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PROPOSED CONCEPT AND PRELIMINARY DESIGN FOR THE SENTINEL-5 UVNS SPECTROMETER

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I. INTRODUCTION

Sentinel-5 is an atmospheric monitoring mission within the European Copernicus programme, formerly GMES (Global Monitoring for Environment and Security). Its main objective is trace-gas and aerosol optical depth measurements for air quality and climate monitoring and forecast with daily global coverage. Constituents of interest are O_3, SO_2, HCHO (formaldehyde), BrO, NO_2, CHCHO (glyoxal), O_2, CH_4 (methane), and CO. Sentinel-5 will complement the Sentinel-4 GEO data over Europe. Both Sentinel-4 and -5 are intended to start operation in 2020.

The space segment of Sentinel-5 is implemented by an imaging UVNS (Ultraviolet Visible Near-Infrared Shortwave (infrared)) spectrometer, in the following referred to as S5 UVNS. It is carried on a MetOp-SG (second generation) satellite A, flying on a sun-synchronous polar low-Earth orbit at 817 km height. S5 UVNS is intended to provide an unprecedented spatial resolution of 7 km x 7 km on Earth (at Nadir) at a field of view (FOV) of 108.4° in across-track (ACT) direction corresponding to a ground swath width of about 2670 km. The instrument is implemented as a push broom spectrometer, scanning the Earth by measuring one row of ground pixels ACT at a time, and providing the respective spectrum for each pixel. The image dimension along-track (ALT), i.e. in scan direction, is acquired by the scan motion.

This paper describes concept and preliminary design of the S5 UVNS as developed by Kayser-Threde (KT) during Sentinel-5 project phase A/B1, and proposed to ESA for phase B2/C/D. Note that on 1 September 2014 Kayser-Threde merged with OHB System under the name of OHB System AG.

II. SENTINEL-5 MISSION REQUIREMENTS

The main requirements relevant for the optical design may be distinguished with respect to *spectral properties*, *imaging geometry*, and *optical and radiometric performance*. The following provides a short overview. See also e.g. [1], [2] for further information.

The spectral range is divided into 7 bands for each of which specific requirement parameter values apply. These bands are depicted in Fig. 1, and listed in Table 1. UV1, UV2, and VIS represent a contiguous range. Note that NIR1 may be omitted if NIR2 is implemented with a “breakthrough” resolution of $\Delta\lambda = 0.12$ nm. A SWIR2 band, existing in the early stage of the project, was later removed. The number of bands, their relative spectral positions, required spectral resolutions, power densities etc. determine the number of separate spectrometers to capture the specified bands. In the given case a minimum of 5 spectrometers is required. Note that the UV and VIS bands, although contiguous, cover a too diverse range with respect to parameter values, and a too large spectral range to allow implementation by a single spectrometer under the given requirements.

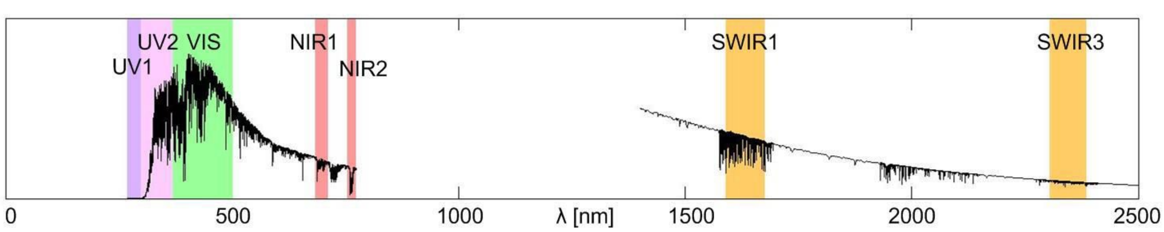


Fig.1. Spectral Bands specified for Sentinel-5

The extremely large ACT FOV of 108.4°, combined with requirements for low distortion of the FOV (smile), f-theta imaging behaviour, and image field flatness constitutes the main driver for telescope design. Another demanding requirement is the spatial resolution with a ground pixel size of 7 km x 7 km at Nadir which is much smaller than those of previous missions (see Fig. 2). Because of the high spatial resolution the requirements for co-registration and geo-location become drivers for the optical system design. Co-registration defines the match of two separate image pixels with respect to their true spatial position on ground or their spectral location. Intraband co-registration basically refers to the imaging distortion of the respective spectrometer, while inter-band co-registration refers to the mutual spatial pixel-by-pixel match between different spectrometers. Because of the small ground pixel size the inter-band co-registration requirement of 1.4 km (20% of the pixel width) represents a main driver for instrument alignment and stability.

