF	Diffuser
FOV	Field of view
FW	Filterwheel
FWHM	Full width at half maximum
MAXDOAS	Multi-Axes Differential Optical Absorption Spectroscopy
ND filter	Neutral density filter
OPEN	Open hole
Pandonia	ESA Ground-Based Air-Quality Spectrometer Validation Network
Pandora	Pandora spectrometer system
Pandora-2S	Pandora dual spectrometers system
PAZ	pointing azimuth
PZA	Pointing zenith angle
ROE	Readout electronics
SkyFOV	Field of view for sky observations
SkyFOV1	SkyFOV for spectrometer 1
SkyFOV2	SkyFOV for spectrometer 2
Spec1	Pandora-2S spectrometer 1
Spec2	Pandora-2S spectrometer 2
SunFOV	Field of view for direct sun observations
SunFOV1	SunFOV for spectrometer 1
SunFOV12Dist	Distance of the centers of the SunFOV1 and the SunFOV2
SunFOV2	SunFOV for spectrometer 2
SunSkyFOVDist	Distance of the centers of the SunFOV and the SkyFOV
TEC	Temperature control system
U340	Colored glass bandpass filter with maximum transmission at 340 nm

1 Introduction

This report is deliverable D03 of the ESA Ground-Based Air-Quality Spectrometer Validation Network (Pandonia) project [2, 1]. As decided in the project's kick-off meeting, the selected network instrument will be the Pandora dual spectrometers system (Pandora-2S), which is an enhanced version of the existing Pandora spectrometer system (Pandora).

Pandora is composed of an array spectrometer housed in a temperature control box and connected by fiber optics to a telescope. Mounted on a tracker with full azimuth motion and zenith angle 0 to 100° range, Pandora has full direct sun and Multi-Axes Differential Optical Absorption Spectroscopy (MAXDOAS) observation capability. The technology to retrieve total ozone (O_3) columns and total nitrogen dioxide (NO_2) columns from direct sun measurements, as well as NO_2 slant columns from sky radiances by Pandora has already been successfully demonstrated [5, 13, 10, 8, 11, 7, 9, 12, 6].

The current state of design and evolution of Pandora-2S is described here. Each section describes a hardware part of Pandora-2S: section 2 the spectrometers, section 3 the head sensor, section 4 the tracker, section 5 the fiber, and section 6 the temperature controller. Section 7 describes upgrades in the instrument control software needed to run Pandora-2S.

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

[3] A. Cede. *Manual for Pandora Software Suite Version 1.5*, 2012. URL `http://avdc.gsfc.nasa.gov/pub/tools/Pandora/install/PanSoftwareSuite1.5_Manual.pdf`.

[4] A. Cede and M. Tiefengraber. Inter-calibration of ground-based spectrometers and Lidars – Minispectrometer Intercalibration and Satellite Validation, LuftBlick Report 2013003: Mid-term progress Report, 2013.

[5] J. Herman, A. Cede, E. Spinei, G. Mount, M. Tzortziou, and N. Abuhassan. NO_2 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.

[6] T. Knepp et al. Estimating surface NO_2 and SO_2 mixing ratios from fast-response total column observations and potential application to geostationary missions. *Journal of Atmospheric Chemistry*, pages 1–26, 2013. ISSN 0167-7764. doi: 10.1007/s10874-013-9257-6. URL `http://dx.doi.org/10.1007/s10874-013-9257-6`.

[7] G. Pinardi et al. MAX-DOAS formaldehyde slant column measurements during CINDI: intercomparison and analysis improvement. *Atmospheric Measurement Techniques*, 6(1), 2013.

[8] A. J. M. Piters et al. The Cabauw Intercomparison campaign for Nitrogen Dioxide measuring Instruments (CINDI): design, execution, and early results. *Atmospheric Measurement Techniques*, 5:457–485, 2012.

[9] A. J. Reed, A. M. Thompson, D. E. Kollonige, D. K. Martins, M. A. Tzortziou, J. R. Herman, T. A. Berkoff, N. K. Abuhassan, and A. Cede. Effects of local meteorology and aerosols on ozone and nitrogen dioxide retrievals from OMI and pandora spectrometers in Maryland, USA during DISCOVER-AQ 2011. *Journal of Atmospheric Chemistry*, pages 1–28, 2013.

[10] H. K. Roscoe et al. Intercomparison of slant column measurements of NO_2 and O_4 by MAX-DOAS and zenith-sky UV and visible spectrometers. *Atmospheric Measurement Techniques Discussions*, 3(4): 3383–3423, 2010.

[11] M. Tzortziou, J. R. Herman, A. Cede, and N. Abuhassan. High precision, absolute total column ozone measurements from the Pandora spectrometer system: Comparisons with data from a Brewer double monochromator and Aura OMI. *Journal of Geophysical Research (Atmospheres)*, 117:D16303, August 2012. doi: 10.1029/2012JD017814.

[12] M. Tzortziou, J. R. Herman, A. Cede, C. P. Loughner, N. Abuhassan, and S. Naik. Spatial and temporal variability of ozone and nitrogen dioxide over a major urban estuarine ecosystem. *Journal of Atmospheric Chemistry*, pages 1–23, 2013. ISSN 0167-7764. doi: 10.1007/s10874-013-9255-8. URL `http://dx.doi.org/10.1007/s10874-013-9255-8`.

[13] S. Wang, T. J. Pongetti, S. P. Sander, E. Spinei, G. H. Mount, A. Cede, and J. Herman. Direct Sun measurements of NO_2 column abundances from Table Mountain, California: Intercomparison of low-and high-resolution spectrometers. *Journal of Geophysical Research (Atmospheres)*, 115(D13), 2010.

2 Spectrometer

2.1 Pandora spectrometer

The standard spectrometer used in Pandora is the AvaSpec-ULS2048x64 (`http://avantes.com/products/spectrometers/sensline/item/817-avaspec-uls2048x64`). The detector of this minispectrometer is the Hamamatsu image sensor S11071-1106 (`http://www.hamamatsu.com/jp/en/product/alpha/C/4206/4214/S11071-1106/index.html`), a non-cooled back-thinned CCD with 2048x64 effective pixels and a total size of 29 mm wide and 1 mm high. The detector is driven by readout electronics (ROE) made by Avantes, where the 64 CCD-rows are binned, so that a 2048 elements array of data is returned at each measurement. This detector has a quantum efficiency above 50 % for the entire wavelength range 200 to 900 nm.

The optical bench is a Symmetrical Czerny-Turner design with 75 mm focal length. Equipped with a 1200 lines/mm holographic grating, which is blazed at 250 nm, and a 50 μm wide slit, it has a wavelength range from 280 to 530 nm, a step of 0.13 nm per pixel, and a resolution of about 0.6 nm (figure 1). The slit function is symmetric (figure 2) and varies little over the entire wavelength range (figure 1). The temperature dependence of the dispersion is less than 10 pm/°C and no significant change in resolution with temperature is seen.

