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In-field and Out-of-field stray light analysis for the COPERNICUS Sentinel 4 instrument

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ABSTRACT

Sentinel-4 is an imaging UVN (UV-VIS-NIR) spectrometer, developed by Airbus Defence and Space as prime contractor under ESA contract in the frame of the joint EU/ESA COPERNICUS program. The mission objective is the operational monitoring of trace gas concentrations for atmospheric chemistry and climate applications. Stray light, which is unwanted light captured by the detectors, is one of the major contributors to such important instrument performance metrics as absolute and relative spectral and spatial radiometric accuracies. Amongst the different sources of stray light, Out-of-Band stray light can not be corrected. It is thus important to ensure its impact is limited. The main scope of this paper is to describe the stray light simulations performed in the frame of the Sentinel-4 project: the models, analysis approach and the results. Also, the technical challenges faced in building the models and performing the analysis and the solutions found to solve them are presented.

Keywords: Sentinel 4, Copernicus, stray light, spectrometer, geostationary

1. INTRODUCTION

Sentinel-4 is an imaging UVN (UV-VIS-NIR) spectrometer which will provide accurate measurements of key atmospheric constituents such as ozone, nitrogen dioxide, sulfur dioxide, methane, and aerosol properties over Europe and adjacent regions from a geostationary orbit (see Fig. 1) – hence the motto of Sentinel-4 “Knowing what we breathe”.

In the family of already flown UVN spectrometers (SCIAMACHY, OMI, GOME & GOME 2) and of those spectrometers recently launched (TROPOMI) and currently under development (Sentinel-5), Sentinel 4 is unique in being the first geostationary UVN mission, together with very similar geostationary UVN missions over other continents, which are being developed in parallel by NASA (TEMPO) and KARI (GEMS). Furthermore, thanks to its 60-minutes repeat cycle measurements and high spatial resolution (8x8 km^2). Sentinel-4 will increase the frequency of cloud-free observations, which is necessary to assess troposphere variability.

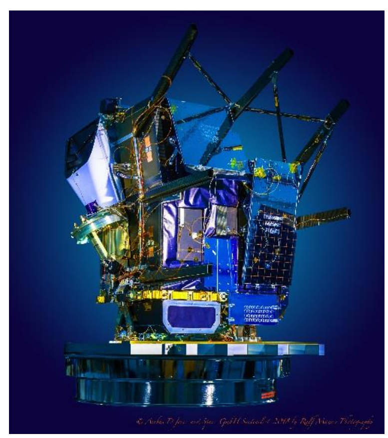

Fig. 1: **Left**: artistic impression of Sentinel-4 embarked on Meteosat Third Generation-Sounder. **Right:** photo of the instrument e-EM (without MLI) currently under testing.

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Two identical Sentinel-4 instruments (PFM and FM-2) will be embarked, as Customer Furnished Item (CFI), fully verified, qualified and calibrated respectively onto two EUMETSAT satellites: Meteosat Third Generation-Sounder 1 & 2 (MTG-S1 and MTG-S2), whose Flight Acceptance Reviews are presently planned respectively in Q4 2021 and Q1 2030.

2. SENTINEL-4 REQUIREMENTS AND OPTICAL CONCEPT OVERVIEW

2.1 Sentinel-4 driving requirements

Table 1 below gives an overview of the Sentinel-4 instrument main design and performance requirements.

Table 1: Main design and performance parameters of Sentinel-4

Spectral			
Parameter	**UV-VIS values**	**NIR values**	**Comments**
Wavelength range	305-500 nm	750-775 nm	
Spectral Resolution / Spectral Oversampling	0.5 nm / 3	0.12 nm / 3	Oversampling is Resolution divided by spectral pixel sampling
Spectral Calibration Accuracy	0.0017 nm	0.0020 nm	
Geometric and Temporal Coverage			
Parameter	**Value(s)**		**Comments**
Spatial Sampling Distance (SSD)	8 km x 8 km (E/W) (N/S)		On-ground-projected SSD at reference point in Europe (45°N latitude; sub-satellite-point longitude)
Integrated Energy	70% over $1.47SSD_{EW}*1.13SSD_{NS}$ 90% over $1.72SSD_{EW}*1.72SSD_{NS}$		Integrated energy is a measure for the spatial resolution of the instrument
N/S slit field-of-view (swath)	4.0°		
Daily Earth observation time	Summer max: 01:40 – 21:40 Winter min: 03:40 – 19:40		Adjusted to seasonally varying solar Earth illumination on monthly basis
Spatial co-registration	Intra-detector: 10% of SSD Inter-detector: 20% of SSD		2-dimensional (E/W & N/S) absolute co-registration
Radiometric			
Parameter	**UV-VIS values**	**NIR values**	**Comments**
Optical Throughput	~50% (in UV)	~60%	End-to-end scanner-to-detector
Radiometric Aperture	70 mm	44 mm	Circular diameter
Earth Signal-to-Noise-Ratio (SNR)	UV: >160 VIS: >1600	759-770nm: >90 Rest NIR: >600	For specified Earth radiance Reference scene
Earth Absolute RA	< 3%	< 3%	For Earth radiance & reflectance
Sun Absolute RA	< 3%	< 3%	For sun irradiance
Polarization Sensitivity	< 1%	< 1%	
Relative Spectral RA	< 0.05%	< 0.5%	For a spectral window of 3nm (UVVIS) and 7.5nm (NIR) and for reflectance only
Relative Spatial RA	< 0.25%	< 0.25%	For Earth radiance & reflectance
Power	212 W (average in operating mode)		
Mass	200 kg		
Data	25.1 Mbps (instantaneous, during acquisition)		
Number of units	Three (3): • Optical Instrument Module (OIM), which contains the optical and detection part • Instrument Control Unit (ICU) • Scanner Drive Electronic (SDE)		

