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SPEX THE DUTCH ROADMAP TOWARDS AEROSOL MEASUREMENT FROM SPACE

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I. INTRODUCTION

SPEX is developed as part of the roadmap for optical instruments of the Netherlands Space Office to support environment and climate research [1]. SPEX is a compact and highly accurate polarimeter to measure atmospheric aerosol based on a novel method for measuring the state of linear polarization: spectral modulation [2]. When operated from space, it can provide global monitoring of aerosols and clouds. This is important for society because these aerosol measurements allow for a more accurate prediction of climate [3]. Furthermore, aerosol pollution in urban areas significantly reduces life expectancy [4]. Developed by a consortium of knowledge institutes and industry under scientific guidance of SRON Netherlands Institute for Space Research, the SPEX instrument has gone through lab, field and airborne testing [5, 6, 7]. The air campaign was carried out on NASA's ER-2 high-altitude airborne science aircraft. These tests have shown that SPEX is accurate enough to determine, not only the well-known aerosol optical thickness (AOT), but also particle specific properties such as the aerosol mean size, the single scattering albedo (SSA) and the complex refractive index. These measurements can be used to discriminate between natural and man-made aerosol.

Recently, we have initiated a conceptual design and technology development phase to bring SPEX into low Earth orbit. The very high accuracy of our innovative polarization measurement combined with its spectral resolving power allows for a reduction of the spectral bandwidth compared to existing polarimeter solutions, without loss of performance. By limiting the spectral range, it is possible to incorporate a commercial detector and to include the polarimeter in an optical bench that is currently under development by TNO and Airbus DS NL (which in turn is based on the ESA Sentinel-5 Precursor instrument TROPOMI, to be launched this year), thereby increasing design heritage [8]. The modular approach, the absence of mechanisms, and the manufacturing concept are "designed for scale". This means that small-volume production is possible, bringing the cost of recurring models down without compromising on performance. We therefore call this concept SPEXlite.

Opportunities for the application of SPEXlite are for example as supporting payload on the NASA PACE (Plankton, Aerosol, Cloud, ocean Ecosystem) mission, or as a supporting instrument for future CO₂ missions. In addition, scale production could open the way to a range of commercial instruments dedicated to provide climate and air-quality services from ground, air or space. In this contribution we report on first results of the SPEX Airborne flights and the design concept for SPEXlite for a low-earth-orbit satellite platform.

II. SCIENCE CASE

Anthropogenic aerosols are believed to cause a forcing of climate change comparable in magnitude but opposite in sign to greenhouse gases. In contrast to the climate effect of greenhouse gases, which is understood relatively well, the negative forcing (cooling effect) caused by aerosols represents the largest reported uncertainty in the most recent assessment of the International Panel on Climate Change (IPCC). This uncertainty severely hampers future predictions of climate change. Strong aerosol cooling in the past and present would imply that future global warming may proceed at, or even above, the upper extreme of the range projected by the IPCC. Aerosols are also known to strongly affect air quality, especially in regions with high industrial activity and large amounts of traffic, or in regions that are influenced by biomass burning. Exposure to particulate matter air pollution has major adverse human health impacts, including asthma attacks, heart and lung diseases, and premature mortality.

The high-level primary science goals of SPEX and the corresponding geophysical data products to address these science goals are summarized in Figure 1. Aerosol absorption (SSA), composition / type and layer height are considered as the most important aerosol characteristics that are needed to advance our understanding of the role of aerosols in climate change. See for example [9]. This has been confirmed during a SPEX user workshop organized by SRON and NWO on 27 November 2015 in The Hague.