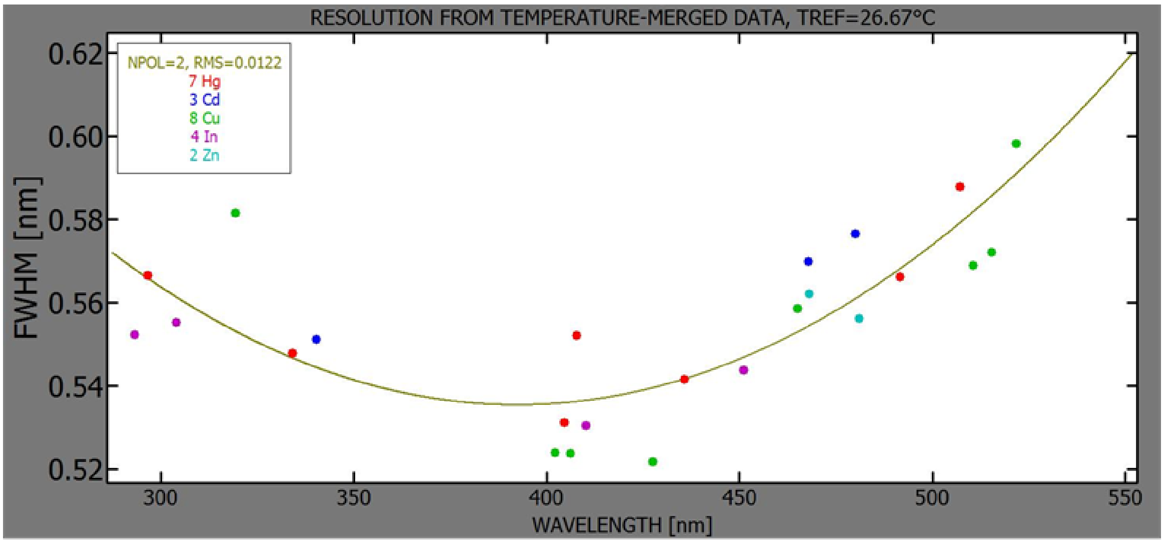

Figure 1: Resolution of a typical Pandora. Dots are the FWHM of the slit functions measured with mercury, cadmium, copper, indium, and zinc lamps (see legend) as a function of wavelength. Line is a 2nd order polynomial fit in the data.

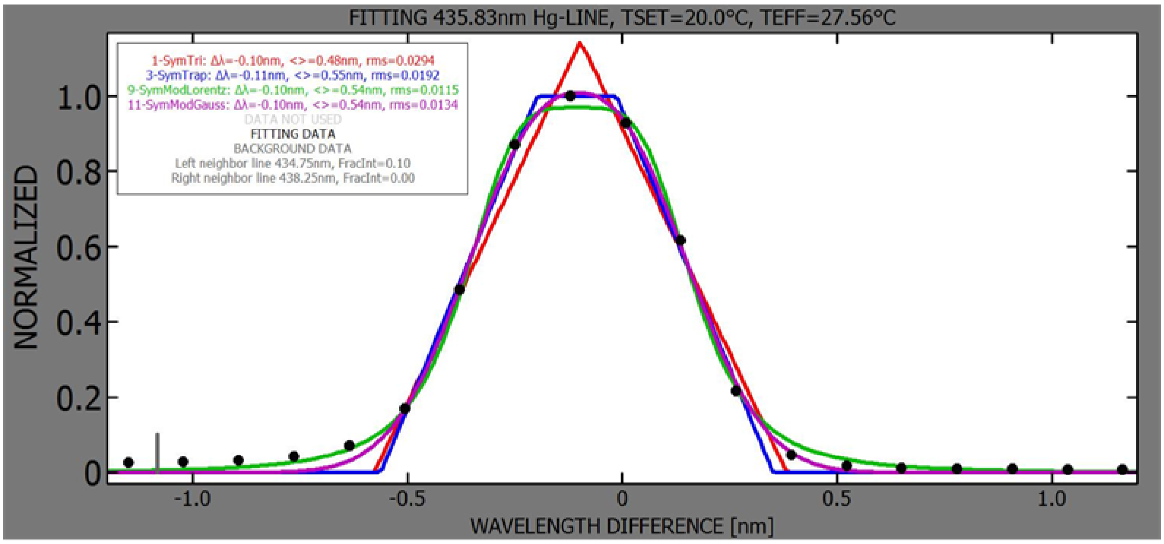

Figure 2: Slit function of a typical Pandora for the 436 nm mercury line. Black dots are measurements and colored lines are fitted mathematical functions.

2.2 Pandora-2S spectrometers

Pandora-2S will include two spectrometers. Pandora-2S spectrometer 1 (Spec1) has the same configuration as the spectrometer in Pandora. Pandora-2S spectrometer 2 (Spec2) will have the same optical bench and detector as Spec1, but will be equipped with a 600 lines/mm grating, which is blazed at 500 nm. The slit width is also 50 μm and the wavelength range goes from 380 to 900 nm. This gives a step of 0.25 nm per pixel and a resolution of about 1.1 nm. We have tested this configuration on a unit with similar settings, with a wavelength range shifted to lower values (280-800 nm instead of 380-900 nm). The slit function was symmetric (figure 3) and varied little over the entire wavelength range (figure 4). As for Spec1, the temperature dependence of the dispersion was less than 10 pm/°C and no significant change in resolution with temperature was seen.