Fig. 2. Spatial ground pixel size (at Nadir) of Sentinel-5 as compared to other missions

In order to attain the precision and resolution desired for the chemical component concentration analysis from the measured spectra, demanding requirements are given for high relative spectral and spatial radiometric accuracy, very low polarisation sensitivity, low stray light, and high accuracy of the knowledge of the instrument spectral response function, as well as very high long-term stability.

II. INSTRUMENT CONCEPT

As already mentioned, the width of the total spectral range to be covered and the differing requirements for the 7 spectral bands necessitate an implementation using at least 5 separate spectrometers. This number may be attained by concatenating 2 of the 3 UV-VIS bands into one, e.g. UV1 with UV2, and by dropping NIR1 in favour of NIR2 with a spectral resolution $\Delta\lambda \leq 0.12$ nm. This has been the choice made by Kayser-Threde.

Table 1. Spectral bands specification and chosen implementation. (Note: T, B, G denote implementation alternatives proposed by ESA, termed “threshold”, “breakthrough” and “goal”, respectively)

Spectral band	Spectral range [nm]	Spectral resolution Δλ [nm]	Implementation by KT	
			Spectrometer	Assembly
UV1	270 - 300	1	UV	UV
UV2	300 - 310	1.0 (T) – 0.5 (G)		
	310 - 370	0.5		
VIS	370 - 500	0.5	VIS	VIS-NIR
NIR1	G: 685 - 710	0.4 (T)	–	
	T: 710 - 750	0.2 (G)	–	
NIR2	T: 755 - 773	0.4 (T)	–	
		0.12 (B)	NIR	VIS-NIR
	G: 750 - 775	0.06	–	
SWIR1	1590 - 1675	0.25	SWIR1	SWIR
SWIR3	2305 - 2385	0.25	SWIR3	

The second fundamental optical component beside the spectrometer itself is the telescope that images the ground swath onto the spectrometer slit. In the case of an implementation with several spectrometers, one usually splits the beam path behind the telescope accordingly by means of dichroic beam-splitters, and illuminates the entrance slits of each of the spectrometers separately. While this is not a difficult task in case of 2 spectrometers, it starts to get complicated with 3, 4 or more channels. It typically requires the introduction of cascaded relay optics that complicate design and alignment significantly, not to mention the deteriorating impact on transmission, stray light and ghosts, spectral features, as well as envelope, and mass. The routing of the beam paths, starting more or less from a single point, often leads to an entangled arrangement of optical assemblies with components that are at times hardly accessible and difficult to align. An alternative method for beam splitting consists in the use of a laterally replicated slit usually consisting of two parallel slits, either real or virtual, in close vicinity of each other but distant enough to allow for beam separation by micro mirrors or the like (e.g. EnMap, TROPOMI). Typically, this method is used to separate a contiguous spectral range to into different bands measured by separate spectrometers when the split needs to be performed without loss of spectral values at the respective band edges (e.g. UV1-UV2-VIS). The drawback of it is the resulting image field separation which in the case of extreme wide-field projections as with S5 UVN entails image field incongruence impairing co-registration in the first place, and possibly necessitating interpolation and resampling of the measured data. Due to the small dimensions of the optical elements required for beam separation manufacture, alignment, and stray light requirements etc. tend to be demanding issues.

In order to avoid the described difficulties, the concept proposed by KT for S5 UVNS divides the instrument up into 3 separate modules, each comprising the respective spectrometer assembly combined with its own telescope directly mounted onto the spectrometer box, and each supplemented with its own on-board calibration unit (OBCU). This leads to a highly modular design, - optically, mechanically, and thermally. The advantages of such a setup are obvious: Assembly, alignment and calibration may to the most part be performed on spectrometer assembly level. Alignment on instrument level reduces to aligning the modules with respect to the satellite reference and mutually for co-registration. This allows for a high degree of parallel processing, e.g. in separate facilities, or for subcontracting including a substantial part of the AIT process. The latter is very advantageous e.g. in the case of the SWIR assembly, where Thales Alenia Space France (TAS-F) as subcontractor developed the optical design, and proposed to implement the spectrometer assembly. Furthermore, complex alignment inter-dependencies are practically eliminated. Due to the fact that beam splitting is reduced to the use of simple dichroic beam splitters, no complex splitting and relay optics are needed, and the overall number of optical elements can be reduced to a minimum, thereby substantially reducing the alignment effort, and enabling superior instrument performance.

