

# Topsoil clay content mapping in croplands from Sentinel-2 data: Influence of atmospheric correction methods across a season time series

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1	Topsoil clay content mapping in croplands from Sentinel-2 data: influence
2	of atmospheric correction methods across a season time series
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16	Abstract
17	Recent studies demonstrated the capability of Sentinel-2 (S2) data to estimate topsoil
18	properties and highlighted the sensitivity of these estimations to soil surface conditions
19	depending on the S2 acquisition date. These estimations are based on Bottom Of Atmosphere
20	(BOA) reflectance images, obtained from Top Of Atmosphere (TOA) reflectance values using
21	Atmospheric Correction (AC) methods. AC of optical satellite imagery is an important pre-
22	processing stage before estimating biophysical variables, and several AC methods are
23	currently operational to perform such conversion. This study aims at evaluating the sensitivity
24	of topsoil clay content estimation to atmospheric corrections along an S2 time series. Three
25	AC methods were tested (MAJA, Sen2Cor, and LaSRC) on a time series of eleven Sentinel-2

images acquired over a cultivated region in India (Karnataka State) from February 2017 to 26 27 June 2017. Multiple Linear Regression models were built using clay content analyzed from topsoil samples collected over bare soil pixels and corresponding BOA reflectance data. The 28 29 influence of AC methods was also analysed depending on bare soil pixels selections based on two spectral indices and several thresholds: the normalized difference vegetation index 30 (NDVI below 0.25, 0.3 and 0.35) and the combination of NDVI (below 0.3) and Normalized 31 32 Burned Ratio 2 index (NBR2 below 0.09, 0.12 and 0.15) for masking green vegetation, crop residues and soil moisture. 33

First, this work highlighted that regression models were more sensitive to acquisition 34 35 date than to AC method, suggesting that soil surface conditions were more influent on clay content estimation models than variability among atmospheric corrections. Secondly, no AC 36 method outperformed other methods for clay content estimation, and the performances of 37 38 regression models varied mostly depending on the bare soil pixels selection used to calibrate the regression models. Finally, differences in BOA reflectance among AC methods for the 39 same acquisition date led to differences in NDVI and NBR2, and hence in bare soil coverage 40 identification and subsequent topsoil clay content mapping coverage. Thus, selecting S2 41 images with respect to the acquisition date appears to be a more critical step than selecting an 42 43 AC method, to ensure optimal retrieval accuracy when mapping topsoil properties assumed to be relatively stable over time. 44

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Keywords: clay content; Sentinel-2; atmospheric correction; multiple linear regression; soil
property mapping; India.

48

## 49 **1. Introduction**

Soils are key to meeting global environmental sustainability challenges for food security, 50 51 water security, energy sustainability, climate stability, biodiversity, and ecosystem service delivery (McBratney et al., 2014). An accurate and spatially referenced characterization of 52 soil properties over cultivated areas, including soil organic matter, soil texture, or iron 53 content, is essential for meeting these global environmental sustainability challenges and 54 would also allow to help for planning agricultural engineering work such as land 55 56 consolidation, drainage management, and soil erosion prevention. Particle-size distribution, also called soil texture, refers to relative amounts of sand, silt, and clay in grams per kilogram 57 (g kg<sup>-1</sup>) in a soil, the sum of these particle size fractions equaling 1000 g kg<sup>-1</sup>. Soil texture is a 58 59 major component of soil, as it has an important influence on water infiltration and soil stabilization (Le Bissonnais et al., 2007, 2018). To ensure soil security, adequate decisions 60 both at global and local levels are required to favor the beneficial roles of soil (Rodrigo-61 62 Comino et al., 2020). Such decisions require accurate spatially referenced soil information systems that can be used in environmental modeling. 63

Spectroscopy covering the Visible, Near Infrared, and Short Wave Infrared domains 64 (VNIR/SWIR, 400 – 2500 nm) is a technology that proved its relevance for the estimation of 65 soil properties (Viscarra Rossel et al., 2006) as the soil reflectance spectrum results from the 66 position and shape of absorption features of chemical constituents ("peaks") (e.g., water 67 molecules influence the absorption features at specific wavelengths that are the results of 68 overtone and combination modes from the IR region) and overall spectral shape of the 69 physical properties (e.g., texture) (Ben-Dor and Banin, 1995a, 1995b). Most of the 70 71 absorptions in the VNIR/SWIR region are characteristic of clay and organic matter, and are dominated by C-H, O-H, N-H and metal-OH bonds (e.g., Clark et al., 1990). Soil physical 72 73 properties, including particle size, scatter the light in a way that the spectrum shape and base line are changing (Wetzel, 1983; Chabrillat et al., 2019). According to Ben-Dor et al. (2002), 74

an accurate estimate of a soil property can be expected from VNIR/SWIR data if the targeted
soil property i) is related to a chemical species that impacts soil surface reflectance values
through absorption bands (e.g., OH- ion for clay) or ii) is highly correlated with the latter
(e.g., CEC correlated with clay content). In addition to these two rules, a minimum level of
variability of the targeted soil property across study regions is required to be accurately
estimated (Gomez et al., 2012a).

81 VNIR/SWIR airborne spectroscopy was successfully used to map a large range of soil properties such as iron, soil organic carbon (SOC), and clay contents over bare soil surfaces 82 with high accuracy (e.g., Ben-Dor et al., 2002; Stevens et al., 2010; Gomez et al., 2008, 83 2012b; Chabrillat et al., 2019). More recently, the VNIR/SWIR multispectral satellites 84 Sentinel-2 (S2) enabled mapping topsoil properties over bare soil surfaces, such as SOC (e.g., 85 Gholizadeh et al., 2018; Vaudour et al., 2019a, b, 2021; Žížala et al., 2019; Castaldi et al., 86 87 2021; Dvorakova et al., 2021; Urbina-Salazar et al., 2021) and texture (e.g., Gholizadeh et al., 2018; Gomez et al., 2019; Bousbih et al., 2019). Despite lower accuracy of S2 estimates 88 89 compared to airborne imaging spectroscopy, the global coverage and high revisit frequency of 90 S2 (five days at the equator) opened perspectives for regional mapping. However, the selection of an S2 acquisition over a multi-temporal series in order to have an optimal 91 92 estimation of soil properties, such as clay content, raises questions due to multiple factors influencing surface reflectance, and possibly statistical models adjusted to estimate soil 93 properties (Vaudour et al., 2019b; Gomez et al., 2019; Castaldi et al., 2019). Indeed soil 94 surface conditions such as soil moisture and roughness (e.g., due to tillage operations) 95 96 influence soil reflectance (Chabrillat et al., 2019). The Normalized Difference Vegetation Index (NDVI, based on Red and NIR spectral bands) and the Normalized Burned Ratio 2 97 (NBR2) index (based on spectral bands around 1600 nm and 2200 nm) have been widely used 98 as indicators for photosynthetic vegetation and dry crop residues, respectively (e.g., for 99

Landsat 8 by Demattê et al., 2018 and S2 by Castaldi et al. 2019). Nevertheless, while NBR2 100 101 follows a linear relationship with crop residue cover over dry soils, no correlation with residue cover could be found over moist soils (Dvorakova et al., 2020). So it is assumed that NBR2 102 103 reacts both to crop residues and soil moisture, where high values of NBR2 indicate soils that are moist and/or are covered by crop residues. In the way of creating a composite multi-date 104 105 bare soil image based on S2 images for soil organic carbon (SOC) prediction, Dvorakova et 106 al., (2021) and Vaudour et al. (2021) developed strategies that allow selecting S2 pixels with 107 minimal influence of crop residues, surface roughness or soil moisture, using spectral indices, especially NDVI and NBR2 indices for detecting these disturbing factors. 108