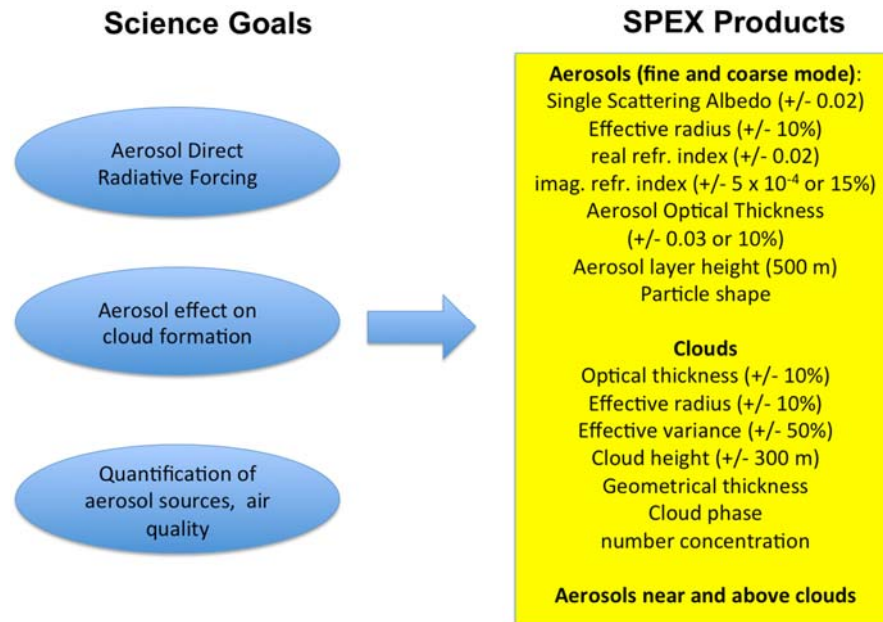


Figure 1: High level primary science goals and foreseen aerosol and cloud data products of the SPEX instrument.

In addition to the primary science objectives outlined above, the SPEX instrument has the capabilities to meet a number of secondary science objectives, the most important being 1) Providing an atmospheric correction for ocean color remote sensing, 2) Providing a light path correction for retrieval of Greenhouse gases CO₂ and CH₄ and other trace gases, 3) Providing information on reflection properties of the Earth surface. The ability to attribute natural and man-made aerosols provides a wealth of information servicing different users with examples being general air quality services and regulatory compliance services. Airbus DS NL and SRON are jointly working to set-up the processing chain that will enable the delivery of value added services.

III. INSTRUMENT REQUIREMENTS

The aerosol and cloud products that are mentioned above can only be unambiguously determined from an instrument that measures radiance and polarization spectrally resolved and at multiple viewing angles for one ground pixel [10, 11].

The instrument specifications that are required for the retrieval of the relevant aerosol and cloud products are listed in Table 1. These requirements are based on extensive retrieval simulations performed at SRON [12, 13, 14]. Here, in order to make the needed step forward compared to the planned operational 3MI mission in characterization of key aerosol properties like SSA (absorption), refractive index (aerosol typing) and aerosol height, it is essential to improve the accuracy of the measured degree of polarization by about an order of magnitude.

The baseline requirements in Table 1 correspond to an instrument that flies in tandem with a separate cloud imager. Such instrument has significantly improved aerosol retrieval capabilities compared to 3MI. In particular, capabilities to retrieve aerosol absorption (SSA) and aerosol layer height are improved because of the availability of near UV measurements down to 385 nm and spectrally resolved measurements with 4 nm resolution combined with the high polarimetric accuracy. Retrieval capabilities for aerosol refractive index (highly relevant for aerosol typing) are significantly improved because of the high polarimetric accuracy. Also, the spatial sampling is a factor 2 higher. For an instrument with the baseline capabilities it is required to fly on the same platform (or in formation) with a cloud imager that is needed to provide cirrus cloud screening and to provide the cloud properties needed to address the science questions related to the indirect aerosol forcing. This cloud imager should at least have spectral bands at 1380 nm (for cirrus screening / characterization) and 1600 nm (for droplet size retrieval). Further spectral bands at 1880 nm (for improved cirrus screening / characterization) and 2250 nm (for improved droplet size retrieval and cloud phase retrieval) are desired.

The extended requirements in Table 1 correspond to a stand-alone instrument providing all relevant aerosol and cloud properties. The extended swath and angular range maximize the coverage. The extended wavelength range allows for standard cloud retrievals and cirrus characterization / screening. For aerosols, the extension to 1600 nm provides improved AOT retrievals over land and is also important to provide aerosol corrections for retrieval of Greenhouse gases CO₂ and CH₄ which have absorption lines around 1600 nm.