KT uses an identical 4-mirror design for all 3 telescopes. Differences arise only due to the wavelength dependencies of depolarisation components integrated in the internal telescope beam-path. As all spectrometer slits are implemented as real apertures in the telescope image field, the across-track slit length is identical for all spectrometers (37.3 mm). For the UV, VIS and NIR2 (for short UVN) spectrometer channels using the same spectrometer magnification and along-track slit-width (110 µm) allows for using the same CCD detector chip for all 3 UVN channels. The SWIR assembly features magnification and an along-track slit width (130 µm) different from the UVN channels but the same number of across-track pixels in order to comply with the co-registration requirements. Both SWIR1 and SWIR3 use the same MCT detector. As parts of the 3 on-board calibration units (OBCU), 3 identical calibration wheel assemblies in front of the telescope apertures allow for sun and white-light calibration via diffuser plates, as well as for closing the observation beam path. Further optical components deserving special mention are the polarisation scrambler positioned in the telescope beam path, and the slit homogeniser as an optional replacement of the regular slit.

Fig. 3 shows an optical functional block diagram of the instrument with the 3 different temperature regimes required: While most part of the optics can be operated at 293 K, the detectors and the SWIR spectrometer assembly need to be cooled to attain the required detector SNR, and to reduce the IR instrument background.

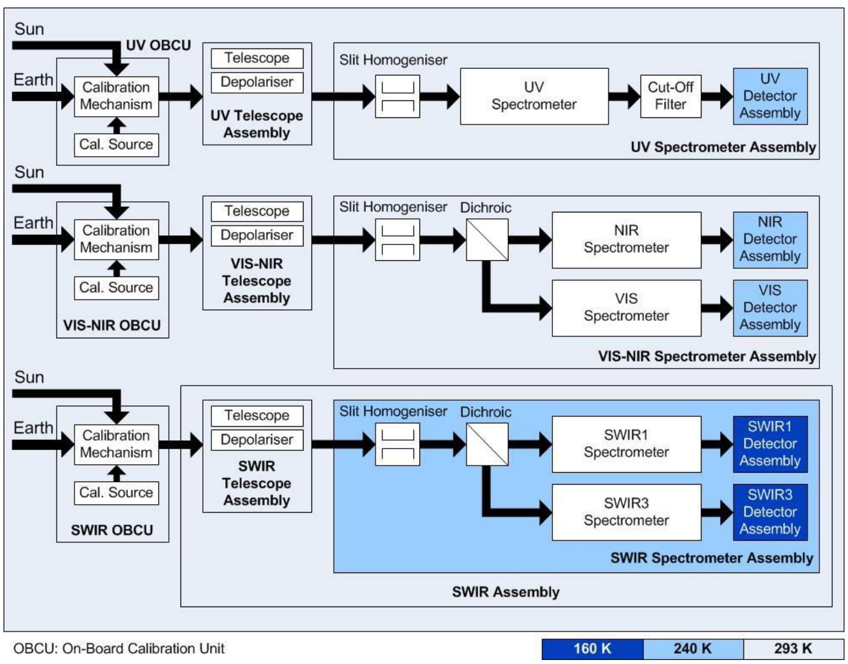


Fig. 3. Optical functional block diagram of the instrument.

Fig. 4 provides a 3D view of the mechanical layout of the instrument, and shows the basic structural configuration. Telescope baffles and instrument cover have been omitted for a better view of the structural details. The 3 optical modules are separately mounted on the optical bench. The stiff centre box of the optical bench and the mounting of the spectrometer assemblies close to each other ensure that the assemblies maintain the highest possible stability against each other. While the telescope assemblies are mounted onto the respective spectrometer assemblies, thereby yielding rigid mechanical units, the comparatively low requirements on alignment accuracy of the calibration mechanisms allows mounting them directly on the optical bench. Note that the fixation points of the spectrometer assemblies on the optical bench are still accessible after integration in order to be able to align the spectrometers for co-registration. The optical bench is fixed via bipods to the instrument base plate. The base plate also carries the instrument cover (not shown) which supports the radiator, the baffles, and the thermal equipment, e.g. MLI (multilayer insulation). The cover is thermally and structurally decoupled from the optical bench.

