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SPEXone, the multi-angle spectropolarimeter for PACE, adjusted and improved for new space applications

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ABSTRACT

Aerosol quantification is of paramount importance for climate research, health and many other fields. The best method for measuring and characterizing aerosol from space is the application of a multi-angle polarimeter. A Dutch consortium has developed and delivered the so called SPEXone instrument for the NASA PACE (Plankton, Aerosol, Cloud, ocean Ecosystem) mission, to be launched early 2024.

SPEXone is based on the polarization modulation of the spectrum, allowing full characterization of the state of linear polarization of the incoming light. Earth is viewed under five angles, producing ten modulated spectra, projected on a single detector. A polarimetric accuracy of 0.3% is achieved, with the instrument of about 10 dm^3 volume and 10 kg mass.

Based on the SPEXone design and experience, an upgraded instrument is being developed. Main change is the wider swath applied, from the 100 km swath for PACE to the present 250 km. This impacts the five telescopes, being integrated in one telescope unit.

Other changes in the design are based on lessons learned, in particular the reduction and avoidance of stray light. The detector readout is adjusted for higher frame rate and more robust readout. These changes do not impact the instrument's budgets for mass, volume and power.

In this paper, we will explain the principle of the SPEXone multi-angle spectropolarimeter instrument, the improvements with respect to the PACE version and its development status. The instrument can be flown as a stand-alone instrument for aerosol detection, as well as a support instrument where aerosol corrections are relevant, e.g., for high accuracy detection and quantification of methane and CO_2.

Keywords: Earth Observation satellite, aerosol, CO_2, spectropolarimetry, spectral modulation, telescope, stray light, SPEXone.

1. INTRODUCTION

Aerosol quantification is of paramount importance for climate research, air quality and health and many other fields. In climate research, the contribution of atmospheric aerosol presently has the largest uncertainty [1]. Climate change due to atmospheric aerosols is determined by the kind and size of aerosol, its altitude, the time of day etc. Aerosol has a double role in the Earth atmosphere: the direct absorption and scatter of light by aerosol, as well as an indirect effect as condensation nuclei for water vapor, and thus as an initiator in cloud formation. In addition to its direct and indirect effects on the climate, detailed knowledge of aerosol is required when very accurate measurements are taken from space e.g. CO_2 [2][3]. It is commonly known that CO_2 is the main driver of the current climate change. Because the gas is practically inert in the Earth atmosphere, it is very well mixed. To learn about the sources and sinks of CO_2, very accurate global measurements are needed, well below 1 ppm, on an average atmospheric concentration of about 420 ppm CO_2 [4]. Reaching this 10^{-3} accuracy level is the major

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challenge of the present satellite-based CO_2 sensors. Essential in accurate trace-gas retrieval is the detailed knowledge of the light path between the sun and the sensor. Ideally, the light goes through the atmosphere, is reflected by the Earth surface, travels back through the atmosphere and is detected by the satellite spectrometer. The measured absorption spectrum allows retrieval of the trace-gas total column. Concentrations are deduced taking many factors into account such as surface pressure, surface elevation etc. However, in addition to the ideal situation, light can also be scattered by the atmosphere itself, e.g. by molecules, clouds, aerosol, etc. In general, this would be interpreted as a lower-than-real CO_2 column. But multiple reflections, can also lead to a longer than normal light path and thus to a higher-than-real retrieved CO_2 column. A first order correction is applied by co-measuring the oxygen column at 760 nm. As the oxygen concentration is constant and well known, this gives a good first order correction for the light path, sufficient for the determination of most trace gases. But the correction relies on the assumption that the scatter of light is identical at 760 nm, and the wavelength at which the trace gas is detected. For the high accuracy required for CO_2, the assumption is not completely valid: CO_2 is generally determined in the Short-Wave InfraRed (SWIR) bands around 1.6 μm, and 2.0 μm. Scatter due to molecules, aerosol and water droplets is in general decreasing for longer wavelength. The detailed knowledge of aerosol, as derived from a dedicated sensor, improves the accuracy of CO_2 column determination typically by a factor of 2 - 3 [3], in particular in areas with significant aerosol loading, e.g., in populated areas with anthropogenic aerosols, regions of biomass burning, and regions with desert dust.