109 Atmospheric conditions also strongly influence the Top of Atmosphere (TOA) reflectance (Level-1C products), and the choice of atmospheric correction (AC) method used 110 111 to convert S2 Level-1C into Level-2A products may result in differences in terms of Bottom 112 of Atmosphere (BOA) reflectance. These AC methods use different atmospheric models and hypotheses, which may affect the resulting BOA reflectance depending on the season, clouds, 113 sun azimuth, and elevation, and therefore the soil property estimations. Several AC methods 114 115 have been developed for multispectral images (e.g., Multi-sensor Atmospheric Correction and Cloud Screening -MACCS, Hagolle et al. (2015a), updated and renamed « MACCS-ATCOR 116 joint algorithm » or MAJA, Lonjou et al. (2016); Sen2Cor, Gascon et al. (2017), Louis et al. 117 (2016); Land Surface Reflectance Code -LaSRC, Vermote et al. (2016)). MAJA and Sen2Cor 118 methods were both developed specifically for Sentinel-2 and have become widely used 119 standard products available from Copernicus and other platforms. LaSRC, originally 120 developed by NASA for Landsat, has been adapted recently for Sentinel-2, so it may also 121 become a standard product in the future (e.g., considered in the Brazil Data Cube, Ferreira et 122 al., 2020). These methods use quite different processing paths, from the atmospheric 123 parameter estimation to the radiative transfer model and temporal information, justifying 124

interest in their comparison. A first Atmospheric Correction Inter-comparison Exercise 125 126 (ACIX) was carried out under an international collaborative initiative to compare a set of AC methods for optical sensors, including S2 (Doxani et al., 2018). However, because the 127 exercise continued, Doxani et al. (2018) did not draw common conclusions from all the 128 algorithms. In addition, Sola et al. (2018a, 2018b) evaluated four AC methods for S2 images, 129 highlighting minor differences between these AC methods. Finally, to the best of our 130 knowledge, no work has been conducted on the impact of AC methods on soil property 131 estimation. 132

Following, on the one hand, the studies from Doxani et al. (2018) and Sola et al. 133 (2018a, 2018b) evaluating AC methods for S2 images, and those from Gomez et al. (2019) 134 and Vaudour et al. (2019b) studying the impact of acquisition dates on prediction 135 performances of texture and SOC contents, the objective of this study is to evaluate the 136 137 impact of three major AC methods (Sen2Cor, MAJA, and LaSRC) along an S2 time series on clay content estimation in the topsoil. The influence of these AC methods was also analysed 138 depending on bare soil pixels selections based on two spectral indices and several thresholds: 139 the NDVI (below 0.25, 0.3 and 0.35) and the combination of NDVI (below 0.3) and NBR2 140 (below 0.09, 0.12 and 0.15). Eleven S2 images covering a cropping cycle in 2017 in a 141 cultivated region in India (Karnataka State) were selected for this study. Soil samples were 142 collected over the study area and analyzed in a laboratory. Clay content was then estimated 143 from each BOA S2 image, corrected by the three AC methods, using multiple linear 144 regression models. 145

146

- 147 **2. Materials and Methods**
- 148 **2.1.** Study area

The Berambadi catchment is a subcatchment of the South Gundal located in the Deccan 149 Plateau of Southern India (Figure 1a), extending over 84 km<sup>2</sup> (Figure 1b). Our study area is 150 located in the eastern part of the Berambadi catchment, of which 60% of the surface is 151 dedicated to agriculture, with a high diversity of crops (e.g., sunflower, marigold, sorghum, 152 turmeric, maize, etc.) and high seasonal variability. The western part of the Berambadi 153 catchment is covered by forest (not shown in Figure 1b). The Berambadi catchment belongs 154 to the Kabini Critical Zone Observatory (AMBHAS, BVET, Tomer et al., 2015; Sekhar et al., 155 156 2016), which is part of the OZCAR network (Gaillardet et al., 2018). The climate is tropical subhumid with an average rainfall of 800 mm/year and a PET of 1100 mm (aridity index 157 158 P/PET of 0.7). The monsoon dynamics drive three main seasons: dry season (winter in January and February, summer from March to May), Kharif (southwest monsoon season, 159 from June to September), and Rabi (north-east monsoon season, from October to December). 160 Red soils (Ferralsols and Chromic Luvisols) cover the uplands and hillslopes, while black 161 soils (Vertisols and Vertic intergrades) are mostly found in the valley bottom (Barbiero et al., 162 2010). Uplands and hillslopes are mainly characterized by coarse soil texture (sandy loam) 163 due to erosion processes, whereas valleys bottoms are mainly characterized by finer soil 164 texture (clay) mainly caused by deposition processes (Gunnell and Bourgeon, 1997; Barbiero 165 et al., 2010). 166

167 Three cropping seasons regulate the farm system (Robert et al., 2017). During the 168 Kharif season (from June to September) corresponding to the rainy season, most of the 169 cropping area are cultivated with sorghum, maize, sunflower, marigold, as well as crops 170 grown in irrigated conditions, such as turmeric, onion, garlic, and banana. During the Rabi 171 season (from October to January) corresponding to the winter season, most irrigated plots are 172 cultivated with maize, horse gram, and vegetables. Finally, during the Summer season (from February to May) corresponding to the hot and dry season, only few plots are cultivated, andalmost 90% of the cropland is bare land.

175

# [Figure 1]

176

## 177 2.2. Soil dataset

A total of 164 topsoil samples were collected over Berambadi in November 2019 (Figure 1b). 178 All samples were composed of five sub-samples collected to a depth of 5 cm within a 10 m 179 ×10 m square (one at the center and four at each corner) centered on the geographical position 180 of the sampling plot, as recorded by a Garmin GPS instrument. After sample homogenization, 181 approximately 20 g was devoted to soil property analysis. The samples were then air-dried 182 and sieved with a 2 mm sieve prior to being analyzed in the laboratory. The clay fraction was 183 determined using the pipette method as described by Piper (1966). The clay content ranged 184 between 58 and 622 g kg<sup>-1</sup> (mean = 252 g kg<sup>-1</sup>, standard deviation = 124 g kg<sup>-1</sup> and skewness 185  $= 5 \text{ g kg}^{-1}$ ). 186

187

## 188 2.3. Sentinel-2 images

Launched in 2015 and then 2017 the combination of both Sentinel-2 satellites (S2A and S2B) delivers a revisit period of five days at the equator. The multispectral sensors acquired information over thirteen spectral bands in the VNIR/SWIR spectral domain, with spatial resolution ranging from 10 m to 60 m.

Twenty-six images from the S2 tile 43PFP were acquired over Berambadi between February 1<sup>st</sup> and June 30<sup>th</sup> 2017. This corresponds to the summer season and beginning of Kharif season in South India, when both a maximum of bare soil pixels and a minimum of clouds can be encountered. As clay content is a perennial property in topsoil horizons, we can assume that the clay content analyzed from soil samples collected in 2019 remained unchanged compared to 2017, as assumed in previous studies (e.g., Gomez et al., 2008;
Loiseau et al., 2019).

200

#### 201 2.3.1. Atmospheric correction method

Atmospheric corrections were performed on the 26 images using three AC methods described 202 in the next subsections (MAJA, Lonjou et al., 2016; Sen2Cor, Louis et al., 2016; LaSRC; 203 Vermote et al., 2016) providing three time series of atmospherically corrected images (Figure 204 205 2a). After atmospheric correction, only ten bands were retained for spectral modeling, corresponding to the four 10 m resolution bands (B2, B3, B4 and B8, see Table 1 in 206 207 Dvorakova et al., 2021) and the six 20 m resolution bands (B5, B6, B7, B8A, B11 and B12, see Table 1 in Dvorakova et al., 2021). The BOA products were provided with reflectance 208 \*10000. 209

210

# [Figure 2]

211

#### 212 a. Sen2Cor

Since 2015, the Copernicus Open Access Hub has provided Level-2A products of S2 imagery
data over Europe, using the Sen2Cor processor developed by European Space Agency (ESA)
(ESA, 2015; Gascon et al., 2017; Louis et al., 2016). The Sen2Cor processor performs
atmospheric correction, terrain and cirrus correction, and scene classification applied to TOA
data.

The Sen2Cor 2.8 was applied to produce Level-2A images from Level-1C images using default settings (available in the Ground Image Processing Parameters files delivered with Sen2Cor official release, https://step.esa.int/main/snap-supportedplugins/sen2cor/sen2cor\_v2-8). The Planet Digital Elevation Model was used, and cirrus and Bidirectional Reflectance Distribution Function (BRDF) corrections were deactivated. All other parameters were set to their default value. In addition to Level-2A reflectance data,
Sen2Cor also produces an Aerosol Optical Thickness (AOT) map, a Water Vapour (WV)
map, and a Scene Classification Map (SCM) together with Quality Indicators (QI) for cloud
and snow probabilities. After conversion to Level-2A reflectance, Sen2Cor provides the four
VNIR spectral bands with their native spatial resolution of 10 m and the six 20 m resolution
bands, which were resampled to 10 m using nearest-neighbor interpolation.