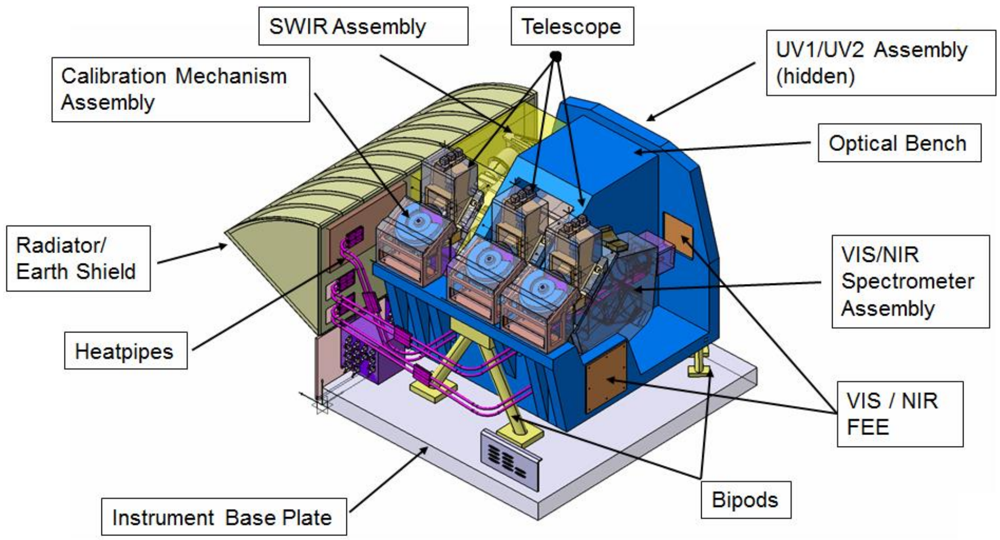


Fig. 4. Mechanical Layout (without baffles and instrument cover)

III. OPTICAL SYSTEM DESIGN

A. Telescope and Depolarisation Concept

The telescope, shown in Fig. 5, is basically a three mirror anastigmat (TMA) with an additional fold mirror for accommodation with respect to viewing orientation and envelope. It features an aperture of F/4, and anamorphic focal lengths of 17 mm and 21 mm. The mirror surfaces are spherical and aspherical. For UV and VIS-NIR, coating by aluminium is mandatory to achieve optimum broad-band reflectivity, while for SWIR gold is a better choice. The coatings are overcoated by a thin (10 to 20 nm) protective layer of Al_2O_3 or SiO_2. In the image field, the telescope is telecentric, and features a very low field curvature, with the image plane well within the depth of focus range. This enables perfect interfacing to the subsequent spectrometer slit. The telescope implements a near-f-theta projection and an almost constant étendue over the full field. Entrance pupil and intermediate image field are accessible which allows for effective stray light suppression and contamination control by appropriate stops and baffles.

All 3 telescopes possess an identical geometrical design, the only difference being the positions of mirror M4 and of the slit which differ by values in the range of less than 0.2 mm. This deviation is due to the presence of refractive depolarisation components with optical and geometrical parameters that are individually adapted to the respective wavelength bands. The main depolarisation component is the polarisation scrambler. It effectively reduces the polarisation sensitivity of the subsequent part of the optical system. Note that very low overall polarisation sensitivity is mandatory for successful air quality data retrieval. The polarisation introduced by the preceding optical components, however, is not affected. Therefore, the scrambler should be placed at the foremost position possible. In the presented preliminary design, the scrambler is positioned subsequent to M4. Uncoated plates of fused silica were added between M3 and M4 with tilt angles yielding minimum overall polarisation sensitivity. The associated refraction at oblique incidence angles leads to chromatic lateral focal spot shifts representing the major source of co-registration error. The scrambler, placed in the telecentric beam path, does not introduce any chromatic lateral errors.