Both trace gases and aerosol are measured from space using the reflected sunlight. While the detection of trace gases is based on the gas-specific absorptions in the spectrum, the detection of aerosol is less trivial. Light reflection by aerosol does not show distinct spectral features. Several aerosol properties such as size, shape and refractive index give rise to a much stronger variation of scattered light as a function of scattering angle and in the spectral dependence of the degree of linear polarization. Therefore, the best method for measuring and characterizing aerosol from space is the application of a multi-angle polarimeter. In this case, light reflected off a part of the atmosphere is detected under several viewing angles, and the light is analyzed for its state of polarization as a function of wavelength [5].

In principle, several instrument concepts are possible, that do the same job. Instruments like the French POLDER on ADEOS I and II, and PARASOL, or 3MI on Metop Second Generation image the Earth with a wide field of view. A filter wheel with polarization and color filters is applied to set the polarization and spectral band pass.

Instruments such as HARP2 on NASA's PACE mission and MAP on ESA's CO2M mission employ advanced techniques where images are taken in which the color and the polarization is set by static filters in the optical design. This allows for up to 60 viewing angles, three polarization angles and 4 spectral bands. JPL's MSPI instrument employs yet another detection principle where dual photo-elastic modulators time modulate the intensity of the light according its polarizational state.

A Dutch consortium consisting of Airbus Defense and Space Netherlands , SRON Netherlands Institute for Space research, with support from the Netherlands Organization for Applied Scientific Research (TNO), has developed an instrument based on a different approach where the linear polarization of the light causes a modulation on the spectrum, which is observed with moderate spectral resolution. A limited number of viewing angles (typically 3 – 9) are observed by different telescopes. The viewing angles are combined and the modulated spectra are measured using one single spectrometer and detector system. This results in fewer viewing angles, but more spectral information, leading to the same information on aerosol [6]. The principle of SPEX has been proven by several instruments: iSPEX, SPEX-airborne, and recently the SPEXone instrument for the NASA PACE (Plankton, Aerosol, Cloud, ocean Ecosystem) mission, to be launched early 2024, has been delivered. More on the SPEXone instrument for PACE can be found in [6][7], its calibration in [8], and its data retrieval in [5] and [9].

2. PRINCIPLE OF SPEX

The SPEXone instrument is mounted on a sun synchronous satellite platform. It is composed of three components: The telescope collecting light from five viewing angles: Nadir looking, 20° looking forward and backward and 50° forward and backward. Each viewing angle has the same across track field of view, or swath, as projected on Earth. The telescope module contains five telescopes, each composed of three mirrors. The primary, secondary and ternary mirrors are machined in three compound mirror elements, , each containing five individual sub mirrors. The telescope module co-aligns the five viewing angles. Five Entrance Apertures, defining the pupils, are placed between before the primary telescope mirror. The five apertures are machined in one single Entrance

Aperture Module. Each viewing angle has its own optimized baffle, reducing out-of-field stray light. The telescope module is under patent US20200319026A1.

The third set of telescope mirrors focus the five telecentric beams on five slits in a common slit plate.

The pupil-averaged angles on the telescope mirrors has been kept low (typically below 16°), such that the polarization induced by the telescope mirrors is minimized. It is typically well below 0.007, while calibration reduces the error to typically < 0.001.

Between telescope mirror 3 and the spectrometer is the Polarization Modulation Optics (PMO) Module. It consists of several optical components: a fused-silica Mooney Rhomb achromatic quarter-wave retarder transforms the +/- 45° linear-polarization component into circular polarization (in the Stokes parameters, transform the U polarization into V polarization, while leaving Q unchanged). The next element is an a-thermal Multiple Order Retarder (MOR), made out of a combination of MgF2 and Quartz, and placed with its optical axes at 45° with respect to the quarter wave retarder. Together, these elements encode the linear polarization of the light as a polarization modulation on the spectrum. A polarizing beam splitter results in two beams with s and p polarization. Two wire grid polarizers boost the polarization purity to well above 1000. Now the polarization modulation is transformed in an amplitude modulation on the resulting spectra, where the modulation amplitude is a measure for the Degree of Linear Polarization (DoLP), and its phase a measure for the Angle of Linear Polarization (AoLP). It is assumed that the incoming reflected light contains no circular polarization. This is a justified assumption.

Finally, two fold mirrors and a roof-top mirror bring the two sets of five beams in the same plane, virtually doubling the number of spectrometer slits , and directing the ten beams to the collimator of the spectrometer.

