S4 Surface Reflectance Map Conceptual Development

SURMACED

Final Report

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List of abbreviations and acronyms

AMF	Air Mass Factor
ATBD	Algorithm Theoretical Basis Document
BRF	Bidirectional Reflectance Factor
BSA	Black Sky Albedo
CA	Coverage Area
DOAS	Differential Optical Absorption Spectroscopy
EUMETSAT	European Organization for the Exploitation of Meteorological Satellites
FCI	Flexible Combined Imager
GRASP	Generalized Retrieval of Aerosol and Surface Properties
HSS	
JMA	Japanese Meteorological Agency
LER	Lambertian equivalent reflectance
LUT	Look-Up Table
MRD	Mission Requirement Document
MTG	Meteosat Third Generation
NOAA	National Oceanic and Atmospheric Administration
RA	Reference Area
RPV	Rahman-Pinty-Verstaete
SSD	Spatial Sampling Distance
SSP	Sub-Satellite Point
UVN	Ultraviolet, Visible, Near infrared
VIS	Visible

Reference Documents

RD1 RD1: GMES Sentinels-4 and-5 Mission Requirements Document (MRD), EOP-SMA/1507/JL-dr, v3.2, (2011).

RD2 Statement of Work, ESA, Algorithm Concept Development for the Daily Surface Reflectance Map Product for Sentinel-4, EOP-SM/2336/BV-bv, Issue 1.1

RD3 SURMACED Technical Note 1, ESA Contract 40000106521/12/NL/MP

RD4 SURMACED Technical Note 2, ESA Contract 40000106521/12/NL/MP

RD5 SURMACED Technical Note 2, ESA Contract 40000106521/12/NL/MP

RD6 SURMACED S4-GRASP ATBD, ESA Contract 40000106521/12/NL/MP

RD7 Dubovik, O. 2010. Study on Improved Retrieval Method Od Detailed Aerosol Properties from MTG/FCI, Part 1, Theoretical Concept. EUMETSAT ITT No 09/992.

1 Introduction

The objective of the SURMACED study is to describe an algorithm for the retrieval of surface reflectance map from Sentinel-4 observations [RD1] that would meet user requirements [RD2]. Specifically, the study includes the following major tasks

- A review of the accuracy of the surface reflectance and its directionality required for meeting the Level-2 requirements of the main target species of Sentinel-4 (Section 2);
- A review of existing heritage concepts in view of their relevance to Sentinel-4 taking into account the specific capabilities of the Sentinel-4/UVN instrument (Section 3);
- Generation of an Algorithm Theoretical Baseline Document (ATBD), and recommendations on the development approach of the daily UVN surface reflectance product for Sentinel-4 (Section 4).

The elaboration of surface reflectance map from Sentinel-4 observations requires addressing a series of technical and physical issues. Among the physical issues, the radiative coupling between aerosols and surface scattering is certainly one of the most challenging problems to be solved. Indeed, aerosols modify differently the amount of radiation reflected by the surface and observed from space as a function of the wavelength and the viewing directions.

The need to accurately document the surface reflectance anisotropy is triggered by the S4 mission objective to monitor the daily cycle of trace gas species such as O_3, SO_2, HCHO, and NO_2, *etc*… The Generalized Retrieval of Aerosol and Surface Properties (GRASP) method is proposed to provide accurate surface reflectance maps. This approach retrieves simultaneously surface reflectance and aerosol properties.

2 Requirements elaboration

The first SURMACED task is the accuracy review of the surface reflectance and its directionality required for meeting the Level-2 requirements of the main target species of Sentinel-4 [RD3]. In the UV-Vis region, systematic retrieval errors are generally dominated by the uncertainty in tropospheric air-mass factor (AMF). One of the key input parameters for the calculation of the AMF is the surface reflectance which affects retrievals directly through the clear-sky AMF and indirectly through the cloud retrievals. In this study, AMF calculations are performed assuming non-Lambertian surface conditions represented by the Bidirectional Reflectance Factor (BRF) field in combination with atmospheric radiative transfer model simulations to test the sensitivity of the AMF to different surface reflectance treatments for the typical observational conditions of Sentinel-4.