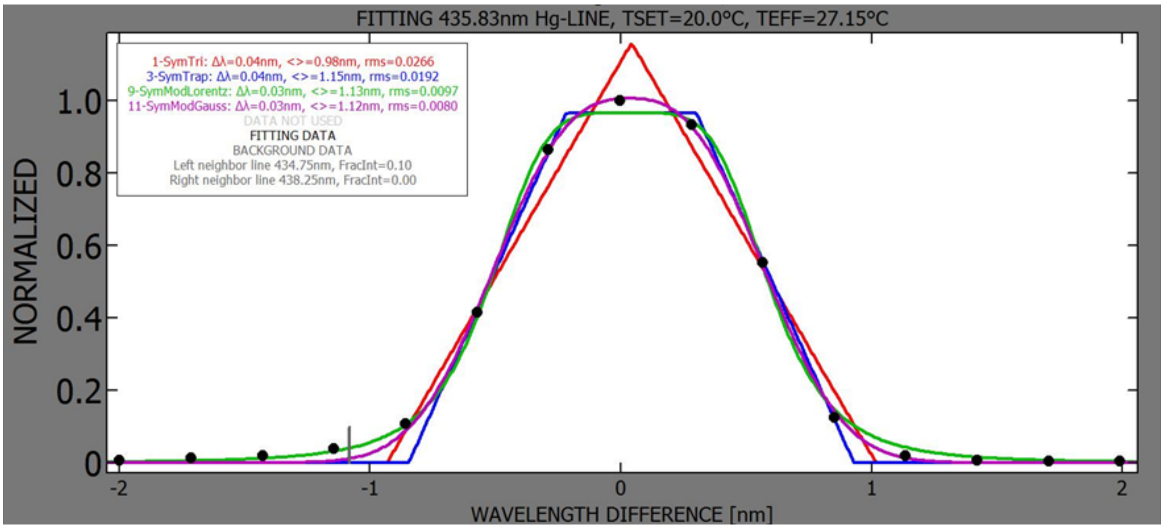

Figure 3: Slit function of a spectrometer configured similarly to Spec2 of Pandora-2S for the 436 nm mercury line. Black dots are measurements and colored lines are fitted mathematical functions.

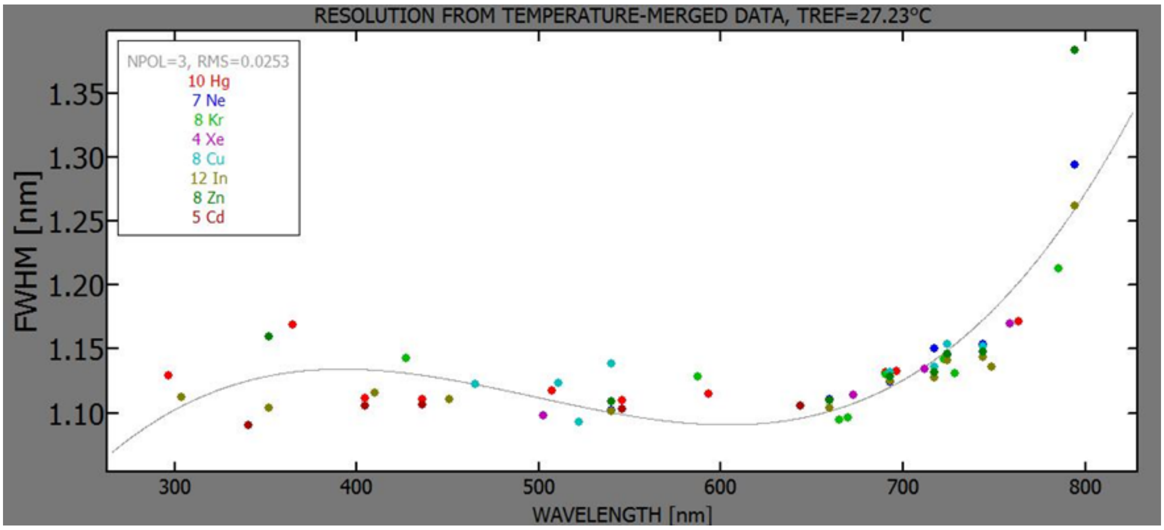

Figure 4: Resolution of a spectrometer configured similarly to Spec2 of Pandora-2S. Dots are the FWHM of the slit functions measured with mercury, neon, krypton, xenon, copper, indium, zinc, and cadmium lamps (see legend) as a function of wavelength. Line is a 3rd order polynomial fit in the data.

While we are very pleased with the overall optical performance of the Avantes spectrometers, we have been experiencing systematic issues in the quality of the Pandora spectra, which might be related to the Avantes ROE in the form of:

1. temporary enhanced scatter in the data as described in section 3.3 of *Cede and Tiefengraber* [4].
2. temporary additional spectral signal in the data as described in section 3.3 of *Cede and Tiefengraber* [4].
3. dark offset is dependent on illumination, which should not be the case (see figure 5).

Item 3 may be attributed to the Avantes ROE; possibly items 1 and 2 as well. While exploring other potential providers for the ROE, we have found a better performing ROE from JETI (`http://www.jeti.com/cms/`) and observed that the key element for good ROE is a CCD mounted directly on the main electronics board or at least a smaller auxiliary electronics board, which is then connected to the main board by a data line. In the Avantes ROE setup, a data line is used between the CCD and the board probably causing the problematic features described above. At this time the superior performing Jeti ROE is too large to fit within the provided Avantes optical bench. Since the mandatory data products of Pandonia are hardly affected by this issue, we will continue using the current hardware, until we possibly find a better solution in the future.

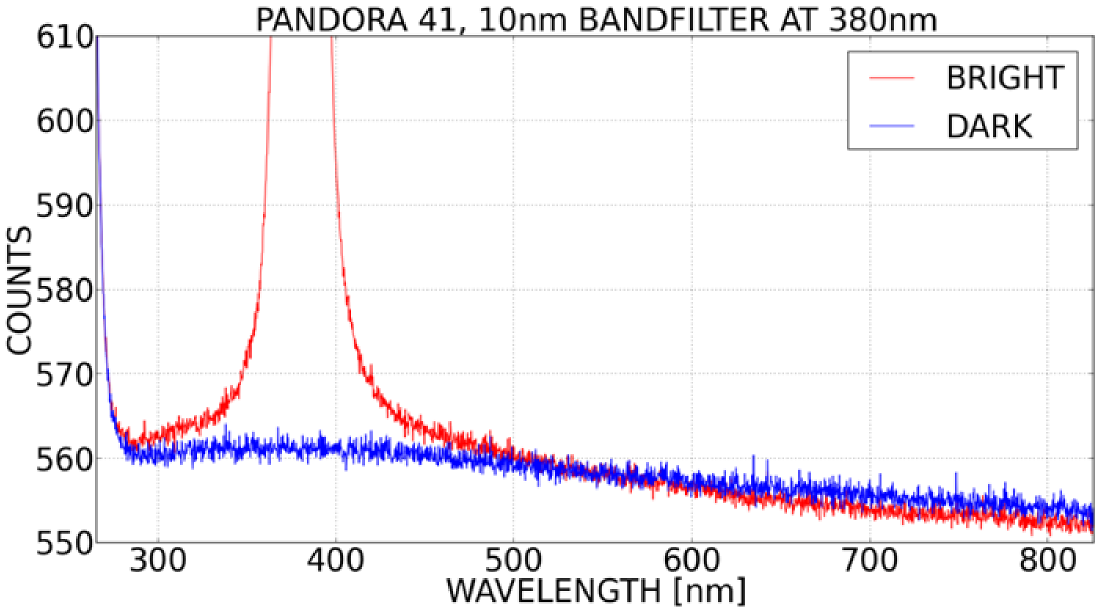

Figure 5: Measurements of a spectrally narrow signal with a Spec2-like spectrometer. Red line is the signal with light, blue line is the dark signal. Due to issues with the dark offset, the dark signal is larger than the bright signal above 500 nm. This makes a stray light calibration impossible.