The spectrometer consists of two collimator free-form mirrors and a fold mirror, a holographic grating with 500 lines/mm, operating in first order, and an imager consisting of two free-form mirrors and a fold mirror.

Just before the Detector Module (DEM) an order-sorting filter (OSF) is placed to block any light from the higher orders of the grating. In the PACE instrument, the backside of the OSF is used for a low-pass filter, limiting light from beyond the optical band from reaching the detector. In the new application this filter is repositioned, see section 3.2.

3. ADJUSTMENTS AND IMPROVEMENTS

It does not happen too often that the second version of a scientific instrument is developed. In the case of SPEXone, the same consortium develops a very similar instrument that is candidate for application on the ESA CO2M platform. Next to delivering an aerosol product on its own, the primary task on CO2M is to improve the accuracy of the CO_2 column determination. The new application asks for adjustments and improvements of the instrument. Adjustments are either driven by changes in requirements and interfaces, and by improvements based on the lessons learned to improve the performance, and to improve the AIT.

The most pronounced hardware changes are discussed below. Other changes pertain to the test and calibration procedures, where lessons learned are implemented to increase the quality of the measurements, and increase the efficiency of the campaigns.

3.1 Change in telescope design

The most important change is the across track field of view, from 100 km for PACE to 250 km for CO2M. This is to get a good overlap between the SPEXone instrument and the main CO2M spectrometer instrument. To this end, the sizes of all 3 telescope mirrors were adjusted, and the effective focal length was decreased, such that the image size at the spectrometer entrance slit plane remained the same. In order to also achieve the same F/#'s for the telescopes, the size of the entrance apertures was reduced. A comparison of the telescopes is shown in Figure 1.

The thickness of the entrance aperture has been significantly reduced as the larger angles in the telescope would give rise to more vignetting due to the entrance aperture, as well as ghost images caused by reflections off the inner walls. To facilitate AIT, the entrance apertures of the five beams have also been integrated in one single piece.

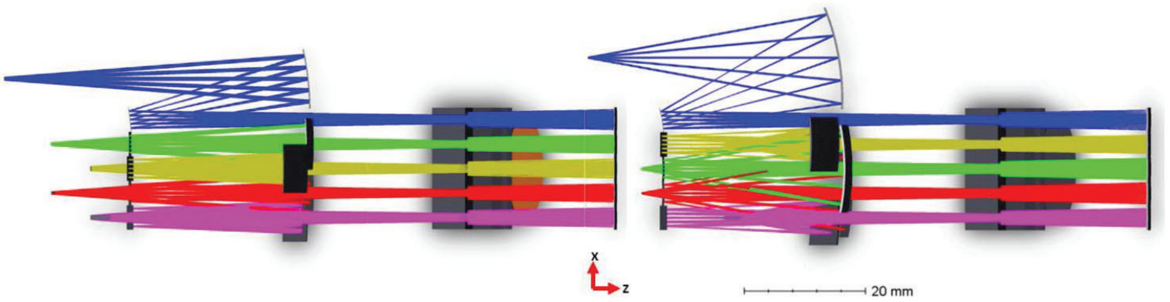

Figure 1: Side view of the SPEXone telescopes. Left PACE, right CO2M. Blue is nadir looking, red and green are +/- 20°, pink and beige are +/-50° viewing angle.