2.2 Sentinel-4 measurement Concept

The instrument measurement concept, illustrated in Fig. 2 (left), can be described as follows: A scanning mirror, operating in push-broom mode, selects a strip of land whose “white light”, reflected by the Earth and transmitted through the Earth atmosphere, is collected by the telescope. The collected “white light” is split into two 2 wavelength ranges (i.e. the Ultraviolet & Visible-UVVIS and the Near-Infrared-NIR ranges) by a dichroic beam-splitter mirror and focused onto the two slits of the two separate spectrometers. Afterwards the light is first collimated onto the dispersing optical elements of the two spectrometer channels (either a grating or a grism) and dispersed in the spectral direction.
The generated spectra are re-imaged onto two 2-dimensional charge coupled device (CCD) detector arrays. One dimension features the spectrum, the other dimension the spatial (North/South) direction corresponding to the selected strip on Earth (ground swath). At the end of this scanning process which lasts about 1 hour, spectra of multiple strips of land, which make up the complete field of view, are acquired and a complete spectral image of the Earth atmosphere over Europe is created. The process is repeated daily n-times so long as the relevant strip of land is illuminated by the Sun.

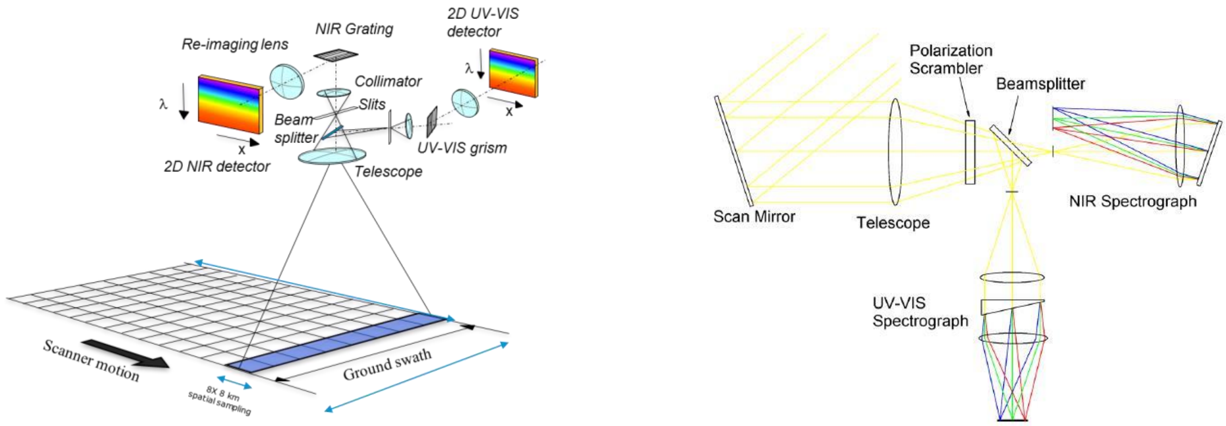

Fig. 2: Sentinel4 instrument measurement principle (left) and Optical design sketch (right).

2.3 Sentinel-4 Optical Design

The Sentinel-4 core optical layout scetch is shown in Fig. 2 (right). It consists of the following optical modules: Scanner, Telescope Module (including beamsplitter & slits), UVVIS and NIR Spectrograph Modules.
The Focal plane of Sentinel-4 features two CCDs detectors (UV-VIS and NIR), which are both frame-transfer CCDs. The CCDs are covering the range 305-500nm and 750-775nm respectively.

The main end-to-end performances driving the optical design are the polarization (polarization sensitivity and its spectral & spatial features), the stray light and the co-registration.
One of the main optimization criterion of the optics design is the minimization of stray light: the main sources of stray light are scattering from surface roughness and particulate contamination, as well as ghosts. The term ghosts encompasses a variety of false light effects, such as multi-reflections from anti-reflection (AR)-coated surfaces, unwanted reflections from mechanical surfaces outside the nominal optical path (lens mounts, optical stops, baffles, etc.), and unwanted or multiple diffractions from the dispersers. All these stray light sources are mitigated by minimization of the number of optical elements. Furthermore, ghosts are suppressed by dedicated optimization of the optics design in all areas, e.g. spectrograph and disperser architectures, as well as by a sophisticated stray light baffling architecture; namely the beam splitter-slits-assembly and in the FPAs.