3 Head sensor

3.1 Pandora head sensor

The Pandora head sensor is shown in figure 6. The light enters through a collimator tube, passes the flat fused silica entrance window, passes the two filterwheels (FWs) with nine positions each, and reaches the fused-silica plano-convex lens, which focuses the photons on the fiber. The standard settings for the FWs are shown in figure 7. For direct sun observations, FW 1 is positioned at DIFF, U340+DIFF or BP300, while for sky observations the options are OPEN or U340. FW 2 is OPEN for sky measurements and uses an appropriate ND filter for direct sun observations.

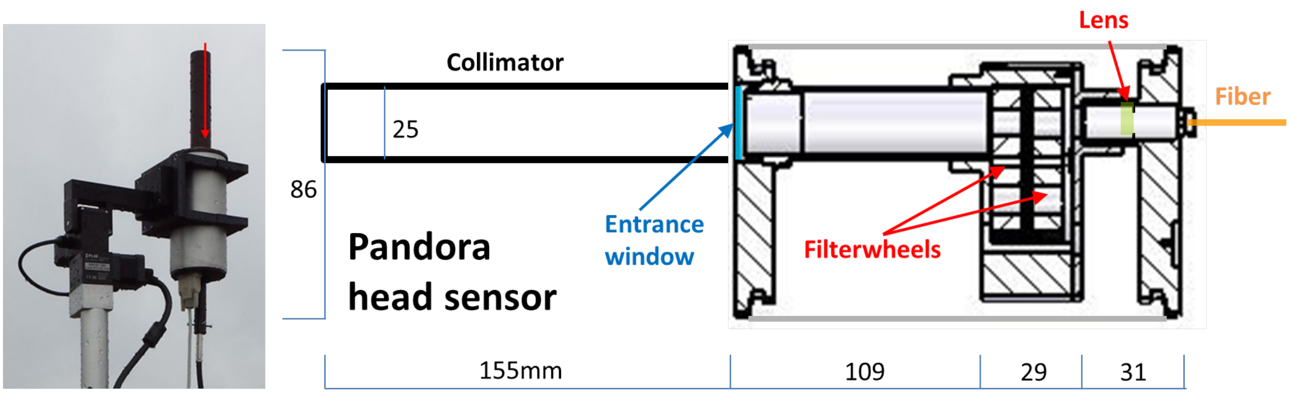

Figure 6: Left panel: Picture of Pandora head sensor pointing upwards and mounted on the tracker. Red arrow shows the direction of incoming light. Right panel: Schematics of Pandora head sensor. Entrance quartz window is in blue. Fused silica plano-convex lens in green. Single core fiber in orange. Dimensions are in mm.

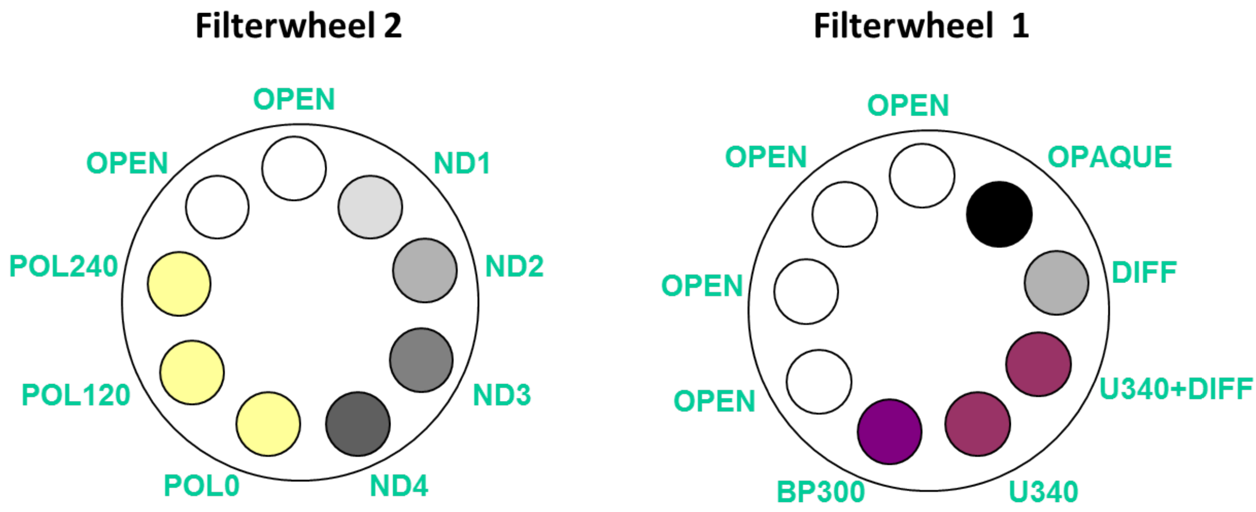

Figure 7: FW settings for the standard Pandora configuration. OPEN is an open hole. ND1 to ND4 are neutral density filters. POL are optional linear polarizers. DIFF is a ground quartz diffuser. U340 is a colored glass bandpass filter with maximum transmission at 340 nm. BP300 is an interference bandpass filter with maximum transmission at 300 nm.

3.2 Pandora-2S head sensor

The Pandora-2S head sensor will have two optical paths included: There will be two collimators, two entrance windows, two lenses and two fiber ports. The paths are designed with 4 FW-positions between them. If the optical path of Spec1 passes position 1 (2, 3, 4, 5, 6, 7, 8, 9) of a FW, then the optical path of Spec2 passes at the same time position 5 (6, 7, 8, 9, 1, 2, 3, 4). This requires the FW-settings to be coordinated (see figure 8). Here we assume that Spec1 has in general less light input than Spec2. Therefore we are including e.g. the option to measure Spec1 at OPEN and Spec2 at ND1, but not the opposite.

Another change in the Pandora-2S head sensor is that the power and transmission connection will be changed from the current RS232 cable to the connector, which has improved weather resistance thus preventing corrosion of the surrounding metal components eg. connector pins. The most likely choice of connector is the Amphenol Industrial PT06E-12-10P (see e.g. `http://ex-en.alliedelec.com/search/productdetail.aspx?SKU=70011061`).