The SURMACED study investigated the impact of surface reflectance uncertainties on trace gas DOAS-type retrievals of O_3, SO_2, HCHO, and NO_2, using the RPV surface BRF model. The sensitivity of the AMF to surface reflectance uncertainties was found to be larger in the visible region than at shorter wavelengths. Also uncertainties were found to be dominated by the mean amplitude and asymmetry parameter in the RPV model. Concentrating on these two parameters, the corresponding surface reflectance uncertainty requirements for trace gas retrieval have been estimated. Furthermore, the uncertainty requirements on equivalent Lambertian albedos commonly used in operational trace gas retrieval were also estimated. Using black-sky albedos (BSA) as a proxy for Lambertian albedos we found that this approximation is sufficiently accurate in most cases. However larger errors (up to 20%) can be encountered in polluted cases justifying the need for a full BRF model.

Table 1: Summary of uncertainty requirements on surface reflectance for use in trace gas retrieval

Wavelength		325nm		320nm		340nm	450nm	
Data Product		Total O_3	Tropo. O_3	Volcanic SO_2	Tropo. SO_2	Tropo. HCHO	Total NO_2	Tropo. NO_2
PM	a_{bs}	0.09	>0.1	>0.1	0.089	0.059	0.017	0.005
	ρ_0	0.056	0.075	>0.1	0.055	0.036	0.01	0.003
	κ, θ, h_0	>50%	>50%	>50%	>50%	>50%	30%	7%
NRT	a_{bs}	>0.1	>0.1		0.073	0.03	0.017	0.005
	ρ_0	0.093	0.075		0.047	0.018	0.01	0.003
	κ, θ, h_0	>50%	>50%		0>50%	32%	30%	7%

Table 1 summarizes the main outcome of this first task, *i.e.* it lists the surface reflectance uncertainty requirements that match user requirements on trace gas data products defined in the S4/S5 Mission Requirement Document (MRD) [RD1].

As can be seen, in most cases except for NO_2, the uncertainty requirements on surface albedo are larger than 0.03, and the requirements on amplitude and anisotropy parameters are larger than 0.01 and 30%. For the tropospheric NO_2 case however, the requirements on surface albedo, amplitude and anisotropy parameters are much more demanding, respectively of 0.005, 0.003 and 7%.

The driving case assumed for tropospheric NO_2 is a polluted scenario where the bulk of the NO_2 is located in the boundary layer, while 50% of the allowed uncertainty in the NO_2 column is allocated to surface in surface albedo. According to the S4/S5 MRD the user requirement applicable to this case is 10%, which is extremely strict as compared to the typical accuracy of current satellite NO_2 products (40%-80% for polluted conditions, Valks et al., 2011). Even in the ideal case where the albedo requirement would entirely consume this allowed uncertainty on NO_2 retrieval, an uncertainty requirement of ~0.01 is obtained. This is significantly smaller than the accuracy of the current albedo products from satellite measurements and therefore puts strong constraints on S4 BRF retrieval algorithms. The surface reflectance uncertainty requirements derived from the tropospheric NO_2 case with the abovementioned assumptions could therefore not be adopted as threshold requirements but were taken as a goal.

Accordingly, the present study focuses on obtaining the best achievable accuracy. Possible approximations and simplifications to the code that would enhance computational efficiency to the cost of accuracy are not investigated.