229

230 **b.** MAJA

The MAJA processor (Lonjou et al., 2016; Hagolle et al., 2019) was initially developed to 231 perform cloud detection and atmospheric correction over time series of optical images 232 acquired at high resolution and under quasi constant viewing angles. MAJA combines Multi-233 Mission Atmospheric Correction and Cloud Screening (MACCS) developed by the French 234 235 Centre National d'Études Spatiales (CNES) and ATCOR developed by the German Aerospace Center (DLR). This spectro-temporal AC method was developed to process images 236 237 from Formosat-2, Landsat, VENµS, and S2 satellites. MAJA is based on a spectral 238 assumption of the link between red and blue spectral bands and a temporal assumption assuming that a given neighborhood separated by a few days should yield similar surface 239 reflectance (Hagolle et al., 2015a; 2015b). In the current study, the MAJA correction was 240 processed with on-demand PEPS (Plateforme d'Exploitation des Produits Sentinel) processing 241 service, which uses eight S2 acquisitions prior to each acquisition of interest to meet the 242 temporal assumption (https://labo.obs-mip.fr/multitemp/on-demand-sentinel2-l2a-processing-243 with-maja-on-peps, last access on 2021-07-01). As Sen2Cor, MAJA provides spectral bands 244 with their native spatial resolution. After Level-2A conversion, we used nearest-neighbor 245 interpolation to convert all 20 m bands to 10 m resolution. 246

249 Landsat Surface Reflectance Code (LaSRC) is an AC method initially developed to convert TOA radiance to BOA reflectance for Landsat 8 collection, which was recently adapted to 250 251 Sentinel-2 (Vermote et al., 2018). The algorithm performs atmospheric correction, assuming a Lambertian-plane-parallel atmosphere, and using the Second Simulation of the Satellite 252 Signal in the Solar Spectrum (6S) "Urban Clean" model (Vermote et al., 2016; USGS, 2016). 253 The atmospheric parameters required for the inversion include surface pressure (from the 254 255 National Center for Environmental Prediction Global Data Assimilation System-NCEP GDAS weather model), water vapor (derived from the MODIS near-infrared channels), ozone 256 257 (from NCEP GDAS), and aerosol properties (AOT and Angstrom exponent) (Claverie et al., 2018). The aerosol properties are estimated using the comparison between assumed surface 258 reflectance ratios computed from MODIS time series and Sentinel-2 TOA reflectance ratios. 259 260 The correction algorithm is applied at a spatial resolution of 10 m, which is the output resolution for all bands. Therefore, the L1C bands with a resolution of 20 and 60 m are 261 resampled with a nearest-neighbor method in a pre-processing step. 262

263

#### 264 **2.3.2.** Cloud mask

265 Pixels identified as clouds or cloud shadows were masked over the S2 time series, using the cloud mask product provided by MAJA (Figure 2a). The MAJA cloud mask is computed with 266 a combination of mono-temporal and multi-temporal approaches (Hagolle et al., 2010) and 267 accounts for different types of clouds (low, high, thin) and corresponding projected shadows 268 (Baetens et al., 2019). Recent cloud mask algorithms inter-comparisons highlighted that the 269 MAJA cloud mask algorithm provided similar to better performances over other cloud and 270 271 shadow mask algorithms on a large variety of environments (Baetens et al., 2019; Tarrio et al., 2020). 272

273

# 274 2.3.3. Bare soil selection

S2 pixels identified as non-cultivated land were masked using a land-use map available for the study area (AMBHAS Team, 2015) (Figure 2a). These pixels correspond to urban areas, bodies of water, and natural vegetation (forest). Among the 26 images available over the study area, eleven were finally kept for this study, for which the surface of cultivated land outside clouds and cloud shadows covered more than 95% of the Berambadi catchment.

After masking pixels corresponding to non-cultivated land, bare soil were 280 discriminated from photosynthetic vegetation, based on a thresholding applied on the 281 282 normalized difference vegetation index (NDVI) calculated using the red band B04 (665 nm) and the NIR band B08 (842 nm) (Figure 2a). Three NDVI thresholds common to all images 283 were defined based on visual interpretation from an expert with field knowledge and literature 284 285 (e.g., Stevens et al., 2008; Vaudour et al., 2016; Lu et al., 2013), : (i) below 0.25, (ii) below 0.3 and (iii) below 0.35. Pixels corresponding to bare soil were also differentiated from crop 286 287 residue and moist soil, applying thresholding on the Normalized Burned Ratio 2 index (NBR2) calculated using the SWIR1 band B11 (1610 nm) and the SWIR2 band B12 (2202 288 nm) (Figure 2a). As setting a threshold for the NBR2 index might be difficult without relevant 289 290 field observation (Dvorakova et al., 2020 and 2021), four thresholds of NBR2 were tested: (i) no threshold, (ii) below 0.15, (iii) below 0.12 and (iv) below 0.09. . This study focused on the 291 common pixels identified as bare soil for all images to compare clay predictions obtained for 292 the different acquisitions and AC methods. 293

Topsoil water content is directly related to the time since last precipitations. As soil moisture affects spectra (Diek et al., 2016; Vaudour et al., 2019b) and in order to compare the NBR2 response with rainfall events, we calculated the number of days from the last rain for each S2 image to hint at the topsoil humidity conditions, based on daily rainfall measured in

the Maddur village, on the West part of the Berambadi catchment. Among these eleven 298 selected images, two images were acquired following heavy rainfall (cumulative rainfall of 299 25.5 mm and 18.4 mm over the last two days before the S2 data acquisition on 08-03-2017 300 and 04-04-2017, respectively), three images were acquired following moderate rainfall 301 (cumulative rainfall of 6.5 mm, 5.5 mm and 9 mm over the last five days before the S2 data 302 acquisition on 25-03-2017, 24-04-2017, and 07-05-2017), and six images were acquired after 303 304 more than five days without rain (03-02-2017, 16-02-2017, 23-02-2017, 26-02-2017, 28-03-2017, and 27-04-2017). 305

306

# 307 2.4 Spectral Measures

The BOA reflectances produced with the three different AC methods were compared pairwise to estimate the spectral similarity between AC methods over the eleven dates (Figure 2b). These spectral similarity analysis were performed using R software (R Development Core Team, 2015). The coefficient of correlation  $r_{i,t}$  was calculated between the BOA reflectance values as follows:

$$r_{i,t} = cor(Refl_{i,t}^{AC1}, Refl_{i,t}^{AC2})$$
(1)

where  $Ref l_{i,j}^{AC1}$  and  $Ref l_{i,j}^{AC2}$  are the BOA reflectance values obtained from AC methods 1 and 2, at band *i* for the S2 image acquired at date *t*. The coefficient of correlation *r* was calculated over the *N* bare soil pixels, for which soil sample was collected and clay content was analyzed.

318 As the coefficient of correlation  $r_{i,t}$  does not reflect the bias in the data (due to change 319 in albedo in our case), the bias  $Rbias_{i,t}$  between two AC methods at band *i* for the S2 image 320 acquired at date *t* was calculated as follows:

321 
$$Rbias_{i,t} = \sum_{k=1}^{N} \frac{Refl_{i,t,k}^{AC1}}{N} - \sum_{k=1}^{N} \frac{Refl_{i,t,k}^{AC2}}{N}$$
(2)

where  $Refl_{i,t,k}^{AC1}$  and  $Refl_{i,t,k}^{AC2}$  are the BOA reflectance values for pixel k, at band i for the S2 image acquired at date t, obtained from one AC and another, respectively, and N is the number of considered pixels. The bias  $Rbias_{i,t}$  was calculated over the N bare soil pixels for which soil sample was collected and clay content was analyzed.