Still, stray light cannot be completely excluded per design and the remaining stray light level is driving the instrument performance. As such it shall be minimized per design (at Level-0) or corrected per post processing (at Level 1b).
In the following the stray light simulation performed in the frame of the Sentinel-4 project is presented: the models, analysis approach and the results. Also, the technical challenges faced in building the models and performing the analysis and the solutions found to solve them are presented

3. SENTINEL-4 STRAY LIGHT SIMULATIONS APPROACH

Stray light, which is unwanted light captured by the detectors, is one of the major contributors to such important instrument performance metrics as absolute and relative spectral and spatial radiometric accuracies. There are two physical mechanisms responsible for stray light generation, which are scatter and reflections (ghost images) from optical or mechanical surfaces.
Different types of stray light in the instrument are distinguished based on the origin, impact and potential for correction by image processing. Those are In-Field (IF), In-Band (IB), Out-Of-Field (OOF) and Out-Of-Band (OOB). Typically, if an instrument opto-mechanical design is optimized for stray light reduction, IF-IB stray light is the one with the highest intensity. Luckily, it can be (partially) corrected, as the sources that generate it are captured in the images. The opposite is true for other combinations such as IF-OOB, OOF-IB and OOF-OOB.

On system level, the performance requirements impacted by stray light are formulated with a reference to a nominal scene to be observed by the instrument as shown in Fig. 3. Thus, the objective of the stray light simulations is to calculate the irradiance on the detector due to stray light assuming that the instrument observes the reference scene.

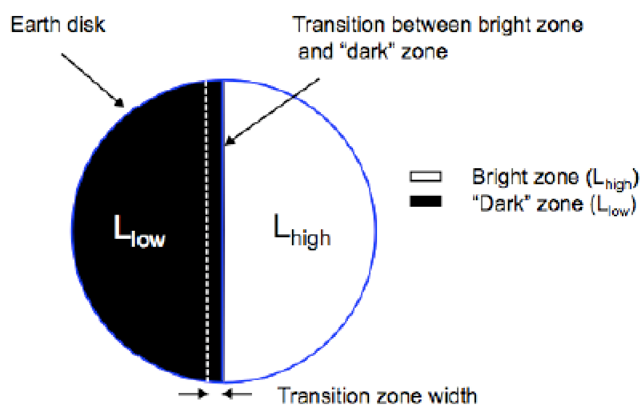

Fig.3 : Reference scene defined for S4 performance requirements.

In Sentinel-4 a set of optical models has been developed in Zemax and Python to assess the impact of stray light on optical performance. These models and the achieve results are presented in the following sections.

The approach to calculate stray light irradiance for a given reference scene is based on using a set of so-called kernels. A kernel in this case is a geometrical Point Spread Function which does not include light propagated via a nominal path, but includes all the stray light. A convolution of the reference scene with a grid of kernels results in the stray light irradiance. Thus, the objective of the simulations described in this article is to calculate such a set of kernels, as dense and as accurate as possible, given constraints on the simulation computing time (days, rather than months).

3.1 IF stray light modelling approach

In-Field and In-Band simulations of the stray light due to scattering and ghosts are based on an analytical model and a Zemax non-sequential model respectively.

Zemax non-sequential ghosts modelling is relatively simple and the principles of such an analysis are reviewed in literature. That is why it is left out of scope of this article as less interesting.

IF and IB stray light simulations are based on an approach proposed by G. Peterson [1]. Using paraxial optics laws, G. Peterson showed that the image plane irradiance due to scattered light in an optical system generated by a point source is given by a linear combination of BSDFs of the optical surfaces. The coefficients in this combination are defined by the coordinates of the marginal ray on the respective optical surfaces of the system. The equations derived in [1] can be used to calculate scattered stray light kernel for a given wavelength. Accounting for paraxial optics approximation used in [1], there is no dependence of the kernel on the Field Of View.

Both Airbus DS and ESA [2] have developed software tools for scattered stray light simulation based on Peterson model, and the tools have been cross-validated with respect to each other.

When calculating a kernel, one has to know what data to use as BSDFs of the surfaces. In an early phase of the project BSDF models such as Harvey Shack (HS) are typically used. In this case the b-coefficient of the model is scaled according to the Total Integrates Scatter of the surface with a roughness according to the manufacturing specification.

However, as the S4 is already in the manufacturing phase, the representative optical samples were available, and their BSDFs have been measured in ESA TEC-MMO optical laboratory. The BSDF models describing scatter due to roughness have been derived from those BSDF measurements. Figure 4 shows an example of such a BSDF raw data and a HS model fitting some of the curves. The orange and grey curves in Fig. 4 show the instrument signature of the BSDF measurement setup. The coefficients of the fitting HS model have been subsequently substituted in the stray light simulation tool.

The BSDF optics samples were clean, which means that an additional BSDF model is needed to simulate the scatter effect of contamination. Such a model has been implemented based on Mie scatter theory and MIL1246 cleanliness standard [3 – 5].