A promising next extension of the instrument capabilities, not listed here, is to include hyperangular measurements (e.g. 50 angles) for one wavelength band. This facilitates advanced cloud droplet size distributions for multi-layer clouds and improved determination of cloud phase, making use of the rainbow in polarization [15].

Table 1: Baseline and extended requirements for SPEX instruments

Parameter	Baseline requirements (in tandem with cloud imager)	Extended requirements (stand-alone instrument)
Swath	50°	90°
angular range (on ground)	+/- 55°	+/- 60°
# viewing angles	5	5
spectral range	385 - 770 nm	385 - 1600 nm
spectral resolution intensity	4 nm	4 nm
spectral resolution DoLP	20 – 40 nm	20 – 40 nm
spatial resolution (for all angles)	4×4 km ²	4×4 km ²
spatial sampling	2×2 km ²	2×2 km ²
polarimetric accuracy	0.002	0.002
radiometric accuracy	2%	2%
SNR for ocean scene at SZA = 70°	300	300

IV. SPEXLITE CONCEPT

A. Maximizing design heritage: integration of SPEX and Spectrolite

To deliver a cost-effective high-performance instrument, the SPEXlite concept combines the design heritage of two earlier instruments: Firstly, the spectro-polarimeter *SPEX* employing the spectral modulation technique, as developed in the Netherlands over the past decade [2, 5, 6, 7]. Major steps in this program have been the development, characterization, and field-testing of a *SPEX* Prototype. Absolute polarimetric accuracy measurements, performed with the prototype instrument demonstrated a performance in the lab of the polarimetric accuracy far beyond the design target, and already compatible with the more stringent requirements set out for an Earth observing instrument. Retrieval of aerosol micro-physical properties such as refractive index using ground-based measurements at Cabauw Experimental Site for Atmospheric Research with the *SPEX* prototype showed excellent agreement with local AERONET data. Subsequently, the *SPEX* prototype was upgraded to act as a stand-alone instrument for operating on a NASA ER-2 research aircraft.

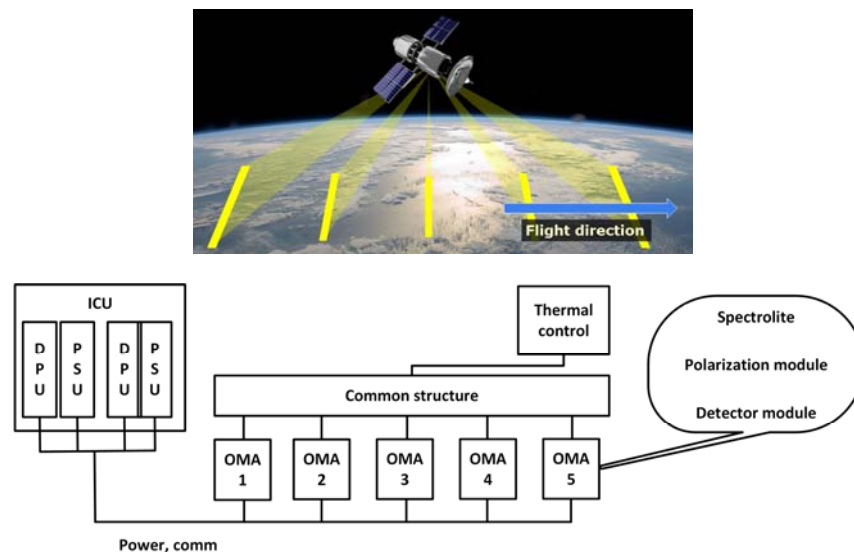


Figure 2 Top: *SPEX*lite observation concept with five viewing directions along track. Bottom: configuration of the main elements of the instrument. Each of the five OMAs consists of a spectrolite, a polarization module and a detector module.