The spectral angle was used to analyze the spectral similarity between BOA reflectance spectra. The spectral angle  $SA_{k,t}$  considers the whole spectra and not a single band as  $r_{i,t}$  and  $Rbias_{i,t}$  (Kruse et al., 1993). It was calculated between the BOA spectrum obtained from one AC and another, for pixel *k* and the S2 image acquired at date *t*, as follows:

330 
$$SA_{k,t} = \frac{\sum_{i=1}^{nb} Refl_{i,t,k}^{AC1} * Refl_{i,t,k}^{AC2}}{\sqrt{\sum_{i=1}^{nb} Refl_{i,t,k}^{AC1^2}} \sqrt{\sum_{i=1}^{nb} Refl_{i,t,k}^{AC2^2}}}$$
(3)

where  $Refl_{i,t,k}^{AC1}$  and  $Refl_{i,t,k}^{AC2}$  are the BOA reflectance values at band *i* obtained from one AC method and another, respectively, for pixel *k*, and *nb* is the total number of spectral bands (10 in our case).  $SA_{k,t}$  ranges between 0 and 1, with low values corresponding to low spectral similarity and high values corresponding to high spectral similarity. The spectral angle mapper  $SA_t$  was finally calculated for the S2 image acquired at date *t*, over the *N* bare soil pixels for which soil sample was collected and clay content was analyzed, as follows:

337 
$$SA_t = \frac{1}{N} \sum_{k=1}^N SA_{k,t}$$
 (4)

338 where  $SA_{k,t}$  was calculated from Equation (3).

339

# 340 2.5. Regression model

Regression models and analysis were performed using R software (R Development Core Team, 2015), and both the ade4 (Dray and Dufour, 2007) and pls packages (Mevik and Wehrens, 2007) were used.

A Multiple Linear Regression (MLR) method was used to produce clay maps estimated from S2 images. MLR is a multivariate approach adjusting a linear relationship

between a dependent (response) variable (Y-variable, i.e., clay content in the present case), 346 347 and a set of predictor variables (X-variables, i.e., S2 spectra in the present case) (Tenehaus, 1998) (Figure 2d). A restrictive selection of pixels corresponding to bare soil may result in 348 small sample size available to train and validate regression models using independant 349 datasets. In this work, a k-fold cross-validation (CV) was used. The original dataset was 350 351 randomly divided into k sub-datasets. Then, k-1 sub-datasets were used as training data, and the remaining one was used as validation data. The CV process was repeated k times, and the 352 model performance was evaluated by averaging prediction error obtained for the k sub-353 datasets. The k-fold CV method can take full advantage of data, as each part of the original 354 355 dataset is randomly divided and used for both training and testing. Here, 10-fold crossvalidation (CV) was used to build robust methods for estimating the accuracy of MLR models 356 and repeated 5 times. 357

Finally, three statistical criteria were used to assess model performances: mean absolute error (MAE), root mean square error ( $RMSE_{cv}$ ), and Pearson correlation coefficient ( $R^2_{cv}$ ) of cross validation (Figure 2e). These statistical criteria were calculated taking into account the 10-fold CV and 5 repetitions.

362

## **363 3. Results**

# 364 **3.1 Bare soil coverage analysis**

The distribution of NDVI values calculated over all unmasked pixels showed positive skew for all acquisition dates and AC methods with values lower than 0.25 (Figure 3). Larger differences in NDVI distributions between the three AC methods were obtained for the S2 image acquired on 08-03-2017 (Figure 3). The median value of NDVI distributions obtained using the LaSRC method (around 0.21) was slightly higher than the median obtained using Sen2Cor and MAJA methods (around 0.19) regardless of the date (Figure 3). 371

## [Figure 3]

372

The distribution of NBR2 values calculated over all unmasked pixels showed positive skew 373 374 for all acquisition dates and AC methods with values lower than 0.2 (Figure 4). The median value of NBR2 distributions obtained using the LaSRC (around 0.12 along the dates) method 375 376 was slightly higher than the median obtained using Sen2Cor and MAJA methods (around 0.9 and 0.10 along the dates, respectively), regardless of the date (Figure 4). The AC methods 377 affected the NBR2 values (Figure 4) more than NDVI values (Figure 3) as NBR2 378 distributions differed from an AC method to another, especially for the S2 images acquired on 379 380 08-03-2017, 04-04-2017, 24-04-2017, 27-04-2017 and 07-05-2017. [Figure 4] 381 382 383 Bare soil coverage selected using both NDVI and NBR2 thresholding varied depending on both acquisition dates and AC methods (Table 1). The acquisition date providing the 384 385 maximum bare soil coverage varied among AC methods. As an example, using a NDVI 386 below 0.3, the S2 image providing the maximum bare soil coverage was the one acquired on 26-02-2017 from MAJA-corrected S2 images (with 85.9%), on 08-03-2017 from Sen2Cor-387 corrected S2 images (with 85.9%), and on 23-02-2017 from LaSRC-corrected S2 images 388 (with 82.7%) (Table 1). The acquisition date providing the minimum bare soil coverage also 389 varied from an AC method to another. Still using a NDVI below 0.3, the S2 image providing 390 the minimum bare soil coverage was the one acquired on 07-05-2017 along MAJA-corrected 391 392 S2 images (with 76.3%), on 03-02-2017 along Sen2Cor-corrected S2 images (with 73.4%) and on 08-03-2017 along LaSRC-corrected S2 images (with 75.1%) (Table 1). Regardless of 393 394 the NDVI and NBR2 thresholds, the image acquired on 08-03-2017 presented maximum bare soil coverage for all AC methods (range from 5.7 to 20.75%, Table 1). Regardless of the 395

NDVI and NBR2 thresholds, the Sen2Cor method provided the highest range of bare soil
coverage along the acquition dates (range from 9.18 to 18.49%, Table 1). Finally, a majority
of LaSRC-corrected S2 images provided slightly less bare soil coverage than those corrected
by Sen2Cor and MAJA, regardless of the NDVI threshold or the combination of NDVI and
NBR2 thresholds (Table 1).

401

# [Table 1]

402

The bare soil pixels that were common for all S2 images corrected by MAJA, Sen2Cor and 403 LaSRC covered from 67.3% of the surface based on a NDVI below 0.35 to 1.2% based on 404 NDVI and NBR2 below 0.3 and 0.09, respectively (Table 2). This resulted in varying sample 405 sizes of bare soil locations with clay content information, which ranged from 122 samples 406 based on NDVI below 0.35 to 2 samples based on NDVI and NBR2 below 0.3 and 0.09, 407 408 respectively (Table 2). Due to the poor bare soil coverage on 08-03-2017 using NBR2 below to 0.12 or lower, especially from the LaSRC method (Table 1, Figure 4), the bare soil 409 410 coverage common to all dates did not exceed 7%, which allowed 12 or less samples (Table 2). 411 As the combinations of NDVI below 0.3 and NBR2 below 0.09 or 0.12, were too restrictive, this study used the four datasets reaching more than 45 collected samples 412 identified as bare soil pixels (i.e. extracted using NDVI below 0.25, 0.3, 0.35 and using the 413 combination of NDVI and NBR2 below 0.3 and 0.15, respectively) to train MLR models 414 (Figures 2c and d) and apply them to the corresponding bare soil coverage. These four dataset 415 displayed close distributions with a range between 58 and 592 g kg<sup>-1</sup>, a mean around 220 g kg<sup>-1</sup> 416 <sup>1</sup>, and skewness from 7 to 8.7 g kg<sup>-1</sup> (Table 2). 417

418

[Table 2]

419

# 420 **3.2 BOA reflectance analysis based on bare soil pixels identified with NDVI below 0.3**

The effect of AC methods on BOA reflectance values was investigated based on the 111 bare 421 422 soil pixels for which a measured clay content value was available for training the regression models, identified with a NDVI below 0.3 (Table 2). The BOA reflectance values obtained for 423 each image corrected by the three AC methods were compared based on these 111 bare soil 424 pixels. Reflectance obtained with LaSRC showed lower values for almost all bands, except 425 for B04 on 08-03-2017 (Figure 5C) and for B03 (Figure 5B). Reflectance obtained with 426 427 Sen2Cor from bands B04 to B12 (665 nm to 2190 nm, red boxplots, Figures 5 from C to J) showed systematically higher values than reflectance obtained with MAJA and LaSRC 428 (yellow and blue boxplots, respectively, Figures 5 from C to J), except on 08-03-2017 for 429 430 Band 04. The largest difference in BOA reflectance obtained among the three AC methods at the same date was observed on 08-03-2017 and mainly over the visible spectral bands 431 (Figures 5A, B, and C). The  $SA_t$  values (Equation (4)), computed for pairwise comparison 432 433 among AC methods over the 111 topsoil spectra, are high, up to 0.994, showing high similarities between spectra corrected by different AC methods (data not shown). 434

