

# End-to-end simulations to optimize imaging spectroscopy mission requirements for seven scientific applications

Xavier Briottet, Karine Adeline, T. Bajjouk, V. Carrere, Malik Chami, Yohann Constans, Yevgeny Derimian, Alice Dupiau, Marie Dumont, Stéphanie Doz, et al.

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Keywords: imaging spectroscopy, signal-to-noise ratio, spectral sampling, image quality,
mineralogy, soil moisture content, tree species, leaf functional traits, bottom classification,
shallow water, bathymetry, seabed, urban land cover, plume, aerosols, methane, cryosphere,
water vapor, aerosols

#### 43 Highlights:

Assess the impact of instrumental design on various end-user hyperspectral
applications,

- Evaluation of the main sources of error, namely the signal-to-noise ratio (SNR), the
   radiometric calibration and the spectral sampling strategy,
- Analysis of sensibility to the instrumental configurations for each application.
- 49 Journal: ISPRS Open Journal of Photogrammetry and Remote Sensing

#### 50 • Abstract

51 CNES is currently carrying out a Phase A study to assess the feasibility of a future hyperspectral 52 imaging sensor (10 m spatial resolution) combined with a panchromatic camera (2.5 m spatial 53 resolution). This mission focuses on both high spatial and spectral resolution requirements, as 54 inherited from previous French studies such as HYPEX, HYPXIM, and BIODIVERSITY. To 55 meet user requirements, cost, and instrument compactness constraints, CNES asked the French 56 hyperspectral Mission Advisory Group (MAG), representing a broad French scientific 57 community, to provide recommendations on spectral sampling, particularly in the Short Wave 58 InfraRed (SWIR) for various applications.

59 This paper presents the tests carried out with the aim of defining the optimal spectral sampling 60 and spectral resolution in the SWIR domain for quantitative estimation of physical variables 61 and classification purposes. The targeted applications are geosciences (mineralogy, soil 62 moisture content), forestry (tree species classification, leaf functional traits), coastal and inland 63 waters (bathymetry, water column, bottom classification in shallow water, coastal habitat 64 classification), urban areas (land cover), industrial plumes (aerosols, methane and carbon dioxide), cryosphere (specific surface area, equivalent black carbon concentration), and 65 atmosphere (water vapor, carbon dioxide and aerosols). All the products simulated in this 66 67 exercise used the same CNES end-to-end processing chain, with realistic instrument parameters, enabling easy comparison between applications. 648 simulations were carried out
with different spectral strategies, radiometric calibration performances and signal-to-noise
Ratios (SNR): 24 instrument configurations × 25 datasets (22 images + 3 spectral libraries).

71 The results show that a 16/20 nm spectral sampling in the SWIR domain is sufficient for most 72 applications. However, 10 nm spectral sampling is recommended for applications based on 73 specific absorption bands such as mineralogy, industrial plumes or atmospheric gases. In 74 addition, a slight performance loss is generally observed when radiometric calibration accuracy 75 decreases, with a few exceptions in bathymetry and in the cryosphere for which the observed performance is severely degraded. Finally, most applications can be achieved with the lowest 76 SNR, with the exception of bathymetry, shallow water classification, as well as carbon dioxide 77 78 and methane estimation, which require the higher SNR level tested. On the basis of these results, 79 CNES is currently evaluating the best compromise for designing the future hyperspectral sensor 80 to meet the objectives of priority applications.

## 81 **1. Introduction**

82 Imaging spectroscopy (IS) is now recognized as a powerful tool for satellite-based Earth 83 observation. Several sun-synchronous space missions such as Gaofen 5 (Liu et al., 2019), 84 PRISMA (Meini et al., 2015) or EnMap (Guanter et al., 2015) are already operational (Oian, 85 2021). They offer global coverage with a revisit time from 4 to 29 days. All these sensors have a ground sampling distance (GSD) of 30 m which reduces the range of applications due to the 86 87 presence of mixed pixels in heterogeneous scenes (Zhao et al., 2014; Transon et al., 2018). 88 Spatial resolution is considered the « Achille heel » for the recovery of fine-scale surface 89 parameters. Other authors have mentioned these limitations for crop disease detection (Dutta et al., 2006; White et al., 2007), forest functional traits estimation (Miraglio et al., 2022), urban 90

area classification (Cavalli et al., 2008; Heldens et al., 2011), clay mineral mapping (Gomez et
al., 2015), characterization of acid mine drainage (Davies and Calvin, 2017), monitoring of
industrial gas plumes (methane, carbon dioxyde), smoke (Nesme et al., 2021; Deschamps et al.,
2013), or early detection of coral bleaching (Yamano and Tamura, 2004). Ustin and Middleton
(2021) reported that a 10 m GSD is justified to improve the mapping capabilities of crops,
minerals, snow/ice, water resources, vegetation type and condition.

97 There is therefore a real need to complement existing IS sensors with a new sensor with better 98 spatial resolution. A number of IS missions are currently under study, such as SHALOM 99 (Feingersh et Ben-Dor, 2016) and PRISMA-NG (Ansalone et al., 2021). For many years, 100 French researchers supported by CNES/DGA have been working on specifications of a new 10 101 m GSD IS sensor under several names: HYPXIM (Briottet et al., 2011; Carrère et al., 2013), 102 HYPEX-2 (Briottet et al., 2017) and BIODIVERSITY (Briottet et al., 2022). A phase A, led by 103 CNES was completed in mid-2022 with the aim of proposing an instrument combining 104 hyperspectral imaging (10 m GSD, spectral range 0.45-2.40 µm, 10 km swath) with 105 panchromatic imagery (2.5 m GSD) with a revisit time of 5 days. One of the aims of this study 106 was to define the optimum signal-to-noise ratio (SNR), radiometric image quality and spectral 107 sampling for different applications, within the constraint of instrument compactness: 108 geosciences, forestry, coastal and inland waters, urban areas, industrial plumes, cryosphere, and 109 atmosphere. All these applications have been selected because they require high spatial 110 resolution, on the order of 10 m, and correspond to the themes identified by Taramelli et al. 111 (2020). The aim of this work is therefore to present the results of a cross-analysis of these 112 scientific fields, which will help consolidate the mission requirements and the payload design.

After describing the input data in §2, the end-to-end simulator for calculating radiance at the top of the atmosphere is presented in §3, along with the insertion of specific sensor characteristics (spectral strategy, SNR, radiometric calibration accuracy), the choice of surface reflectance and the methods used to extract the relevant parameters for each application. The results are presented in §4, followed by a discussion in §5 and a conclusion in §6.

## 118 2. Materials

Two types of input data were used to cover these seven scientific domains: reflectance spectra measured in the laboratory or simulated using dedicated models, presented in §2.1, and hyperspectral images (§2.2).

#### 122 **2.1. Laboratory, field and simulated spectra**

The use of laboratory measured spectra concerns applications in mineralogy and soil moisture content (SMC) estimation (geosciences), while the use of simulated spectra concerns applications in leaf functional traits estimation (vegetation), spectral surface area (SSA) and equivalent black carbon (eBC) estimation (cryosphere), and atmospheric aerosol and gas estimation (atmosphere).

For mineralogy estimation, 38 reflectance spectra of 16 minerals of interest (clays, carbonates, sulphates, rare earth elements (REE), oxy-hydroxides, etc.) with a wide range of chemical composition and grain size were selected from the United States Geological Survey (USGS) Spectral Library (<u>https://crustal.usgs.gov/speclab/).</u> The results presented here are limited to the 11 most typical minerals whose spectral characteristics are given in Table 1. 133 Table 1. Diagnostic absorption characteristics of 11 representative minerals. Bastnaesite, monazite, and 134 xenotime have specific absorption peaks in the visible and near-infrared (VNIR) due to varying proportions of rare 135 earth elements: only the four main absorption peaks are shown.

Mineral	USGS Reference	Wavelength positions of diagnostic absorption features
Gypsum	Gypsum_HS333.3B	~1.75 μm; secondary absorption ~2.21 μm
Calcite	Calcite_WS272	~2.34 μm; secondary absorption ~2.16 μm
Kaolinite	Kaolinite_CM9	Doublet ~2.16 µm and ~2.21 µm
Alunite	HS295-3B	~1.76 μm, ~2.16 μm; secondary absorption ~2.32 μm
Goethite	Goethite_GDS134	~0.66 μm, ~0.91 μm; secondary absorption ~0.50 μm
Hematite	Hematite_HS45.3	~0.86 μm; secondary absorption ~0.66 μm
Jarosite	Jarosite_GDS635_Na_Cyprus	~0.43, ~0.92, 2.21 and 2.27 μm
Montmorillonite	Montmorillonite_SAz-1	~2.22 μm
Bastnaesite	Bastnaesite_REE_WS320	~ 0.58 ,0.74, 0.80 and 0.86 μm
Monazite	Monazite_REE_GDS947_Calif	~ 0.58, 0.75, 0.80 and 0.87 μm
Xenotime	Xenotime_GDS966_Iveland_REE	~ 0.66, 0.75, 0.81 and 0.91 μm

136 For coastal habitat classification, a library of field spectra was acquired using an ASD FieldSpec 137 4 Hi-Res spectroradiometer, which covers the wavelength range from 350 and 2500 nm with 138 spectral resolution ranging from 3 nm (VIS-NIR) to 8 nm (SWIR). The spectra recorded over 139 2151 bands were calibrated using a Spectralon to provide reflectance factor measurements. 140 Three to five spectra were recorded on each target to account for intra-target variability. These 141 targets have different benthic characteristics: vegetation types (green, red, brown algae and 142 microphytobenthos) and substrate types (mud, sand, shells and rocks), Sabellaria alveolata 143 bioconstructions, oyster reefs, etc. This spectral library will enable us to access the potential of 144 the SWIR for discriminating intertidal benthic feature, given that we have no images in the 145 coastal zone in this wavelength range.

For SMC, reflectance spectra of 32 soils measured for different gravimetric water contents
ranging from 5% to 85% were extracted from the Les08 database (Lesaignoux et al., 2013;
Figure 1) used to validate the Multilayer rAdiative tRansfer Model of soll reflectance
(MARMIT) model (Bablet et al., 2018, Dupiau et al., 2022).