Three successful flights have been undertaken this year, of which data analysis is currently being performed by a consortium consisting out of SRON and Airbus DS NL. Early results are presented below. Secondly, the compact and lightweight all-reflective imaging spectrometer *Spectrolite*, designed for cost-effective manufacturability and adaptability to specific earth observation tasks [8]. Its design traces its lineage to the TROPOMI and OMI instruments. The TROPOLITE-version of Spectrolite has recently flown in atmospheric observation campaigns [16].

B. Instrument configuration

The combination of a Spectrolite imaging spectrometer and SPEX polarisation optics forms an imaging spectropolarimeter that can observe a single swath on Earth. In the context of the SPEXlite instrument, one such module is called an Opto Mechanical Assembly (OMA). For SPEXlite, five OMAs will be combined, one for each along-track viewing direction, see Figure 2, top. The basic envisaged configuration of the polarimeter is shown in Figure 2, bottom. The main elements are:

- A cold redundant Instrument Control Unit (ICU) that contains cold-redundant Power and Data Processing capabilities (DPU = Data Processing Unit ; PSU = Power Supply Unit)
- 5 Polarimeter Modules (OMA) , each consisting of: An optical bench, based on the Spectrolite design; a polarization module, based on the SPEX design; a commercial Detector Module.

All the OMAs are placed on a common structure. The ICU is separate, and can be placed inside the spacecraft.

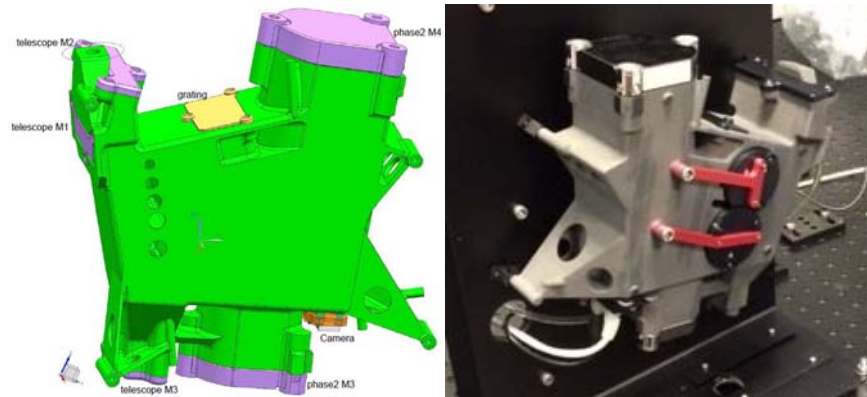


Figure 3 Left: Design of the Spectrolite spectrometer module. Right: Photograph of an assembled Spectrolite prototype.

C. Opto mechanical assemblies

The Spectrolite-based optical bench is an all-reflective, off-axis design, including four free-form mirrors and a flat grating in the spectrometer [8]. It is designed for ease of assembly, see Figure 3. The mechanical housing is manufactured using 3D printing. The contact pads to which the mirrors need to be mounted are machined to arrive at the right accuracy and flatness. The design of the spectrolite prototype will be slightly modified to accommodate the polarization optics right after the telescope and in front of the entrance slit and the polarization splitter directly after the slit. The telescope was designed to minimize instrumental polarization by ensuring that the angle of incidence of all light rays is smaller than 10 degrees.

The SPEX polarimetry concept is based on spectral polarization modulation; the degree and angle of linear polarization are encoded in a modulation of the radiance spectrum. This is achieved through a set of dedicated optical crystals: an achromatic quarter-wave retarder (QWR), an athermal multiple order retarder (MOR) and a polarizing beamsplitter. The QWR and MOR ensure that incident linearly polarized light is modulated in the spectral domain. The polarizing beam splitter transforms the spectral polarization modulation into two spectrally modulated intensities, such that amplitude and phase of the modulation are proportional to the degree and angle of linear polarization respectively. In the present concept, the QWR will be implemented as a superachromatic waveplate or Fresnel rhomb, while the MOR will be an athermal combination of MgF2 and Quartz. Baseline concept for the polarizing beam splitter is a Wollaston-prism in combination with a total internal reflection prism in order to direct the split beams towards the slit. As the polarization optics require proper mechanical mounting, a breadboard program will be executed in order to demonstrate the compatibility of the optical design with the telescope and spectrometer, and to increase the technology readiness level of the mounting concept by thermal and vibrational cycling of the breadboard model. The spectrometer has a reflection grating as the dispersive element. Long- and short-pass filters will be used to block out-of-band light. To minimize cost and maximize commonality, the five Opto Mechanical Assemblies that are combined into the SPEXlite instrument are identical. As each OMA corresponds to a different along-track viewing direction, the along- and across-track