3 Selection of the retrieval method

The second SURMACED task consists in reviewing the existing approaches for the retrieval of surface reflectance from space observations [RD4]. This analysis is performed in light of the physics of the signal observed by S4, the constraints of the retrievals and the mission objectives, *i.e.*, the requested surface BRF accuracy to document the daily cycle of atmospheric composition as defined in Table 1. The goal accuracy in the surface albedo near 450 nm is better than 0.005 in order to exclude significant errors in tropospheric NO_2 retrievals. Such an accuracy requirement is extremely tight as compared to the performance achieved by standard dataset such as the NASA MODIS surface albedo one which has a recognised surface albedo uncertainty of about 0.01 – 0.03. The objective is therefore to determine which approach and associated assumptions is most appropriated for the retrieval of surface reflectance from S4. This analysis suggests using the GRASP algorithm which is based on a physically-based joint surface-aerosol retrieval approach relying on an OE inversion technique, as already prototyped by [RD7] for the processing of MTG-I/FCI observations. As already stressed in the first SURMACED task, the use of a Lambertian Equivalent Reflectance (LER) surface approximation leads to error magnitude equal to the accuracy requirements for NO2 in polluted cases (Figure 1). The joint retrieval of surface reflectance and aerosol properties has proven to be very robust and has been implemented at EUMETSAT, JMA and NOAA for the systematic processing of archived geostationary observations for the retrieval of surface reflectance from any archived geostationary observations.

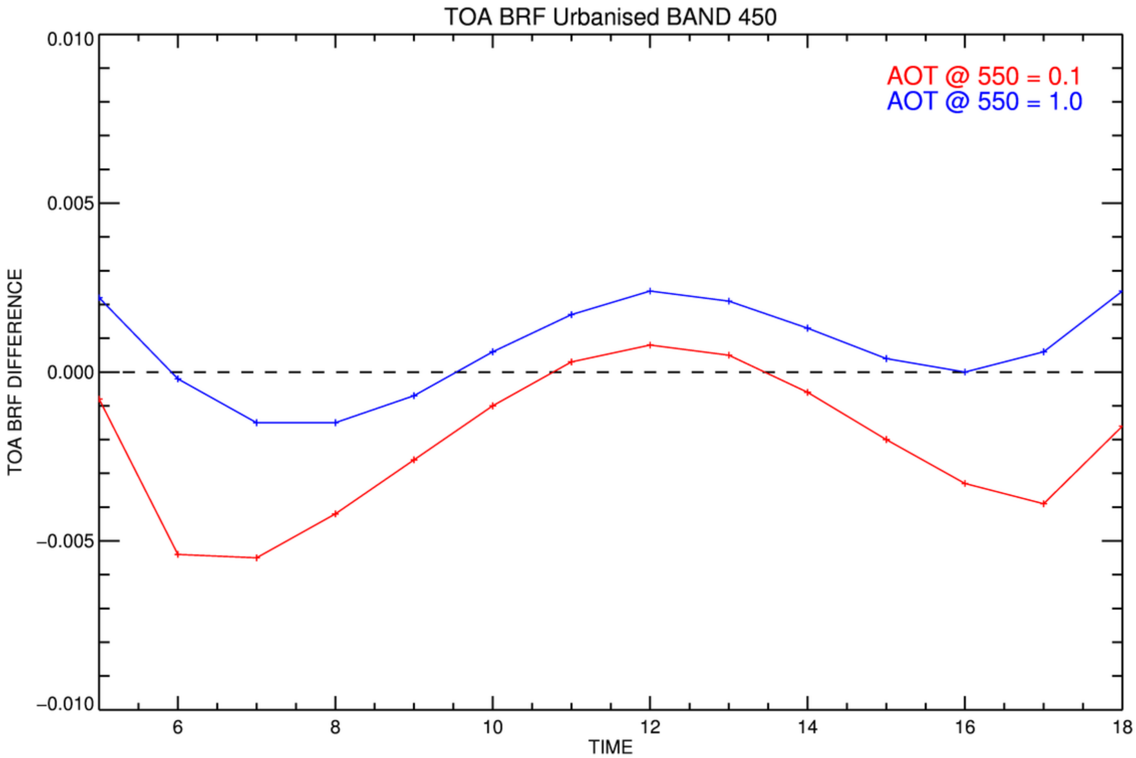

Figure 1: Difference between the simulated TOA S4 signal at 450nm over the urbanised surface type with an Lambertian Equivalent Reflectance (LER) equal to the BRF value at the local time and a simulation with a BRF surface.