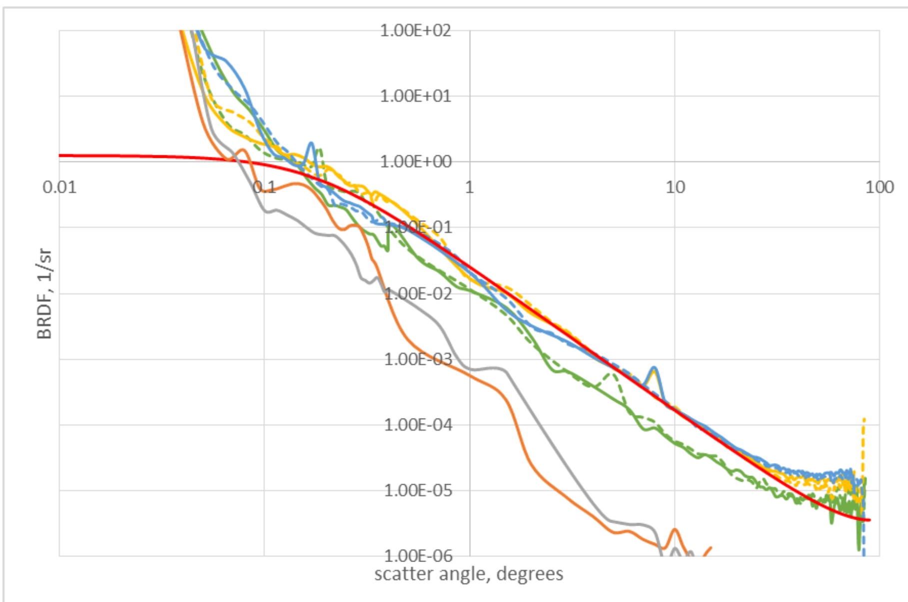

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Fig.4 : Example of measured BSDF raw data of several samples with a superimposed a HS model.

3.2 OOF stray light modelling approach

This article focuses on the simulation of the stray light impact on the performance requirements at system level. This is not a typical stray light analysis aimed at investigating critical objects and possible stray light paths. Such an analysis has been performed in the past as an effort to support opto-mechanical design. Detailed models of the instrument subsystems (telescope and spectrometers) have been developed in ASAP, and each subsystem has been analysed independently to identify potential high energy stray light paths. This activity, a so-called hot spot analysis, resulted in modification of the internal baffling in order to block the dangerous stray light trajectories.

The approach to the simulations described in this article includes using Zemax as a non-sequential raytracing engine combined with Python software controlling the simulation. The software in Python communicates with Zemax model of the instrument via DDE interface and performers such functions as setting simulation parameters, starting a simulation, retrieving simulation results and data post-processing.

Three optical modules of the instrument have been simulated separately: telescope (including beamsplitter assembly), UV and NIR spectrometers. This separation was made to simplify simulations, assuming that the stray light is generated in the telescope and spectrometers independently. One of the consequences is that the stray light generated in the spectrometers by the telescope stray light is neglected. Also, it is assumed that the stray light paths do not include contributions in the spectrometers and telescope at the same time. This is a valid assumption considering that the telescope is separated from the spectrometers by the slit. Figures 5, 6 and 7 show the cross-sections of the Zemax models of the telescope, UV and NIR spectrometers respectively. One can see the optical as well as mechanical components of the models.

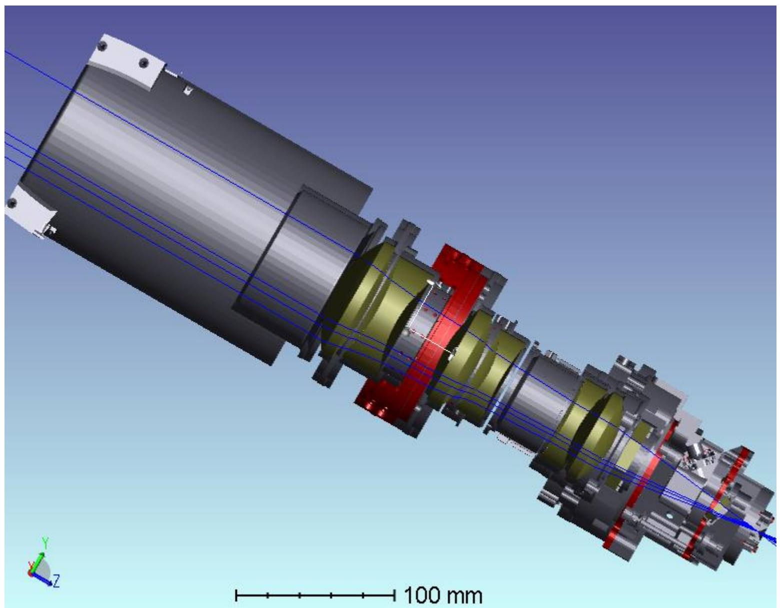


Fig.5 : Cross-section of the non-sequential Zemax telescope model.