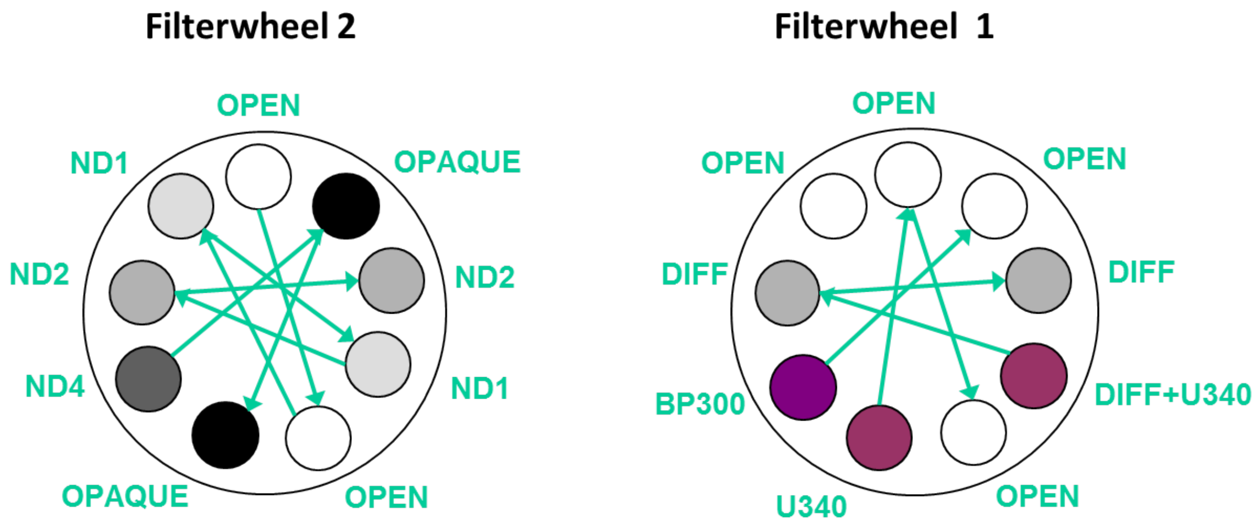

Figure 8: Planned FW settings for Pandora-2S. The filter names are as in figure 7. The green arrows indicate 'useful' combinations. For a given FW-position of Spec1, the arrow points to the position for Spec2.

4 Tracker

Pandora-2S will use the same tracker as Pandora, which is Pan-Tilt Unit-D46-70 from FLIR Motion Control Systems, Inc. (`http://www.flir.com/mcs/view/?id=53712`). The main disadvantages of the current Pandora tracker are:

- The gears loosen over time, thus requiring periodic maintenance.
- It uses stepper motors without optical encoders, which means it does not 'notice' if steps are lost during the positioning.

Independently of this project, Pandora manufacturer SciGlob Instruments and Services (`http://sciglob.com/`) is currently developing an improved tracker. Once their new tracker is finished we will also use it for the instruments in this project.

5 Fiber

5.1 Pandora fiber

Pandora uses a 400 μm core and 440 μm clad diameter single strand fused silica fiber with a silicone jacket and SMA connectors on both ends. The numerical aperture of the fiber is 0.22 and the fiber length can vary from 3 m to 20 m, typically 10 m.

5.2 Pandora-2S fiber

Pandora-2S will use two separate fibers, one for each spectrometer. We have tested fibers with larger diameter (up to 1000 μm core diameter) and could verify that the throughput increases approximately linearly with the diameter as expected. The increased throughput would certainly be an advantage for sky observations, where we have rather low light input. However an increased fiber diameter also has disadvantages:

- The focal length of the lens must be modified, which requires a change of the length of the head sensor.
- The minimum bend radius (typically 40 times the core diameter) increases. Therefore it is harder to pack the fiber and also there is more risk to over-bend and break it.

A final decision on the best choice of fiber diameter has not yet been made.

6 Temperature controller

6.1 Pandora temperature controller

The Pandora spectrometer is temperature controlled by a bi-polar (heat and cool) proportional-integral-derivative temperature controller drawing currents of up to 25 A. The temperature control system (TEC) used is model TC-36-25-RS232 from TE Technology, Inc. (https://tetech.com/products/tc-36-25-rs232/). This system includes two temperature sensors. Sensor 1 is used for the temperature control and sits on the Peltier element (blue data in figure 9). Sensor 2 gives auxiliary temperature information and is placed inside the optical bench (green data in figure 9). The control temperature for Pandora is typically 15 °C.

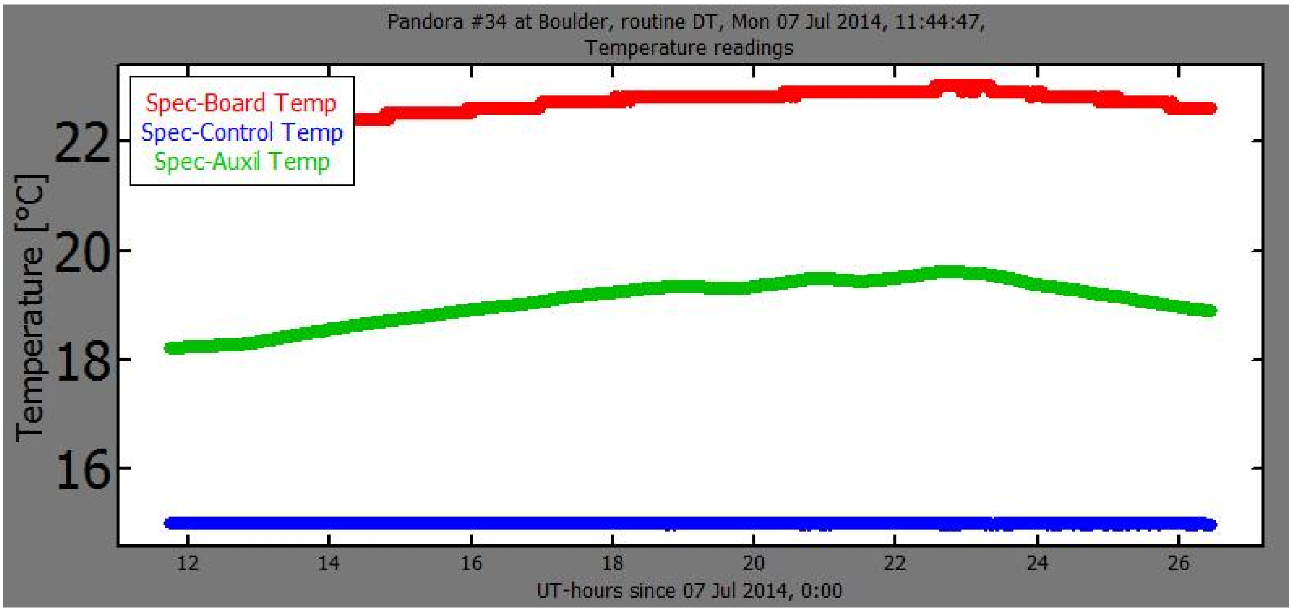

Figure 9: Measured temperatures of Pandora 34 on 7-Jul-2014 as a typical temperature behavior of Pandora. The control temperature (blue, measured by the TEC) is stable at 15 °C. The temperatures on the optical bench (green, measured by the TEC) and on the ROE (red, measured by the ROE) are a few degrees higher and vary for about 1.5 °C over the day.