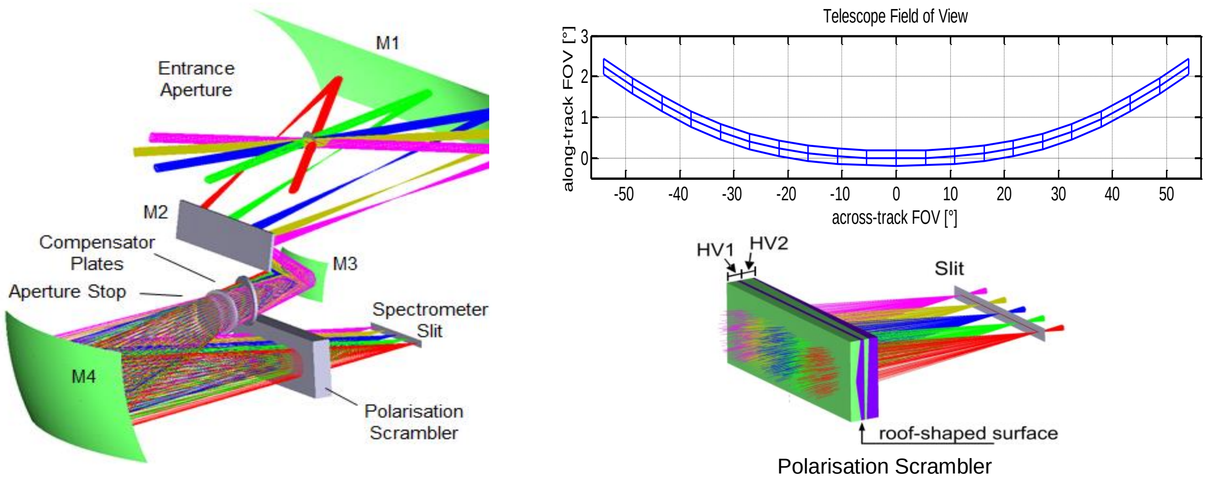


Fig. 5. Telescope optical layout including depolarisation components, and a graph showing the FOV. Note the scaling of the FOV ordinate axis (ALT FOV angle).

The used polarisation scrambler is derived from the Dual Babinet Compensator Pseudo-Depolariser (DBCP) [3]. It avoids the co-registration error generated by the DBCP by replacing the frontmost block of the DBCP with a block with a roof shaped internal surface, effectively representing the lateral combination of two blocks with opposing wedge angles. Fig. 6 illustrates construction and functional principle.

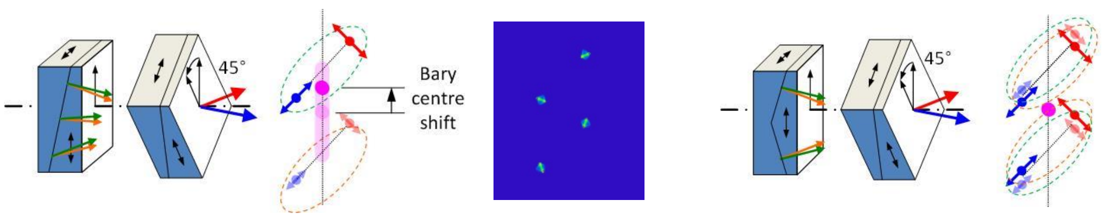


Fig. 6. Construction principle of a Dual Babinet Compensator Pseudo-Depolariser (DBCP, left), resulting far-field distribution, and the derived scrambler (right). Arrows on the wedges indicate the crystal axis orientation.

The DBCP consists of 4 birefringent wedges (e.g. from crystalline quartz) that are combined into 2 blocks à 2 wedges with orthogonally oriented crystal axes. Both blocks are rotated against each other by a specific angle, e.g. 45°. The DBCP splits the incident light in 4 mutually diverging linearly polarised beams with a far-field distribution as depicted in Fig. 6, corresponding to a split of each image point into a pattern of four. For the DBCP the barycentre of the point pattern intensity profile shifts with polarisation angle. The derived scrambler eliminates this shift by superimposing 2 mutually mirror-inverted patterns. See also [4] for a similar design.