ground pixel sizes differ for the $\pm 50^\circ$, $\pm 20^\circ$ and nadir modules. The OMAs will be designed such that all viewing directions meet or exceed the resolution requirements.

The fully reflective architecture of the spectrometer is intrinsically achromatic and can therefore be readily extended into SWIR wavelength range. This only requires replacing the grating and detector units. Such extension could be interesting for future extension of the cloud science capabilities of the spectropolarimeter.

D. Detector and instrument control unit

Advanced CMOS detector development applicable for SPEXlite, is ongoing within Cosine and at other partners. Our current effort for the detector and related electronics is based on a high sensitivity CMOS image sensor with megapixel resolution. The electronics comes with an FPGA, volatile and non-volatile memories for full-resolution operation, making it suitable for a large range of applications while ensuring outstanding image quality. Operation of the detector includes capturing megapixel images at ~ 15 frames per second in 10 or 12 bit mode. Cosine measurement systems BV develops the *Commercial Operational Instruments* family. The first In Orbit Demonstration of the technology is foreseen in 2017, as part of the maiden space flight of a miniaturized hyperspectral instrument with onboard analytics called HyperScout[®] [20].

The Instrument Control Unit acts as the interface unit between the platform on one side and the SPEXlite instrument on the other. The ICU performs Command execution and configures and synchronises the Detectors within the system. Once image data is available in the Detectors, the ICU will retrieve the digitized output from the five detector interfaces and packetize the data, and forward the packets to the spacecraft for recording or direct downlink through a dedicated interface. The ICU also provides pre-conditioned power to the Detectors and is capable of controlling the temperatures of the instrument units to within sufficiently stable limits.

From an operational point of view, the ICU can provide functionality for event reporting and event action. In addition, specific operation procedures, memory management control and fault management control functions could be implemented to match the operational needs at platform level.

VI. PERFORMANCE MODEL

A preliminary assessment of the performance in terms of signal-to-noise ratio (SNR) has been carried out using a simplified instrument performance model. This model takes as input spectral radiance files that in this case are forward model calculations of the expected radiance for ocean and land scenes with different aerosol optical thickness. The model calculates the detector response based on several instrument and detector parameters, most notably: spatial resolution, spectral dispersion, spectral range, transmission, quantum efficiency, pixel pitch, pixel size and detector noise parameters.

The SNR is calculated for a scene with minimum radiance but for which the requirement still holds. This scene is a combination of a Lambertian Equivalent Radiance (LER) of 0.03 and spectral radiance of an ocean scene with low aerosol optical thickness, as shown in Figure 4-top. The main driver of the SNR of this low radiance scene is the read noise of the detector associated with multiple detector reading per observation time. The number of detector readings per observation time is driven by the maximum expected radiance for which the requirements must hold. This maximum radiance scene is taken to be a thick, bright, unpolarized cloud that is modeled as a LER = 1.0 scene, see Figure 4-top. The frame rate is set such that the pixel saturation does not exceed 0.75 in order to avoid too large non-linearity effects.