6.2 Pandora-2S temperature controller

Initial tests with a Pandora-2S prototype indicate that the same TEC can be used to control both spectrometers of Pandora-2S, if the two units are packed appropriately. As of this writing, extreme temperature situations have not been tested; therefore, a decision on the exact method of temperature control is yet to be finalized.

7 Instrument control software

7.1 Pandora operating software

The Pandora operating software [3] reads the instrument operation file, connects to the instrument hardware, changes filterwheel positions, moves the tracker, operates the camera, controls the temperature box, takes spectroscopic measurements, saves the raw signals, and provides a graphical interface for the user to display current data and operate Pandora (figure 10). The software is written in the open source programming language Python (`http://python.org/`) and the current official version is 1.5.

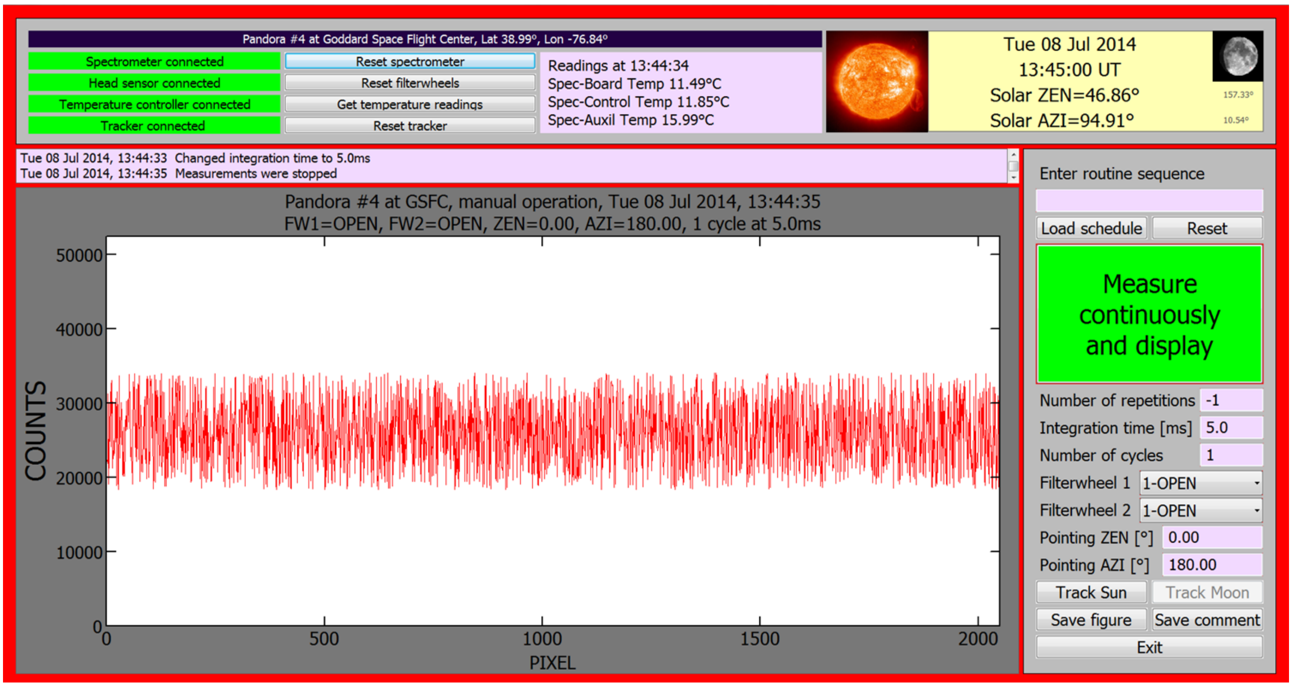

Figure 10: Screen shot of Pandora operating software [3].

7.2 Pandora-2S operating software

The operating software for Pandora-2S needs to be able to simultaneously run two spectrometers and possibly two temperature controllers. A prototype of this software has already been started and tested. The design is based on the Pandora operating software, with modified controls on the interface to deal with the additional hardware (figure 11).

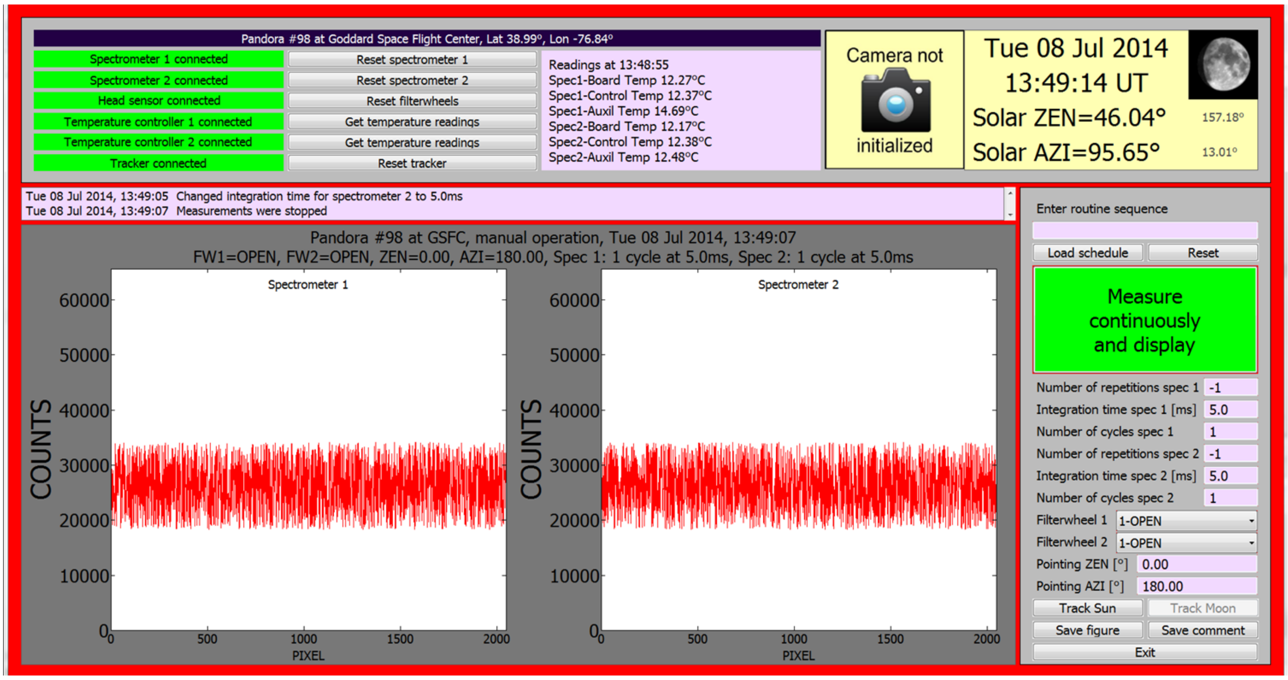

Figure 11: Screen shot of Pandora-2S operating software prototype.