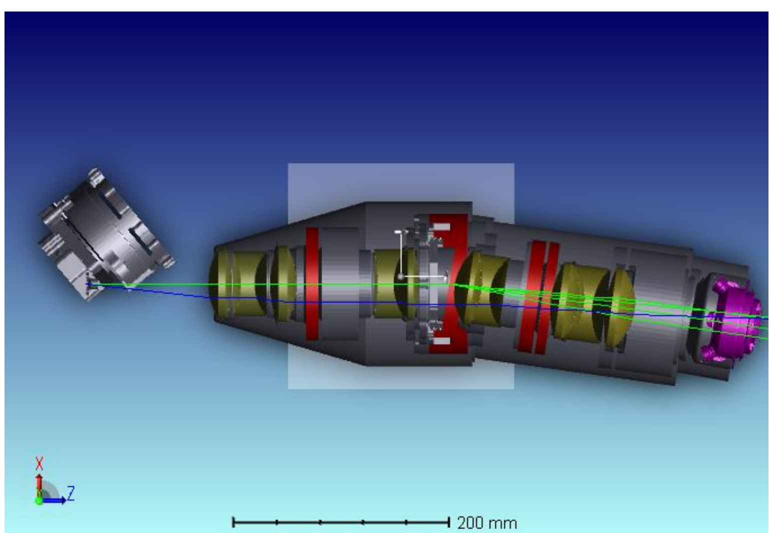


Fig.6 : Cross-section of the non-sequential Zemax UV spectrometer model with the slit assembly on the left.

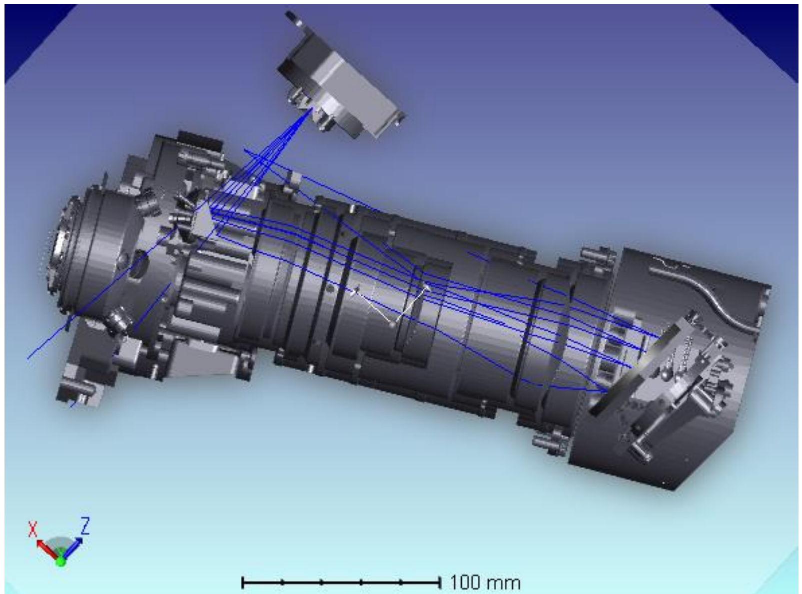


Fig.7 : Cross-section of the non-sequential Zemax NIR spectrometer model with the slit assembly.

Several technical problems have been solved in the process of building the representative Zemax models after implementing optical elements including antireflection coatings.

Firstly, the mechanical components (lens holders, baffles, screws, etc.) can not be imported in Zemax from the mechanical design CAD files, even though Zemax allows such an import. One reason is that a large number of complex-shaped objects would make the model too heavy and the ray tracing slow. Another reason is that Zemax treats imported CAD objects as a whole. That is why it is not possible, for example, to apply different coatings to different surfaces of the object. It is always one coating applied to the object as a whole. The solution was to simplify the mechanical CAD design for the optical model, in such a way that it is still representative optically, but as simple as possible from the mechanical point of view.

Second problem solved was the implementation of the coating model applied to the mechanical parts. Some mechanical parts are coated by the Acktar black coating, for which the coating model is available in Zemax BSDF format from the manufacturer. Other parts are coated by Aeroglaze Z307 coating, for which no model exists for Zemax. However, such a model has been implemented for the ASAP software and is described in one of the ASAP software tutorials. This model is defined in an analytical form as a polynomial ASAP model. Using a dedicated Matlab script, polynomial coordinates used in ASAP have been converted in to the coordinates of Zemax BSDF format and a set of data has been created for Zemax BSDF file representing Z307 model. The resulting BSDF is illustrated in Fig. 8 for the 15 degrees angle of light incidence.