435

#### [Figure 5]

436

The Pearson's correlation coefficient  $r_{i,t}$  (Equation (1)) computed between the 111 topsoil 437 spectra corrected by MAJA and Sen2Cor were very high for all bands and dates, ranging from 438 0.93 to 0.99 (Figure 6A1). The lowest correlations were obtained for B02 (490 nm) and B03 439 (560 nm), with a mean of 0.97, while the NIR and SWIR bands showed a very high 440 correlation (> 0.99) (Figure 6A1). Along the eleven dates, the lowest correlations were 441 obtained for the S2 image acquired on 08-03-2017 (mean of 0.99 over the spectral bands), 442 while the highest correlations were obtained for the S2 image acquired on 16-02-2017 (mean 443 up to 0.999 over the spectral bands) (Figure 6A1). 444

The correlations  $r_{i,t}$  between the 111 topsoil spectra corrected by MAJA and LaSRC followed similar patterns to correlations  $r_{i,t}$  calculated between the 111 spectra corrected by Sen2Cor and LaSRC (Figures 6A2 and A3). The correlations  $r_{i,t}$  were very high varying from 0.90 to 0.99, except for B02 (from 0.52 and 0.90) and B03 (from 0.79 and 0.97). Along the eleven dates, the lowest correlations were obtained for the S2 image acquired on 08-03-2017 (mean of 0.88 over the spectral bands, Figures 6A2 and A3).

451

The  $Rbias_{i,t}$  (in absolute value) between the 111 spectra corrected by MAJA and Sen2Cor 452 ranged from 2.5 (B02 at 490 nm, on 23-02-2017) to 400.0 (B12 at 2190 nm, on 24-04-2017) 453 454 for all the bands and dates (Figure 6B1). Along the 10 spectral bands, the highest  $Rbias_{i,t}$ were obtained for the B12 (2190 nm) (mean of 302.2 in absolute value) while the lowest 455 Rbias<sub>i,t</sub> were obtained for the B02 (490 nm) (mean of 68 in absolute value) (Figure 6B1). 456 Along the eleven dates, the highest  $Rbias_{i,t}$  were obtained for the S2 image acquired on 04-457 458 04-2017 (mean of 220.5 in absolute value), while the lowest *Rbias<sub>it</sub>* were obtained for the S2 image acquired on 16-02-2017 (mean of 76.3 in absolute value) (Figure 6B1). 459

The Rbias<sub>i,t</sub> (in absolute value) between the 111 spectra corrected by MAJA and 460 LaSRC varied from 0.00 (B8A at 865 nm, on 28-03-2017) to 249.6 (B02 at 490 nm, on 08-461 03-2017) for all bands and dates (Figure 6B2). Along the 10 spectral bands, the highest 462  $Rbias_{i,t}$  were obtained for the B02 (490 nm) (mean of 112.3 in absolute value) while the 463 lowest Rbias<sub>i,t</sub> were obtained for the B08A (865 nm) (mean of 10.9 in absolute value) (Figure 464 6B2). Along the eleven dates, the highest  $Rbias_{i,t}$  were obtained for the S2 image acquired on 465 08-03-2017 (mean of 135.9 in absolute value), while the lowest  $Rbias_{i,t}$  were obtained for the 466 S2 image acquired on 25-03-2017 (mean of 33.2 in absolute value) (Figure 6B2). 467

468 The *Rbias<sub>i,t</sub>* (in absolute value) between the 111 spectra corrected by Sen2Cor and 469 LaSRC varied from 20 (B02 at 490 nm, on 03-02-2017) and 460.8 (B05 at 705 nm, on 08-03-

2017) for all the bands and dates (Figure 6B3). Along the 10 spectral bands, the highest 470 Rbias<sub>it</sub> were obtained for the B05 (705 nm) (mean of 310.9 in absolute value), while the 471 lowest biases were obtained for the B08A (865 nm) (mean of 128.8 in absolute value) (Figure 472 473 6B3). Along the eleven dates, the highest  $Rbias_{i,t}$  were obtained for the S2 image acquired on 08-03-2017 (mean of 308.4 in absolute value), while the lowest *Rbias<sub>i,t</sub>* were obtained for the 474 S2 image acquired on 16-02-2017 (mean of 100.8 in absolute value) (Figure 6B3). 475 [Figure 6] 476 477 3.3 Clay predictions based on bare soil pixels identified with NDVI below 0.3 478 The effect of AC methods on clay content estimations was firstly investigated based on bare 479 soil pixels obtained with NDVI below 0.3. MLR models were built from each S2 image and 480 each AC method using the 111 topsoil samples identified with NDVI below 0.3, providing 33 481 MLR models. Performances for the prediction of clay content strongly varied depending on 482 the acquisition date, with  $R^2_{cv}$  ranging from 0.49 to 0.72 for MAJA, from 0.45 to 0.71 for 483 Sen2Cor, and from 0.43 to 0.71 for LaSRC (Table 3). 484 The difference in  $R^2_{cv}$  obtained when comparing dates of acquisition for each AC 485 method varied from 0.23 (obtained from MAJA-corrected S2 images) to 0.29 (obtained from 486 LaSRC-corrected S2 images) (Table 3), suggesting a strong impact of the acquisition date on 487 clay content estimation. Based on MAJA- and Sen2Cor-corrected S2 images, the best MLR 488 model was obtained from the S2 image acquired on 24-04-2017 ( $R^2_{cv} > 0.71$  and  $RMSE_{CV} >$ 489 6.50%, Table 3), while based on LaSRC-corrected S2 images, the best MLR model was 490 491 obtained from the S2 image acquired on 25-03-2017 ( $R^2_{cv}$  of 0.71 and  $RMSE_{CV}$  of 6.38%, Table 3). The MLR models built from the S2 image acquired on 04-04-2017 provided poor 492 performances for clay content prediction ( $R_{cv}^2 \le 0.55$  and  $RMSE_{CV} \ge 6.50\%$ , Table 3) for all 493 494 AC methods.

The difference in  $R^2_{cv}$  obtained when comparing the three corrected S2 images for a 495 496 given date of acquisition varied from 0.00 (obtained on 27-04-2017) to 0.07 (obtained on 08-03-2017) (Table 3), suggesting a poor impact of the AC method selection on clay content 497 estimation. The three AC methods provided very close regression performances for six S2 498 images (03-02-2017, 26-02-2017, 25-03-2017, 28-03-2017, 24-04-2017 and 27-04-2017, 499 Table 3). Considering the five remaining S2 images, MAJA provided corrected S2 images 500 501 associated to the best clay content estimations for four acquisition dates, while LaSRC 502 provided corrected S2 images associated to the best clay content estimations for only one acquisition dates (04-04-2017, Table 3). 503

Finally, the largest difference in  $R^2_{cv}$  obtained when comparing AC methods for a given date of acquisition was 0.07, while the largest difference in  $R^2_{cv}$  obtained when comparing dates of acquisition for each AC method was 0.29 (Table 3). So it suggested a stronger impact of the acquisition date on clay prediction performance compared to the AC method.

509

[Table 3]

510

# 511 **3.4 Influence of bare soil pixels identification on clay predictions**

The analysis of AC influence on clay content estimations was extended to varying bare soil pixels identifications: with NDVI below 0.25 and 0.35, and with the combination of NDVI and NBR2 below 0.3 and 0.15, respectively. Based on these bare soil pixels identifications, MLR models were built from MAJA-, Sen2Cor- and LaSRC-corrected images.