The proposed GRASP approach relies on the daily accumulation of S4 data to form a multi-angular and multi-spectral observation vector. While the surface properties and aerosol composition are assumed temporally invariant during the course of the day, the aerosol concentration will be retrieved for each clear-sky processed slot. The GRASP algorithm has been originally designed for the processing of PARASOL observations relying on a similar approach as used for AERONET. The GRASP algorithm benefits from several decisive advantages for the retrieval of surface reflectance:

- Surface reflectance and aerosol properties are jointly retrieved, offering accurate atmospheric correction as these two quantities are intimately radiatively coupled as shown in [RD4].
- All state variables, including aerosol single scattering properties are allowed to vary continuously within the solution space. This advantage prevents the use of LUT which always limit the solution space boundaries and retrieval accuracy. The GRASP algorithm has proven to be the most accurate one.
- The GRASP algorithm inverts simultaneously a block of pixels, applying temporal, spatial and spectral smoothness constraints on the state variables.
- The GRASP algorithm is physically-based and can therefore be applied to any observation system with enough degree of freedom. It has already been proven possible to be applied on MTG/FCI observations for an accurate retrieval of aerosol properties [RD7].

4 Algorithm concept description

The third major task concerns the sensitivity analyses performed to elaborate the S4 surface reflectance daily product ATBD. This task explores the possibility to meet the requirements defined in [RD3] with the proposed GRASP algorithm in order to generate the S4 daily surface reflectance map. Five spectral bands centred on 342, 374, 417, 456and 756 nm have been selected for the retrieval of reflectance and atmospheric properties. It has been demonstrated that there is no need to perform spectral interpolation between these bands to characterise surface reflectance at any wavelength in the S4 spectral domain. Analysis of the variability of the surface parameters have shown that, on average, daily variations of surface albedo is about 0.0018 and 0.0023 in the 600 and 800 nm spectral regions respectively over the S4 coverage area. Such information is critical to provide temporal smoothness constraints on the surface reflectance retrieval. Monthly statistics of cloud coverage have shown that number of daylight cloud-free hourly observations is close to zero around 60^{o}N and about 5 around 35^{o}N in wintertime (Figure 2). In summertime, these numbers are close to 8 for both locations. It is therefore needed to accumulate about 5 days of consecutive observations in order to collect enough cloud-free information to perform the inversion in summertime. In wintertime, an accumulation period of 10 days might be necessary in order to collect enough daylight clear-sky observations.

The GRASP algorithm is proposed to derive both surface reflectance and atmospheric properties from S4 observations in the five selected spectral bands. This algorithm relies on L1c S4 reflectance data. It is recommended to generate the L1c data from the HSS observation that should be spectrally located at the place of the five selected bands.

The strategy originally proposed for the adaptation of the GRASP algorithm to S4 observations has been modified in order to cope with the very demanding surface reflectance goal requirement in the 450 band resulting from the retrieval of the tropospheric NO_2 daily cycle. The new objective was therefore to demonstrate whether such demanding requirement would be achievable at all. It has been shown than in cloud-free and noise-free conditions such objective would be achievable in summertime. When 3% of random noise is added to the data, the objective is only achievable over dark surfaces. In order to improve the performance of the GRASP algorithm, the joint processing of S4 and FCI data is highly recommended. The GRASP algorithm is capable of dealing with such synergy.

An implementation concept is also proposed for the GRASP algorithm. It relies on the division of the S4 CA in a series of sub-regions, each one hosting an accumulation file including all input data. Such strategy eases a parallel processing of the input data minimizing also the required memory.