8 Optical alignment

A critical issue for Pandora-2S is the co-alignment of the two optical paths. We require that when Spec1 points to a specific position in the sky, also Spec2 points to the same position within a certain tolerance. In other words the centers of the fields of view (FOVs) of Spec1 and Spec2 should overlap closely. This section describes the optical alignment procedure for Pandora and the plan for Pandora-2S.

8.1 Optical alignment Pandora

Pandora has actually two separate FOVs, one for direct sun observations (SunFOV) and one for sky observations (SkyFOV). The FWHM of the SunFOV is about 2° and is determined by the diameter of the aperture on top of the collimator, the diameter of the aperture behind the diffuser, and the distance of these two apertures (figures 12 and 13). The FWHM of the SkyFOV is about 1.5° and is determined by the diameter of the fiber and the distance between lens and fiber, which equals the focal length of the fiber at 350 nm.

If the centers of the aperture on top of the collimator, of the aperture behind the diffuser, of the lens, and of the fiber are not perfectly aligned along a straight line, then the centers of the SkyFOV and the SunFOV will not be the same. In order to align them, we use the fiber connector at the back of the head sensor, which can be tilted for a few degrees and also shifted for about 1 mm in each direction relative to the central position. The current procedure to co-align the SunFOV and the SkyFOV of a Pandora is an iterative process to minimize the distance of the centers of the SunFOV and the SkyFOV (SunSkyFOVDist). The fiber connector is fixed in a certain position and SunSkyFOVDist is measured in the laboratory. Then the position of the fiber connector is changed until SunSkyFOVDist is minimized. Our experience has shown that SunSkyFOVDist without the above described adjustment process can be as much as 0.4°. After adjustment we reach SunSkyFOVDist <0.2°, which is our tolerance. In most cases we obtain SunSkyFOVDist <0.1°.

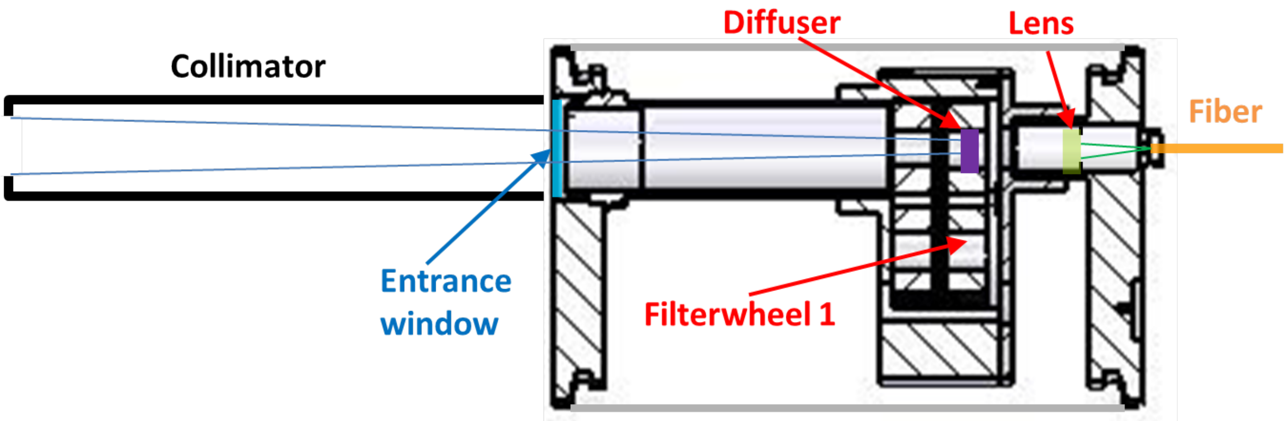

Figure 12: Schematics of the Pandora head sensor as in figure 6. The SunFOV is determined by the aperture on top of the collimator and the aperture behing the diffuser (see thin blue lines). The SkyFOV is determined by the focal length of the lend and the diameter of the fiber (see thin green lines).

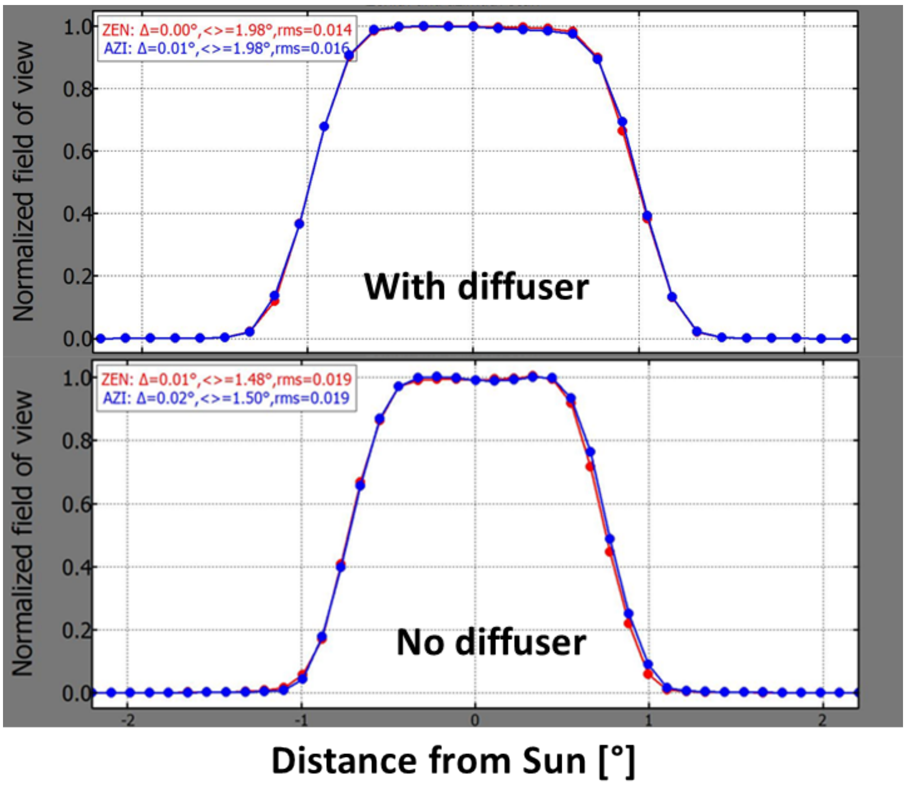

Figure 13: FOV of Pandora 26 with the diffuser in the filterwheel (SunFOV, top) and without diffuser (SkyFOV, bottom). Note that this is measured using the Sun. Therefore it is convoluted with the 0.5° direct sun beam and the slopes on each side are 2/°. The true, unconvoluted FOV has much steeper slopes.