Regardless of the AC methods and thresholdings, the poorest performances were obtained from the S2 image acquired on 08-03-2017 (Table 3). Using MAJA-corrected S2 images, the best performances were obtained from the S2 image acquired on 24-04-2017, independently from thresholding. Using Sen2Cor- and LaSRC-corrected S2 images, the best

performances were obtained from S2 images acquired on 25-03-2017 and 24-04-2017,
depending on thresholding (Table 3).

Regression models performances obtained based on bare soil coverage selected using 522 NDVI below 0.3 and 0.35, were similar. Using such NDVI thresholds, the largest difference 523 in  $R^{2}_{cv}$  obtained when comparing AC methods for a given date of acquisition was 0.07, while 524 the largest difference in  $R^2_{cv}$  obtained when comparing dates of acquisition for each AC 525 526 method was 0.29 (Table 3). Using the 84 topsoil samples identified with NDVI below 0.25, the largest difference in  $R^2_{cv}$  obtained when comparing AC methods for a given date of 527 acquisition was 0.04, while the largest difference in  $R^2_{cv}$  obtained when comparing dates of 528 529 acquisition for each AC method was 0.31 (Table 3). Using the 47 topsoil samples identified with NDVI below 0.3 and NBR2 below 0.15, the largest difference in  $R^2_{cv}$  obtained when 530 comparing AC methods for a given date of acquisition was 0.08, while the largest difference 531 532 in  $R^{2}_{cv}$  obtained when comparing dates of acquisition for each AC method was 0.26 (Table 3). These results suggest that the acquisition date has stronger influence than the AC method on 533 clay prediction performance. Finally, applying restrictive NDVI thresholds or combining 534 NDVI and NBR2 thresholds did not systematically improve the models performance for a 535 given acquisition date (Table 3). 536

537

#### 538 **4. Discussion**

## 539 Variation in bare soils coverage

The extent of bare soil coverage varied depending on acquisition date, AC method and index thresholds (Table 1), with more variability due to dates and index thresholds than AC methods. While the non-cultivated lands mask (urban areas, bodies of water, and natural vegetation forest) was unique regardless of AC methods and date of acquisition, the cloud, and land masks were consistent only among the three AC methods but not among the eleven dates, and the photosynthetic vegetation masks varied between AC methods and the date of
acquisition. Indeed, the clouds were masked using one cloud mask specific to each S2 date
provided by MAJA (Table 1, Section 2.3.2), and the photosynthetic vegetation was masked by
applying a threshold on the NDVI calculated using the red band B04 (665 nm) and the NIR
band B08 (842 nm) of each S2 image.

550 As clouds only affected three dates (08-03-2017, 04-04-2017, and 27-04-2017, Table 551 1) and bands B04 and B08 differed slightly depending on the S2 acquisition date (Figures 5C 552 and G, respectively), the variability of bare soil coverage along the dates was mainly due to the cut-off induced by NDVI and NBR2 values, which may vary according to some changes 553 554 in soil surface conditions (due to humidity, roughness), new crop growing within the dates (Vaudour et al., 2019b) or crop residues (Dvorakova et al., 2021). The variability of NDVI 555 values for the same date depending on AC methods was also previously observed by Sola et 556 557 al. (2018a, 2018b).

The choice of an AC method showed very minor influence on bare soil coverage, 558 559 except for the image acquired on 08-03-2017 (e.g., from 58.22% to 78.97% using NDVI < 560 0.25 and LaSRC- and Sen2Cor-corrected S2 images, Table 1). For this specific date, such difference may be due to some unmasked clouds (including cirrus) over the Berambadi (Table 561 562 1) affecting the reflectance along the spectra, hence the NDVI values. Tarrio et al. (2020) showed that although MAJA detects clouds and cloud shadows fairly well, producing few 563 errors of omission, the majority of omitted clouds for MAJA was composed of high cirrus 564 clouds. 565

566

# 567 Variation in BOA spectra (based on bare soil pixels identified with NDVI below 0.3)

568 Atmospheric corrections performed with Sen2Cor resulted in higher reflectance values for 569 bands B04 to B12 (665 nm to 2190 nm, red boxplots, Figures 5 from C to J), except for the

date 08-03-2017 in Band 04 (Figure 5C), compared to others AC methods. These results are 570 571 in agreement with those obtained by Sola et al. (2018a, 2018b), who reported higher BOA reflectance obtained by Sen2Cor compared to MAJA and the 6S model. Li et al. (2018) also 572 573 observed an overestimation of surface reflectance by Sen2Cor, especially for bright pixels, and suggested that may be due to an AOT overestimation. Reflectance obtained with LaSRC 574 showed systematically lower values for almost all bands, with the exception for B04 on 08-575 576 03-2017 (Figure 5C) and generally for B03 (Figure 5B), than reflectance obtained with MAJA 577 and Sen2Cor. These results are still in agreement with Sola et al. (2018a), who reported lower BOA reflectance obtained by the 6S model compared to MAJA and Sen2Cor. Moreover, 578 579 reflectance values obtained on 08-03-2017 from bands B05 to B12 (705 nm to 2190 nm, Figure 4) were the lowest of the time series, which may be explained by a higher soil moisture 580 content on the 08-03-2017 image due to previous rainfall, likely to cause a general decrease in 581 582 reflectance (Minasny et al., 2011) or some unmasked clouds (including cirrus).

Variations in performances between AC methods might be explained by several 583 factors: i) MAJA is based on a multitemporal approach, while other methods are based on 584 individual acquisitions and ii) the computation of AOT and water vapor as well as the 585 radiative transfer model differs among methods, iii) each AC method uses its own cloud mask 586 method to screen the main cloudy pixels for which AC parameter estimations (such as AOT) 587 would probably not converge. Regarding this last factor, a gap-filling operation was 588 performed to fill AOT values for cloudy pixels (either by using a constant value for MAJA or 589 interpolation for Sen2Cor and LaSRC) before applying atmospheric correction with radiative 590 591 transfer models. Such differences in cloudy pixels may result in local differences in correction accuracy, especially in the surroundings of shadowed or clouded pixels, and therefore 592 593 contribute to a small part of the difference between the accuracy of MAJA and the other methods. However, considering the low rate of omission of MAJA cloud detection exposed in 594

Baetens et al. (2019), as well as the spatial homogeneity of the atmospheric correction parameters, this cannot fully explain the differences in accuracy observed between the methods.

Despite these differences observed for BOA reflectance produced by the three AC methods (Figures 5 and 6), the spectra were highly correlated regardless of the date of acquisition, except for 08-03-2017, and regardless of the bands, except the B02 (490 nm). Such high correlations are in accordance with the results obtained by Padró et al. (2017), who compared BOA reflectances obtained by several AC methods, including Sen2Cor, with in situ reflectances, and obtained high correlations regardless of the AC methods ( $r^2 > 0.9$ ).

604

# 605 AC method as minor driver of prediction performances

Our MLR regression models for clay content estimations provided performances (Table 3) in accordance with the performances obtained by Shabou et al. (2015) and Gasmi et al. (2021) using multispectral Landsat images over Mediterranean contexts, and by Bellinaso et al. (2021) and Vaudour et al. (2019a) using S2 images over tropical and temperate/Mediterranean contexts, respectively.

Regardless of the bare soil coverage selection, the AC method had a limited influence on MLR performances for clay content prediction (Table 3). Indeed the MLR models built from MAJA-, Sen2Cor- and LaSRC-corrected S2 images provided close performances (Table 3). This is in accordance with Marujo et al. (2021), who expected that LaSRC and Sen2Cor would converge to produce consistent and comparable data from both sensors. However, this is not in accordance with Sola et al. (2018a), who showed MAJA provided better performances in the analysis per land cover compared to Sen2Cor.

618

#### 619 S2 acquisition date as the main driver of prediction performances

Regardless of the bare soil coverage selection, the date of S2 image acquisition showed a stronger influence than the AC method on the performances for clay content prediction (Table 3). As previously shown by Demattê et al. (2018) and then Castaldi et al. (2019), Vaudour et al. (2019b) and Dvorakova et al. (2021), soil surface conditions impact the accuracy of SOC prediction models. This seems the case through our observed time-series, for which the dates acquired shortly after a rainfall event resulted in the lowest performance (on 08-03-2017 and 04-04-2017, Table 3), presumably due to higher soil moisture.