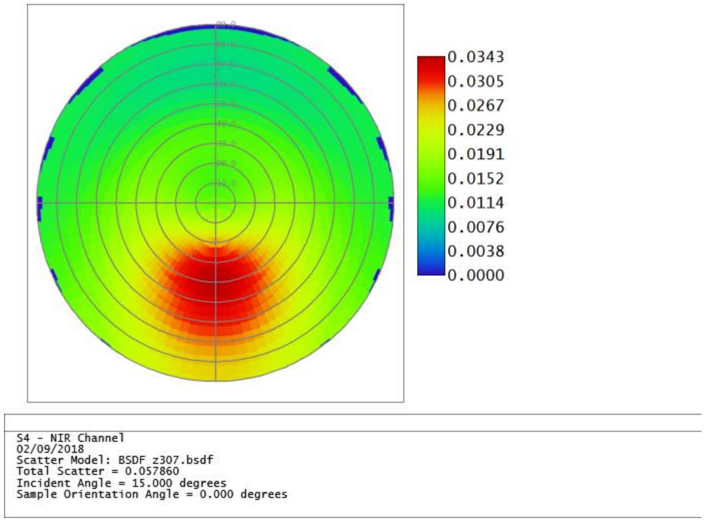


Fig.8 : Z307 BSDF model in Zemax for angle of incidence of 15 degrees. One can see a strong forward scattering.

When setting a simulation up, one has to approach the settings of Zemax non-sequential raytracing carefully.

It is not uncommon that when one runs a non-sequential raytracing in Zemax involving a complex model, Zemax reports about an error and stops. Then one has to mark a check-box “ignore errors” in the raytracing control dialog.

In this case, as also mentioned in Zemax tutorials, one has to look at the value of energy lost due to errors that Zemax reports in the end of the raytracing. To be confident in the correct results, this energy must be negligible as compared to the energy collected on the detector (or any other relevant surfaces).

In a complex system the energy lost due to errors can quickly go out of control. Very often, the cause of errors is a too low number of the maximum allowed ray segments. However, even setting this number to a maximum value allowed by Zemax may not help. Also, increasing this number can result in a very long time needed to complete the raytracing. In this case, one can investigate the ways to reduce the probability of Zemax generating too many ray paths, while still ensure that the relevant stray light paths can not be missed.

For the simulation of OOF stray light reported in this article, we considered that the ray can not reach the detector along the nominal path. Thus, there are three options for an OOF ray to propagate to the detector: by two scatter events, by a scatter and a reflection and by two reflections. For each of these options we can make a conservative estimate of the energy lost by a ray and set a respective limit for the “Minimum relative ray intensity” in Zemax non-sequential settings. This approach reduces the number of ray segments considerably and allowed us to reduce the energy lost due to errors to an acceptable limit.

Another important parameter is the number of scattered rays that Zemax generates when simulating scattering. Each of the new scattered rays means a new branch of ray segments. That is why, the number of scattered rays has been set to 2 for scatter from mechanical surfaces and to 1 for scatter from optical surfaces.

4. SENTINEL-4 STRAY LIGHT ANALYSIS RESULTS

4.1 IF stray light modelling result

Figures 9 and 10 show the simulation of the reference scenes projected on the instrument focal planes (of UVVIS and NIR spectrometers respectively). The irradiance is expressed as a photon flux.

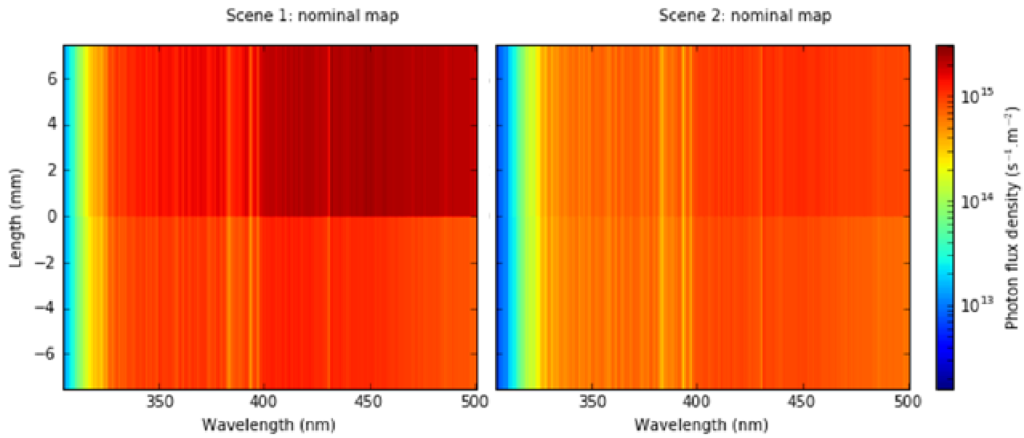


Fig.9 : Reference scenes projected on the UVVIS spectrometer focal plane.