150 151

Figure 1. Reflectance spectra of two soil samples (81StJulien and 31FaugaX1) extracted from the Les08 152 database (Lesaignoux et al., 2013). https://pss-gitlab.math.univ-paris-diderot.fr/marmit/marmit

153 For the estimation of leaf functional traits, a spectral database was generated using the DART

154 ray-tracing model (Gastellu-Etchegorry et al., 2012) coupled to the PROSPECT leaf radiative

155 transfer model (Jacquemoud et al., 1996) with the input variables described in Table 2. The

156 objective is to simulate top of canopy reflectance images similar to those acquired by an

157 airborne hyperspectral sensor (see Miraglio et al., 2022).

158 Table 2. Range of variation in biochemical and physical properties of trees. FVC: fractional vegetation cover, 159 LAD: leaf angle distribution, ALA: average leaf angle, LAI: leaf area index, Cab: chlorophyll content, Car: 160 carotenoid content, EWT: equivalent water thickness, and N: leaf structure parameter in PROSPECT.

Canopy parameter	Value and range	
FVC (%)	30, 50, 70, 90	
LAD (°)	Ellipsoidal	
ALA (°)	55-65	
LAI (m <sup>2</sup> /m <sup>2</sup> )	1-4	
Cab (µg/cm²)	5 - 70	
Car (µg/cm <sup>2</sup> )	4 - 20	
EWT (g/cm <sup>2</sup> )	0.001 - 0.025	
LMA (g/cm <sup>2</sup> )	0.001 - 0.025	
N	1.5 – 2.1	

161	To estimate the specific surface area (SSA) and the equivalent black carbon (eBC)
162	concentration, snow reflectance spectra were simulated with the Two-streAm Radiative
163	TransfEr in Snow model (TARTES, Libois et al., 2013) with the input parameters detailed in

164 Table 3. SSA and eBC values were determined using *in situ* hyperspectral measurements

165 (Libois et al., 2013; Picard et al., 2016; Dumont et al., 2017; Tuzet et al., 2019, 2020).

**Table 3**. Definition of the variation ranges of the inputs for the TARTES simulations.

Variable	Range
Spectral range	350-3000 nm at 1 nm resolution
Specific surface area (SSA)	3-100 kg m <sup>-2</sup>
Sun zenith angle	0-80° by 10° step
Dust	11 values between 0 and 500 $10^{-6}$ g g <sup>-1</sup>
Equivalent black carbon (eBC) concentration	11 values between 0 and 300 10 <sup>-9</sup> g g <sup>-1</sup>

167 To estimate the composition of the gaseous atmosphere (water vapor, carbon dioxide), 168 performance is assessed on the basis of a standard mid-latitude summer atmosphere, with a  $CO_2$ 169 concentration of 400 ppm. The observation is at nadir and the solar zenith angle is 20°, while 170 the ground reflectance corresponds to a bright desert-like surface.

171 For atmospheric aerosols, synthetic TOA radiances were generated using the Generalized 172 Retrieval of Aerosol and Surface Properties (GRASP, Dubovik et al. 2021) algorithm for a 173 fixed geometry corresponding to a scattering angle of 150° and selected nominal wavelengths 174 in the atmospheric windows (419, 441, 492, 546, 669, 770, 865, 2312 nm). Only a subset of 175 wavelengths was selected, as the spectral characteristics of aerosols vary little in the solar 176 domain. A mixture of two aerosol types with different size distributions, chemical compositions 177 and shapes was used for the simulations: a fine mode for pollution particles and a coarse mode 178 for desert dust. The influence of gases is negligible in this study, as the spectral bands were 179 selected outside the main gas absorption peaks. The top of atmosphere reflectance ranged from 180 0.09 to 0.11 at 419 nm and around 0.01 at 2190 nm, representing different aerosol 181 concentrations over a dark surface (water). Only one scenario is presented here, corresponding 182 to a constant SNR of 200 in the 400-550 nm spectral range and 100 in the 600-2400 nm spectral 183 range.

#### 184

### 2.2. Airborne hyperspectral imaging

185 Images were acquired by airborne sensors with different spectral resolutions: NEO-HySpex (4-

186 7 nm, <u>https://www.neo.no/</u>), NEO-ODIN (3-6 nm, <u>https://www.neo.no/</u>), AVIRIS-C (10 nm,

187 <u>https://aviris.jpl.nasa.gov/</u>), and AVIRIS-NG (3.7 nm, <u>https://aviris.jpl.nasa.gov/</u>). They all

- 188 cover the 0.4-2.5  $\mu$ m spectral range. Table 4 lists the images and variables of interest for each
- 189 scientific field.

190 **Table 4.** IS images used in this study, with  $\theta_s$  sun zenith angle applied in subsequent simulations and all the images are acquired at nadir.

Scientific	Acquisition	Location	Sensor	Applications: Variable of interest		
domain	date		characteristics	••		
	Sept. 2019	Cherves-	HySpex:			
	$\theta_s = 50.5^{\circ}$	Richemont,	$GSD_{VNIR} = 0.5 \text{ m}$	Mineralogy: gypsum, calcite		
		France	$GSD_{SWIR} = 1 \text{ m}$			
	Sept. 2019	Chevanceaux,	$\frac{1}{2} \frac{1}{2} \frac{1}$	Minoralogy kaolinita		
Geosciences	$\theta_s = 50.2^{\circ}$	France	$GSD_{VNIR} = 0.5 \text{ III}$	Mineralogy. Kaomine		
	Jupo 2020	Cuprite NV	AVIRIS-NG	Mineralogy: alunite kaolinite iron		
	$\theta_{\rm c} = 15.8^{\circ}$	USA	GSD = 2.9  m	oxy-hydroxides		
	<u>1010</u> June 2014	Mountain Pass.	AVIRIS-NG	Mineralogy: bastnaesite (carbonate-		
	$\theta_s = 76.1^\circ$	CA, USA	GSD = 3.7  m	fluoride mineral, REE)		
	0 1 0015	Eslas Esuat	HySpex:	Tree species classification		
	Sept. 2015 $a = 47.2^{\circ}$	Fabas Forest,	$GSD_{VNIR} = 4 m$	(temperate forest, LAI = $3 \text{ m}^2/\text{m}^2$ ): 20		
Vocatation	$\theta_{S} = 47.5$	France	$GSD_{SWIR} = 4 m$	species		
vegetation	$J_{\rm MDO} 2014$	Tonzi Ranch,	AVIRIS NC	Mediterranean woodland savannah,		
	$\theta_{c} = 17.9^{\circ}$	CA, USA	GSD = 4  m	$(LAI = 0.8 \text{ m}^2/\text{m}^2)$ : Cab, Car, LMA		
		(Figure 11)		and EWT		
	July 2016	Decesff From es	HySpex	De theory of the		
	$\theta_s = 31.3 - 32.3^{\circ}$	Roscon, France	$GSD_{VNIR} = 0.5 \text{ m}$	Bathymetry		
		Porquerolles		Bathymotry		
	Sept. 2017	Island, France	HySpex	Water column estimation:		
Coastal waters	$_{S}\theta_{S} = 42.4^{\circ}$	(Figure 13)	$GSD_{VNIR} = 1 m$	phytoplancton, SPM, CDOM		
		0		–Bottom classification of shallow		
	July 2019	Camargue,	HySpex	water.		
	$\theta_S = 22.5^{\circ}$	France	$GSD_{VNIR} = 1 \text{ m}$	Classification of intertidal coastal		
	June, 2019 $A_{-} = 25.5^{\circ}$	France	$CSD_{VAUR} = 0.5 \text{ m}$	habitate (10 classes)		
	$\frac{0_{s}}{1_{s}} = 20.5$	1101100	NEO-ODIN	10 (10 (10))		
Urban area	$\theta_{\rm s} = 20.5^{\circ}$	Toulon, France	GSD = 0.5  m	Urban land cover (10 classes)		
	Sept. 2015	Eas our Mar	Unchov			
Industrial site	$\theta_{s} = 58.2 - $	Fos-sur-mer, France	GSD = 1.4  m	Aerosol plume		
	60.7°	TTALLE	0.00 - 1.4 III			

Oct. 2019	New Mexico,	AVIRIS-C	Mathana laaka
$\theta_S = 15.0^\circ$	USA	GSD = 6.6 m	Wethane leaks

192 The Fabas forest is composed of six distinct dominant species, including *Quercus* sp., Douglas 193 pine (*Pseudotsuga menziesii*), Laricio pine (*Pinus nigra*), maritime pine (*Pinus pinaster*), 194 Weymouth pine (*Pinus strobus*) and black locust (*Robinia pseudoacacia*). These six species 195 are included in the classification process, along with two additional classes: other conifer and 196 deciduous trees.

- 197 For urban areas, ten classes were considered: tile, vegetation, shadow, high reflectance, asphalt,
- 198 bare soil, pavement, road, stadium and stone.
- 199 For shallow water bottom classification, three classes were considered for the Porquerolles site
- 200 (sand, Posidonia oceanica and Caulerpa taxifolia), and four classes for Camargue site
- 201 (sediments, zosters, green algae and red algae).

## 202 **3.** Method



203 The processing chain is detailed in Figure 2.

- 204
- 205 **Figure 2.** Overview of the end-to-end simulator.

Each application targets one or several variables of interest. For each, a reference value is defined and hyperspectral data (spectra or images) are produced. The end-to-end simulator propagates this data at the top of the atmosphere, just as it would have been acquired by a 209 satellite. Various satellite performances can be simulated. Next, a specific method is applied to 210 retrieve the variable of interest from the satellite data. Finally, the estimated value is compared 211 with the reference value. The discrepancy between the estimation and the reference indicates if 212 the satellite performances meet the application requirements or not. The end-to-end simulator 213 and the processing of each application are detailed below. Figure 3 gives the processing orders and the main parameters used in our simulations. 214





219 The End-to-End simulator and the processing for each application are detailed in the following.

220

#### 3.1. End-to-end simulator

221 The aim of the end-to-end simulator (Figure 2) is to simulate the output signal, in spectral 222 radiance unit, that a sensor can acquire, taking into account its own errors, and then to carry out 223 the atmospheric correction to retrieve the spectral reflectance of the surface.