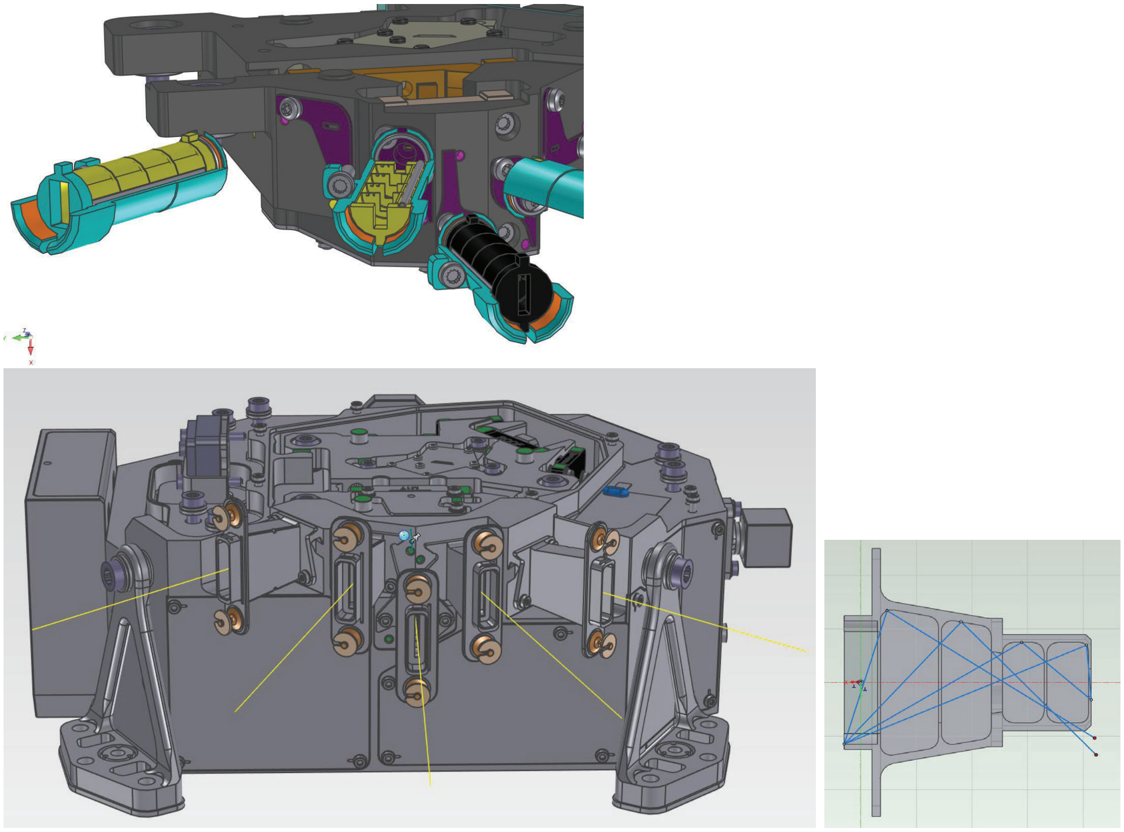

Figure 2: illustration of the adapted telescopes: above the telescopes of SPEXone for PACE, below the new version. The small graph at the lower right shows the internal baffles (of the nadir view port).

The larger Field of View also led to adjustments of the stray light baffles, see Figure 2. The new baffles are now also used as MLI attachment points.

Although the telescope has been adjusted, the Polarization Modulation Optics (PMO) has remained unchanged (apart from coatings, see section 3.2).

3.2 Stray light reduction measures

In any instrument, stray light is a challenging topic to deal with, and this is not any different in SPEXone, see ref (Rietjens ICSO 2022). Although stray light can be largely corrected for in the data processing, residuals after correction remain a significant part of the instrument's error budget, in particular in the error in the degree of linear polarization (DoLP). The best approach is to avoid stray light as much as possible.

There are several sources of stray light, and different measures have been taken for each. The surface roughness of the telescope mirrors mainly leads to spatial stray light, with the net result that light from bright scenes is scattered, and ends up polluting the dark scenes. In the spectrometer, the surface roughness of the mirrors leads to spectral-spatial stray light, polluting both the dark scenes as well as spectral parts with low intensity. This component of stray light can be reduced by the production of smoother surfaces. The production of high quality surface finish on the telescope mirrors is particularly challenging since the mirrors for the five telescopes are produced as five segments of a monolithic part, each segment with a different surface shape. The surface roughness of the SPEXone for PACE telescope mirrors was determined to be between 2 and 5 nm rms. For the present application, a refined design and manufacturing process has produced a surface roughness less than 2 nm for all telescope mirrors. As straylight scales with the square of the surface roughness, this should have a major impact.

The surface roughness of the spectrometer mirrors was already less than 2 nm for the PACE implementation. However, the mirror production, polishing, and coating was a multi-company effort, requiring excessive transportation and handling. The current production plan involves a single company effort, such that there is significantly less risk involved in the production, and the final quality of the mirrors is expected to be improved with respect to PACE.

In the existing instruments, several ghost reflections of low intensity were found. The most severe ghost images were caused by higher-order reflections from the grating, that could reach the detector via extra reflections off the mounts and walls of the spectrometer. In general, these reflections are hard to correct for in the data processing. Ray tracing of these ghosts revealed the optical paths. Measures have been taken to prevent these reflections from reaching the detector. Mainly by the introduction of mechanical baffles, and by extending the black anodized inner walls of the spectrometer, such that higher grating diffraction orders cannot re-enter the optical path, and light paths between the mirrors other than the intended light path are blocked, see Figure 3.