Due to the small SunSkyFOVDist, it is possible to determine only one set of 'leveling angles' for a Pandora at a specific location. The leveling angles say how much the instrument is inclined relative to a perfectly horizontal position and are determined during the first days at a site (see appendix I of *Cede* [3] for details). Currently we determine the leveling angles using the SkyFOV only. This means that Pandora is pointing to the correct position in the sky, but has an offset of SunSkyFOVDist when pointing at the sun. However since the SunFOV has a flat top for a region of ±0.5° (see figure 13), this offset does not matter.

8.2 Optical alignment Pandora-2S

Pandora-2S will have four FOVs. The SunFOV for Spec1 and Spec2 (SunFOV1 and SunFOV2) and the Sky-FOV for each spectrometer (SkyFOV1 and SkyFOV2). We can align the SkyFOV towards the SunFOV of each spectrometer individually with the technique described in the previous section, but this does not necessarily mean that the co-alignment of SunFOV1 and SunFOV2 is also given. Out planned procedure for the co-alignment is as follows:

- Measure the distance of the centers of SunFOV1 and SunFOV2 (SunFOV12Dist) in the field. This cannot be done in the laboratory, since the optical paths are at a spatial distance to each other.
- If SunFOV12Dist is above the tolerance (0.3°), then the head sensor has to be checked and possibly the apertures shifted.
- Align SkyFOV1 to SunFOV1 and SkyFOV2 to SunFOV2 respectively using the technique outlined in the previous section.

We have reason to believe that SunFOV12Dist is below or close to the tolerance to begin with in most cases. When a regular Pandora is aligned in the field, the first step is a rough alignment using the external sun pointer (see figure 14). After the projection of the sun beam is centered on the target, the alignment is checked by scanning the sun, i.e. obtaining a graph as shown in figure 13. We noticed that in most cases the center of the FOV is within 0.3°.

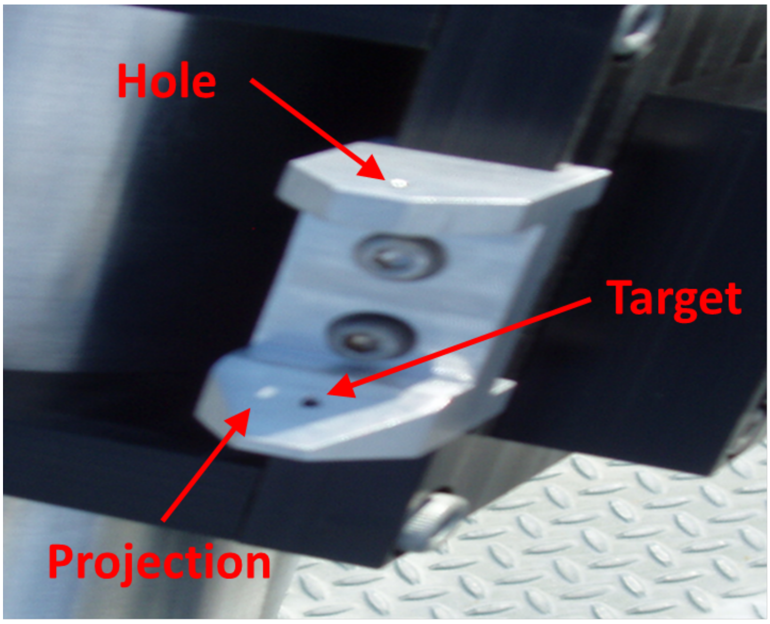

Figure 14: External sun pointer attached to the head sensor. When pointing to the sun the projection of the sun beam should fall on top of the target.

The Pandora-2S alignment technique also requires changes in the operating software:

- A field calibration routine to determine the relative offsets of all fours FOVs has to be written.

- The instrument operation file has to be modified to include an entry with the obtained offsets.
- The operation software has to determine the leveling angles based on the mean offset over all four FOVs.
- The software has to write different pointing angles for Spec1 and Spec2 in the raw data file.

The main consequence of this is that if the user sets Pandora-2S to point to a certain position in the sky (e.g. pointing zenith angle (PZA) 80.0° and pointing azimuth (PAZ) 180.0°), then the true pointing angles (and the numbers written in the raw data file) for Spec1 and Spec2 will be slightly difference, e.g. PZA=80.11°, PAZ=179.97° for Spec1 and PZA=79.94°, PAZ=180.20° for Spec2. This possibly requires some flexibility in the algorithms to retrieve trace gas profiles from Pandora-2S sky observations.

9 Schedule

This section gives an overview of the current status and the planned schedule for Pandora-2S. At this stage we still expect the Pandora-2S prototype to be delivered in 2014. The item 'Plans for 2015' lists planned actions in addition to the 'default action', which is to test the Pandora-2S prototype in laboratory and field. Note that these planned actions are done outside of this project by LuftBlick and SciGlob, but will potentially benefit the project.

9.1 Pandora-2S spectrometers

Development team: SciGlob, Alexander Cede, Martin Tiefengraber

Current status: The spectrometers are finished and the packing into the temperature controller has been designed.

Plans for 2014: Pack the spectrometers into the new temperature control system.

Plans for 2015: Investigate new options for the detector, optical bench, and ROE.

9.2 Pandora-2S head sensor

Development team: SciGlob, Alexander Cede

Current status: The Pandora-2S head sensor has been built. The co-alignment of the optics for Spec1 and Spec2 is being tested.

Plans for 2014: Finish the head sensor alignment.

Plans for 2015: Reconsider the option of including a camera in the head sensor by default.

9.3 Pandora-2S tracker

Development team: SciGlob, Alexander Cede

Current status: The tracker is finished.

Plans for 2014: None

Plans for 2015: SciGlob builds and tests a prototype of the new tracker.

9.4 Pandora-2S temperature controller

Development team: SciGlob, Alexander Cede

Current status: The temperature controller is finished.

Plans for 2014: Pack the spectrometers into the new temperature control system and test the performance in the field.

Plans for 2015: None

9.5 Pandora-2S software

Development team: Alexander Cede, Marc Schwärz, Martin Tiefengraber

Current status: The software of Pandora-2S has been started.

Plans for 2014: Finish a first version of the Pandora-2S operation software.

Plans for 2015: Make a first version of the complete software for Pandora-2S (i.e. operation software, processing software, analysis software, etc.).