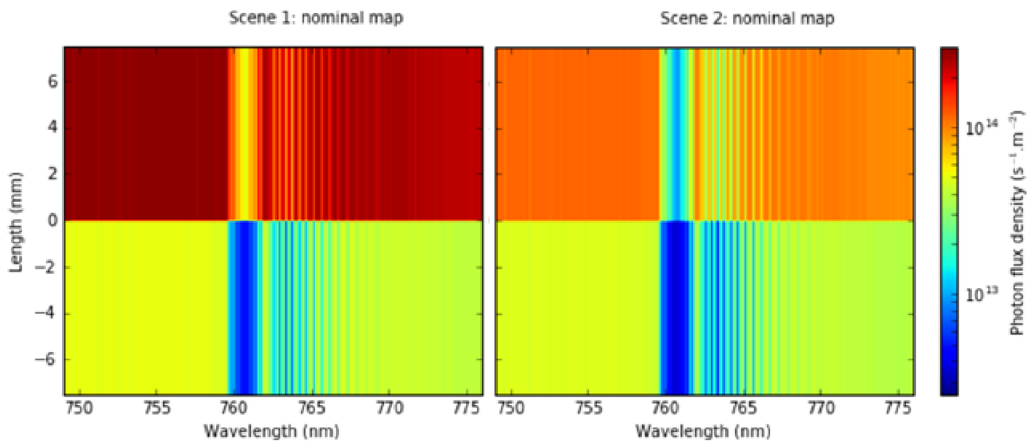
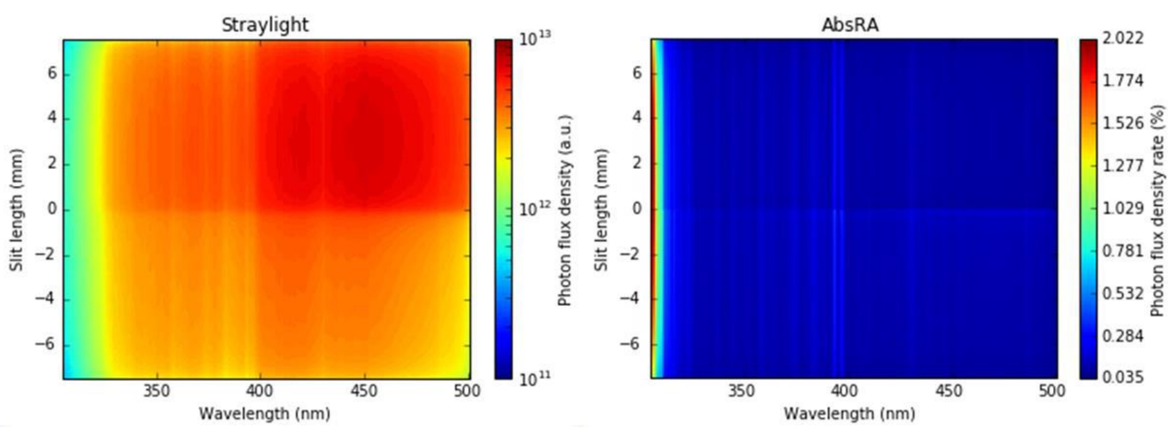


Fig.10 : Reference scenes projected on the NIR spectrometer focal plane.

As an example, Figs. 11 and 12 show the stray light irradiance and respective radiometric error due to stray light (Radiometric Accuracy) map for UVVIS and NIR spectrometers respectively.



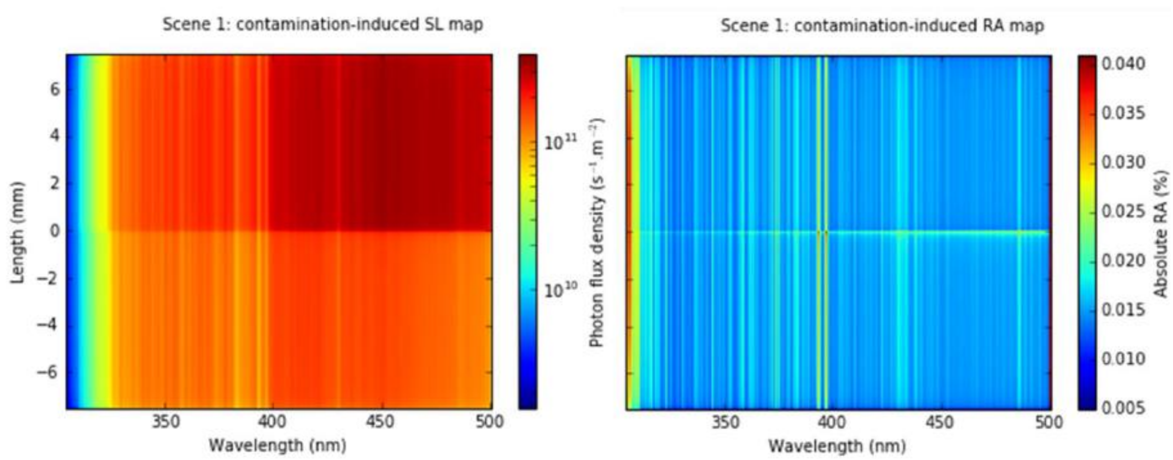


Fig.11 : Resulting stray light irradiance and induced radiometric error in the UVVIS spectrometer due to roughness (top) and contamination (bottom).