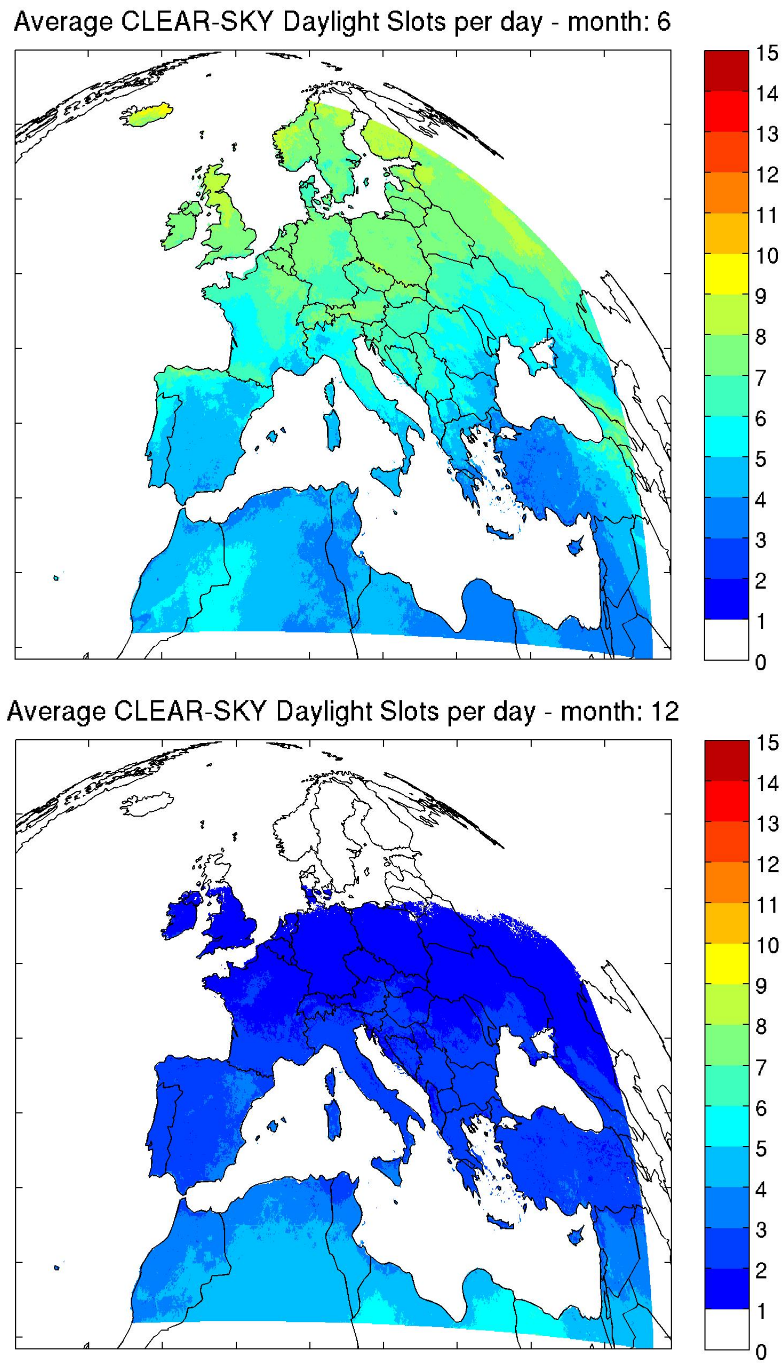

Figure 2: Average number of clear-sky daylight hourly observations for the month of June (top) and December (below) over the S4 coverage area.

This analysis has lead to a series of specific recommendation for the GRASP algorithm prototyping

1. Spectral band selection

- The following five spectral bands (342, 374, 417, 456and 756 nm) are proposed for the retrieval of reflectance and atmospheric properties
- In order to minimize S4 radiometric and spectral noise, it is recommended to bin these bands at a resolution of 4nm. There are no strict constraints concerning the exact width and location of the selected bands as long as the total gaseous transmittance remains higher than 0.995 in the polluted atmospheric profile used in this study.
- It is not necessary to interpolate the retrieved surface reflectance values at the nominal atmospheric wavelengths.
- It is recommended to based the S4 surface product on HSS observations provided these observations spectrally encompasses the selected bands.