224 All data processing was carried out using an end-to-end simulator developed and operated by the French Space Agency (CNES), so that results could be compared (Figure 2). This 225 226 simulator allows two types of input to be taken into account, depending on the data available for each application: surface reflectance spectra or airborne images expressed in radiance units. 227

228

#### 3.1.1. Input top-of-atmosphere spectral radiance

229 The COMANCHE code (Poutier et al., 2002), based on MODTRAN 5.3 (Berk et al., 2005),

230 was used to calculate the top-of-atmosphere (TOA) radiance. We chose the MODTRAN standard parameters which were coherent with the case studies, i.e. a mid-latitude summer atmosphere and a rural aerosol type with a 23 km horizontal visibility. The solar angular conditions were deduced from the input acquisition conditions (Table 4). A nadir viewing angle was applied for all images since they were all acquired at nadir. The resulting TOA spectral radiance is then processed further to simulate the acquired signals in the hyperspectral and panchromatic channels.

#### 237 **3.1.2. Output top-of-atmosphere spectral radiance**

238 Several scenarios were explored to quantify the instrumental effects on the final products:

• Two signal-to-noise ratios: *optimistic* (O) [100-400] @Lref and *realistic* (R) [50-250] @L<sub>ref</sub>

240 (Figure 4), with  $L_{ref}$  the reference radiance. Gaussian noise with a zero mean and a standard 241 deviation  $\sigma$  was added to the input radiance.  $\sigma$  is equal to:

242 
$$\sigma(\lambda) = \sqrt{a(\lambda) + b(\lambda) \cdot L(\lambda)}$$

with *a* a constant noise and *b* a noise associated to the radiance, both depending on the
spectral width, *L* the TOA radiance, and λ the central wavelength of the spectral band. *L<sub>ref</sub>*is defined for an albedo of 0.3, a sun zenith angle of 60° and nadir viewing, a standard midlatitude winter atmosphere, and a continental aerosol type with a 23 km horizontal visibility.
Two absolute and interband calibration performances (Figure 5): *threshold* (t) [5% absolute,
2% interband] and *target* (T) [3% absolute, 1% interband].

• Six instrumental spectral response functions (ISRF) defining different sampling strategies, 1 labelled from #1 to #6 (Table 5). Note that the spectral configurations differ only in the 251 SWIR. The ISRF defines how sensible are each spectral channel to every incoming 252 wavelength. The TOA equivalent radiance acquired in a given spectral band *i* is computed 253 by:  $L_i = \frac{\int ISRF_i(\lambda) L(\lambda) d\lambda}{(ISRF_i(\lambda) d\lambda}$  where  $L(\lambda)$  is the TOA radiance computed in Paragraph 3.1.1 and

 $ISRF_i(\lambda)$  the spectral response of band *i*.  $ISRF_i(\lambda)$  is modeled as a Gaussian function with 254 255 a central wavelength  $\lambda_{C_i}$  and a full width at half maximum  $FWHM_i$ . Table 5 provides the spectral step (i.e. the distance between  $\lambda_{C_i}$  and  $\lambda_{C_{i+1}}$ ) and the spectral width (FWHM) of 256 257 each sampling strategy. Note that strategy #5 is a sum of Gaussian functions with a linear 258 increasing FWHM. Several ISRFs were tested as the matrix detector might have a limited 259 number of lines to record all the spectral bands. This disadvantage can be overcome by 260 widening the channels spectral width and thus reducing their number. To take into account that the central wavelength of each band may not be known precisely, the calculation 261 262 includes a constant spectral shift of 1 nm, typical from a spectral calibration error.

Note the instrument parameters used are realistic and that the sensor is technologically feasible. In summary, a scenario is defined by a spectral strategy (#1 to #6), a calibration performance (t for *threshold* or T for *target*) and a SNR (O for *optimistic* or R for *realistic*). Each scenario is then referred to as the triplet (spectral strategy, calibration, SNR). A star indicates that the comment applies to all possibilities in the triplet component. The reference scenario is (#1, T, O), i.e. 10 nm wide spectral channels with the lower calibration errors and the best SNR.



Figure 4. Top: reference spectral radiance, L<sub>ref</sub>, used to define SNR. Bottom left: optimistic SNR. Bottom right: realistic SNR.



274 **Figure 5.** Absolute and interband calibration errors: threshold and target.

	VNII	R (400 – 90	0 nm)	SWIR (9	000 – 1850 nm / 1950 – 2400 nm)	
Sampling Strategy	Spectral step (nm)	Spectral width (nm)	Number of channels	Spectral step (nm)	Spectral width (nm)	Number of channels
#1	10	10	51	10	10	136
#2	10	10	51	20	20	68
#3	10	10	51	16	16	85
#4	10	10	51	22 for $\lambda \le 1.95$ 10 for $\lambda > 2.05$	22 for $\lambda \le 1.95$ 10 for $\lambda > 2.05$	86
#5	10	10	51	12	Linear increase from 14 to 17 nm over [0.9 – 1.3], [1.3 – 1.8], and [1.95 – 2.4],	112
#6	8	16	63	10	20	136

Table 5. Spectral sampling strategies. The spectral range from 1850 to 1950 nm is unused.

In addition, the instrument introduces some blurring into the image, the magnitude of which depends on the wavelength and is modelled by the modulation transfer function (MTF). Due to the push-broom acquisition mode, the MTF is not equivalent along and across the satellite track (Figure 6). When processing the spectral libraries, the MTF simulation is not activated as only one pixel is processed.

When processing the spectral libraries, MTF simulation is not activated as only one pixel is processed.



Figure 6. Modulation transfer function (MTF) of five spectral bands of the instrument in the frequency domain. The instrument also features a panchromatic channel (PAN). Four additional images were generated with two SNR (realistic or optimistic, Figure 4) and two instrumental calibration performances (threshold or target). Figure 7 shows the normalized sensitivity of the panchromatic channel and its point spread function at 639 nm.



Wavelength [µm]
Position [m]
Figure 7. (Left) Normalized sensitivity of the panchromatic channel. (Right) Point spread function at 639 nm.
To summarize the end-to-end processing chain, the input TOA radiance is first affected by the
MTF (reduction of the input spatial resolution), then by the ISRF (reduction of the input spectral

resolution). At this point, the absolute calibration error as well as the inter-band calibrationerror are applied. The last step corresponds to the instrumental noise simulation.

In the end, for each input image, this experimental design produced twenty-four simulated images representative of various instrumental performances. However, the sensor design does not yet allow us to take into account other potential defects, such as stray light, geometric errors (geolocation, band registration, etc.), across-track variations in instrument characteristics (MTF, ISRF, etc.) including the smile effect, polarization sensitivity, directional effects induced by slowing down the satellite during acquisition or, and detector defects (remanence, dead pixels, etc.).

302

#### **3.1.3. Spectral surface reflectance**

The complexity of atmospheric correction algorithms allow them to be adapted to different situations. In this study, simulated data or images have been corrected for atmospheric effects with high performance so as not to interfere with the other parameters of interest (i.e., instrument configuration). However, some typical sources of error are accounted for:

An error of 5 km in horizontal visibility: the upward transfer is performed with a visibility
 of 23 km and the downward transfer with a visibility of 18 km. Aerosol type remains
 unchanged.

A 5% error in the water vapor content: the downward transfer is calculated with 95% of the
water vapor content simulated on the upward transfer.

312 As the upward transfer is done numerically, the atmospheric correction can be carried out with 313 the same performance whatever the target. This choice makes it possible to compare images 314 from one application to another.

315

#### **3.2. Description of methods by scientific field**

- 316 For each scientific field covered by this study, Table 6 provides the variables of interest, the
- 317 input format, the method used to estimate these variables, the bibliographic reference detailing
- 318 the method and the evaluation criteria.

# Table 6. Methods used to retrieve application-related variables. SA: Spectral Analyst, SAM: Spectral Angle Mapper, SD: standard deviation, SFF: Spectral Feature Fitting, SVM: Support Vector Machine, PLS: Partial Least Square, ACE: Adaptive Coherence Estimator, RMSE: Root-Mean-Square Error, PM: Particle Matter.

Scientific domain	Variable of interest	Type of IS inputs (unit)	Method and author	Reference value of the variable of interest	Evaluation criteria
Geosciences	Mineral composition	Image (surface reflectance)	Visual assessment SAM (Kruse et al., 1993) SFF (Clark et al., 1990)	Mineralogical maps of the site	Position and shape of absorption features Identification if SA > 0.7 and SAM < 0.2 Identification if SA > 0.7 and max(RMSE of SFF) > 0.1
	Soil moisture content	Spectra (surface reflectance)	MARMIT model (Bablet et al., 2018)	Laboratory measurements	RMSE between laboratory input and satellite outputs
Vagatation	Tree species classification	Image (surface reflectance)	Supervised classification: SVM with Radial Basis function (Gimenez et al., 2022)	In situ measurements	Mean, RMSE values of Overall Accuracy, F-score over the 24 scenarios and 30 iterations each
vegetation	Leaf functional traits	Image (surface reflectance)	Hybrid method using DART/PROSPECT simulations and PLSR (Miraglio et al., 2022)	Traits maps from a high spatial resolution image	RMSE by comparing ISRF #1 and the others ISRF
	Bathymetry	Image (surface reflectance)	HYPIP processing chain (Lennon et al., 2013)	Lidar measurements	SD and RMSE / bathymetric Lidar
Coastal	Bathymetry and bio- optical aquatic parameters	Image (surface reflectance)	Hybrid method based on the Lee model (Lee et al., 1999, Minghelli et al., 2020)	Lidar measurements, in situ water characterization	RMSE / in situ data $RE(\%) = \frac{100}{N} \sum_{i=1}^{N} \frac{ \hat{y}_i - y_i }{y_i} / \text{ in situ data}$
zones	Classification of intertidal coastal area	Image (surface reflectance )	With and without IS Pansharpening + Fully Constrained Least Square – the endmembers are known (Heinz and Chang, 2001)	Manual in situ classification map	Normalized RMSE on abundance
	Intertidal coastal area	Spectra (surface reflectance)	PLS and discriminant analysis (Lee et al., 2018)	In situ field spectra	Kappa coefficient Overall Accuracy
Luban area	Urban Land Cover 1	Image (TOA radiance)	IS Pansharpening, Random Forest classification (Loncan et al., 2015)	Manual classification	Good classification rate / reference image
UIDall alea	Urban Land Cover 2	Image in TOA radiance unit	Upsampling of the IS image, SVM classification, fusion with PAN (Ouerghemmi et al., 2017)	Manual classification	Mean F-Score over the classes
PM1 Flux of industrial aerosol Industrial plume		Image (TOA radiance)	Multitemporal algorithm (Foucher et al., 2019)	In situ measurements	Estimated error High objective: < 80 μg/m³ Low objective: < 150 μg/m³
site	Methane concentration of industrial plume	Image (TOA radiance)	Plume detection with ACE detector, quantification of the concentration (Nesme et al., 2021)	JPL estimation	Estimated error High objective: < 1000 ppm.m Low objective: < 1500 ppm.m