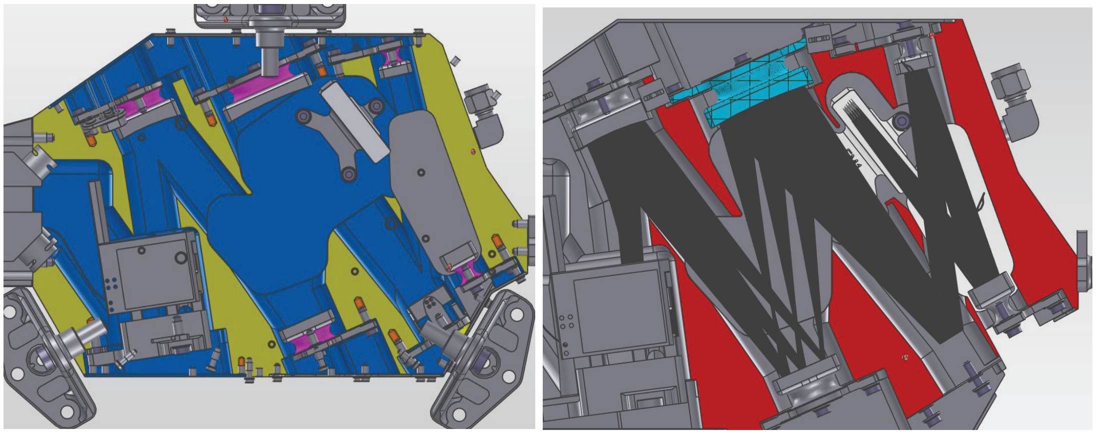

Figure 3: Top view of the spectrometer optics for PACE (left) and the new design (right). Subtle changes are implemented to block ghosts from higher order grating reflections.

A final major improvement is introduced by the repositioning of the low-pass filter in the system. The optical band of 385 nm – 770 nm needs to be limited. On the short wavelength, this is achieved by the spectrum of the Earth reflected sunlight, as well as the coatings of the transmissive elements of the system, the grating diffraction efficiency, and the quantum efficiency of the detector.

The operational spectral band of the spectrometer spans a full octave, such that the long wavelength end of the first diffraction order overlaps with the short wavelength end of the second diffraction order. To avoid mixing these optical signals, a filter is introduced just before the detector. On the front side of it is a graded filter that acts as an order sorting filter. However, this would still allow light from beyond the optical band from hitting the edge of the detector. Directly outside the optically active area of the detector are highly reflective structures. Long-wavelength light could thus cause stray light in the direct vicinity of the detector pixels. A short-pass filter (SPF) on the backside of the order-sorting filter prevents the long wavelength light from reaching the detector. The SPF coating recipe is a proprietary coating recipe provided by producer Optics Balzers Jena, but a ZEMAX encrypted coating file was provided, so that full wavelength and angle-dependent optical properties could be ascertained. The optical characteristics of the short-pass filter are shown in Figure 4.

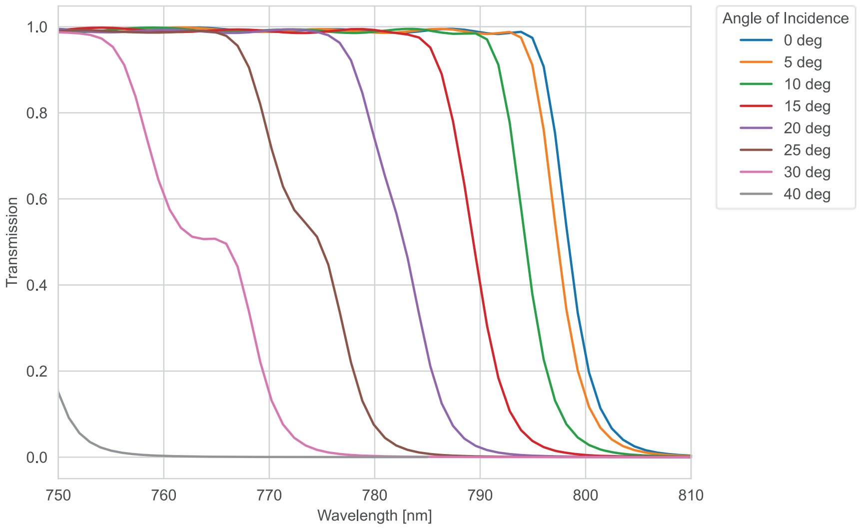

Figure 4: Optical characteristics of the short-pass filter, as applied on the backside of the order-sorting filter in the SPEXone for PACE instrument.