As the date of S2 image acquisition appears to be very important for soil property estimation, and this even more compared to the AC method, future researches could focus on identifying rules for selecting the best date of image acquisition. This was started by selecting dates with average driest condition or lower crop residues over bare soils based on NDVI and NBR2 spectral indices and enabled to obtain the best prediction performances using singledates images (Castaldi et al., 2019; Vaudour et al., 2019b; Urbina-Salazar et al., 2021).

Similarly, rules for date selection may be used to create multi-temporal image 633 composites composed of multidate images stacked over the same tile. From now, multi-634 635 temporal image composites are built from either pixelwise thresholding based on the minimum pixel value (Loiseau et al., 2019; Vaudour et al., 2021), average reflectance value 636 (e.g., Demattê et al., 2018; Gasmi et al., 2019; Dvorakova et al., 2021), median reflectance 637 value (Castaldi et al., 2021; Luo et al., 2022), or considering a trade-off between average per 638 date-indices and maximum bare soil coverage (Vaudour et al., 2021) along a multidate 639 satellite series. Multiple studies suggested using multi-temporal image composites to 640 641 maximize bare soil coverage for soil property prediction (e.g., Demattê et al., 2018; Vaudour et al., 2021; Dvorakova et al., 2021). However, current researches do not converge towards a 642 common conclusion about their benefits compared to single-date images, especially in terms 643 of soil property prediction accuracies. While Gasmi et al. (2019) showed that multi-temporal 644

image composites based on mean spectral reflectance from bare soil pixels along a Landsat-TM time series allowed to increase both the prediction accuracy of soil clay content and mapping coverage, Vaudour et al. (2021) showed that none of the multi-temporal image composites based on pixelwise or per-date bare soil reflectance along a S2 time series improved model performance for SOC prediction compared to the best single-date image. Therefore, benefit and methodologies for multi-temporal mosaicking are critical questions remaining to be explored.

652

# 653 **5.** Conclusions

654 The influence of three atmospheric corrections, namely MAJA, Sen2Cor and LaSRC, on eleven S2 images was evaluated based on clay content estimation over bare soil pixels. Our 655 study highlighted the influence of the S2 acquisition date and AC method on model 656 657 performances adjusted for clay content estimations, with more variability induced by the acquisition date than the AC method. Thus, the influence of the choice of an AC on the 658 659 estimation of soil properties can be considered as moderate compared to soil surface 660 conditions, such as moisture, crop residue or roughness, which may be strongly variable in space and time. As regression models performances were close from one AC method to 661 another, this work did not allow to consider one AC method to be the best method prior 662 estimating clay content. As Sen2Cor provided performances for clay content estimations close 663 to MAJA and LaSRC methods, and since ESA provides corrected imagery with Sen2Cor, this 664 AC method might be a satisfactory choice. Finally, as soil properties such as organic carbon 665 666 and iron are key properties influencing soil radiometric properties in a different manner than clay, the impact of AC methods on the estimation of such topsoil properties could be further 667 investigated to test the robustness of our conclusions. 668

669

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**Figure 1**: a) Location of the Berambadi catchment in India (red dot) and b) the 164 collected soil surface samples (red dots) plotted over the S2 image acquired on 03-02-2017 (colored composite of bands 08 (R), 04 (G), and 03 (B)). White pixels correspond to masked pixels (non-bare soils).



**Figure 2**: Workflow. a) Preparation of the BOA S2 images restricted to bare soil pixels, b) spectral analysis of BOA images across the time-series and obtained from the 3 AC methods, c) preparation of both calibration and validation datasets for d) model building and e) validation of clay predictions.



Figure 3: Histograms of NDVI values calculated for each S2 image corrected by the MAJA (yellow), Sen2Cor (orange), and LaSRC (cyan) AC methods.



Figure 4: Histograms of NBR2 values calculated for each S2 image corrected by the MAJA (yellow), Sen2Cor (orange), and LaSRC (cyan) AC methods.



**Figure 5**: Distribution of BOA reflectance obtained with MAJA (yellow), Sen2Cor (orange) and LaSRC (cyan) at each spectral band and for each date.



**Figure 6**: Coefficient of correlation  $r_{i,t}$  (A1, A2 and A3) and *Rbias*<sub>*i*,t</sub> (BA, B2 and B3) calculated between the BOA reflectance obtained by MAJA and Sen2Cor (A1 and B1), by MAJA and LaSRC (A2 and B2), and by Sen2Cor and LaSRC (A3 and B3) for the 111 spectra.

**Table 1:** Proportion of masked cloud surface (%) over each S2 image. Proportion of bare soil (%) over each S2 image obtained by each AC method and the tested combinations of NDVI and NBR2 thresholds. The range (difference between the largest and smallest values of bare soil coverage) was also calculated along both AC methods and S2 dates. Highest ranges of bare soil pixels along both AC methods and S2 dates are highlighted in bold.

			S2 acquisition date (DD-MM-YYYY)											
		03-02-	16-02-	23-02-	26-02-	08-03-	25-03-	28-03-	04-04-	24-04-	27-04-	07-05-		
		2017	2017	2017	2017	2017	2017	2017	2017	2017	2017	2017	_	
	% of masked cloud surface	0	0	0	0	3	0	0	0.3	0	1.4	0	Range along the dates (%)	
	% of bare soil with MAJA	66.45	74.5	75.18	78.7	71.78	70.43	72.16	68.42	67.69	68.38	65.03	13.67	
	% of bare soil with Sen2Cor	60.48	67.85	74.6	77.42	78.97	70.59	70.28	76.4	73.96	71.97	68.89	18.49	
NDVI <	% of bare soil with LaSRC	61.01	66.78	72.74	70.09	58.22	69.26	67.64	67.79	66.3	65.92	62.7	14.52	
0.25	Range of bare soil along the 3 AC methods (%)	5.97	7.72	2.44	8.61	20.75	1.33	4.52	8.61	7.66	6.05	6.19		
	% of bare soil with MAJA	77.9	83.4	83.8	85.9	80.5	80.8	81.8	79.8	79.1	78.6	76.3	9.6	
	% of bare soil with Sen2Cor	73.4	79.9	83.5	85.6	85.9	81.1	80.9	85.1	83.3	81.3	79.5	12.5	
	% of bare soil with LaSRC	75.2	79.1	82.7	82	75.1	80.9	80.2	80.5	78.7	79.2	75.3	7.6	
0.5	Range of bare soil along the 3 AC methods (%)	4.5	4.3	1.1	3.9	10.8	0.3	1.6	5.3	4.6	2.7	4.2		
	% of bare soil with MAJA	84.36	88.44	88.56	90.03	85.37	86.69	87.27	86.28	85.58	84.77	83.22	6.81	
	% of bare soil with Sen2Cor	80.97	86.12	88.4	90.15	89.58	87.02	86.77	90.13	88.74	86.9	85.92	9.18	
0.35	% of bare soil with LaSRC	82.71	85.27	87.99	87.85	83.81	87	86.67	87.29	85.82	86.46	82.93	5.28	
0.55	Range of bare soil along the 3 AC methods (%)	3.39	3.17	0.57	2.3	5.77	0.33	0.6	3.85	3.16	2.13	2.99		
	% of bare soil with MAJA	23.69	20.73	27.24	17.57	5.11	40.7	26.07	22.37	21.42	18.42	15.34	35.59	