	Specific Surface Area,				
Cryosphere	equivalent black	Spectra (surface	Hybrid method with TARTES (Dumont et al. 2017)	Simulations	Bias, standard deviation of the estimates / reference
cryosphere	carbon content of	reflectance)	Tryona methoa whit mittee (Damont et al., 2017)	ominutions	inputs
	snow				
	Water waper and COa	Spectra (TOA	Optimal actimation theory (Harbin at al. 2013)	Simulations	DMCE
A transmission	Water vapor and CO2	radiance)	Optimal estimation theory (Herbin et al., 2013)	Simulations	NIVI3E
Aunosphere	Aaracala	Spectra (TOA	GRASP and optimized fitting following the multi-	Cimulations	DMCE
	Aerosois	radiance)	term Least Square Method (Dubovik et al., 2021)	Simulations	KIVIJE
321					

#### 322 **3.2.1. Geosciences**

323 A first assessment of the impact of instrument characteristics was carried out qualitatively on 324 spectra of representative minerals extracted from the spectral library and image pixels. The 325 positions and shapes of their absorption features enabled us to visually evaluate the different 326 scenarios, in particular with regards to the spectral strategy. Next, a quantitative assessment 327 was carried out using the Spectral Analyst (SA) algorithm in the ENVI software 328 (https://www.nv5geospatialsoftware.com/). This compares the spectra of representative 329 minerals with those of a reference spectral library at the same spectral resolution, resampled 330 according to the spectral characteristics (band positions and full width at half maximum) of the 331 different strategies. This procedure enabled us to assess the impact of instrument calibration 332 and SNR. To compare the spectra, we used two well-known spectral matching techniques called 333 Spectral Angle Mapper (SAM) (Kruse et al., 1993) and Spectral Feature Fitting (SFF) (Clark 334 et al., 1990). SAM determines the spectral similarity between two spectra by treating them as 335 two vectors in a space whose dimensionality is equal to the number of bands, and calculating 336 the angle between these vectors. This technique is insensitive to illumination and albedo effects 337 when used on calibrated reflectance spectra. SFF is based on the least squares method. The 338 reference spectra are scaled to match the unknown spectra after the continuum is removed from 339 both (Clark et al., 1990; Mars and Rowan, 2010). SAM and SFF values are calculated on VNIR 340 (0.4-1.3 µm), SWIR1 (1.3-2.0 µm) and SWIR2 (2.0-2.5 µm) to avoid as far as possible 341 problems associated with atmospheric corrections in the two main water vapor absorption bands 342 around 1.4 and 1.9 µm. This also allows us to focus on spectral ranges where the selected 343 minerals exhibit diagnostic absorption features, which is recommended with these spectral 344 matching techniques. The SA result is a ranked or weighted score, with higher scores indicating 345 greater confidence.

Soil moisture content is estimated by inversion of the MARMIT model, which represents a wet soil as a dry soil covered by a thin layer of liquid water of thickness *L* (Bablet et al., 2018). The dry soil can be fully or partially covered with water, with a coverage fraction equal to  $\epsilon$ . The two input parameters of MARMIT, *L* and  $\epsilon$  are estimated by minimizing the cost function:

$$\chi^{2}(L,\epsilon) = \sqrt{\frac{\sum_{\lambda_{1}}^{\lambda_{2}} (R_{meas}(\lambda) - R_{mod}(\lambda, L, \epsilon))^{2}}{n_{\lambda}}}$$

with  $n_{\lambda}$  the number of wavelengths (or channels),  $R_{meas}$  the measured soil reflectance, and  $R_{mod}$  the soil reflectance estimated by MARMIT. The lower and upper bounds of the model parameters are 0 and 1 for  $\epsilon$ , 0 and 0.2 cm for *L*. A calibration step is required to establish a statistical relationship between the mean water thickness (mean light path) defined as  $\varphi = L \times$   $\epsilon$  and the measured SMC. The evaluation of the method consists in retrieving SMC by applying the relation found in the calibration step and comparing it with the measured values. The RMSE is calculated on 160 SMC values ranging from 5 to 85%.

**357 3.2.2. Vegetation** 

358 A supervised support vector machine (SVM) classification is applied together with a radial 359 basis function (RBF) kernel to classify tree species on the basis of spectral signatures extracted 360 from the HySpex image and corresponding to the field inventory. Two subsets are randomly 361 generated, a training one (70%) and a validation one (30%). The training subset is used to 362 optimize the RBF-SVM hyper-parameters, C and Gamma. The strategy followed is based on 363 an exhaustive grid search strategy with 5-fold cross validation aimed at maximizing the overall accuracy (OA) of the classifier. The space defined by C values ranging from  $10^{-2}$  to  $10^{9}$  and 364 Gamma values ranging from  $10^{-7}$  to 10 is explored. The model is then trained using the 365 parameters obtained and the training subset. Next, the trained SVM classifier is applied to the 366 367 validation subset. The method's performance is evaluated using the OA and F-score, the user and producer accuracy for each class. As the scores can depend on initial conditions, the whole procedure is repeated 30 times and the mean and RMSE of each accuracy score is calculated. Thirdly, the tree species map is produced using the same scheme with the spectral signature dataset for the training and the image for application. Ultimately, the relevance of each of the twenty-four scenarios is evaluated using this classification scheme, and compared using the mean and standard deviation of the accuracy scores obtained.

374 Leaf functional traits are estimated using a hybrid method based on training a PLSR on the previously described spectral database generated by DART. An automatic determination of the 375 376 optimal number of latent variables and a selection of the most important variables in the 377 projection design are performed for the PLSR parameterization. To optimize trait extraction, 378 the spectral range is adapted to the influence of each trait: 0.5-0.8 µm for chlorophyll (Cab) and 379 carotenoids (Car), and 1.5–2.4 µm for leaf mass per area (LMA) and equivalent water thickness 380 (EWT) (Miraglio et al., 2022). Then, the optimal trained PLSR is applied on the airborne image 381 to derive inversion maps of leaf traits, and the RMSE is calculated by comparing the reference 382 scenario (#1) with the others (#2 to #6).

#### **383 3.2.3. Coastal zones**

Shallow water bathymetry is estimated in the 400-900 nm range using the SWIM® software developed by Hytech-imaging (Lennon et al., 2013). SWIM® includes modules for the correction of the sun glint at the surface and for the correction of the air/water interface. Both SWIM and HYPIP include modules for uncertainty propagation from the sensor to the final products. Another method is applied to simultaneously estimate bathymetry and bio-optical parameters and perform shallow water bottom classification (Lee et al., 1999; Minghelli et al., 2020). The aquatic bio-optical parameters are chlorophyll, suspended particulate matter (SPM), 391 colored dissolved organic matter (CDOM), depth, bottom sediment abundance, zosters, green392 and red algae.

A fully constrained least squares (FCLS) unmixing method is also applied to the airborne VNIR image to estimate the abundance of the several seabed species. PLS-DA analysis (Lee et al., 2018) is then used for VNIR-SWIR field spectra to evaluate the discrimination performance of BIODIVERSITY configurations. This method can be applied to datasets with few observations and many explanatory variables (spectral reflectance), as is the case with the spectral library used in this study.

399

#### 3.2.4. Urban area

400 Considering that a GSD of 10 m is not sufficient to classify an urban area, a hyperspectral 401 pansharpening method called Gain is first applied (ULC1). It is inspired by the Brovey 402 transform applied to the RGB+PAN case (Saroglu et al., 2004), but has been generalized to the 403 HS+PAN case (Loncan et al., 2015). A supervised classification method (random forest) is then 404 applied to the resulting image. Ten classes are selected, each composed of twenty spectra. The 405 calibration and validation phases follow the k-fold method: random selection of five groups 406 with a uniform distribution of each class, then four groups are used for calibration and the last 407 one for validation. A second urban land cover (ULC2) method is applied. First, a hyperspectral 408 image is oversampled (bilinear interpolation) to a GSD of 2.5 m corresponding to the 409 panchromatic band. Then, a supervised SVM classification is performed. Ten classes are 410 considered. Fifty training samples were selected for each class, to provide a model unbiased by 411 the unbalanced distribution of classes. This number is considered sufficient to obtain efficient 412 classification models, while keeping a sufficient number of validation samples. For each 413 classification, ten iterations of the classification process (involving random selection of training samples) are performed. Then, a fusion process is then applied. The classification results areevaluated by averaging the F-scores over the classes.

416 **3.2.5. Industrial site** 

417 Characterization of PM1 aerosols in an industrial plume uses a multi-temporal algorithm 418 (Foucher et al., 2019). The objective is to determine the difference between two images 419 corrected for illumination and viewing angles, acquired in two wind directions to enhance the 420 PM1 plume signature. The differential model depends on aerosol properties, such as radius, 421 single scattering albedo, and concentration. A correlation map (adaptive coherence estimator, 422 ACE) between the temporal differential and the a priori plume signature from different aerosols types is then calculated. The model assumes a constant layer height of 100 m: for a GSD of 10 423 m, a mass of 1 g would correspond to a concentration of  $100 \,\mu\text{g/m}^3$ , or a column concentration 424 of  $10^{-2}$  g/m<sup>2</sup>. Pixel concentration is estimated using a linear formalism. To validate the estimate, 425 426 the error must be below a given threshold (Table 5).

Industrial methane plumes are characterized in two stages (Nesme et al., 2021). To validate the estimate, the error must be below a given threshold (Table 5): a low threshold associated with a flow rate of around 30 g/s, a high threshold associated with a flow rate of around 50 g/s. The detection map is built from thresholds on the ACE detector, on the residuals, and on a priori sensitivity. The amount of excess methane is associated with the transmission  $\tau_{gaz}$  deduced by inversion of the equation:

$$L_g^* = L_{ng}^* \tau_{gaz} \tag{2}$$

433 with  $L_g^*$  the sensor radiance corresponding to excess gas in the optical path and  $L_{ng}^*$  the sensor 434 radiance of the same pixel without excess gas, both corrected for atmospheric path radiance.



The snow surface is characterized by two properties accessible from imaging spectroscopy (Dumont et al., 2017): the specific surface area (SSA), the ratio between the surface area of airice and the snow mass and the equivalent black carbon concentration (eBC). The extraction method finds optimal values for the two variables that minimize the difference between a large set of measured reflectance data and TARTES simulations.