B. Spectrometers

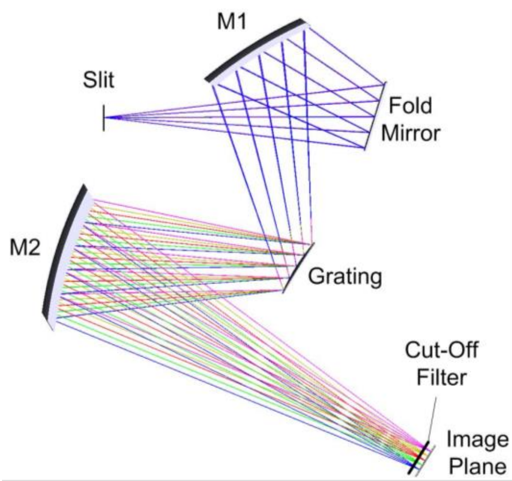
For the *UV spectrometer*, an Offner design with a blazed convex spherical holographic grating used in the -1st order was chosen. Spectrometer layout and details are shown in Fig. 7. The Offner design combines superior imaging quality for the given high aspect ratio wide field with a minimum number of elements, and accordingly low diffuse stray light levels. In order to shield the UV1 sensor area from stray light originating in the UV2 band with an up to 4 orders of magnitude larger spectral radiant power, a special cut-off filter is placed in close vicinity of the detector chip. By means of baffling (not shown in Fig. 7), ghosting could be completely eliminated. The imaging performance (spot size, keystone, smile, etc.) is well within the required limits.

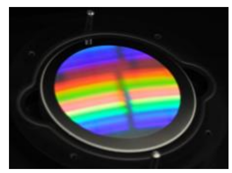
First bread board samples of the grating were manufactured by Zeiss in Jena. They feature an efficiency of more than 60% in the used order. The manufacturing process uses holographic recording followed by reactive ion beam etching to create the blazed grating profile. Thereby the artefacts (ghosts) typical for ruled gratings can be avoided. A recent description of the technology can be found in [5].

The *VIS-NIR spectrometer assembly*, shown in Fig. 8, combines the VIS and NIR spectrometers in one assembly with a common slit. Beam path separation is obtained by means of a dichroic beam splitter positioned in the diverging beam path subsequent to the slit. Both spectrometers share the first 2 lenses. Except for the fold mirrors, both spectrometers are fully refractive with transmissive binary gratings used with their -1st order in

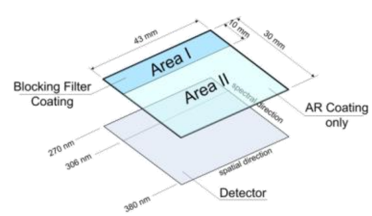
Littrow condition. All transmissive optical elements are made of fused silica only, endowing the design with superior properties with respect to radiation hardness, thermal insensitivity and stability, as well as manufacturability. Complications and difficulties known e.g. from the use of calcium fluoride (CaF_2) are completely avoided. Except for a very small number of regular aspherics, all surfaces are either plane or spherical, and all of the lenses are combined in pre-alignable doublet or triplet assemblies. For both spectrometers diffuse scatter and ghosts are in compliance to the requirements. Due to the low number of non-evanescent grating orders, only a comparably small number of ghosts appears and can easily be controlled.

The gratings are manufactured by e-beam structuring and subsequent ion-etching on plane fused silica wafers. Each grating substrate is combined with 2 prisms. Ideally, both prisms should be bonded to the grating, creating an immersed transmission grating. Because of the technological uncertainties of bonding a grating structure to a second surface, a preliminary design was chosen, bonding only one prism to the grating substrate base, and leaving an air gap between the structured grating surface and the adjacent prism. For the diffraction gratings bread board samples were manufactured by Fraunhofer IOF in Jena. Measurements yielded diffraction efficiencies larger than 63% for VIS, and between 84% and 95% for NIR, as well as low polarisation sensitivities of less than 3%. For a description of the technology see e.g. [6].





Holographic convex grating (photograph)



Layout of the cut-off filter for stray light suppression. Filter area I is coated for strongly blocking UV2 light while transmitting at UV1 wavelengths.