NDVI <	% of bare soil with Sen2Cor	33.89	35.86	44.66	32.25	14.81	55.19	41.83	44.34	51.25	38.96	44.38	40.38
0.3 and	% of bare soil with LaSRC	20.22	17.26	21.82	10.42	2.08	37.83	19.17	15.16	11.83	9.65	8.53	35.75
NBR2 < 0.09	Range of bare soil along the 3 AC methods (%)	13.67	18.6	22.84	21.83	12.73	17.36	22.66	29.18	39.42	29.31	35.85	
	% of bare soil with MAJA	58.51	57.64	64.29	57.21	17.21	73.28	64.02	55.51	59.32	54.8	50.48	56.07
NDVI <	% of bare soil with Sen2Cor	62.82	67.21	73.72	69.59	36.37	77.75	72.56	73.38	77.52	70.72	72.09	41.38
0.5 anu NBR2 <	% of bare soil with LaSRC	55.24	52.96	59.46	47.06	10.15	71.79	57.71	48.09	47.64	42.63	39.64	61.64
0.12	Range of bare soil along the 3 AC methods (%)	7.58	14.25	14.26	22.53	26.22	5.96	14.85	25.29	29.88	28.09	32.45	
	% of bare soil with MAJA	74.78	78.25	80.58	79.76	40.01	80.35	79.75	74.97	77.06	75.21	72.43	40.57
NDVI <	% of bare soil with Sen2Cor	72.51	78.5	82.55	83.55	63.42	80.87	80.17	83.84	82.75	80.05	78.9	20.42
0.3 and NBR2 < 0.15	% of bare soil with LaSRC	72.13	74.04	78.71	74.72	27.63	80.29	77.53	73.13	73.89	72.1	68.22	52.66
	Range of bare soil along the 3 AC methods (%)	2.65	4.46	3.84	8.83	35.79	0.58	2.64	10.71	8.86	7.95	10.68	

**Table 2:** Proportion of common bare soil surface (%) for all S2 images corrected by MAJA. Sen2Cor and LaSRC. Number of collected topsoil samples located over these common bare soil pixels and statistics calculated for each dataset of topsoil samples. These values were calculated for each tested combinations of NDVI and NBR2 thresholds.

		Statistics on collected topsoil samples located over common bare soil pixel									
	% of common bare soil	Number of samples	min (g kg <sup>-1</sup> )	max (g kg <sup>-1</sup> )	mean (g kg <sup>-1</sup> )	Standard deviation (g kg <sup>-1</sup> )	skewness (g kg <sup>-1</sup> )				
NDVI < 0.25	40.0%	84	58	592	212	117	8.7				
NDVI < 0.3	57.2%	111	58	592	224	120	7.8				
NDVI < 0.35	67.3%	122	58	592	228	190	7.0				
NDVI < 0.3 and NBR2 < 0.09	1.2%	2	58	64	61	3.9	0				
NDVI < 0.3 and NBR2 < 0.12	7%	12	58	449	147	109	18.0				
NDVI < 0.3 and NBR2 < 0.15	21%	47	58	592	228	119	7.0				

				S2 acquisition date (DD-MM-YYYY)									
			03-02- 2017	16-02- 2017	23-02- 2017	26-02- 2017	08-03- 2017	25-03- 2017	28-03- 2017	04-04- 2017	24-04- 2017	27-04- 2017	07-05- 2017
		$\boldsymbol{R}^{2}_{cv}$	0.62	0.63	0.62	0.61	0.52	0.74	0.71	0.62	0.80	0.73	0.72
	MAJA	RMSE <sub>cv</sub>	7.77	7.56	7.82	7.66	8.74	6.44	6.94	7.86	5.68	6.56	6.47
-		MAE	5.55	5.84	5.97	5.72	6.88	5.02	5.45	6.29	4.68	5.23	5.22
		$\boldsymbol{R}^{2}_{cv}$	0.62	0.63	0.62	0.60	0.50	0.76	0.72	0.62	0.80	0.74	0.72
0.25	Sen2Cor	RMSE <sub>cv</sub>	7.86	7.68	7.77	7.81	8.93	6.34	7.00	7.74	5.70	6.52	6.59
0.20		MAE	5.54	5.89	5.88	5.71	7.09	4.94	5.48	6.21	4.70	5.20	5.30
		$\boldsymbol{R}^{2}_{cv}$	0.63	0.62	0.62	0.59	0.50	0.75	0.72	0.63	0.77	0.72	0.68
	LaSRC	RMSE <sub>cv</sub>	7.61	7.58	7.61	7.91	8.94	6.21	6.84	7.64	6.16	6.50	6.99
		MAE	5.39	5.66	5.85	5.99	7.09	4.79	5.47	6.02	5.07	5.35	5.73
	MAJA	$\boldsymbol{R}^{2}_{cv}$	0.62	0.65	0.64	0.65	0.49	0.71	0.66	0.51	0.72	0.68	0.68
		<b>RMSE</b> <sub>cv</sub>	7.57	7.29	7.44	7.34	8.77	6.60	7.19	8.56	6.50	6.98	6.89
-		MAE	5.67	5.57	5.62	5.41	6.98	5.18	5.68	6.79	5.17	5.53	5.73
		$\boldsymbol{R}^{2}_{cv}$	0.61	0.64	0.61	0.64	0.45	0.71	0.67	0.48	0.71	0.68	0.67
NDVI < 0.3	Sen2Cor	<b>RMSE</b> <sub>cv</sub>	7.68	7.35	7.54	7.38	9.15	6.63	7.15	8.73	6.56	6.97	6.98
		MAE	5.70	5.63	5.66	5.40	7.30	5.20	5.62	6.89	5.24	5.48	5.84
		$\boldsymbol{R}^{2}_{cv}$	0.62	0.62	0.62	0.64	0.43	0.71	0.66	0.55	0.71	0.68	0.64
	LaSRC	RMSE <sub>cv</sub>	7.43	7.31	7.38	7.44	9.26	6.38	7.17	8.20	6.62	6.70	7.10
		MAE	5.50	5.54	5.61	5.51	7.40	4.94	5.68	6.44	5.34	5.39	5.88
		$R^2_{cv}$	0.63	0.64	0.61	0.65	0.51	0.74	0.71	0.55	0.75	0.70	0.70
NDVI <	MAJA	RMSE <sub>cv</sub>	7.47	7.42	7.59	7.42	8.51	6.32	6.72	8.27	6.14	6.68	6.79
0.35		MAE	5.59	5.60	5.69	5.59	6.76	4.91	5.28	6.55	4.79	5.22	5.61
	Sen2Cor	$\boldsymbol{R}^{2}_{cv}$	0.62	0.63	0.62	0.62	0.47	0.73	0.70	0.51	0.75	0.70	0.69

**Table 3:** Validation performances for the estimations of soil clay content obtained from the MLR models built from MAJA- Sen2Cor- and LaSRCcorrected S2 images. Best performances in terms of both  $R_{cv}^2$  and  $RMSE_{cv}$  for each date are highlighted in bold.

		RMSE <sub>cv</sub>	7.61	7.51	7.55	7.57	8.88	6.34	6.77	8.42	6.22	6.68	6.81
		MAE	5.68	5.69	5.72	5.65	7.04	4.91	5.26	6.62	4.87	5.20	5.68
		$\boldsymbol{R}^{2}_{cv}$	0.60	0.61	0.61	0.63	0.45	0.74	0.70	0.58	0.74	0.69	0.66
	LaSRC	RMSE <sub>cv</sub>	7.55	7.42	7.45	7.59	8.97	6.21	6.80	7.92	6.30	6.81	7.03
		MAE	5.58	5.54	5.53	5.76	7.11	4.80	5.35	6.24	4.97	5.32	5.75
	MAJA	$R^2_{cv}$	0.70	0.73	0.71	0.70	0.58	0.75	0.66	0.62	0.77	0.73	0.73
		RMSE <sub>cv</sub>	6.91	7.22	7.06	7.69	9.03	6.98	7.93	8.84	6.82	7.48	7.36
_		MAE	5.73	6.14	5.94	6.28	7.65	5.80	6.47	7.32	5.60	6.31	6.34
NDVI < 0.3		$\boldsymbol{R}^{2}_{cv}$	0.70	0.73	0.71	0.72	0.54	0.78	0.67	0.62	0.77	0.73	0.72
and NBR2	Sen2Cor	<b>RMSE</b> <sub>cv</sub>	6.97	7.09	7.26	7.54	9.50	6.88	7.77	8.29	7.03	7.63	7.23
< 0.15		MAE	5.80	5.99	6.24	6.14	7.97	5.71	6.42	6.82	5.75	6.43	6.14
	LaSRC	$\boldsymbol{R}^{2}_{cv}$	0.73	0.74	0.72	0.71	0.52	0.78	0.68	0.67	0.69	0.71	0.74
		<b>RMSE</b> <sub>cv</sub>	5.98	6.77	6.46	7.11	9.53	6.81	7.78	8.43	8.41	8.04	7.49
		MAE	4.99	5.71	5.43	5.70	7.86	5.38	6.50	7.17	7.11	6.80	6.37