441

#### 3.2.7. Atmosphere

442 The method for quantifying water vapor and carbon dioxide used the Shannon information 443 content with the formalism proposed by Rodgers (2000). It introduces the theory of optimal 444 estimation, widely described by Herbin et al. (2013). The a priori errors of the CO<sub>2</sub> and H<sub>2</sub>O profiles are set at 5% and 10% respectively. The covariance matrix of measurement errors is 445 446 deduced from instrument performance and accuracy. The latter is related to the radiometric 447 noise expressed by the SNR defined as Optimistic-Target, and Realistic-Threshold. The accuracy of non-retrieved parameters is set to  $\delta T = 1K$ , compatible with the typical values used 448 449 by the European Centre for Medium-Range Weather Forecasts on each layer of the temperature 450 profile for assimilation, and to an uncertainty of  $0.5^{\circ}$  on the optical path.

The atmospheric aerosol retrieval method uses the GRASP algorithm. The inversion procedure is based on a statistically optimized least squares method and combines the advantages of a variety of approaches (Dubovik, 2004). This method has already been applied to PRISMA images (Litvinov et al., 2021).

## 455 **4. Results**

#### 456 **4.1. Geosciences**

Table 7 presents only a representative subset of the results focusing on cases with spectral strategies (#1, #2, #5 and #6) and with *realistic* SNR conditions representing medium and extreme scenarios.

All diagnostic gypsum absorption bands (Table 1) are observed visually. As expected, there is also an impact of smoothing due to a lower spectral resolution on the shape of the secondary 2.21  $\mu$ m absorption for # 2 and # 6. In terms of quantitative evaluation (Table 7), the SAM score (respectively SFF) is above 0.75 (resp. 0.61) in SWIR1 except for (#2, T, R), and 0.90 (resp. 0.73) in SWIR2. Whatever the scenario, good scores are obtained with SWIR1 except for (#2, T, R) where gypsum is not identified despite a higher SNR (150:1).

Diagnostic absorption of calcite at ~ 2.34  $\mu$ m is visible for all scenarios but smoothing (#2, #5, and #6) has an impact on shape and position, leading to possible confusion with dolomite, another carbonate, whose absorption is located at ~ 2.33  $\mu$ m. For all scenarios, secondary absorption at ~ 2.16  $\mu$ m is very low. Whatever the scenario (Table 7), the SAM score is > 0.88 and the SFF score > 0.73.

The kaolinite doublet (Table 2) is visible for #1 and slightly visible for #5 and #6 for which the weaker absorption at ~ 2.16  $\mu$ m is attenuated (Figure 8). Confusion with other clay minerals is possible and the crystallinity of kaolinite cannot be characterized because the relative strength of the doublet absorptions is modified. Unfortunately, the kaolinite doublet is no longer visible with #2. According to Table 7, in all scenarios, SAM remains > 0.88 and SFF > 0.76.



477 Figure 8. Three kaolinite spectra extracted from the Chevanceaux image, from left to right: (#1,T,R), (#5,T,R),
478 (#2,T,R).

For gypsum, the diagnostic absorption of alunite at 1.76  $\mu$ m is visible. The other absorptions are visible whatever the scenario, except for (#2, T, R) and (#5, T, R) for which there is a small difference in the right-hand side of the absorption at ~2.16  $\mu$ m that could hamper identification when using a feature fitting approach. However, high scores are obtained (SAM > 0.85 and SFF > 0.77).

484 Diagnostic absorptions in the VNIR for goethite and hematite can be identified visually 485 whatever the scenario; meanwhile residual peaks related to atmospheric correction can be 486 corrected. This is confirmed by the fact that SAM can detect goethite (score > 0.73) but hematite 487 detection remains more challenging (score > 0.64). In contrast, SFF cannot detect the 488 corresponding absorption bands (score < 0.53).

All jarosite absorption bands can be detected visually in the infrared, regardless of the scenario tested, leading to SAM scores > 0.79 in the VNIR and > 0.91 in the SWIR. High scores > 0.71 are also achieved with SFF except for (#6,T,R). However, whatever the scenario, the jarosite absorption at ~ 0.45  $\mu$ m is not clearly visible because it is partially cut off, being located at the edge of the VNIR; this could be a problem for jarosite identification.

494 The montmorillonite absorption band is clearly visible for all scenarios except for (#2,T,R),

495 where a shape change is detected. SAM and SFF scores are high, > 0.9 and > 0.73, respectively.

Finally, rare-earth elements (bastnaesite, monazite and xenotime) spectra show clear diagnostic absorptions in the VNIR for all scenarios (Figure 9). However, instrument calibration and atmospheric correction errors induce "peaks" located in the absorption bands of dioxygen (~ 0.76  $\mu$ m) and water vapor (~ 0.94 and ~ 1.13  $\mu$ m). This explains the poor SFF scores. On the contrary, SAM scores are > 0.67, the lowest score being obtained for (#6,T,R).



501

Figure 9. Representative rare-earth elements spectra extracted from the Mountain Pass image. Left: Reference
 USGS reflectance spectrum. Right: Reflectance for scenario (#1,t,R) after atmospheric correction.

504 In general, SAM gives better results than SFF, with scores close to 0.9 in the SWIR2. This

505 difference can be explained by the fact that SFF compares the shape of spectra that have

506 undergone continuum removal.

**Table 7.** SAM/SFF scores from Spectral Analyst (SA) tool (scenario #, t for threshold, T for Target, R for Realistic). Note that SA was performed on a subset of the SWIR2 to avoid the problem caused by CO<sub>2</sub> absorption peaks. In the SWIR1, gypsum and alunite scores are estimated by excluding atmospheric water vapor absorption at 1.4 μm.

Mineral		(#1, T, R)			(#1, t, R)		(#2,	T, R)	(#5,	T, R)	(#6, T,R)
	VNIR	SWIR 1	SWIR 2	VNIR	SWIR1	SWIR 2	SWIR1	SWIR 2	SWIR 1	SWIR 2	VNIR
Gypsum		0.77/0.64	0.90/0.77		0.75/0.61	0.90/0.84	0.00/0.58	0.94/0.92	0.96/0.94	0.93/0.88	
Calcite			0.91/0.73			0.88/0.82		0.94/0.92		0.94/0.89	
Kaolinite			0.91/0.78			0.88/0.76		0.92/0.85		0.92/0.85	
Alunite		066/0.49	0.89/0.80		0.43/0.00	0.85/0.77	0.00/0.57	0.88/0.84	0.72/0.94	0.90/0.84	
Goethite	0.73/0.47			0.77/0.53							0.84/0.10
Hematite	0.68/0.27			0.65/0.18							0.64/0.00
Jarosite	0.80/0.71		0.91/0.70	0.79/0.70		0.87/0.71		0.95/0.91		0.93/0.87	0.85/0.01
Montmorillonite			0.90/0.73			0.90/0.79		0.95/0.91		0.94/0.88	
Bastnaesite	0.68/0.40			0.67/0.40							0.61/0.03
Monazite	0.75/0.40			0.75/0.43							0.74/0.15
Xenotime	0.69/0.60			0.71/0.70							0.64/0.21

511 Estimated soil moisture content is unaffected by the scenarios, with a mean RMSE of 2.6% and

512 a standard deviation of 0.1%.

#### **4.2. Vegetation**

514 The overall accuracy (OA) performance is summarized in Table 8 for tree classification.

	Opti	mistic	Rea	listic
	Target	Threshold	Target	Threshold
#1	$0.82 \pm 0.03$	$0.83 \pm 0.03$	$0.76 \pm 0.04$	$0.76 \pm 0.03$
#2	$0.81 \pm 0.02$	$0.81 \pm 0.03$	$0.74 \pm 0.03$	$0.74 \pm 0.04$
#3	$0.82 \pm 0.03$	$0.81 \pm 0.03$	$0.75 \pm 0.03$	$0.77 \pm 0.02$
#4	$0.82 \pm 0.03$	$0.81 \pm 0.03$	$0.75 \pm 0.03$	$0.75 \pm 0.03$
#5	$0.82 \pm 0.03$	$0.82 \pm 0.03$	$0.78 \pm 0.03$	$0.76 \pm 0.03$
#6	$0.83 \pm 0.04$	$0.84 \pm 0.02$	$0.77 \pm 0.03$	$0.79 \pm 0.04$

515 **Table 8**. Overall accuracy performance of tree classification.

516 The overall accuracy of *optimistic* simulations (mean OA value 0.82) is better than that of 517 *realistic* simulations (mean OA value 0.76), whatever the sampling strategy. Performance 518 depends only on the SNR (7% loss between *optimistic* and *realistic*), but not on calibration.

For the estimation of leaf functional traits, the optimistic and realistic scenarios perform 519 520 similarly regardless of the trait studied, and are not further discriminated in the following. 521 Figure 12 shows the Cab, Car, LMA and EWT maps obtained with scenario (#1, T, O). 522 Comparison of leaf trait estimation performance for sampling strategies #2 to #6 versus #1 leads 523 to an average RMSE of 2.2  $\mu$ g/cm<sup>2</sup> for Cab (average standard deviation of 0.5  $\mu$ g/cm<sup>2</sup>), 0.8 524 µg/cm<sup>2</sup> for Car (resp. 0.1 µg/cm<sup>2</sup>), 0.0008 g/cm<sup>2</sup> for LMA (resp. 0.0003 g/cm<sup>2</sup>) and 0.0014 525 g/cm<sup>2</sup> for EWT (resp. 0.0000 g/cm<sup>2</sup>). In fact, the same RMSE values are found for EWT 526 whatever the scenario. The performance of *threshold* compared with *target* deteriorates slightly, 527 with an average increase in RMSE of 0.5 µg/cm<sup>2</sup> for Cab, 0.1 µg/cm<sup>2</sup> for Car and 0.0004 g/cm<sup>2</sup> for LMA. Overall, irrespective of calibration performance and SNR level, the quality of leaf 528 529 trait estimation with scenarios #2 to #6 is similar to that of scenario #1.