Fig. 7. UV spectrometer and special elements: holographic convex grating, and cut-off filter

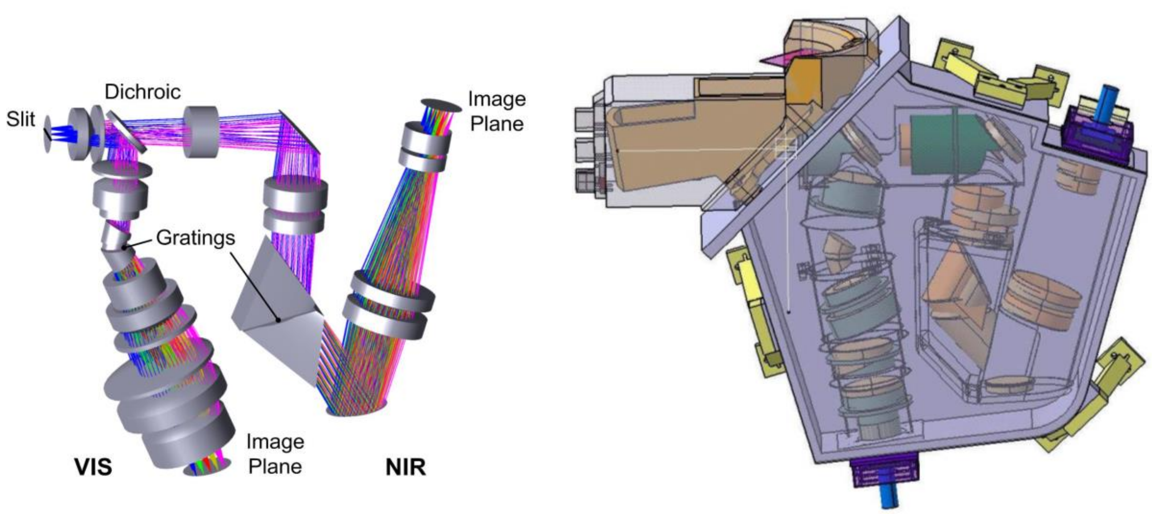


Fig. 8. VIS-NIR spectrometer assembly. Left: Optical layout. Right: Module with telescope and detector

The *SWIR spectrometer assembly*, shown in Fig. 9, was designed by Thales Alenia Space France as subcontractor. The design features immersed blazed reflective gratings used in -6th order. The grating structure is created by anisotropic wet etching of a flat wafer of mono-crystalline silicon cut at a specific angle with respect to the crystal orientation. The blaze angle naturally results from the associated etch rate anisotropy on the wafer [7]. The flat grating substrate is combined by molecular bonding and thermal fusion with a prism block of silicon to yield the final grating component. The described technology has already been used for TROPOMI. Based on simulations, a diffraction efficiency of more than 60% was expected.

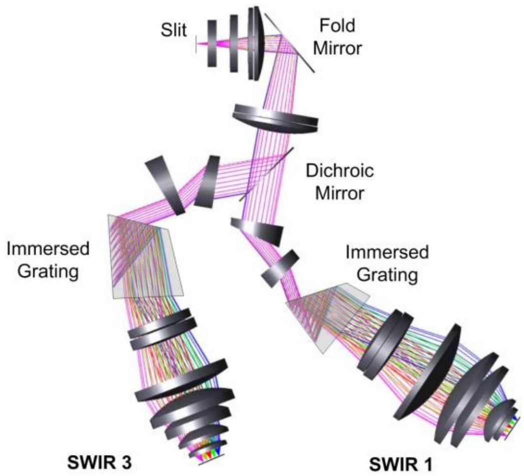


Fig. 9. SWIR spectrometer assembly (by Thales Alenia Space France)

C. On-Board Calibration

Fig. 10 depicts the main components of an on-board calibration unit (OBCU), consisting of a diffuser wheel mechanism and a calibration source assembly using a quartz tungsten halogen lamp.