The SNR is calculated per modulation period and per final science pixel and plotted Figure 4-bottom. The SNR per science pixel is thus the combined SNR of many detector pixels of several detector readings. E.g. at 550 nm the total number of pixels that are combined into a single science pixel exceeds 1000 as a result of several tens of pixels per modulation period in the spectral direction, of several co-addings per science observation, and oversampling in both time and space. The latter is necessary in order to be able to process all data from different viewing angles onto a common grid. The SNR for the minimum scene exceeds the requirement of 300 over the full spectral range from 385-780 nm. Several options to increase the SNR near the edges of the wavelength range are under consideration. For example the use of a spectral filter or adapted detector settings to increase the spectral uniformity of the response. The relatively high spectral sampling of a modulation period, in combination of oversampling in time and space, contribute to the high polarimetric accuracy of the SPEX concept. The concept is relatively insensitive for pixel-to-pixel gain variations (or pixel-response non-uniformity) as remaining post-calibration variations are averaged out significantly. Also, the concept can tolerate a substantial loss of detector pixels, e.g. due to radiation effects over the mission lifetime, with very limited impact on the polarimetric accuracy and SNR.

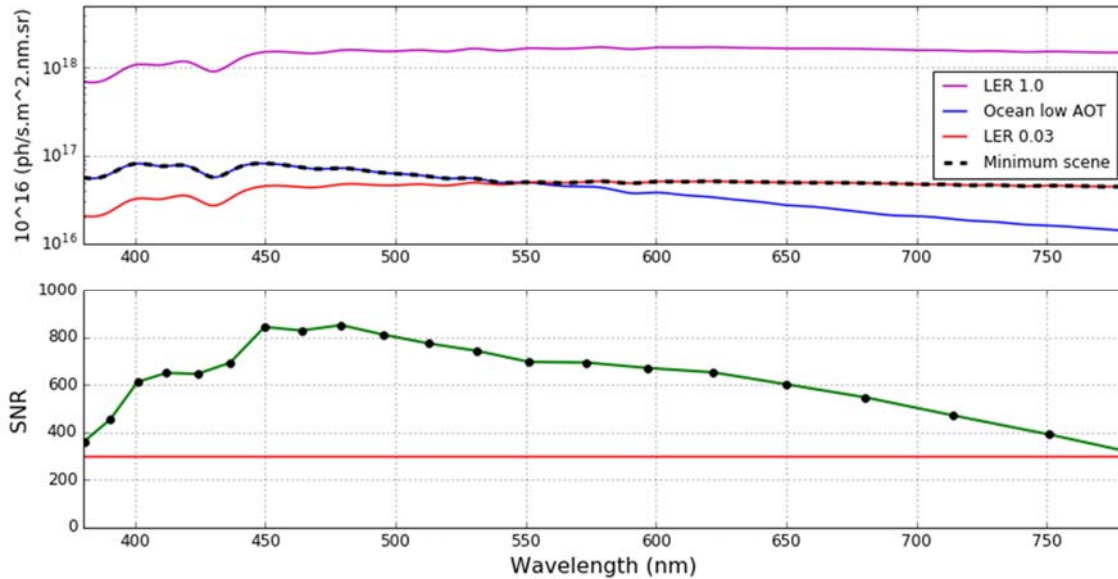


Figure 4: Top: minimum and maximum radiance spectrum used for the SNR calculation. Bottom: SNR per modulation period per science pixel. The dots in the bottom figure indicate the center wavelength of each modulation period. The red line indicated the SNR requirement.

VII. SCIENCE DATA PROCESSING

A. Level 0-1

Level 0-1 processing includes three main steps. First, detector specific corrections are applied to the raw data like dark current correction, offset and gain corrections, and photo response non-uniformity. In the second step, time series of polarization and radiance values are determined for ground pixel elements along the swath, as a function of wavelength, for each of the five OMA modules. This step involves the application of wavelength calibration, line-of-sight calibration, polarization calibration, and radiometric calibration data. In particular, to determine the Degree and Angle of Linear Polarization (DoLP and AoLP), the spectra are ‘demodulated’. This is achieved by respectively subtracting and adding two spectra emerging from the beam-splitter such that the difference contains only the modulations, and the sum is modulation free. The ratio of these two is fitted in the spectral domain at a number of preselected wavelengths to deliver the modulation amplitude. DoLP and AoLP are then obtained from the modulation amplitude by applying polarization calibration data. Radiometry is obtained from the modulation-free sum-spectrum by the application of radiometric calibration data. Note that radiance and polarimetry are derived from the same image, in a single snapshot. This is unique to SPEX. The third step is the co-location of polarimetric and radiance measurements. The time series obtained in the second step are projected onto a geographical long-latitude grid and overlapping data are combined to provide multi-angular data at each groundpixel. This step involves the application of line-of-sight calibration data, which provide the direction of incoming light relative to the instrument frame, and also the application of platform attitude data, to determine the direction of incoming light relative to an Earth-fixed frame.