530 These results can be compared to absolute RMSE values of 8.5  $\mu$ g/cm<sup>2</sup> for Cab under the same 531 conditions (Miraglio et al., 2020), or to an RMSE of 8.1 µg/cm<sup>2</sup> for a sparse coniferous forest 532 (Zarco-Tejada et al., 2019). For Car, Miraglio et al. (2020) found an RMSE of 2.24 µg/cm<sup>2</sup>, 533 Zarco-Tejada et al. (2013) an RMSE of 0.9 µg/cm<sup>2</sup> on crops and Asner et al. (2015) an RMSE 534 of  $0.2 \,\mu$ g/cm<sup>2</sup> on tropical forests. On tropical forests, Chadwick et Asner (2016) found an RMSE 535 of 0.0020 g/cm<sup>2</sup> and Asner et al. (2015) an RMSE of 0.0023 g/cm<sup>2</sup> for LMA. Buddenbaum et 536 al. (2015) estimated EWT on European beech seedlings with an RMSE of 0.0007 g/cm<sup>2</sup>, within 537 a range of 0.001 to 0.008 g/cm<sup>2</sup>. Li et al. (2008) retrieved EWT with an RMSE of 0.0132 g/cm<sup>2</sup> 538 from optical libraries and simulated data.

539 4

#### 4.3. Coastal zones

For bathymetry, since scenarios #1 to #5 have the same spectral strategy in the VNIR, only
scenarios #1 and #6 will be compared. Table 9 summarized the results for the three images used
to estimate bathymetry.

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$\mathcal{I}$	4	J

**Table 9.** Bathymetry performance obtained on the three images.

			]	RMSE (m)		
Site	Ro	scoff	Porquero	lles Island	Camarg	ue
Scenario	#1-5	#6	#1-5	#6	#1-5	#6
Optimistic, Target	1.0	1.2	1.5	1.2	0.3	0.4
Optimistic, Threshold	1.7	1.8	2.0	1.6	0.4	0.5
Realistic, Target	1.2	1.2	2.2	1.4	0.3	0.4
Realistic, Threshold	1.8	1.8	2.8	1.7	0.4	0.5

Water depth is estimated at between 0 and 10 m in Porquerolles Island and between 0 and 2.5
m in Camargue.

For Roscoff, the (\*,T,\*) scenarios give better results than the (\*,t,\*) scenarios (decrease of around 0.7 m). Scenario #6 tends to smooth out the results, with a noise distribution similar to that of scenario #1. The impact of calibration is therefore the most critical factor. The performance of bathymetric products calculated with the *target* calibration is consistently better than that calculated with the *threshold* calibration. Using the best configuration (#1,T,\*), bathymetric product performance is close to that calculated with the original HySpex data. The SNR effect is insignificant, but caveats can be made about the impact of noise inherent in the source data, which could have an impact on the calibration present value and noise effects.

554 For Porquerolles, the *target* calibration gives better results than the *threshold* calibration (Figure 555 14). The difference between derived bathymetry and the in-situ data is small (RMSE < 2.8 m) 556 corresponding to a relative error < 30%). Note, however, that retrieval in *threshold* calibration 557 remains acceptable. Retrieval performance is better for #6 than for #1. For Camargue, the *target* 558 calibration provides 20% better bathymetry retrieval than that obtained with the threshold 559 calibrations. The latter is not acceptable: the relative difference between bathymetry retrieval 560 and in-situ data is ~ 80%. Performance is consistently better for sampling strategy #1 than for 561 sampling strategy #6.

For remote sensing of coastal ecosystems, the retrieval of bathymetry using simulated data is always of interest. A relative error < 30% remains satisfactory and is generally accepted by the community (Dekker et al., 2011). A relative error < 20% should ideally be sought to significantly improve understanding of these ecosystems. For the classification of shallow water bottoms, Tables 10 and 11 give the classification results obtained for Porquerolles Island and Camargue.

Scenario	Sand (%)	Posidonia oceanica (%)	Caulerpa taxifolia (%)
(#1,O,T)	29	33	8
(#6,O,T)	28	32	4
(#1,O,t)	30	33	4
(#6,O,t)	29	33	4
(#1,R,T)	38	46	24
(#6,R,T)	29	34	11
(#1,R,t)	30	35	4
(#6,R,t)	28	32	4

568 **Table 10.** RMSE error for bottom abundance fraction retrieval in Porquerolles Island.

Scenario	SPM (%)	Zoster (%)	Green algae (%)	Red algae (%)
(#1,O,T)	11.	19.	23.	23.
(#6,O,T)	15.	2.	17.	26.
(#1,O,t)	20.	7.	25.	49.
(#6,O,t)	34.	5.	10.	49.
(#1,R,T)	14.	17.	15.	27.
(#6,R,T)	17.	6.	16.	32.
(#1,R,t)	2.	11.	18.	49.
(#6,R,t)	31.	9.	9.	49.

569 **Table 11.** RMSE error for bottom abundance fraction retrieval in Camargue.

570 For Porquerolles, the average RMSE found for retrieval of bottom abundance fractions varies 571 according to the background (Figure 14): sand (30-28%), Posidonia oceanica (32-46%) and Caulerpa taxifolia (4-24%). The lowest RMSE is obtained on the latter with an RMSE < 10% 572 573 except for (#1,T,R) and (#6,T,R). The best scenarios are (#6,T,O), (#6,T,O), (#1,t,O), (#6,t,O), 574 (#1,t,R) and (#6,t,R). For Camargue, the RMSE error is between 2% and 49% for all scenarios. 575 The retrieval of zoster species (between 2% and 19%) leads to the best results. Overall, the best 576 scenario for estimating the four variables is (#6,T,O). Inversion performance is globally higher 577 for Camargue than for Porquerolles Island. As the bathymetry of Camargue is much lower than 578 that of Porquerolles Island, the TOA radiance is higher, which reduces the influence of sensor 579 noise on retrieval performance. A degradation in sensor calibration induces a significant 580 decrease in inversion performance and thus reduces the ability to correctly derive bathymetry 581 in shallow water. Sensitivity to SNR shows that a strategy involving wider spectral bands is 582 preferred (i.e., Porquerolles Island). The narrow spectral band strategy only has an advantage 583 when SNR is not the limiting factor, typically for shallow water sites such as Camargue. 584 Estimates of abundance fraction of bottom species proved to be inconsistent and non-585 exploitable (RMSE > 3 m) for bottom depths > 10 m.

586 For coastal habitat classification, unmixing performance was evaluated on the VNIR 587 hyperspectral image and compared with the reference. RMSE performance is very similar 588 across all scenarios (average RMSE 4.65%, average standard deviation 3.73%). A slight 589 improvement is obtained using pansharpened images (4.26% and 3.40%, respectively). This is 590 not surprising given the high spatial heterogeneity of these areas and the need for fine spatial 591 resolution to improve the accuracy of biological component estimates. The best performances 592 were obtained with (#6,T,O) and (#1,T,O), and the worst with (#1,t,R) with or without prior 593 pansharpening.

Finally, PLS-DA applied to the VNIR-SWIR spectral library on a limited number of scenarios
(#1,T,R), (#2,T,R), (#5,T,R), (#1,t,R) led to better performances than those obtained with VNIR
images (Kappa ranging from 0.76 to 0.92). Among the four scenarios tested, the best
performance is obtained with (#2,T,R), underlining the importance of SNR in the discriminant
process.

599 **4.4. Urban land cover** 

Whatever the scenario, performance is very similar. With the ULC1 method (Figure 15), overall accuracy performance is between 66 and 67% with *target* calibration and ~ 65%  $\pm$  0.1 with *threshold* calibration. With the ULC2 method, all scenarios are similar, with an F-score of ~ 54%  $\pm$  0.1. This classification is based primarily on the overall spectral shape of the reflectance and is therefore insensitive to spectral strategies.

605 **4.5. Industrial site** 

To estimate PM1 aerosols, only the VNIR is used. Consequently, only sampling strategies #1 and #6 are considered. First, the detection performance of the aerosol plumes present in the images is evaluated by estimating the percentage of true positives and false positives compared with the airborne image used as a reference (Table 12). As performance does not depend on calibration, only an average value is given.

	True positive (%)	False positive (%)
#1, Optimistic	56	19
#6, Optimistic	64	23
#1, Realistic	64	21
#6, Realistic	67	23

612 The detection rate varies from 56% to 67% and the false detection rate from 19% to 23%. There 613 is no trend between these values and changes in the instrument specifications, especially with 614 the optimization of segmentation parameters. Table 13 shows the average sensitivity to aerosol 615 properties estimated from the differential image for #1 and #6. This includes uncertainty due to 616 instrumental mode, native noise, registration errors and radiative transfer model assumptions. 617 This image was acquired with a high sun zenith angle and a low spatial extent of the plume. 618 With this particular geometry, the downward solar flux does not pass through the plume, 619 leading to poor soot estimation whatever the strategy.

Scenario	Concentration (µg/m³) Known aerosol type	Radius (nm)	Absorptance (%)	Concentration (µg/m³) Unknown aerosol type
(#1,T,O)	73	42	30	140
(#6,T,O)	74	43	40	160
(#1,t,O)	91	90	5	145
(#6,t,O)	92	57	4	140
(#1,T,R)	82	45	30	280
(#6,T,R)	79	53	40	190
(#1,t,R)	106	100	50	260
(#6,t,R)	98	70	50	170

620 **Table 13.** Average sensitivity to PM1 mass concentration for the aerosol model studied.

When the aerosol model is known, the high objective of 80  $\mu$ g/m<sup>3</sup> is reached for (\*,T,O), and the acceptable low objective of 150  $\mu$ g/m<sup>3</sup> is reached for all scenarios. However, when the aerosol model is unknown (uncertainties in radius and soot fraction), the increase in uncertainty depends on the sensitivity of the estimate of aerosol radius and soot content. Only scenarios (#1,T,O), (#1,t,O) and (#6,t,O) meet the low objective.

626 Table 14 presents the methane estimates.

	Opt	imistic	Rei	alistic
Sampling	Target	Threshold	Target	Threshold
#1	900	980	1330	1490
#2	980	1050	1300	1510
#3	900	1120	1310	1420
#4	930	1020	1330	1410
#5	890	1000	1250	1450
#6	800	860	1070	1160

627 **Table 14**. Methane abundances (ppm.m) for each scenario. Note that the reference value obtained from the airborne image is 510 ppm.m.

In the case of a *realistic* SNR and a *threshold* value for calibration, sampling strategy #3 should achieve the low objective of 1500 ppm.m. Sampling strategy #1 is better than #3 in the case of high SNR (*optimistic*), but has no advantage in the case of low SNR (*realistic*). Sampling strategy #6 performs better at all SNRs and should provide results within the high objective of 1000 ppm.m. However, due to the low spectral resolution, it leads to an increase in false alarms compared to the other strategies, which induced a bias in the flow rate estimation. For sampling strategies #1 to #5, the high objective is only achieved in the case of high SNR (*optimistic*).