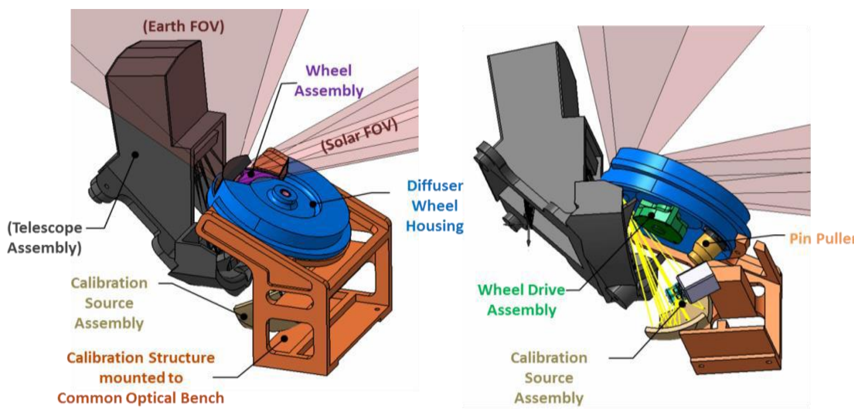


Fig. 10. On-Board calibration unit

A diffuser wheel carries two quasi volume diffusers that are used in transmission for sun calibration (one for regular operation, and one for monitoring the degradation of the first), and one backside diffuser in reflection to be used with the white light source (WLS). In a forth position, the wheel provides a shutter for the beam path. The three OBCUs show only slight differences in diffuser parameters, coatings and operational modes of the white light sources. The diffuser wheel functions and its design are similar to the MERIS and OLCI calibration mechanisms [8], [9]. Further elements of the OBCUs are calibration LEDs positioned close to the detectors.

D. Slit Homogeniser

The slit homogeniser (SH) was proposed as an optional replacement for the regular spectrometer slit. The reason for introducing the SH lies in the fact that the illumination pattern on a spectrometer slit varies according to the viewed object field. But variations of the illumination profile across the slit result in variations of the instrumental line shape (ILS) and thereby cause line shape distortions of measured spectra. Their impact on the measurement accuracy may be more or less severe depending on the chemical species and the spectral region. The SH basically consists of two opposing mirrors. The light entering from each point on the entrance multiply reflects, mixes, and eventually fills the exit aperture (Fig. 11 a)). The (wrong) assumption of an incoherent superposition of light rays yields a rather smooth and almost constant exit illumination profile (Fig. 11 b)) while in reality, due to the high dispersion of the grating, a monochromatic coherent model must be assumed, yielding interference patterns that vary with source position (see Fig.11 c)) and with wavelength. Investigations show that despite the strong non-uniformity of these patterns, ILS stability substantially improves.

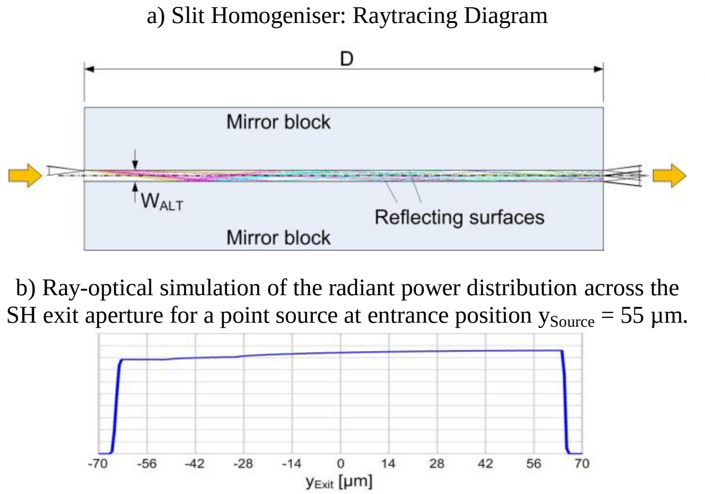


Fig. 11. Slit homogeniser and radiant power simulation results (W_{ALT} = 130 µm, λ = 2345 nm, D = 5 mm)

In the proposed instrument, SH and regular slit can be exchanged without affecting the optical design: The SH is placed with its exit aperture at the position of the regular slit. A positive cylindrical lens in front of the SH, realised e.g. by a cylindrical surface shape of the polarisation scrambler, astigmatically splits the telescope's back focal point, and positions the created along-slit focal line onto the SH entrance. Possible implementations of the SH may be e.g. polished blocks of aluminium, or aluminium- or gold-coated blocks of silicon, or comparably hard materials allowing the fabrication of precise aperture edges without breakouts.

IV. SUMMARY

The UVNS instrument concept proposed by Kayser-Threde to ESA for Sentinel-5, phase B2/C/D has been described, providing a rationale for the chosen concept, and describing its main components, as well as novel optical elements, such as the polarisation scrambler and slit homogeniser, that are important to be able to comply to the demanding performance requirements.

ACKNOWLEDGEMENTS

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