With an ~F/5 focus on the detector and wavelength-dependent incident angle, the angles of the ray through the SPF for wavelengths near the cutoff wavelength are between 0 and 20°, reflecting the light beyond about 800 nm. Light between 775 nm and 800 nm is partially transmitted. And it is this light that causes an extra straylight problem. The light hits the detector and is mostly converted into an optical signal. However, the detector features a micro-lens array, see Figure 5, to concentrate the light onto the photo-diode part of the detector unit cell, thereby increasing the sensitivity of the sensor. A small fraction is reflected off the surface of the micro-lens array of the detector.

In this extra reflection, the angle of the light is significantly increased for the light at the extremes of the light cone and/or the edges of the micro lens. When the reflected light reaches the low-pass filter for a second time, the increased angle of the light shifts the filter cutoff to shorter wavelengths, which causes the filter to act as a reflection filter, returning the long-wavelength light a second time to the detector. In the PACE instrument this reflection was found in the calibration phase. In Figure 6, the extra red stray light can be seen when the source is 785 nm. This stray-light contribution disappears quickly when going to shorter wavelengths. Some is visible at the in-band wavelength of 768 nm, and even at 750 nm, some hints can be seen. At a source of 732 nm, the extra straylight is absent. All in line with the transmission plots of Figure 4. Ray-tracing simulations indeed show this stray light, with the distinct feature that it only appear far from the source.

Note that the stray light ends up at the detector far away from its source, leading to cross talk between polarizations and viewing angles. This straylight is very difficult to correct for in the data processor. Therefore, a solution in hardware is by far preferred.

As the straylight is caused by a high-incident angle double reflection between the detector lens array and low-pass filter, the solution is to move the low-pass filter to a position far away from the detector. The only transmissive optics of the instrument are found in the PMO. Here, the Mooney Rhomb and the wire-grid polarizers are the most obvious candidates as these are made of the same material (fused silica) and are not bi-refringent. The entrance surface of the Mooney Rhomb was selected for practical reasons: the backside of the wire-grid polarizer is also used for its adhesive bonding leading to areas that have to remain uncoated. A relatively simple anti-reflection coating is not a problem, but for a delicate low-pass filter with a sharply determined cut-off wavelength the masking off was considered too risky. Shadowing by the mask during the coating process would have produced a region near the mask where the coating performance was not well defined. This region potentially extended into the clear aperture of the component.

As the F-number of the beams in the PMO is much higher, typically F/20, and the beams themselves are telecentric, the angles of incidence are much smaller. Therefore, the recipe of the low-pass filter needed to be adjusted to shift the cut-off wavelength to 779 nm (50% transmission point), taking some production margin into account.

At the backside of the order-sorting filter, the low-pass filter will be replaced by an anti-reflection coating. Its reflection will be typically 1%, up to 10% for the most extreme angle, resulting in an order of magnitude improvement with respect to the low-pass filter.

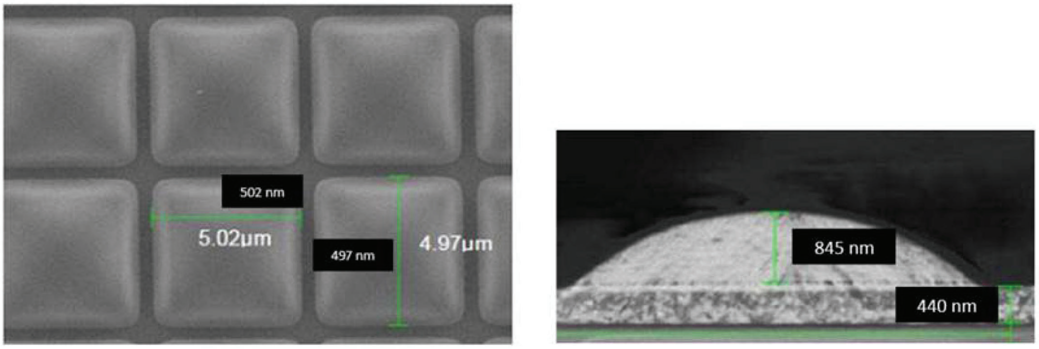

Figure 5: Electron microscope images of the micro-lens array on the detector surface. The micro lenses concentrate the light onto the photo-diode part of the detector unit cell, taken from [10].