**4.6. Cryosphere** 

Table 15 shows the retrieval results for specific surface area (SSA) and equivalent black carbon(eBC) concentration.

639**Table 15.** Mean bias and standard deviation on retrieved SSA and eBC. The SSA reference value is  $2 \pm 1$ 640m²/kg. The black carbon reference value is  $18 \pm 14$  ng/g.

	Opt	imistic	Reali	istic
Variable	(*,T,O)	(*,t,O)	(*,T,R)	(*,t,R)
SSA (m²/kg)	$4\pm 2$	$7\pm4$	$4\pm3$	$8\pm4$
eBC ( ng/g)	$84 \pm 56$	$102 \pm 64$	$83 \pm 56$	$101 \pm 64$

The results show that instrumental noise and sampling strategy have a negligible effect compared to calibration errors. SSA retrieval is generally satisfactory, while eBC concentration retrieval is more challenging. In some cases, degradation of the spectral strategy slightly modifies sensitivity to other errors. Thus, a high-performance calibration should enable these two key parameters to be estimated, whereas a low-performance calibration will only give

access to SSA. The retrieval of SSA and eBC concentration is not affected by the change inspectral resolution from 10 to 20 nm in the SWIR.

648

#### 4.7. Atmosphere

Table 16 summarizes the total uncertainties of the  $H_20$  and  $CO_2$  atmospheric columns. As the variations in performance are not very large, only the two extreme cases (\*,T,O) and (\*,t,R) are shown.

652**Table 16.** Mean error and standard deviation on H20 and CO2 estimates calculated for the six sampling653strategies.

		H <sub>2</sub> 0 (%)	C	O2 (%)
Scenario	(*,T,O)	(*,t,R)	(*,T,O)	(*,t,R)
	$4.5 \pm 0.8$	$5.7 \pm 1.0$	$2.3 \pm 0.2$	$2.5 \pm 0.1$

654 For water vapor, whatever the sampling strategy, the degradation in SNR and image quality 655 leads to a slight increase in the average uncertainty from 4.5 to 5.7%. Total uncertainty on the 656 tropospheric CO<sub>2</sub> profile is minimum at around 2.0 with (#1,T,0), corresponding to an 657 uncertainty of 8 ppm on the estimated tropospheric CO<sub>2</sub> column. It is maximum at around 2.6 658 with (#2,T,R), corresponding to an uncertainty of 10.5 ppm on the estimated tropospheric CO<sub>2</sub> 659 column. Thus, sampling strategy #1 is the best option, while #2 is the least favorable. In contrast 660 to H<sub>2</sub>O, the best SNR is preferable to spectral resolution for a better estimation of the 661 tropospheric CO<sub>2</sub> column. Finally, in the case of simultaneous restitution of both gas 662 concentrations, the choice of spectral strategy will depend mainly on the measurement noise.

Figure 10 shows retrieved versus assumed AOT in the forward radiance simulations, the former thus representing the reference (true) values, at 492 nm and 865 nm. Consistently good spectral retrieval indicates correct aerosol model identification. The figure shows the AOT correlations for SNR =200 (spectral bands centered on 419, 441, 492 and 546 nm) and SNR = 100 (spectral bands centered on 669, 770, 865 and 2190 nm) for the scenario (#1,T,R). A slight degradation compared to the noise-free case (not presented here) was noted in the simulations. At the same time, the retrieved AOT values and spectral dependence are reasonably good: R is ~ 0.99 and RMSE from 0.023 to 0.036. These performances are considered to be of reasonable quality, since the same simulations, but without noise, led to RMSEs of 0.015 and 0.025, demonstrating that intrinsic GRASP uncertainty explains a large part of the RMSE. With an SNR of 50, the retrieval convergence algorithm is very poor for all channels.



674

**Figure 10.** Top: Correlation between retrieved and assumed aerosol optical thickness (AOT) in forward radiance simulations for SNR = 200 (spectral bands centered on 419, 441, 492 and 546 nm) and SNR = 100 (spectral bands centered on 669, 770, 865 and 2190 nm). AOTs are presented at 492 nm and 865 nm. R is the correlation coefficient, RMSE the root mean square error, N the number of points. Bottom: Histograms of absolute differences in AOT (black for all, red for AOT < 0.2 and blue for AOT > 0.2).

## 680 **5.** Discussion

#### 681 **5.1. End-to-end simulation**

These end-to-end simulations were performed with realistic instrument characteristics. All products simulated in this exercise used the same end-to-end processing chain, with similar and realistic instrumentation parameters, which facilitated comparisons between the different 685 applications. This work was based on 24 instrument configurations  $\times$  27 spectral datasets (22 686 images + 5 spectral libraries) leading to 648 simulations with different (spectral strategy, 687 calibration performance and SNR) combinations. However, some limitations were identified. 688 One of the first limitations was that all the instrumental defects were not taken into account 689 such as the straylight, the geometrical errors (geolocation, band co-registration, etc.), the across-690 track variations of the instrument characteristics (MTF, ISRF, etc. including the smile effect for 691 instance), the polarization sensitivity and the detector defects (such as remanence, dead pixels, 692 etc.). Another limitation was the potential overestimation of the performance of the atmospheric 693 correction. Only the water vapor content and the aerosols load errors were considered. The 694 following sources of errors have been neglected: carbon dioxide abundance, aerosol type and 695 the environment effects. Some applications may show better performance here than the ones 696 actually achievable on satellite images. However, the comparison between applications and 697 between different instrumental configurations should remain relevant. Another limitation of 698 this approach was to consider that the performance of the atmospheric correction was constant 699 whatever the performance of the instrument. In practice, the degradation of the instrument will 700 also degrade the atmospheric correction, and will therefore affect the final products even more. 701 The quality of the atmosphere correction was closely related to the calibration performance 702 because the atmospheric water vapor correction uses absorption bands that must be calibrated. 703 But the calibration of bands affected by the atmosphere is more difficult with methods based 704 on ground acquired data (known as vicarious methods), and thus dedicated on-board calibration 705 facilities are required.

706

#### 5.2. Dependence to the application methods and their input datasets

The results of this study were obtained with specific estimation methods on specific inputdatasets. The relative performances observed in this context gave valuable information for the

709 satellite design with seven applications covered; but further work will be required to consolidate 710 the conclusions at an even larger scale. For coastal habitat classification, the SWIR spectral 711 range improved classification performance when using spectral libraries. This observation 712 needs to be evaluated at the image level. SMC was estimated with the MARMIT model (Bablet 713 et al., 2018) but an updated version called MARMIT-2 is now available (Dupiau et al., 2021) 714 and could improve our results. Impurities in snow were not well estimated, one reason being 715 related to the choice of the inverse method, so future work would focus on developing a new 716 and more adapted method. The urban area classification was performed using the hyperspectral 717 pansharpening method named GAIN. The presence of mixed pixels limited the performance of 718 the method. Constans et al. (2021) proposed a new method handling mixed pixels which will 719 be evaluated in the future.

720

#### **5.3.** Synthesis of the results

Table 17 summarizes the results. This is followed by discussions on spectral strategy (§5.3.1),
SNR (§5.3.2) and calibration performance (§5.3.3).

**Table 17.** Summary of thematic performance by strategy. The color code is as follow:  $\Box$  indicates that performance is achieved,  $\Box$  indicates that performance is around the objective threshold,  $\Box$  indicates that performance is below the objective threshold. When necessary, the objective threshold ( $\Delta$ ) is indicated in the first row.

	Opti	mistic	Rea	listic
Thematic	Target	Threshold	Target	Threshold
Mineralogy 11 minerals	<b>1</b> , <b>2</b> , <b>3</b> , <mark>4</mark> , 5, 6	<mark>1</mark> , <mark>2</mark> , <mark>3</mark> , <mark>4</mark> , 5, 6	<b>1</b> , <b>2</b> , <b>3</b> , <mark>4</mark> , 5, 6	<mark>1</mark> , <mark>2</mark> , <mark>3</mark> , <mark>4</mark> , 5, 6
Soil Moisture Content ∆SMC/SMC=10%	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, <mark>4, 5,</mark> 6	1, 2, 3, 4, 5, 6
Tree Species Classification 8 classes	1, 2, 3, 4, 5, 6	1, 2, 3, <mark>4, 5, 6</mark>	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6
Forest EBV				
$\Delta \text{Cab} \sim 8 \ \mu \text{g.cm}^2$	1, 2, 3, 4, 5, 6	1, 2, 3, <mark>4</mark> , 5, 6	1, 2, 3, <mark>4</mark> , 5, 6	1, 2, 3, <mark>4</mark> , 5, 6
$\Delta \text{Car} \sim 1-2 \ \mu \text{g.cm}^2$	<mark>1, 2</mark> , <mark>3</mark> , <mark>4, 5, 6</mark>	<mark>1, 2, 3, 4</mark> , <mark>5, 6</mark>	<mark>1, 2, 3, 4, 5, 6</mark>	<mark>1, 2, 3, 4</mark> , <mark>5, 6</mark>
$\Delta EWT \sim 0.001 \text{ g.cm}^2$	<mark>1</mark> , <mark>2</mark> , <mark>3</mark> , <mark>4</mark> , <mark>5</mark> , 6	<mark>1</mark> , <mark>2</mark> , <mark>3</mark> , <mark>4</mark> , <mark>5</mark> , 6	<mark>1</mark> , 2, 3, <mark>4</mark> , 5, 6	<mark>1</mark> , <mark>2</mark> , <mark>3</mark> , <mark>4</mark> , 5, 6
$\Delta$ LMA~0.002 g.cm <sup>2</sup>	1, 2, 3, 4, 5, 6	1, 2, 3, <mark>4</mark> , 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6
Bathymetry ∆Depth<1 m	1, 2, 3, 4, 5, 6	<b>1</b> , <b>2</b> , <b>3</b> , <b>4</b> , <b>5</b> , 6	<mark>1, 2, 3, 4, 5, 6</mark>	<b>1</b> , 2, <mark>3</mark> , <mark>4</mark> , 5, 6
Bottom Classification of Shallow Water 6	123456	123456	1 2 3 4 5 6	123456
classes				
Classification of Coastal habitats (without	<b>1</b> , <b>2</b> , <b>3</b> , <b>4</b> , <b>5</b> , <b>6</b>	1, 2, 3, 4, 5, 6	<b>1</b> , <b>2</b> , <b>3</b> , <b>4</b> , <b>5</b> , <b>6</b>	<b>1</b> , <b>2</b> , <b>3</b> , <b>4</b> , <b>5</b> , <b>6</b>
Fusion)		2, 2, 0, 1, 0, 0		2, 2, 2, 2, 2, 0
Urban Land Cover 10 classes	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	<b>1</b> , 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6
Industrial Plant Gas $\Delta CH_4 = 1000 \text{ ppm.m}$	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	<mark>1</mark> , 2, 3, 4, 5, 6	1, <mark>2</mark> , 3, 4, 5, 6
Industrial Plant Gas $\Delta CO_2 = 150000$ ppm.m	1, 2, 3, 4, 5, 6	1, 2, 3, <mark>4</mark> , 5, 6	<mark>1</mark> , 2, 3, <mark>4</mark> , 5, 6	1, <mark>2</mark> , 3, 4, 5, 6
Industrial Plant Aerosol: aerosol model				
known	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6
$\Delta AOT=80 \mu g/cm^2$	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6
$\Delta A01=150 \mu g/cm^2$				
Industrial Plant Aerosol: aerosol model not	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6
known $\Delta A01=150 \mu g/cm^2$				
Cryosphere: $\Delta$ SSA=2 m <sup>-</sup> .kg <sup>-1</sup>		1, 2, 3, 4, 5, 6		1, 2, 3, 4, 5, 6
$\Delta eBU=18 \text{ nD.g}^{-1}$		<b>1</b> , <b>2</b> , <b>5</b> , <b>4</b> , <b>5</b> , <b>6</b>	<b>1</b> , <b>2</b> , <b>3</b> , <b>4</b> , <b>5</b> , <b>6</b>	
Autospheric Gas $H_2U$ , $\Delta H_2U/H_2U$ (10%)	1, 2, 3, 4, 5, 6	Not tested	Not tested	1, 2, 3, 4, 5, 6
Atmospheric Gas CU <sub>2</sub>	1, Z, 3, 4, 5, 6	Not tested	Not tested	1, 2, 3, 4, 5, 6
Atmospheric Aerosol with revisit or auxiliary (type, abundance)	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6	1, 2, 3, 4, 5, 6