One can see that spectral features in the contamination stray light map are less blurred as compared to the roughness one. This can be expected if one takes into account that the contamination BSDF is very high at small scattering angles, so that the most energy of the contamination stray light is concentrated within 10 – 15 pixels around the nominal image.

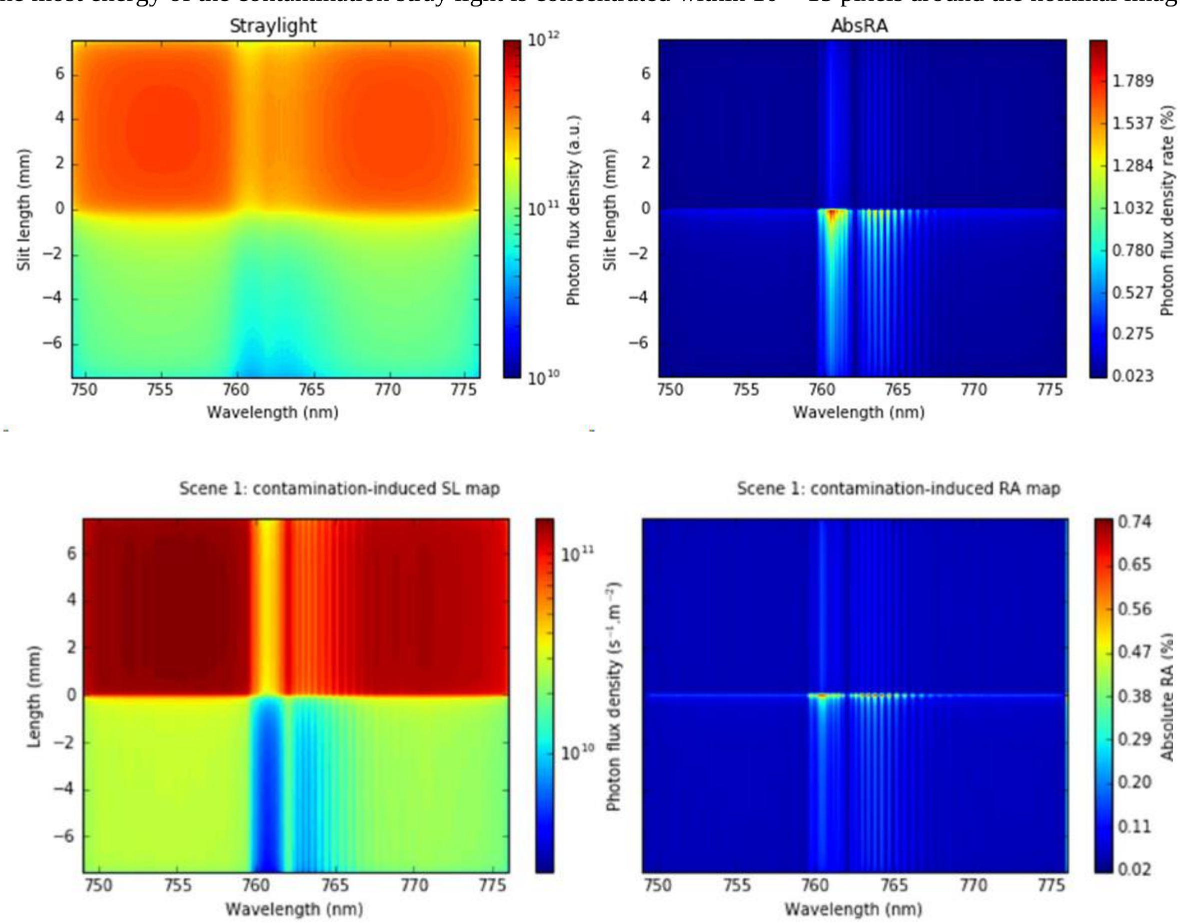


Fig.12 : Resulting stray light irradiance and induced radiometric error in the NIR spectrometer due to roughness (top) and contamination (bottom).

4.2 OOF stray light modelling results

At the moment, the OOF (and also OOB) analysis has been completed for the spectrometers, but for the telescope it is still ongoing. The preliminary results indicate that the OOF - OOB stray light is considerably lower than the IF stray light, which proves a good optomechanical stray light suppression concept.

5. CONCLUSION AND SUMMARY

In conclusion, the status of the Sentinel-4 IF and OOF stray light analysis is reported in this article. The set of models has been developed and is operational. The IF model of industry and a stray light tool developed internally at ESA have been cross-validated to gain additional confidence in the results of the simulations. Measurements of the BSDFs on representative optical samples have been used as an input to the stray light simulation tools. This reduces the simulation uncertainty associated with the BSDF modelling.

The IF analysis have been completed, while the OOF analysis is being finalized. The preliminary results indicate that the main contributor to the performance requirements is the IF stray light while the level of OOF stray light is much lower.

The simulations show that even with a good stray light suppression concept stray light is a driving contributor to the instrument performance. Therefore efficient post processing of the images to further reduce the impact of stray light is implemented to fulfil the challenging radiometric accuracy requirements.

6. ACKNOWLEDGEMENTS

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