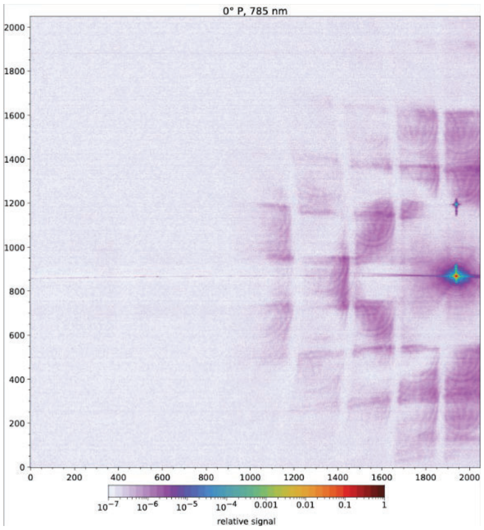

Figure 6: Red straylight as measured in the instrument for PACE. One viewing angle is illuminated with 100% polarized light of 785 nm wavelength. The double reflection from the detector micro-lens array and the low-pass filter results in significant straylight across the detector at long wavelengths.

An assessment has been made for the impact of all stray-light improvements. Quantification of the remaining error is not straightforward, and it also depends on the radiance scenes assumed. However, simulations show that the reduction of the error on the DoLP is between a factor of 1.5 and 3 for the nominal case, or a worst case illumination, respectively. In both cases, the requirement on the DoLP accuracy of 0.35% is met.

3.3 Upgrade of the DEM Firmware

Both SPEXone instruments are equipped with the same off-the-shelf Detector Module (DEM) produced by 3Dplus in France. The DEM model 3DCM734-1W is a very compact unit consisting of an AMS CMV4000 CMOS detector, a Microsemi ProASIC3 FPGA, SDRAM memory, FLASH memory and LVDS inputs and outputs that can be configured as SpaceWire interfaces.

The FPGA is loaded with firmware (F/W) dedicated and optimized for the mission, within the limits of the DEM. Development of the F/W is done in house by SRON. While about half the F/W can be reused from the PACE project, the other half needs an update due to either changed requirements, in particular the increased detector frame rate, or due to its changed interface requirements (CCSDS protocol interface), or due to lessons learned to improve scientific performance.

Most obvious change is the higher sampling rate required, from 3 Hz in PACE to 5 Hz in the new instrument. Internally the detector is read by a maximum of 25 Hz, resulting in a 5 times coadding of frames. To reduce the internal data rate, it is mandatory to apply spectral binning. Binning factors are made flexible now, and can be determined by ground control. The on-board binning requires that anomalous pixels are rejected. A new anomalous-pixel handler is introduced based on a digital pixel map. This elegant method is very efficient and has no limit in the number of anomalous pixels.

Other changes in the F/W pertain to the detector trigger mechanism, the clocking mechanism and synchronization, and the data handling. The latter changed from on demand of the ICU, to automatic offloading. All these changes make the DEM more independent from the ICU functionality, and thereby easier to test as a standalone unit.

4. CONCLUSIONS AND ACKOWLEDGEMENTS

In this paper we've described the background of the SPEXone instrument, and its ability to determine aerosol characteristics. A SPEXone instrument will fly on NASA's PACE mission, with a launch foreseen early 2024. A very similar instrument is under development and is foreseen to fly on ESA's CO2M mission. Its main purpose is to support the CO_2 column measurements and to increase the accuracy of the CO2 column by a factor of two to three.

The similarity of the SPEXone instruments for the two flight opportunities has been maximized. Both have five viewing angles, nadir, +/- 20° and +/- 50°. The Polarization Modulation Optics and the spectrometer are basically unchanged. However, some changes in the requirements led to changes in the instrument. In particular, this holds for the across-track field of view, which is increased from 100 km to 250 km, leading to changes in the telescope module as well as the detector read-out firmware. Other changes are driven by lessons learned. Several measures have been implemented to reduce the stray light.

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