2. S4 Level 1c generation

- It is recommended to use the same equatorial and polar radius values as those that will be used for the generation of MTG/FCI Level 1c images.
- It is recommend that the angular distance between the nominal φ_0 and actual φ_s sub-satellite longitude does not exceed 3 degrees to avoid important differences between the SD of the actual and rectified images.
- It is recommended to limit the reference grid area to the S4 RA, expanding it slightly its western limit.
- It is recommended that the N/S Spatial Sampling Distance (SSD) within the reference grid will be the same as the nominal one. The E/W SSD will be adjustable ranging between the SSD of HSS data, and the nominal SSD The actual value to be used will be determined during commissioning on the basis of i) the data radiometric quality, ii) the navigation accuracy and iii) users' requirements. The distance will however not be larger than the L1b nominal SSD.
- It is recommended to generate the level1c image on the reference grid with the bi-cubic interpolation method not mixing pixels with different status flags values. Should this condition being too restrictive; the closest-neighbour technique shall be used.
- The computation of the observation angles of the level1c pixels shall be performed with respect to the actual SSP (φ_s, λ_s) at the time of acquisition.
- It is recommended that the acquisition absolute UTC time of each level1c pixel is explicitly available in the associated L1c metadata, and not simply the time of a N-S scan line. In case of bi-cubic spline, the weighted mean value should be used.
- There is no need to archive the level1c data once they have been processed by the GRASP algorithm as long as it is possible to regenerate them on demand.

3. Miscellaneous recommendations

- It is recommended to use the MTG/FCI snow mask to verify the presence of recent snowfall, preventing S4-GRASP temporal constraints in such situation.
- In order to minimise the impact of clouds while documenting the surface BRF, S4 hourly observations shall be accumulated during a period of several days, typically 3 to 5.

5 Overall conclusions and recommendations

The SURMACED study concluded that the goal accuracy in the surface albedo near 450 nm is on the order of 0.005; this very demanding accuracy is needed in order to meet the extremely tight user requirements of 10% for NO_2 in polluted scenarios. Such requirement is extremely tight as compared to the performance achieved by standard dataset such as the NASA MODIS surface albedo product which has a recognised uncertainty of about 0.01 – 0.03. The GRASP algorithm has been proposed to meet such requirement. The GRASP algorithm will be used for the processing of other satellite data such as POLDER that will directly benefit to the S4 product.

It has been demonstrated that in noise-free condition it is possible to meet the 450nm requirement in summertime and to some extent with a 3% added random noise. From these results, we can conclude that under very good observation conditions, it will be possible to deliver very accurate surface reflectance information that will permit therefore to analysis the tropospheric NO_2 daily cycle.

The combined use of FCI and S4 L1c data is highly encouraged to improve the aerosol properties characterisation and thereby the accuracy of the retrieved surface reflectance.

The GRASP algorithm is however very complex and time consuming. Further efforts are therefore needed to improve its operability and to reduce its computation time. Several initiatives have already been undertaken in that direction, among other for the processing of the PARASOL data set. During the prototyping phase of the S4-GRASP algorithm, particular attention will have to be paid to the design of the code and its modularity to ease its maintenance. In other words, the algorithm speed-up should not be detrimental to the code maintenance. It is also recommended to adopt a design flexible enough to allow the product generation at a higher frequency than the duration of the accumulation period. Finally, during this prototyping activity, an effort will have to be dedicated to the preparation of the prior information.

The GRASP algorithm prototyping against actual geostationary observations is of paramount importance. Hourly observations acquired by the GOCI radiometer on board the Korean COMS platform would be very useful with this respected, provided access to the daily cycle of observation can be granted. Currently, only three slots per day around noon are publicly available (to be confirmed).

The definition of the GRASP algorithm output still require further analysis in particular with respect to the actual user needs. For instance, the algorithm also derives aerosol properties as a by-product. The opportunity to save this information, including the error covariance matrix, or the possibility to make it available in near-real-time still needs to be defined with Sentinal-4 data users. Along the same line, a specific effort will also have to be dedicated to support users to use a best the derived surface BRF parameters.

It has been demonstrated that the tempting LER simplification should be avoided for the analysis of the tropospheric NO_2 cycle.

Finally, it has demonstrated that high cloud cover and low Sun illumination in wintertime might prevent to deliver an accuracy BRF product or any at all during that season. The SURMACED consortium encourages a southward shift of the Sentinel-4 coverage area close to the winter solstice. A southward shift of 10 degrees would allow the observations of the major CEOS desert targets located in the Sahara desert, easing thereby Sentinal-4 cross calibration over these well documented areas.