B. Level 1-2

The level 1-2 aerosol processing will be based on the algorithm developed at SRON – Netherlands Institute for Space Research. The retrieval approach is described by Hasekamp et al. [2011] and is based on iterative fitting a linearized vector radiative transfer (RT) model, developed at SRON to the multi-angle measurements of intensity and polarization. The state vector of the retrieval (i.e. the unknown parameters) explicitly contains the microphysical aerosol properties corresponding to a bi-modal aerosol model. Here, each mode is separately described by an effective radius and width, complex refractive indices, the column number concentration and for the coarse mode the fraction of spherical particles, for a mixture of spheroids and spheres [Dubovik et al, 2006]. Also the central height of a Gaussian height profile is being retrieved. Surface properties are retrieved simultaneously with the aerosol properties. Over land these properties correspond to parameters describing the directional properties and total reflection of the Earth surface, whereas over the ocean the surface wind speed and oceanic Chlorophyll-A concentration are retrieved. The SRON aerosol retrieval algorithm has been extensively applied and validated for real satellite measurements of the POLDER instrument [17, 18] and airborne measurements of the Research Scanning Polarimeter [13].

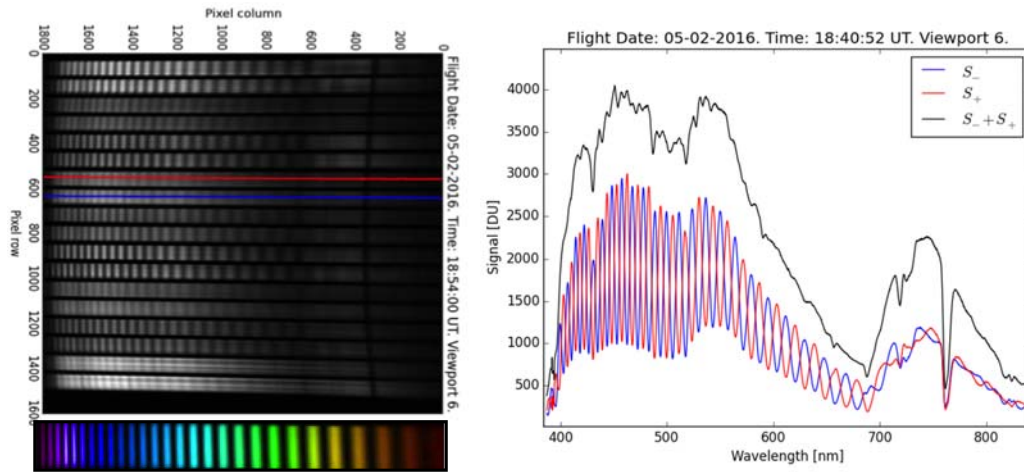


Figure 5. Left: raw detector image displaying nine pairs of modulated spectra. Spectral wavelength increases from left to right, with increasing pixel column. Right: two modulation spectra extracted from the raw image. Red and blue curves correspond with the indicated lines in the left figure.