#### 726 **5.3.1. Spectral strategy**

As Table 5 shows, the different spectral strategies are fairly equivalent over the VNIR and
variable over the SWIR. Two types of results can be distinguished, depending on the variable
to be extracted.

First, when searching for local spectral features characterizing a material, the method's performance is highly dependent on the spectral strategy. This is the case for mineralogy, where the kaolinite doublet can only be discriminated with sampling strategies #1 and #4. Sampling strategies #5 and #6 are acceptable for some minerals, but lead to confusions for others. Sampling strategies #2 and #3 fail to achieve the objectives set for mineralogy. These results confirm the work of Swayze et al. (2003), who predict a spectral resolution of 10 nm to 736 discriminate clays and more specifically kaolinite. Sun et al. (2006) estimate that a spectral 737 sampling interval of 8.2 nm and an SNR > 200 between 1.95 and 2.4  $\mu$ m does not affect the 738 identification of the 15 minerals tested. Furthermore, kaolinite (resp. dickite) cannot not be 739 detected if the spectral sampling interval is > 16.4 nm (resp. 12.3 nm). On the other hand, 740 Chabrillat et al. (2002) showed that a spectral resolution of 17 nm reduces the ability to detect 741 kaolinite in a mixture, as the Al-OH doublet is not well sampled, but allows the detection of 742 smectites or illites. Although the spectral resolution of HyMAP (~17 nm) is almost half that of 743 AVIRIS (~10 nm), Kruse (2002) showed that both sensors can separate calcite from dolomite 744 and the three varieties of sericite present in Northern Grapevine mountains (NV, USA).

Spectral sampling #2 is not recommended for  $H_2O$  and  $CO_2$  estimates, but the best spectral strategy depends strongly on SNR. Spectral sampling #6 is not recommended for bathymetry and aerosol plume. For the gas plume, spectral sampling #5 fails to detect  $CH_4$  accurately (< 1500 ppm.m).

749 Methods based on the use of the global spectral shape do not depend on the spectral sampling 750 strategy. This is the case for SMC, tree species classification, tree functional trait estimation, 751 bathymetry, shallow water bottom classification, coastal habitat classification, urban land 752 cover, snow and ice characterization, and aerosols. They depend on either the SNR (bathymetry, 753 classification in general) and/or instrument calibration (bathymetry, classification, 754 characterization of industrial plant and snow). Gomez et al. (2018) evaluated the predictive 755 performance of clay soil properties as a function of spectral configuration and showed that it 756 did not depend on spectral sampling, which ranged from 5 to 100 nm. For species identification, 757 Jianxin Jia et al. (2022) compared the classification performance of eleven species with 758 different bandwidths, which ranged from 9.6 to 153.6 nm. They conclude that classification 759 performance is similar for a bandwidth ranging from 9.6 to 19.2 nm, and if the bandwidth is 760 widened, leading to a similar SNR, spatial resolution can be improved. Serbin et Townsend

(2020) recommended spectral sampling and FWHM of 10 nm for leaf pigments (Cab, Car), of
20 nm for EWT and LMA. These results are in line with our results.

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#### 5.3.2. Signal-to-noise ratio

For applications using specific absorption bands, performance depends firstly on SNR (*optimistic/realistic*) and secondly on calibration performance. Estimates are slightly degraded between *optimistic* and *realistic*, but most of the applications tested depend little or not on the SNR studied, with the exception of bathymetry and shallow water classification due to low reflectance, carbon dioxide and methane.

769 For mineralogy, according to Kruse et al. (2002), an SNR of at least 100 in the SWIR is required 770 for mineral detection, so the *realistic* SNR is slightly above this limit, while the *optimistic* SNR 771 is higher, as for the PRISMA or EnMap instruments (Peyghambari and Zhang, 2021). Below 772 this value, applications such as calcite-dolomite or clay discrimination, mineral mapping, soil 773 component discrimination or sediment detection is critical (Transon et al., 2018). Thus, such 774 discrimination will be difficult if not impossible with the current SNR of the mission. Sun et al. 775 (2006) estimate that an SNR of at least 200 at 2100 nm is required to map minerals with linear 776 spectral unmixing. Chabrillat et al. (2002) show that detection of dark clays or dark Granero 777 shales requires an SNR > 600 to detect them partially.

778

#### 5.3.3. Calibration performance

Most of the applications tested depend little or not at all on the calibration scenarios, with the exception of bathymetry (not filled for *threshold*) and cryosphere (equivalent black carbon concentration not estimated with *threshold*). A slight loss in performance was observed between *target* and *threshold* calibrations. Whatever the spectral strategy, scenarios with *target* calibration performance and *optimistic* SNR clearly delivered similar performance. Scenarios with *threshold* calibration performance and *optimistic* SNR and scenarios with *target*  calibration performance and *realistic* SNR represent a good compromise. With the SNR used
in this study, the impact of instrument calibration on mineralogy is low. There is no obvious
difference between *target* and *threshold* cases. Spectral calibration and atmospheric correction
errors should be taken with care, as they can induce peaks at H<sub>2</sub>O and CO<sub>2</sub> wavelengths, which
can be problematic for the identification of certain minerals, depending on the algorithm
selected.

## 791 **6.** Conclusion

CNES is working on a hyperspectral mission (0.40-2.45 µm, 10 m GSD, 10 km swath) with a panchromatic camera (2.5 m GSD). A phase A study has just been completed in mid-2022. A large French scientific community has been involved to optimize the instrument design. Taking into account the technological constraints of the SWIR detector, an analysis of several spectral sampling strategies was conducted to assess their impact on end-user applications (mineralogy, vegetation, coastal area, urban area, industrial site, cryosphere and atmosphere).

An end-to-end simulator has been developed to generate the hyperspectral images that the satellite under design will acquire, taking into account the main instrumental effects. It will be improved by including other sources of error when the instrument design matures.

801 It has also been shown that most of applications can be realized with an optimistic SNR level 802 and target calibration, whatever the sampling scenario. With optimistic SNR and threshold 803 calibration, most applications have been achieved, with the exception of bathymetry and 804 cryosphere (eBC). With *realistic* SNR and a *target* calibration, most applications have been 805 achieved, with the exception of industrial aerosols. Finally, with *realistic* SNR and *threshold* 806 calibration, most applications have been achieved, with the exception of bathymetry, bottom 807 classification of shallow water, industrial aerosol and cryosphere (eBC). We also found that 808 some spectral strategies were unable to track certain spectral features for mineralogy and industrial gas estimation. All scenarios tested were simulated with the same atmospheric
uncertainty on water vapor content and aerosol optical thickness, regardless of instrument
configuration.

Based on these results, CNES is studying the best compromise for designing the hyperspectral sensor that will meet the objectives of the priority applications. These preliminary conclusions need to be confirmed by further studies, in particular taking into account the dependence between scenario and atmospheric correction performance, as well as improvements in estimation methods. Other applications will be evaluated, such as crop characterization, pollution monitoring and plastic detection.

## 818 Appendix

819 This appendix completes the results obtained in this work: maps of leaf functional traits,820 shallow water bottom classification and urban land cover.

Figure 11 is an RGB image of the Tonzi site. Figure 12 shows the Cab, Car, LMA and EWT
maps estimated on QUDO with sampling strategy (#1,T,O).



824 Figure 11. Tonzi site (CA, USA)



826

- Figure 12. Leaf functional trait maps obtained with scenario (#1,T,O). Top left: Cab. Top right: Car. Bottom
  left: LMA. Bottom right: EWT.
- 829 Figure 13 is an RGB image of the Porquerolles site. Figure 14 shows maps of water parameters
- 830 (chl, SPM, CDOM), depth and seabed abundance with (#1,T,O).



831

**Figure 13.** The true color hyperspectral image captured by HYSPEX for the Porquerolles site.



833

Figure 14. Estimation of water parameters (chl, SPM, CDOM), depth and seabed abundance with (#1,T,O) at
 Porquerolles site.

- 836 Figure 15 is an RGB image of the Toulon area with the classification map obtained with
- 837 (#1,T,O).



839 **Figure 15.** Left: RGB reference image of Toulon at 2.5 m GSD. Right: Classification map with (#1,T,O).

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