VIII. AIRBORNE RESULTS

A SPEX prototype instrument [5] has been configured for flights on NASA’s high-altitude ER-2 aircraft. This prototype has a polarization modulation unit representative for the SPEXlite design. The employed spectrometer has a conventional design with lenses and a transmission grating. The prototype is limited to a 7° swath but exceeds with 9 viewing angles the minimum of 5. The ER-2 operates at a typical height of 20 km, where atmospheric conditions are calm, allowing the aircraft to maintain a very stable attitude. The SPEX prototype had a maiden flight in February 2016 with cloud-free conditions. The instrument was mounted in the tail cone of the right wing of the aircraft. An example of a raw detector image is shown in Figure 5. The image shows nine pairs of modulated spectra. Each pair corresponds with one of SPEX’s viewing angles. Because at a given snapshot time each viewport collects light from a different scene, the spectra differ in spectral shape and in polarization strength. Note that there is also variation within a spectral band in the row-direction. This corresponds with the change in the scene along the swath direction. From the image, two spectra are extracted, denoted as $S_-(\lambda)$ and $S_+(\lambda)$ – see the right panel in Figure 5. It is clear that the modulations of the two spectra are in anti-phase. The sum $S_-(\lambda) + S_+(\lambda)$ is modulation free (see the black curve in Figure 5) and representative of the spectral radiance. By fitting the scaled difference $S_-(\lambda) - S_+(\lambda) / S_-(\lambda) + S_+(\lambda)$ with a sinusoid, the DoLP is derived as a function of wavelength. Figure 6 shows the DoLP at 550nm, obtained along the flight track of one viewport and the signal strength, with underneath the reconstructed image of the ground as seen at 550nm. The DoLP displays variations down to the 1% level, and is correlated with the ground albedo. This is made explicit in the right panel of Figure 6, where the DoLP is plotted against the signal strength. For homogeneous aerosol scenes, one expects a single trace, and the figure reveals two distinct areas, which are indicative of a change in aerosol optical depth along the flight path.

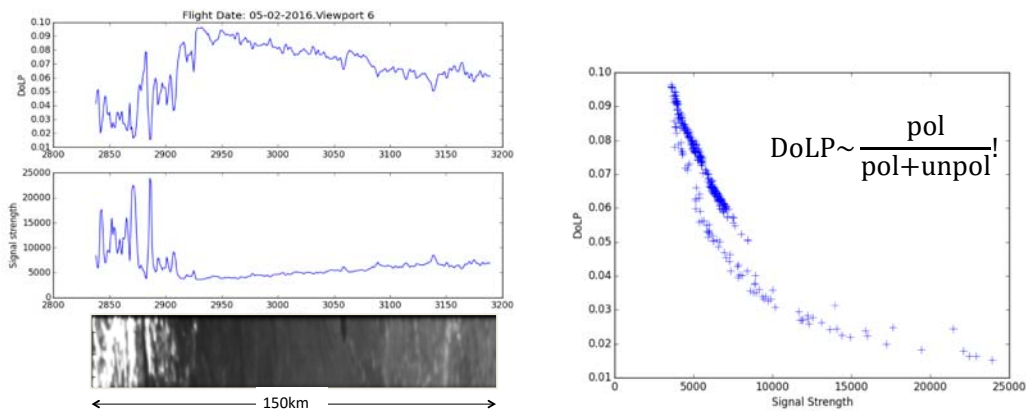


Figure 6. Left top panel: Degree of Linear Polarization along the flight track as a function of time, for 500nm. Left middle panel: Signal strength (intensity) as a function of time. Left bottom panel: ground scene image, reconstructed at 550nm. Right panel: DoLP versus signal strength @550nm

IX. CONCLUSION AND OUTLOOK

Dutch knowledge institutes and industry will collaboratively develop a spectropolarimeter based on SPEX technology for space use to measure Aerosol. The SPEX method of spectral modulation is proven in lab, field and Airborne tests and yields very high accuracy in the degree of polarization. The concept is modular and can be easily configured for wavelength band and number of viewing angles. Moreover, it is cost-effective because it is designed for scale production. This allows for flight possibilities ranging from airborne on research airplanes or UAVs to spaceborne from Low-Earth orbit. SPEXlite could for example match the needs of the NASA Plankton, Aerosol, Cloud, ocean Ecosystem (PACE) and ACE missions planned for launch in the next decade. Also it could be employed as supporting instrument for future missions targeting CO₂ measurements. This greenhouse gas is so well mixed in the atmosphere that polarimetry may be imperative to distinguish direct from scattered sunlight when retrieving the concentrations from spectroscopy of the Earth radiance. The ability to attribute natural and man-made aerosols provides a wealth of information servicing different (commercial) users with examples being general air quality services and regulatory compliance services.

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